Classical & quantum dynamics of information and entanglement properties of fermion systems

by

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I, Claudia Zander, declare that the thesis, which I hereby submit for the degree Doctor of Philosophy in Physics at the University of Pretoria, is my own work and has not previously been submitted by me for a degree at this or any other tertiary institution.

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I said to my soul, be still and wait without hope
For hope would be hope for the wrong thing;
Wait without love for love would be love of the wrong thing;
There is yet faith but the faith and the love and
The hope are all in the waiting.
Wait without thought, for you are not ready for thought:
So the darkness shall be the light, and the stillness the dancing.
T.S. Eliot

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Summary

Due to their great importance, both from the fundamental and from the practical points of view, it is imperative that the various facets of the concepts of information and entanglement are explored systematically in connection with diverse physical systems and processes. These concepts are at the core of the emerging field of the Physics of Information. In this Thesis I investigate some aspects of the dynamics of information in both classical and quantum mechanical systems and then move on to explore entanglement in fermion systems by searching for novel ways to classify and quantify entanglement in fermionic systems.

In Chapter 1 a brief review of the different information and entropic measures as well as of the main evolution equations of classical dynamical and quantum mechanical systems is given. The conservation of information as a fundamental principle both at the classical and quantum levels, and the implications of Landauer's theorem are discussed in brief. An alternative and more intuitive proof of the no-broadcasting theorem is also provided.

Chapter 2 is a background chapter on quantum entanglement, where the differences between the concept of entanglement in systems consisting of distinguishable subsystems and the corresponding concept in systems of identical fermions are emphasized. Different measures of

entanglement and relevant techniques such as majorization, are introduced. To illustrate some of the concepts reviewed here I discuss the entanglement properties of an exactly soluble many-body model which was studied in paper (E) of the publication list corresponding to the present Thesis. An alternative approach to the characterization of quantum correlations, based on perturbations under local measurements, is also briefly reviewed. The use of uncertainty relations as entanglement indicators in composite systems having distinguishable subsystems is then examined in some detail.

Chapter 3 is based on papers (A) and (B) of the list of publications. Extended Landauer-like principles are developed, based amongst others on the conservation of information of divergenceless dynamical systems. Conservation of information within the framework of general probabilistic theories, which include the classical and quantum mechanical probabilities as particular instances, is explored. Furthermore, Zurek's information transfer theorem and the no-deleting theorem are generalized.

Chapter 4 is based on articles (C) and (D) mentioned in the publication list, and investigates several separability criteria for fermions. Criteria for the detection of entanglement are developed based either on the violation of appropriate uncertainty relations or on inequalities involving entropic measures.

Chapter 5 introduces an approach for the characterization of quantum correlations (going beyond entanglement) in fermion systems based upon the state disturbances generated by the measurement of local observables.

Chapter 6 summarizes the conclusions drawn in the previous chapters.

The work leading up to this Thesis has resulted in five publications in peer reviewed science research journals:

(A) C. Zander, A.R. Plastino, A. Plastino, M. Casas and S. Curilef, *Entropy* **11** (4), (2009) pp. 586-597

(B) C. Zander and A.R. Plastino, *Europhys. Lett.* **86** (1), (2009) 18004

(C) C. Zander and A.R. Plastino, *Phys. Rev. A* **81**, (2010) 062128

(D) C. Zander, A.R. Plastino, M. Casas and A. Plastino, *Eur. Phys. J. D* **66**, (2012) 14

(E) C. Zander, A. Plastino and A.R. Plastino, *Braz. J. Phys.* **39** (2), (2009) pp. 464-467.

Zusammenfassung

Aufgrund ihrer großen Bedeutung, sowohl aus der Grundlagenforschung heraus als auch von den praktischen Gesichtspunkten aus gesehen, ist es unerlässlich, dass die verschiedenen Facetten der Begriffe Information und Verschränkung systematisch in Verbindung mit verschiedenen physikalischen Systemen und Prozessen untersucht werden. In dieser Arbeit untersuche ich erst einige Aspekte der Dynamik der Information in klassischen und quantenmechanischen Systemen und fahre dann mit der Erforschung der Verschränkung in Fermionen-Systemen fort.

In Kapitel 1 wird eine kurze Übersicht über die verschiedenen Informations- und Entropiemaße geboten, sowie die wichtigsten Evolutionsgleichungen der klassischen dynamischen und quantenmechanischen Systeme gegeben. Die Erhaltung von Information als Grundprinzip sowohl auf der klassischen Ebene als auch auf der quantenmechanischen Ebene, und die Auswirkungen des Landauer Satzes werden kurz besprochen.

Kapitel 2 ist ein Hintergrundkapitel über Quantenverschränkung, in dem die Unterschiede zwischen dem Konzept der Verschränkung in Systemen bestehend aus unterscheidbaren Subsystemen und dem entsprechenden Konzept in Systemen mit identischen Fermionen hervorgehoben werden. Verschiedene Maße der Verschränkung und relevante Techniken werden vorgestellt. Darüber hinaus bespreche ich die Verschränkungseigenschaften eines genau lösbaren Vielteilchenmodells. Die Verwendung von Unbestimmtheitsrelationen als Verschränkungsindikatoren in zusammengestellten Systemen mit unterscheidbaren Teilsystemen wird dann untersucht.

In Kapitel 3 werden erweiterte Landauer-ähnliche Prinzipien entwickelt, basierend unter anderem auf der Erhaltung von Information in divergenzlosen dynamischen Systemen. Die Erhaltung von Information im Rahmen der allgemeinen probabilistischen Theorien, die die klas-

sischen und quantenmechanischen Wahrscheinlichkeiten als besondere Fälle enthalten, wird ebenfalls untersucht. Außerdem wird in diesem Zusammenhang der Informationsübertragungs-Satz von Zurek verallgemeinert.

Kapitel 4 untersucht mehrere Separabilitätskriterien für Fermionen. Kriterien für den Nachweis von Verschränkung sind entwickelt worden, basierend entweder auf der Verletzung von angebrachten Unbestimmtheitsrelationen oder auf Ungleichheiten, die wiederum die entropischen Maße beinhalten.

Kapitel 5 stellt einen Ansatz zur Charakterisierung von Quanten-Korrelationen (die über die Verschränkung hinausgehen) in Fermionen-Systemen dar, basierend auf den Zustandsstörungen die durch die Messung der lokalen Observablen erzeugt werden.

Kapitel 6 fasst die Schlussfolgerungen zusammen, die in den vorangegangenen Kapiteln gezogen wurden.

Die Arbeiten, die zu dieser These geführt haben, wurden in fünf Publikationen in wissenschaftlichen Fachzeitschriften veröffentlicht.

Resumen

Debido a su gran importancia, tanto desde el punto de vista fundamental como desde el práctico, es imprescindible que las diversas facetas de los conceptos de información y entrelazamiento se exploren de forma sistemática en relación con diversos sistemas y procesos físicos. En esta tesis investigo algunos aspectos de la dinámica de la información en los sistemas mecánicos clásicos y cuánticos, y luego paso a explorar el entrelazamiento de los sistemas de fermiones.

En el capítulo 1 se da una breve revisión de las diferentes medidas de información y medidas entrópicas, así como de las principales ecuaciones de evolución de los sistemas dinámicos clásicos y mecánico-cuánticos. También se discuten brevemente la conservación de la información, tanto a nivel clásico como cuántico, y las implicaciones del teorema de Landauer.

En el capítulo 2 se repasa brevemente el concepto de entrelazamiento cuántico, haciendo énfasis en las diferencias existentes entre el concepto de entrelazamiento en sistemas constituidos por subsistemas distinguibles y el correspondiente concepto en sistemas de fermiones idénticos. Diferentes medidas de entrelazamiento y técnicas relevantes son introducidas. También discuto las propiedades de entrelazamiento de un modelo de muchos cuerpos exactamente soluble. Luego se examina el uso de relaciones de incertidumbre como indicadores de entrelazamiento en los sistemas compuestos por subsistemas distinguibles.

En el capítulo 3 investigo extensiones del principio de Landauer basadas en la conservación de la información en sistemas dinámicos con flujo en el espacio de las fases de divergencia nula. Luego investigo la conservación de la información en el marco de teorías probabilísticas generales, que incluyen a las probabilidades clásicas y a la mecánica cuántica como casos particulares. Además, en este contexto, el teorema de Zurek de transferencia de información es generalizado.

En el capítulo 4 desarrollo varios criterios de separabilidad para sis-

temas de fermiones. Investigo criterios para la detección del entrelazamiento basados tanto en la violación de relaciones de incertidumbre adecuadas o en desigualdades entrópicas.

El capítulo 5 presenta un enfoque para la caracterización de las correlaciones cuánticas (más allá de entrelazamiento) en los sistemas de fermiones, basado en las alteraciones del estado cuántico generadas por la medición de observables locales.

El capítulo 6 resume las conclusiones extraídas en los capítulos anteriores.

Las investigaciones desarrolladas en esta tesis han dado lugar a cinco publicaciones en revistas cientficas sometidas a referato especialitado.

Contents

Chapter 1

Physics and Information

In recent years the physics of information [1–7] has received increasing attention [5, 6, 8–16]. There is a growing consensus that information is endowed with physical reality, not in the least because the ultimate limits of any physical device that processes or transmits information are determined by the fundamental laws of physics [6, 12–14]. That is, the physics of information and computation is an interdisciplinary field which has promoted our understanding of how the underlying physics influences our ability to both manipulate and use information. By the same token a plenitude of theoretical developments indicate that the concept of information constitutes an essential ingredient for a deep understanding of physical systems and processes [1–6]. The physics of information also comprises a set of ideas, concepts and techniques that provide a natural "bridge" between theoretical physics and other branches of Science, particularly biology [17]. Landauer's principle is one of the most fundamental results in the physics of information and is generally associated with the statement "information is physical". It constitutes a historical turning point in the field by directly connecting information processing with (more) conventional physical quantities [18]. According to Landauer's principle a minimal amount of energy is required to be dissipated in order to erase a bit of information in a computing device working at temperature T. This minimum energy is given by $kT \ln 2$, where k denotes Boltzmann's constant [19–21]. Landauer's principle has deep implications, as it allows for the derivation of several important results in classical and quantum information theory [22]. It also constitutes a rather useful heuristic tool for estab-

lishing new links between, or obtaining new derivations of, fundamental aspects of thermodynamics and other areas of physics [23].

Information is something that is encoded in a physical state of a system and a computation is something that can be carried out on a physically realizable device with real physical degrees of freedom. In order to quantify information one will need a measure of how much information is encoded in a system or process. Shannon entropy, Rényi entropy (which is a generalization of Shannon entropy) and Tsallis' $S_q^{(T)}$ power-law entropies will be discussed. Since the universe is quantum mechanical at a fundamental level, the question naturally arises as to how quantum theory can enhance our insight into the nature of information.

Entanglement is one of the most fundamental aspects of quantum physics. It constitutes a physical resource that allows quantum systems to perform information tasks not possible within the classical domain. That is, quantum information is typically encoded in non-local correlations between the different parts of a physical system and these correlations have no classical counterpart. One of the aims of quantum information theory is to understand how entanglement can be used as a resource in communication and other information processes. Two spectacular applications of entanglement are quantum teleportation and superdense coding [7].

Since the outcome of a quantum mechanical measurement has a random element, we are unable to deduce the initial state of the system from the measurement outcome. This basic property of quantum measurements is connected with another important distinction between quantum and classical information: quantum information cannot be copied with perfect fidelity. This is called the no-cloning principle. If it were possible to make a perfect copy of a quantum state, one could then measure an observable of the copy (in fact, we could perform measurements on as many copies as necessary) without disturbing the original, thereby defeating, for instance, the principle that two non-orthogonal quantum states cannot be distinguished with certainty [24]. Perfect quantum cloning would also allow the second principle of thermodynamics [24] to be defeated. It has also been proved that quantum cloning would allow (via EPR-type experiments [25])

information to be transmitted faster than the speed of light.

1.1 Information and entropic measures

Entropy is an extremely important concept in information theory, statistical physics and in other fields as well. The entropy of a probability distribution can be interpreted not only as a measure of uncertainty, but also as a measure of information. The amount of information which one obtains by observing the result of an experiment depending on chance, can be taken numerically equal to the amount of uncertainty concerning the outcome of the experiment before carrying it out [26].

The Shannon entropy, introduced by Claude E. Shannon, is a fundamental measure in information theory [27]. In addition to the above two views of entropy, another complementary view of the Shannon entropy is its application to data compression. In that context the Shannon entropy gives the minimum number of bits needed to store the result of a measurement of a random variable.

1.1.1 Shannon entropy

The most fundamental information measure is Shannon's entropy which gives the amount of uncertainty concerning the outcome of an experiment:

$$H_{Shannon}(p_1, p_2, \ldots, p_n) = -k \sum_{i=1}^{n} p_i \log_2 p_i, \tag{1.1}$$

where p_i is the probability that the discrete variable x will assume the value x_i (out of the n possible values $(x_1, \ldots, x_n)$) and k is a positive constant which when set to one gives the unit "bits" (from the abbreviation of binary digit) for the entropy. Note that entropy is a functional of the distribution $\{x\}$, which means it does not depend on the actual values taken by the random variable x, but only on the probabilities [28]. $H_{Shannon}$ is (for discrete probability distributions) a non-negative quantity: $H_{Shannon} \geq 0$. It measures the lack of knowledge about the precise value of x. Alternatively, $H_{Shannon}$ can be interpreted as a measure of the predictive power of the probability distribution $\{p\}$. The presence

of Boltzmann's constant k in the definition of the thermodynamic entropy is due to historical reasons, reflecting the conventional units of temperature. It is there to make sure that the statistical thermodynamic entropy definition matches the classical entropy of Clausius. In the case of information entropy the logarithm can also be taken to the natural base e. This is equivalent to choosing the "nat" as unit of information or entropy, instead of the usual bits. In practice, information entropy is almost always calculated using logarithms to base 2, but this distinction amounts to nothing other than a change in units. The natural unit of information (nat) is related to the bit as follows: 1 nat = $1/\ln 2$ bits. Two important straightforward features of $H_{Shannon}$ are that it vanishes in the case of "certainty" (that is, when one has $p_i = 1$ for one x_i and $p_j = 0$ for $j \neq i$) and it adopts its maximum value for "uniformity" (that is, where all p_i's are equal to $1/n$).

The three conditions which give rise to the above expression (1.1), are [29]

1. H is a continuous function of the p_i
2. If all p_i's are equal, then $H\left(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}\right)$ is a monotonic increasing function of n
3. The composition law:

$$H\left(p_1, p_2, \ldots, p_n\right) = H\left(w_1, w_2, \ldots, w_r\right) + w_1 H\left(\tfrac{p_1}{w_1}, \ldots, \tfrac{p_k}{w_1}\right) + w_2 H\left(\tfrac{p_{k+1}}{w_2}, \ldots, \tfrac{p_{k+m}}{w_2}\right) + \ldots, \tag{1.2}$$

where $w_1 = (p_1 + \ldots + p_k)$, $w_2 = (p_{k+1} + \ldots + p_{k+m})$, etc.

In the view of Jaynes [29–31], the relationship between thermodynamic and informational entropy is, that thermodynamics should be seen as an application of Shannon's information theory. Thermodynamic entropy is then interpreted as being an estimate of the amount of information that remains uncommunicated by a description solely in terms of the macroscopic variables of classical thermodynamics and that would be needed to define the detailed microscopic state of the system. The increase in entropy characteristic of irreversibility always signifies, both in quantum mechanics and classical theory, a loss of information. The probability distributions corresponding to states of thermodynamical equilibrium are

then determined by Jaynes' maximum entropy principle [29]. That is, these distributions are those that maximize the entropy functional under the constraints imposed by normalization and the available macroscopic data characterizing the equilibrium state.

An important property of entropy is that $S(p)$ is a concave function of its input arguments $p_1, p_2, \ldots, p_n$. This means that for any two probability distributions $\{p'_i\}$ and $\{p''_i\}$ and for any λ such that $0 \leq \lambda \leq 1$, we have

$$S(\lambda p' + (1-\lambda)p'') \geq \lambda S(p') + (1-\lambda)S(p''). \tag{1.3}$$

The physical meaning of this inequality is that mixing different probability distributions can only increase uniformity [24].

One of the most important properties of entropy is its additivity, that is, given two probability distributions $P = (p_1, p_2, \ldots, p_n)$ and $Q = (q_1, q_2, \ldots, q_m)$,

$$H_{Shannon}[P * Q] = H_{Shannon}[P] + H_{Shannon}[Q], \tag{1.4}$$

where by $P*Q$ we denote the direct product of the distributions. Now, one cannot replace condition 3 with eq. (1.4), since the latter condition is much weaker. Actually, there are several quantities other than eq. (1.1) which satisfy conditions 1, 2 and eq. (1.4). The following is one generalization of the Shannon entropy.

1.1.2 Rényi entropy

The *entropy of order* q of the distribution $\mathcal{P} = (p_1, p_2, \ldots, p_n)$ is defined to be [2, 26]

$$S_q^{(R)}(p_1, p_2, \ldots, p_n) = \frac{1}{1-q} \log_2 \left(\sum_{k=1}^{n} p_k^q \right), \tag{1.5}$$

where $q \geq 0$, $q \neq 1$ and $S_q^{(R)}$ is measured in units of bits. That is, the above expression can be regarded as a measure of the entropy of the distribution $\mathcal{P}$ and

in the limiting case $q \to 1$ we recover the Shannon entropy:

$$\lim_{q\to 1} S_q^{(R)}(p_1, p_2, \ldots, p_n) = \sum_{k=1}^{n} p_k \log_2 \frac{1}{p_k}. \tag{1.6}$$

The Rényi entropy is an extensive quantity for statistically independent subsystems (unlike Tsallis entropy) and concave only for $0 < q < 1$.
An interpretation of Rényi entropy is, that the greater the parameter q the greater the dependence of the entropy on the probabilities of the more probable values and hence less on the improbable ones.

In the limit $q \to \infty$ the Rényi entropy becomes very simple and only depends on the largest probability value of the distribution, namely

$$S_\infty^{(R)}(\mathcal{P}) = -\log_2(\max\{p \in \mathcal{P}\}). \tag{1.7}$$

This extreme case constitutes a clear illustration of the previously mentioned interpretation of $S_q^{(R)}$.

Note that in Chapter 4 I will use the equivalent notations $S_q^{(R)}$ or $H_q^{(R)}$ for the Rényi measure.

Closely related to Rényi entropy is another generalization of Shannon's entropy that has been the subject of much interest recently, the Tsallis or $S_q^{(T)}$ power-law entropy.

1.1.3 Tsallis entropy

The power-law $S_q^{(T)}$ entropies, advanced by Tsallis, are non-extensive entropic functionals given by [32–37],

$$S_q^{(T)}(\mathcal{P}) = \frac{1}{q-1}\left(1 - \sum_i p_i^q\right) \tag{1.8}$$

where $\mathcal{P}$ denotes the probability distribution and the parameter q is any real number (characterizing a particular statistics), $q \neq 1$. The probabilities are

thus scaled by q, which means they may be reinforced or weakened. The Tsallis entropy possesses the usual properties of positivity, equiprobability, concavity, irreversibility and it generalizes the standard additivity (eq. (1.4)) as well as the Shannon additivity (eq. (1.2)) [33]. The normal Boltzmann-Gibbs entropy is recovered in the limit $q \to 1$.

The non-extensive thermostatistical formalism based upon the $S_q^{(T)}$ entropies has been applied to a variegated family of problems in physics, astronomy, biology and economics [38]. In particular, the case $q = 2$ constitutes a powerful tool for the study of quantum entanglement [39–41]. Tsallis entropy can also be regarded as a one-parameter generalization of the Shannon entropy.

The characteristic property of Tsallis entropy is *pseudoadditivity*,

$$S_q^{(T)}(A, B) = S_q^{(T)}(A) + S_q^{(T)}(B) + (1 - q)S_q^{(T)}(A)S_q^{(T)}(B), \tag{1.9}$$

with A and B being two mutually independent finite event systems whose joint probability distribution satisfies

$$p(A, B) = p(A)p(B). \tag{1.10}$$

From this it is evident that q is a measure of the non-extensivity of the system.

The Rényi entropy is a monotonic function of the Tsallis entropy,

$$S_q^{(R)}(\mathcal{P}) = \frac{\log_2\left[1 + (1 - q)S_q^{(T)}(\mathcal{P})\right]}{1 - q} \tag{1.11}$$

and furthermore $S_q^{(R)}(\mathcal{P})$ and $S_q^{(T)}(\mathcal{P})$ both decrease monotonically in q.

Note that in Chapter 4 I will use the equivalent notation $H_q^{(T)}$ for the Tsallis measure.

The Shannon entropy, Rényi entropy and Tsallis entropy have found applications in a wide range of physical scenarios. In addition to their role in physics, they

also have several multidisciplinary applications. Apart from its utility in modern information theory, the Shannon entropy has been successfully used amongst others in biology, econophysics and astronomy. Rényi entropy has been used for example in multifractal theory, non-linear chaotic dynamics and cryptography. The Tsallis entropy has been applied for instance to systems with long-range interactions or fluctuating temperature.

1.1.4 Related measures of information

The Shannon entropy can be used to define other measures of information which express the relationship between two discrete random variables X and Y [7, 42]:

- relative entropy $H(X||Y)$: measures the similarity between two random variables
- joint entropy $H(X,Y)$: measures the combined information in two random variables
- conditional entropy $H(X|Y)$: measures the information contained in one of the random variables provided that the outcome of another random variable is known
- mutual information $H(X{:}Y)$: measures the correlation between two random variables, that is, how much information X and Y have in common. In other words, how much knowledge of one random variable reduces the information gained from then learning the other variable.

The definition of the joint entropy follows directly from the definition of the Shannon entropy (1.1),

$$H(X,Y) = -\sum_{x,y} p(x,y)\log p(x,y), \tag{1.12}$$

where $p(x,y)$ is the joint probability distribution. The marginal probability distributions are $p(x) = \sum_y p(x,y)$ and $p(y) = \sum_x p(x,y)$. The expressions for $H(X)$ and $H(Y)$ are then

$$H(X) \;=\; -\sum_{x} p(x)\log p(x)$$

$$H(Y) = -\sum_y p(y)\log p(y). \tag{1.13}$$

Suppose that we know the value of Y, which means we have $H(Y)$ bits of information about the pair (X,Y). The remaining information we can gain about (X,Y) is the remaining information we can acquire about X, even given that we have knowledge of Y. The conditional entropy $H(X|Y)$, that is, the entropy of X conditional on knowing Y, is defined by

$$\begin{aligned} H(X|Y) &= \sum_y p(y)H(X|Y=y) \\ &= -\sum_y p(y)\sum_x p(x|y)\log p(x|y) \\ &= -\sum_{x,y} p(x,y)\log p(x|y), \end{aligned} \tag{1.14}$$

since $p(x,y) = p(y)p(x|y)$ and using this again results in

$$\begin{aligned} H(X|Y) &= -\sum_{x,y} p(x,y)\log\left(\frac{p(x,y)}{p(y)}\right) \\ &= -\sum_{x,y} p(x,y)\log p(x,y) - \left(-\sum_{x,y} p(x,y)\log p(y)\right) \\ &= H(X,Y) - \left(-\sum_y p(y)\log p(y)\right) \\ &= H(X,Y) - H(Y). \end{aligned} \tag{1.15}$$

This also gives a relationship between the joint entropy and the conditional entropy. The mutual information was said to give the amount of information that X and Y have in common. Suppose we add the information contents of X and Y, which means the sum $H(X)+H(Y)$ counts the information common to X and Y twice whereas it counts the information not common only once. If we subtract the joint entropy, we remain with exactly the information common to X and Y,

$$H(X{:}Y) = H(X) + H(Y) - H(X,Y). \tag{1.16}$$

Replacing the joint entropy with the final relation in equation (1.15), one obtains an alternative expression for the mutual information,

$$H(X{:}Y) = H(X) - H(X|Y). \tag{1.17}$$

This can be interpreted as the difference between the information gained from learning X and the information gained from learning X when Y is already known. The mutual information is symmetric, that is, the mutual information between X and Y is the same as the mutual information between Y and X.

Figure 1.1 gives an intuitive illustration of the various useful ways in which the quantities discussed above are related.

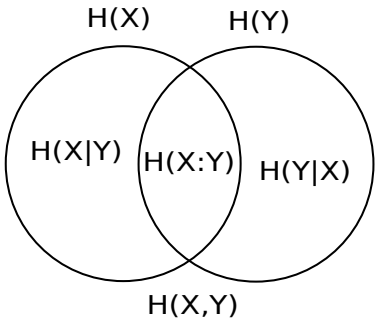


Figure 1.1: Relationship between the joint entropy $H(X,Y)$, the conditional entropy $H(X|Y)$ and the mutual information $H(X{:}Y)$.

When dealing with quantum discord in Section 2.3 we will first give the quantum analogues of the above entropies and then find the corresponding quantum relationships between the different quantum entropic measures.

The relative entropy or Kullback-Leibler distance is discussed in the next Subsection, together with its generalizations. It is a distinguishability measure for discrete or continuous classical probability densities.

1.1.5 Distinguishability measure for classical probability densities: Kullback-Leibler measure and its generalizations

The relative entropy or Kullback-Leibler distance is a measure of the distance between two distributions $p(x)$ and $q(x)$, over the same index set, x. It can be viewed as a measure of the inefficiency of assuming that the distribution is q when the actual distribution is p. The definition of the Kullback-Leibler divergence for probability distributions p and q of a discrete random variable, is [28]

$$H(p||q) = \sum_x p(x) \log \frac{p(x)}{q(x)}. \tag{1.18}$$

Based on continuity arguments, one defines $0 \log \frac{0}{q} = 0$ and $p \log \frac{p}{0} = \infty$. What the above equation says in words, is that the Kullback-Leibler divergence is the average of the logarithmic difference between the probability distributions p and q, where the average is taken using the probabilities p. The Kullback-Leibler measure is only defined for discrete probability distributions with $q(x) > 0$ for all x (among the $p(x)$ there may be zeros) [26]. This quantity is always non-negative and is zero if and only if $p = q$. The relative entropy increases as the distance between p and q increases. It is, however, not a true distance between distributions since it is not symmetric and does not satisfy the triangle inequality. It should be noted that Kullback and Leibler themselves actually defined the divergence as $H(p||q) + H(q||p)$ [43]. One can generalize the Kullback-Leibler measure by replacing the logarithm with an arbitrary function. This will be shown for the continuous case which is discussed next.

All the above information measures can be extended to the case of systems with a continuous phase space. For instance, the Shannon entropy becomes

$$S[f] = -\int f \ln f \, d\Omega, \tag{1.19}$$

where f is a probability density and $d\Omega$ is the volume element in phase space. Thus summations are replaced by integrals.

The generalization of the Kullback-Leibler measure is as follows. Given two probability distributions $\mathcal{P}_1$ and $\mathcal{P}_2$ of continuous random variables, one can define

$$G\big[\mathcal{P}_1, \mathcal{P}_2\big] = \int \mathcal{P}_1 \, g\left[\frac{\mathcal{P}_1}{\mathcal{P}_2}\right] d\mathbf{x}, \tag{1.20}$$

where $g[\ldots]$ denotes an arbitrary function (we assume that the integral in the above equation converges) [16, 44]. This general integral provides a convenient way to measure distances between $\mathcal{P}_1$ and $\mathcal{P}_2$, depending on the explicit choice of the function $g[\ldots]$ [16]. That is, the generalized divergence is intuitively an average, weighted by the function g, of the odds ratio given by $\mathcal{P}_1$ and $\mathcal{P}_2$. Special instances are given by the Kullback-Leibler distance $H(\mathcal{P}_1||\mathcal{P}_2) = \int \mathcal{P}_1 \log \frac{\mathcal{P}_1}{\mathcal{P}_2} \, d\mathbf{x}$, where g is the logarithm, and by the overlap $\mathcal{O}(\mathcal{P}_1, \mathcal{P}_2) = \int \sqrt{\mathcal{P}_1 \mathcal{P}_2} \, d\mathbf{x}$ where $g[z] = z^{-1/2}$. One can also consider a mono-parametric family of functionals based on Tsallis' $S_q^{(T)}$ entropy [45],

$$I_q\big[\mathcal{P}_1, \mathcal{P}_2\big] = \int \mathcal{P}_1 \frac{[\mathcal{P}_1/\mathcal{P}_2]^{q-1} - 1}{q-1} \, d\mathbf{x}, \tag{1.21}$$

parameterized by the real parameter $0 < q \leq 1$, where one has let $g[z] = \frac{1}{q-1}\big(z^{q-1} - 1\big)$. The functional I_q can be interpreted as a non-extensive generalization of the standard Kullback-Leibler distance [44–46].

1.1.6 Mixed states in quantum mechanics

The density operator language gives a description of quantum mechanics that does not take as its foundation the state vector.

This alternative formulation is mathematically equivalent to the state vector approach, however, it provides an extremely useful language for dealing with commonly encountered scenarios in quantum mechanics. Mixed states arise in situations where there is classical uncertainty and so it is unknown by the experimenter which particular states are actually being manipulated. One should not confuse this with the concept of quantum uncertainty, where the results of either some or all measurements cannot be predicted even if the experimenter knows exactly which particular states are being manipulated. This classical uncertainty

could be introduced intentionally, for example by preparing a quantum system in such a way that there is a randomly-varying element in the preparation history or it could also be introduced unintentionally, for example due to the effect of quantum noise which creates ignorance in our knowledge of the quantum state. Another example would be given by the loss of the record/s of a measurement result. A quantum system in thermal equilibrium at finite temperatures is also represented by a mixed state. For a closed system, one can view the mixed state as either representing a single system or as representing an ensemble of systems, which means a large number of copies of the system under consideration, where p_j is the proportion of the ensemble being in the state $|\psi_j\rangle$. If the system is not closed, that is, there may be unwanted interactions due to the environment or the system may be entangled with other systems as part of a composite system, then one cannot say that the system has some definite but unknown state vector, since the density operator records entanglements to other systems. In specific, mixed states which are descriptions of subsystems of composite quantum systems thus have an intrinsic classical uncertainty due to either some or all of the subsystems being entangled. That is, if a quantum system has two or more subsystems that are entangled, then each individual subsystem must be regarded as a mixed state even if the complete system is in a pure state.

A quantum system whose state $|\psi\rangle$ is known exactly is said to be in a pure state. In this case the density operator is simply the projector $\rho = |\psi\rangle\langle\psi|$. Otherwise, ρ is in a mixed state and it is said to be a mixture of the different pure states in the ensemble for ρ [7]. That is, suppose a quantum system is in one of a number of states $|\psi_i\rangle$ (where i is an index) with respective probabilities p_i. This ensemble of pure states is then denoted by $\{p_i, |\psi_i\rangle\}$. It is important to note that the states $|\psi_i\rangle$ do not need to be orthogonal to each other. The density operator for the system is then defined by

$$\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|, \tag{1.22}$$

where $\sum_i p_i = 1$. Now an operator ρ is the density operator associated with an ensemble $\{p_i, |\psi_i\rangle\}$ if and only if it satisfies the conditions [7]:
(a) Hermicity condition: ρ is Hermitian, that is, $\rho^\dagger = \rho$

(b) Normalization condition: ρ has trace equal to one

(c) Positivity condition: ρ is a positive operator, that is, $\langle\phi|\rho|\phi\rangle \geq 0$ for all pure states $|\phi\rangle$.

The above conditions provide a characterization of density operators that is intrinsic to the operator itself: one can define a density operator to be a positive Hermitian operator ρ which has trace equal to one [7]. The set of legitimate statistical operators (and the corresponding family of mixed states) is a convex set and a state is pure when it is an extremal point of that set [47]. The density operator is often known as the density matrix or statistical operator and all these terms are used interchangeably. The basic postulates of quantum mechanics related to unitary evolution and measurement can be completely rephrased in the density operator language. The expectation value of the measurement of an observable M when the system is in the state ρ, is

$$\langle M\rangle_\rho = \sum_i p_i \langle\psi_i|M|\psi_i\rangle = \mathrm{Tr}[\rho M] \tag{1.23}$$

and the variance (or uncertainty) of M is given by

$$\delta^2(M)_\rho = \langle (M - \langle M\rangle_\rho)^2\rangle_\rho = \langle M^2\rangle_\rho - \langle M\rangle_\rho^2. \tag{1.24}$$

Given a density matrix ρ, the decomposition in equation (1.22) is not unique. One may have different $\{p_i, |\psi_i\rangle\}$ leading to the same ρ:

$$\sum_j p'_j |\psi'_j\rangle\langle\psi'_j| = \sum_i p_i |\psi_i\rangle\langle\psi_i|. \tag{1.25}$$

As an illustration consider for instance two decompositions

$$\begin{aligned}\rho &= \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix} = \frac{1}{4}|00\rangle\langle 00| + \frac{1}{4}|01\rangle\langle 01| + \frac{1}{4}|10\rangle\langle 10| + \frac{1}{4}|11\rangle\langle 11| \\ &= \frac{1}{8}\Big(|00\rangle + |11\rangle\Big)\Big(\langle 00| + \langle 11|\Big) + \frac{1}{8}\Big(|00\rangle - |11\rangle\Big)\Big(\langle 00| - \langle 11|\Big)\end{aligned}$$

$$+\frac{1}{8}\Big(|01\rangle + |10\rangle\Big)\Big(\langle 01| + \langle 10|\Big) + \frac{1}{8}\Big(|01\rangle - |10\rangle\Big)\Big(\langle 01| - \langle 10|\Big). \quad (1.26)$$

Thus these two different ensembles of quantum states give rise to the same density matrix. In general, the eigenvalues and eigenvectors of a density matrix just indicate one of many possible ensembles that may give rise to a particular density matrix. Such equivalent ensembles or mixtures cannot be distinguished by measurement of observables alone. This equivalence can be characterized precisely by finding the class of ensembles which give rise to a particular density matrix.

The ensembles $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ and $\rho' = \sum_j p'_j|\psi'_j\rangle\langle\psi'_j|$, where $|\psi_i\rangle, |\psi'_j\rangle$ are normalized states and p_i, p'_j are the probability distributions, define the same density operator (1.25) if and only if there is a unitary matrix $U = (u_{ij})$, that is, $U^\dagger U = \mathbb{I}$ such that

$$\sqrt{p_i}|\psi_i\rangle = \sum_j u_{ij}\sqrt{p'_j}|\psi'_j\rangle, \quad (1.27)$$

where we may extend the smaller ensemble with entries having probability zero in order to make the two ensembles the same size [7]. This unitary freedom in the ensemble for density matrices characterizes the freedom in ensembles $\{p_i, |\psi_i\rangle\}$ that gives rise to a given density matrix ρ.

This non-unique character of the decomposition of ρ as a "mixture" of pure states is very relevant, amongst others, for the discussion of the concept of "entanglement of formation", see equations (2.16) and (2.17).

The main applications of the density operator formalism are the descriptions of quantum systems whose state is only partially known, and the description of subsystems of a composite quantum system, where the latter description is provided by the reduced density operator. The reduced density matrices are an extremely powerful and indispensable tool for the description of individual subsystems and they form the basis of the description of the phenomenon of quantum entanglement. The density matrix of the subsystem is calculated as a partial trace of the density matrix of the whole system. To illuminate the concept of partial trace, suppose we have two systems A and B whose state is described by ρ_{AB}. The reduced density operator for system A is defined by $\rho_A = \mathrm{Tr}_B(\rho_{AB})$,

where Tr_B is the partial trace over system B. The partial trace is defined by [7]

$$\begin{aligned}\mathrm{Tr}_B\big(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|\big) &= \mathrm{Tr}_B\big(|a_1 b_1\rangle\langle a_2 b_2|\big) \\ &= |a_1\rangle\langle a_2|\,\mathrm{Tr}\big(|b_1\rangle\langle b_2|\big) = |a_1\rangle\langle a_2|\big(\langle b_2|b_1\rangle\big) \quad (1.28)\end{aligned}$$

where $|a_{1,2}\rangle$ are any two vectors in the state space of A and $|b_{1,2}\rangle$ are any two vectors in the state space of B. In addition to eq. (1.28) the partial trace is required to be linear in its input. Equation (1.28) leads to the expression for the matrix elements of the reduced (also called marginal) density matrices ρ_A and ρ_B. If we express ρ_A, ρ_B and ρ_{AB} in terms of the orthonormal bases $\{|i\rangle\}$ and $\{|j\rangle\}$ (respectively, of the state spaces of A and B) and the associated product basis $\{|ij\rangle\}$, one has,

$$\begin{aligned}\langle i|\rho_A|j\rangle &= \sum_k \langle ik|\rho_{AB}|jk\rangle \\ \langle k|\rho_B|l\rangle &= \sum_i \langle ik|\rho_{AB}|il\rangle. \quad (1.29)\end{aligned}$$

One sees that the matrix elements of the marginal density matrix of each subsystem are actually obtained by recourse to a trace operation that "acts" upon the labels corresponding to the other subsystem.

Marginal density matrices are the "quantum" analogues of marginal probability distributions in classical probability theory.

The partial trace is used to describe part of a larger quantum system since it is the unique operation which gives rise to the correct description of observable quantities for subsystems of a composite system. That is, the reduced density operator ρ_A provides the correct measurement statistics for measurements made on system A. The partial trace can be regarded as averaging out the information from the subsystem which is not under consideration (in this illustration B) which can nonetheless be entangled with the subsystem whose description we want (which is A in this case).

1.1.7 Quantum entropic measures

A proper extension of Shannon's entropy to the quantum case is given by the von Neumann entropy, defined as

$$S(\rho) \;=\; -\mathrm{Tr}(\rho \log_2 \rho), \tag{1.30}$$

where ρ is the density matrix of the system. Thus quantum states are described by replacing probability distributions with density operators. In order to compute $S(\rho)$, one has to write ρ in terms of its eigenbasis. Since $\lim_{p\to 0} p \log_2 p = 0$ is well defined, we can set $0 \log_2 0 = 0$ by continuity.

If the system under consideration is finite, in other words it has a finite-dimensional matrix representation, the entropy (1.30) describes the departure of our system from a pure state. That is to say, it measures the degree of mixture of our state describing a given finite system.

The following are properties of the von Neumann entropy [7]:

- $S(\rho)$ is only zero for pure states.
- $S(\rho)$ is maximal and equal to $\log_2 N$ for a maximally mixed state, N being the dimension of the Hilbert space.
- $S(\rho)$ is invariant under a change of basis of ρ, that is, $S(\rho) = S(U\rho U^\dagger)$, with U being a unitary transformation.
- Given two density matrices ρ_I, ρ_{II} describing independent systems I and II, we have that $S(\rho)$ is additive: $S(\rho_I \otimes \rho_{II}) = S(\rho_I) + S(\rho_{II})$.
- If ρ_A and ρ_B are the reduced (marginal) density matrices of the general state ρ_{AB}, then
$$S(\rho_{AB}) \;\leq\; S(\rho_A) \;+\; S(\rho_B). \tag{1.31}$$

The last property is known as subadditivity and also holds for the Shannon entropy. However, some properties of the Shannon entropy do not hold for the von Neumann entropy, thus leading to many interesting consequences for quantum

information theory [7]. While in Shannon's theory the entropy of a (discrete) composite system can never be lower than the entropy of any of its parts, in quantum theory this is not the case and can actually be seen as an indicator of an entangled state ρ_{AB}.

Another property is the concavity of the entropy, that is, the entropy is a concave function of its inputs. Given probabilities p_i such that $\sum_i p_i = 1$ and corresponding density operators ρ_i, the entropy complies with the inequality [7]

$$S\left(\sum_i p_i \rho_i\right) \geq \sum_i p_i S(\rho_i). \tag{1.32}$$

The input argument on the left side, $\sum_i p_i \rho_i$, expresses the state of a quantum system that is in an unknown state ρ_i with probability p_i. Thus the uncertainty about this mixture of states has to be greater than the average uncertainty of the states ρ_i, since the state $\sum_i p_i \rho_i$ contains ignorance not only due to the states ρ_i, but also due to the index i [7].

In the framework of quantum information theory the von Neumann entropy is extensively used in different forms such as conditional and relative entropies. The von Neumann entropy is the most fundamental quantum entropic measure. However, other entropic measures, such as the Rényi and the Tsallis one, are very useful in the analysis of several particular problems. For example, the Rényi and the Tsallis entropies lead (for some values of the entropic parameter q) to stronger entropic entanglement criteria for mixed states than the von Neumann entropy.

In the quantum case the Tsallis entropy becomes

$$S_q^{(T)}(\rho) = \frac{1}{q-1}\left[1 - \mathrm{Tr}\left(\rho^q\right)\right] \tag{1.33}$$

and the Rényi entropy

$$S_q^{(R)}(\rho) = \frac{1}{1-q}\log_2\left[\mathrm{Tr}\left(\rho^q\right)\right]. \tag{1.34}$$

The above quantum entropic measures, namely the von Neumann entropy, Tsallis entropy and Rényi entropy are all invariant under unitary transformation, since the trace is invariant under unitary transformation.

1.1.8 Distinguishability measure for quantum mechanical density operators: fidelity distance

A measure of distance between quantum states is the fidelity. It is not a metric on density operators, however, it has many of the properties one expects of a good distance measure. The main properties of this measure that we are going to use are briefly reviewed.

First, the fidelity distance between two quantum states (represented by two density matrices) of a given quantum system is given by [7]

$$F[\,\rho,\sigma\,] \;=\; \mathrm{Tr}\sqrt{\rho^{1/2}\sigma\rho^{1/2}}. \tag{1.35}$$

In the particular case that one of the states is pure, we have

$$F[\,|\psi\rangle,\rho\,] \;=\; \sqrt{\langle\psi|\rho|\psi\rangle}, \tag{1.36}$$

and when both states are pure the fidelity reduces to the modulus of the overlap between the two states.

A fundamental property of the fidelity measure is that it remains constant under unitary transformations,

$$F[\,U\rho\,U^{\dagger},U\sigma U^{\dagger}\,] \;=\; F[\,\rho,\sigma\,]. \tag{1.37}$$

If we have a composite system AB, the distance between two density matrices describing two states of the composite system is smaller or equal to the distance between the marginal density matrices associated with one of the subsystems,

$$F[\,\rho_{AB},\sigma_{AB}\,] \;\leq\; F[\,\rho_{A},\sigma_{A}\,]. \tag{1.38}$$

Finally, the fidelity distance between two factorizable density matrices complies with

$$F[\,\rho_0 \otimes \sigma_0, \rho_1 \otimes \sigma_1\,] \;=\; F[\,\rho_0, \rho_1\,]\,F[\,\sigma_0, \sigma_1\,]. \tag{1.39}$$

The fidelity distance is symmetric in its inputs and it is a number between zero and one, $F = 0$ corresponds to completely distinguishable density matrices, whereas $F = 1$ signifies that the density matrices are identical [7].

1.2 Conservation of information

The conservation of information is a fundamental principle of physics, both at the classical and quantum levels. One of the most important features of the behaviour of closed, isolated physical systems is the conservation of information. A nice description of information conservation in closed, isolated systems is given by Susskind [48]: "There is another very subtle law of physics that may be even more fundamental than energy conservation. It's sometimes called reversibility, but let's just call it *information conservation*. Information conservation implies that if you know the present with perfect precision, you can predict the future for all time. But that's only half of it. It also says that if you know the present, you can be absolutely sure of the past. It goes in both directions."

He goes on to say: "The laws of Quantum Mechanics are very subtle - so subtle that they allow randomness to coexist with both energy conservation and information conservation."

The most complete possible knowledge about the state of a physical system is represented in classical mechanics by a point in the associated phase space, and in quantum mechanics by a vector in the system's Hilbert space. Often one has to deal with an incomplete or partial knowledge about the state of the system. This situation is described classically by a probability density in phase space and quantum mechanically by a density matrix. The amount of knowledge about the system's state associated with these descriptions does not change during the evolution of a closed system. This conservation of information can be expressed in two alternative and complementary ways. On the one hand, we can associate

an entropic functional to the aforementioned probability density or density matrix. These entropic functionals provide a quantitative measure of the lack of knowledge that we have about the precise dynamical state of the system. These measures are preserved during the evolution of the system [49]. In the classical regime this conservation of information is closely related to Liouville's theorem stating the conservation of phase space volume during Hamiltonian evolution. The conservation of information can also be expressed in another way. Let us consider two initial conditions described either by two initial phase space probability densities, or by two initial density matrices. Then, one can consider the degree to which these initial states are distinguishable from each other. A quantitative measure of the amount of "distinguishability" is given classically by an appropriate "distance" or "divergence" between the two probability densities [16]. The most useful ones are the Kullback-Leibler measure and its generalizations. In the quantum case, distinguishability can be quantitatively characterized by recourse to the fidelity measure [7]. In the quantum case this distinguishability measure is also relevant for pure states, in which case it reduces to the modulus of the overlap between the two states. These distinguishability measures are preserved during the evolution of closed physical systems, and this fact constitutes another manifestation of the conservation of information associated with the basic laws of Nature. This distinguishability-based notion of conservation of information is extremely important in quantum information theory and it is at the basis of important features of quantum information, such as those described by the no-cloning and the no-deleting theorems.

Both in the classical and quantum regimes, the information-preserving character of dynamical evolution as given by the Liouville or the von Neumann equation respectively, is one of the fundamental features of the basic laws of nature. That is, in both quantum mechanics and classical mechanics the equations of motion ensure the exact conservation of information for a closed, isolated system. In that regard, I will discuss the main evolution equations, then show in some detail the conservation of information in both the classical and quantum case and finally move on to explain Landauer's principle and its implications.

1.2.1 Main evolution equations

In classical and statistical Hamiltonian mechanics, the Liouville theorem plays an important role. It states that the phase space distribution function, which is a representation of the statistical properties of an ensemble of physical systems, remains constant along the trajectories of the system. In other words, the density of systems in the vicinity of some given system in phase space is constant in time. If we consider a dynamical system with canonical coordinates q_i and conjugate momenta p_i $(i = 1, 2, \ldots, n)$, the dynamical evolution of the phase space distribution function $\rho(p, q, t)$ is governed by the Liouville equation [50]

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right) = 0, \tag{1.40}$$

where the time derivatives (denoted by dots) of the generalized coordinates and momenta are evaluated according to Hamilton's equations,

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{1.41}$$

The Liouville equation is linear and it governs the time evolution of a probability density that describes a statistical ensemble of dynamical systems, all evolving according to the same equations of motion. From this equation it is clear, that the probability distribution function is conserved along the orbit in phase space.

In the case of general classical deterministic dynamical systems whose evolution is determined by the equations of motion

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(\mathbf{x}), \quad \text{with } \mathbf{x}, \mathbf{v} \in \mathcal{R}^N \tag{1.42}$$

where $\mathbf{x}$ indicates a point in the corresponding N-dimensional phase space. The time-dependent probability distribution $\mathcal{P}(\mathbf{x}, t)$ describes the dynamics of a statistical ensemble of such systems. The Liouville equation governs its dynamics [16],

$$\frac{\partial}{\partial t}\mathcal{P} + \nabla \cdot (\mathbf{v}\mathcal{P}) = 0, \tag{1.43}$$

where the ∇-operator is N-dimensional and defined in the standard way,

$$\nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_N} \right). \tag{1.44}$$

Hamiltonian dynamics is a particular instance of (1.42). In that case we have a Hamiltonian system with n degrees of freedom and so $N = 2n$, $\mathbf{x} = (q_1, q_2, \ldots, q_n, p_1, p_2, \ldots, p_n)$, $v_i = \dot{q}_i = \partial H/\partial p_i$ $(i = 1, 2, \ldots, n)$ and $v_i = \dot{p}_{i-n} = -\partial H/\partial q_{i-n}$ $(i = n+1, n+2, \ldots, 2n)$, where q_i and p_i stand for the generalized coordinates and momenta of the Hamiltonian system, respectively. The Liouville equation (1.43) then becomes (1.40) [16].

In the quantum mechanical case, a statistical ensemble of several quantum states is described by the density matrix. The density matrix is thus the quantum mechanical analogue to the classical statistical phase space probability distribution. In classical physics, the only reason for introducing a phase space probability is a lack of detailed knowledge of the state. In quantum mechanics, there is another reason, namely entanglement [49]. The time evolution of pure states is given by the Schrödinger equation. The von Neumann equation describes the evolution of mixed states $\rho(t)$

$$i\hbar \frac{d}{dt}\rho(t) = [H(t), \rho(t)], \tag{1.45}$$

where the brackets denote the commutator and the assumption is that the Hamiltonian of the system $H(t)$ is perfectly well known, unlike the state of the system. The von Neumann equation can be derived from the Schrödinger equation using the linearity of density matrices (1.22) and the Schrödinger equation [51]. Likewise, the Schrödinger equation can be derived from the von Neumann equation, so both are equivalent.

1.2.2 Conservation of information in the classical and quantum case

We now turn our attention to the conservation of information in both the classical and the quantum case. As was already said, this information conservation

can be expressed in two alternative ways. First, let us look at the conservation of the generalized Kullback-Leibler measure in more detail. The evolution of the system is determined by equation (1.42) and the Liouville equation (1.43) governs the dynamics of the time-dependent probability distribution $\mathcal{P}(\mathbf{x},t)$. The idea is to show that the generalized Kullback-Leibler distance $G[\mathcal{P}_1,\mathcal{P}_2]$ as in equation (1.20), remains constant during the time evolution of the system. The two probability distributions $\mathcal{P}_1(\mathbf{x},t)$ and $\mathcal{P}_2(\mathbf{x},t)$ satisfy the Liouville equation (1.43). Since $G[\mathcal{P}_1,\mathcal{P}_2]$ only depends on time (the integration was over $\mathbf{x}$), it means that [16]

$$
\begin{aligned}
\frac{dG}{dt} &\overset{(1)}{=} \int d\mathbf{x}\left[\frac{\partial \mathcal{P}_1}{\partial t}g+\mathcal{P}_1 g'\frac{\partial}{\partial t}\left(\frac{\mathcal{P}_1}{\mathcal{P}_2}\right)\right] \\
&= \int d\mathbf{x}\left[\frac{\partial \mathcal{P}_1}{\partial t}g+\mathcal{P}_1 g'\left\{\frac{\partial \mathcal{P}_1}{\partial t}\frac{1}{\mathcal{P}_2}-\frac{\mathcal{P}_1}{\mathcal{P}_2^2}\frac{\partial \mathcal{P}_2}{\partial t}\right\}\right] \\
&= \int d\mathbf{x}\left[\frac{\partial \mathcal{P}_1}{\partial t}\left\{g+\frac{\mathcal{P}_1}{\mathcal{P}_2}g'\right\}-\frac{\partial \mathcal{P}_2}{\partial t}\frac{\mathcal{P}_1^2}{\mathcal{P}_2^2}g'\right] \\
&\overset{(2)}{=} -\int d\mathbf{x}\left[\nabla\cdot(\mathbf{v}\mathcal{P}_1)\left\{g+\frac{\mathcal{P}_1}{\mathcal{P}_2}g'\right\}-\nabla\cdot(\mathbf{v}\mathcal{P}_2)\frac{\mathcal{P}_1^2}{\mathcal{P}_2^2}g'\right] \\
&\overset{(3)}{=} \int d\mathbf{x}\left[\mathcal{P}_1\mathbf{v}\cdot\nabla\left(g+\frac{\mathcal{P}_1}{\mathcal{P}_2}g'\right)-\mathcal{P}_2\mathbf{v}\cdot\nabla\left(\frac{\mathcal{P}_1^2}{\mathcal{P}_2^2}g'\right)\right] \\
&\quad -\overline{\mathbf{v}}\,\mathcal{P}_1\left\{g+\frac{\mathcal{P}_1}{\mathcal{P}_2}g'\right\}\Big| + \overline{\mathbf{v}}\,\mathcal{P}_2\frac{\mathcal{P}_1^2}{\mathcal{P}_2^2}g'\Big| \\
&= \int d\mathbf{x}\left[\mathbf{v}\cdot\left(\mathcal{P}_1\nabla g+\mathcal{P}_1 g'\nabla\left(\frac{\mathcal{P}_1}{\mathcal{P}_2}\right)+\frac{\mathcal{P}_1^2}{\mathcal{P}_2}\nabla g'-2\mathcal{P}_1\nabla\left(\frac{\mathcal{P}_1}{\mathcal{P}_2}\right)g'\right.\right. \\
&\quad \left.\left.-\frac{\mathcal{P}_1^2}{\mathcal{P}_2}\nabla g'\right)\right]-\overline{\mathbf{v}}\,\mathcal{P}_1 g\Big| \\
&\overset{(4)}{=} \int d\mathbf{x}\left[\mathbf{v}\cdot\left(\mathcal{P}_1\nabla g-\mathcal{P}_1\nabla\left(\frac{\mathcal{P}_1}{\mathcal{P}_2}\right)g'\right)\right] \\
&\overset{(5)}{=} \int d\mathbf{x}\left[\mathbf{v}\cdot\left(\mathcal{P}_1 g'\nabla\left(\frac{\mathcal{P}_1}{\mathcal{P}_2}\right)-\mathcal{P}_1 g'\nabla\left(\frac{\mathcal{P}_1}{\mathcal{P}_2}\right)\right)\right] \\
&= 0.
\end{aligned}
\tag{1.46}
$$

Here we have made use of (1) product and chain rule, (2) Liouville equation, (3) integration by parts, where $\overline{\mathbf{v}}$ denotes the sum of the components of $\mathbf{v}$, (4) the assumption that eventual boundary/surface terms vanish and (5) chain rule $\nabla g = g'\nabla\left(\frac{\mathcal{P}_1}{\mathcal{P}_2}\right)$. Thus $G[\mathcal{P}_1,\mathcal{P}_2]$ is conserved during the dynamical evolution.

The second way of expressing the information conservation is that entropic functionals associated with the probability density $\mathcal{P}(\mathbf{x},t)$ are preserved during the evolution of the divergenceless system (see Subsubsection 3.1.2.1 for more detail on divergenceless dynamical systems). Let the entropic functional be the particular case of Tsallis' family of measures, of which the Shannon entropy is the limit case $q \to 1$. In the continuous case the Tsallis entropy is

$$S_q^{(T)}(\mathcal{P}) = \frac{1}{q-1}\Big(1 - \int \mathcal{P}^q d\mathbf{x}\Big). \tag{1.47}$$

Since the entropy only depends on time, we have that

$$\begin{aligned}
\frac{dS_q^{(T)}}{dt} &= -\frac{1}{q-1}\int q\mathcal{P}^{q-1}\frac{\partial \mathcal{P}}{\partial t}d\mathbf{x} \\
&\overset{(1)}{=} -\frac{q}{q-1}\int \mathcal{P}^{q-1}\big[-\nabla\cdot(\mathbf{v}\mathcal{P})\big]d\mathbf{x} \\
&\overset{(2)}{=} -\frac{q}{q-1}\int\{q-1\}\mathcal{P}^{q-2}\nabla\mathcal{P}\cdot(\mathbf{v}\mathcal{P})d\mathbf{x} + \frac{q}{q-1}\mathcal{P}^{q-1}\mathcal{P}\,\overline{\mathbf{v}}\Big| \\
&\overset{(3)}{=} -q\int \mathcal{P}^{q-1}\nabla\mathcal{P}\cdot\mathbf{v}d\mathbf{x} \\
&\overset{(4)}{=} -\int \nabla(\mathcal{P}^q)\cdot\mathbf{v}d\mathbf{x} \\
&\overset{(5)}{=} -\mathcal{P}^q\,\overline{\mathbf{v}}\Big| + \int \mathcal{P}^q(\nabla\cdot\mathbf{v})d\mathbf{x} \\
&\overset{(6)}{=} \int \mathcal{P}^q(\nabla\cdot\mathbf{v})d\mathbf{x} \overset{(7)}{=} 0,
\end{aligned} \tag{1.48}$$

where one makes use of (1) Liouville equation, (2) integration by parts where $\overline{\mathbf{v}}$ is the sum of the components of $\mathbf{v}$, (3) the assumption that eventual boundary/surface terms vanish, (4) $q\mathcal{P}^{q-1}\nabla\mathcal{P} = \nabla(\mathcal{P}^q)$, (5) integration by parts again, (6) vanishing of boundary terms again and (7) $\nabla\cdot\mathbf{v} = 0$ since we are considering divergenceless dynamical systems. Thus the Tsallis family of measures is preserved during the evolution of the system.

We now move to the quantum case. As mentioned in Subsection 1.1.8, the fidelity is invariant under unitary evolution and hence the distance between two states remains the same. Given a finite-dimensional density matrix $\rho(t)$, a general entropic measure associated with it such as the Tsallis entropy, remains invariant

under unitary evolution, that is, is conserved when $\rho(t)$ evolves according to the von Neumann equation (1.45) with the Hamiltonian being time-independent. The reason for this is that the trace is invariant under unitary transformations and hence the Tsallis entropy is invariant under unitary evolution. Thus quantum mechanics, despite its unpredictability, nonetheless respects the conservation of information.

1.2.3 Landauer's principle

There is a growing consensus that information is endowed with physical reality. Instead of thinking of information as an abstract quantity that has nothing to do with the physical world, we realize that information must be encoded into a physical system and must be processed using the physical dynamical laws. Quoting Landauer [52], "Information is inevitably tied to a physical representation and therefore to restrictions and possibilities related to the laws of physics and the parts available in the universe". This implies that all limitations on information processing or transmission are determined by the restrictions of the underlying fundamental laws of physics. The information theory of Shannon implicitly assumes that information processing is governed by the laws of classical physics. However, a more accurate description of the microscopic world is given by quantum mechanics and so quantum information, which is governed by the laws of quantum mechanics, is a more accurate description of information theory. Since there is a fundamental difference between the classical laws and the quantum laws of physics, the respective resulting information processing is also fundamentally different. Quantum information is a much broader and more general concept and thus allows information-processing protocols that have no classical analogue. This renders the Shannon theory of information a special case of quantum information theory.

Landauer's principle states that by erasing one bit of information, one dissipates on average at least $kT\ln 2$ of energy into the environment, where T is the temperature at which the erasure takes place and k is Boltzmann's constant. Landauer's argument for this is roughly as follows. Erasure or overwriting of data is associated with physical irreversibility since it is a logical function that does

not have a single-valued inverse [21] and thus transforms information from an accessible form to an inaccessible form, known as entropy [18]. He argues that this requires the dissipation of heat of the order of magnitude kT since a bit has one degree of freedom. Before erasure a bit can be in any of the two possible states whereas after being erased it can only be in one state which implies a change in information entropy of $-k \ln 2$. Since entropy in a closed system cannot decrease, Landauer reasons that it must appear somewhere else as heat. Thus Landauer's principle links information in the sense of Shannon's measure [27] with the energy that is required to erase it [19, 53, 54]. There is a crucial assumption implicit in this reasoning, namely that information entropy translates into physical entropy. Landauer's principle is valid both for classical and quantum systems [21].

Landauer's principle holds for any logically irreversible manipulation of information, the erasure of a bit being one case, the merging of two computation paths another one. This is accompanied by a corresponding increase in entropy of non-information-bearing degrees of freedom of either the environment or the information processing apparatus [53]. This increase in entropy typically takes the form of energy transferred into the computing device, converted to heat and thus dissipated into the environment.

Conversely, any logically reversible transformation of information can in principle be accomplished by an appropriate physical mechanism which operates in a thermodynamically reversible manner. Bennett showed that in principle all computation, which is inevitably done with real physical degrees of freedom, could be performed in a logically reversible manner which implies that computation, in principle, requires no dissipation [55]. The reason that real computers dissipate large amounts of heat is solely due to practical engineering concerns, in particular, due to the fact of having only a *finite* memory storage capacity and, consequently, the need to erase lots of information during the computing process.

Landauer's principle is one of the most fundamental results in the physics of information. It constituted a historical landmark in the development of the field by directly connecting information processing with conventional physical quantities [18]. Most remarkably, it played a prominent role in the final defeat of

Maxwell's demon [6, 53]. Landauer's principle has profound implications since it allows for novel, physically motivated derivations of several important results in both classical and quantum information theory [22]. In addition, it is a useful and powerful heuristic tool for obtaining new derivations of, or for establishing new links between, fundamental aspects of thermodynamics and other areas of physics [23].

It has to be said that most derivations of Landauer's principle can be regarded as semi-phenomenological, since they are based on a direct application of the second law of thermodynamics. However, derivations based upon dynamical principles have also been advanced. They assume that the systems under consideration are governed by a Hamiltonian dynamics and are in thermal equilibrium, implying that they can be described by Gibbs' canonical distributions. Piechocinska [21] showed how to derive this principle microscopically for classical systems that are either discrete or continuous in space and time and also for quantum systems, without referring directly to the second law of thermodynamics (Clausius' inequality) in either cases. The derivation utilizes the concavity of the logarithm which leads to an inequality equivalent to Landauer's statement. An alternative derivation based on well-established properties of the Shannon-Gibbs-Boltzmann entropy is given by Daffertshofer and Plastino in [20]. This derivation makes use of the (sub)additivity of the entropy, resulting in a least increase of entropy in the heat bath and thus energy gain even if the information erasure is done adiabatically. The reason for this is that the conservation of the total amount of information implies that the surrounding heat bath must contain the information being erased in the bit-ensemble. This argument also holds in the quantum mechanical case when all the assumptions are adapted accordingly [20].

Information processing can be realized in various physical settings and so more general formulations applicable to non-equilibrium scenarios which involve non-Gibbs ensemble distributions have been advanced [56]. In view of the fundamental character of Landauer's principle it is also highly desirable to explore extensions of it applicable to systems governed by more general kinds of dynamics, that is, by non-Hamiltonian dynamics [57]. This is investigated in Section 3.1.

The ideas and methods from the physics of information lead to important points of contact between physics and biology. In fact, information processing is clearly at the very heart of biology and has been appropriately dubbed the "touchstone of life" [17].

1.3 Quantum no-cloning

The quantum no-cloning theorem constitutes a hallmark feature of quantum information. It states that quantum information cannot be cloned: an unknown quantum state of a given (source) system cannot be perfectly duplicated while leaving the state of the source system unperturbed [58, 59]. No unitary (quantum mechanical) transformation exists that can perform the process

$$|\psi\rangle \otimes |0\rangle \otimes |\Sigma\rangle \longrightarrow |\psi\rangle \otimes |\psi\rangle \otimes |\Sigma_\psi\rangle, \tag{1.49}$$

for arbitrary source states $|\psi\rangle$. In the above equation $|0\rangle$ and $|\Sigma\rangle$ denote, respectively, the initial standard states of the target qubit and of the copy machine, and $|\Sigma_\psi\rangle$ is the final state of the copy machine. In other words, universal quantum cloning is not permitted by the basic laws of quantum mechanics. The impossibility of universal quantum cloning can be proved in two different ways. One can show that it is not compatible with the linearity of quantum evolution or that it is not compatible with the unitarity of quantum evolution.

The above theorem can be generalized for mixed states and is then called the no-broadcasting theorem, for which I will provide an alternative proof which makes use of the fidelity distance between two quantum states (represented by two density matrices) of a given quantum system. The main properties of this measure that we are going to use have been briefly reviewed in Subsection 1.1.8.

1.3.1 No-broadcasting theorem

A general and intuitive proof of the no-broadcasting theorem is presented. This theorem highlights the difference between classical and quantum mechanics and is of great relevance in quantum information theory. It is a generalization of the

no-cloning theorem as one considers general mixed states instead of just pure ones.

Exploring features of quantum mechanics that are purely quantum phenomena is relevant in a theoretical fundamental context [60] and also in a practical context [61], as these features can either enhance quantum computation or place constraints on it. The no-broadcasting theorem says that we cannot copy an unknown mixed state even if we only reproduce it marginally on the two separate quantum systems we are broadcasting onto. Broadcasting is achieved strictly when all the input states are mutually commuting. The no-cloning and no-broadcasting theorems have been of great interest since their initial conception [58, 62]. Several different versions of the proofs have been given over the years [63, 64] and the no-broadcasting theorem has also been extended to more general frameworks [65].

Another proof of the no-broadcasting theorem is provided, where we only initially follow the proof given in [62] but where we do not restrict ourselves to invertible density matrices, as in [64]. The strategy is to assume that there exists a physical process, that is, a unitary evolution such that at least two arbitrary mixed states can be broadcast and then show that they necessarily have to commute. The general problem is as follows: we have a three-partite quantum system ABC, where systems A and B each have an N-dimensional Hilbert space. System A is in either of the two quantum states ρ_0 or ρ_1 and we assume both states can be broadcast. System B is in the standard quantum state Σ which is meant to receive the unknown state. System C is the auxiliary system which acts as the copy-machine and which is in some standard state Υ. The initial state of our system is thus $\rho_s \otimes \Sigma \otimes \Upsilon$ and we do not know whether $s = 0$ or 1. After successful broadcasting which is described by a unitary evolution of the three-partite system, $\Omega_s = U(\rho_s \otimes \Sigma \otimes \Upsilon)U^\dagger$, subsystem AB is in any state $\tilde{\rho}_s$ on the N^2-dimensional Hilbert space such that

$$\mathrm{Tr}_A(\tilde{\rho}_s) = \rho_s \quad \text{and} \quad \mathrm{Tr}_B(\tilde{\rho}_s) = \rho_s. \tag{1.50}$$

Here Tr_A and Tr_B denote partial traces over A and B respectively and $\tilde{\rho}_s = \mathrm{Tr}_C(\Omega_s)$. We show that this is possible only if ρ_0 and ρ_1 commute.

Our proof is based upon the concept of fidelity between two density operators introduced in the previous Subsection 1.1.8. The fidelity between two quantum states is a measure of distinguishability between the two states and is given by eq. (1.35). So in our case we have

$$F[\,\rho_0,\rho_1\,] \;=\; \mathrm{Tr}\sqrt{\rho_0^{1/2}\rho_1\rho_0^{1/2}} \tag{1.51}$$

and making use of properties (1.37) and (1.39) respectively, we have

$$F[\,U(\rho_0\otimes\Sigma\otimes\Upsilon)U^\dagger, U(\rho_1\otimes\Sigma\otimes\Upsilon)U^\dagger\,] \;=\; F[\,\rho_0\otimes\Sigma\otimes\Upsilon,\rho_1\otimes\Sigma\otimes\Upsilon\,] \tag{1.52}$$

and

$$F[\,\rho_0\otimes\Sigma\otimes\Upsilon,\rho_1\otimes\Sigma\otimes\Upsilon\,] \;=\; F[\,\rho_0,\rho_1\,]\,F[\,\Sigma,\Sigma\,]\,F[\,\Upsilon,\Upsilon\,]. \tag{1.53}$$

Combining equations (1.52) and (1.53) results in

$$F[\,\Omega_0,\Omega_1\,] \;=\; F[\,\rho_0,\rho_1\,]. \tag{1.54}$$

A more intuitive way of viewing the fidelity is in terms of generalized measurements or positive operator-valued measures (POVM) $\{E_b\}$. To give a short review of POVM measurements [7], E_b was defined to be $E_b \equiv M_b^\dagger M_b$ where M_b is the measurement operator associated with outcome b of a measurement performed upon a quantum system ρ. The measurement is described by these measurement operators M_b and so the probability of outcome b is given by $p(b) = \mathrm{Tr}(\rho E_b)$. Expressing the fidelity in those terms [7],

$$F[\,\rho_0,\rho_1\,] \;=\; \min_{\{E_b\}}\sum_b \sqrt{\mathrm{Tr}(\rho_0 E_b)}\sqrt{\mathrm{Tr}(\rho_1 E_b)}, \tag{1.55}$$

which gives the minimum overlap between the probability distributions $p_0(b) = \mathrm{Tr}(\rho_0 E_b)$ and $p_1(b) = \mathrm{Tr}(\rho_1 E_b)$. The minimum is taken over all sets of positive operators $\{E_b\}$ such that $\sum_b E_b = \mathbb{I}$. The POVM that achieves the minimum in eq. (1.55) is called the optimal POVM. In light of this, eq. (1.54) means that our ability to distinguish which state we were given remains the same after we

broadcast it.

Let us assume that $\{E_{\lambda_i}\}$ is the optimal POVM for distinguishing ρ_0 and ρ_1. We can construct it in such a way that $E_{\lambda_i} = |\lambda_i\rangle\langle\lambda_i|$. For each s we have that

$$\mathrm{Tr}[\Omega_s(E_{\lambda_i} \otimes \mathbb{I} \otimes \mathbb{I})] = \mathrm{Tr}_A[\mathrm{Tr}_B(\mathrm{Tr}_C\Omega_s)E_{\lambda_i}] = \mathrm{Tr}_A[\rho_s E_{\lambda_i}] = \mathrm{Tr}[\rho_s E_{\lambda_i}] \tag{1.56}$$

and so it follows that

$$\begin{aligned} F_A[\,\rho_0,\rho_1\,] &= \sum_{\lambda_i} \sqrt{\mathrm{Tr}[\Omega_0(E_{\lambda_i} \otimes \mathbb{I} \otimes \mathbb{I})]}\sqrt{\mathrm{Tr}[\Omega_1(E_{\lambda_i} \otimes \mathbb{I} \otimes \mathbb{I})]} \\ &= \sum_{\lambda_i} \sqrt{\mathrm{Tr}[\rho_0 E_{\lambda_i}]}\sqrt{\mathrm{Tr}[\rho_1 E_{\lambda_i}]} = F[\,\rho_0,\rho_1\,] \;=\; F[\,\Omega_0,\Omega_1\,]. \end{aligned} \tag{1.57}$$

The second last equality follows from the assumption that $\{E_{\lambda_i}\}$ is the optimal POVM for distinguishing between ρ_0 and ρ_1 and the last equality follows from eq. (1.54). We can deduce from this that the optimal POVM for distinguishing ρ_0 and ρ_1 (as seen in the marginal sense of subsystem A after broadcasting) is also the optimal POVM (expanded in the product space) for distinguishing Ω_0 and Ω_1. That is, when we perform the optimal measurement on subsystem A, we have at the same time performed the optimal measurement on the entire tripartite system. We have thus performed the best possible measurement on the whole system and there exists no other measurement from which we can obtain more information to discriminate between states Ω_0 and Ω_1.

I am only going to focus on subsystem AB after broadcasting since we are not concerned with what happens to the copy-machine. For subsystem A we choose the basis corresponding to the optimal POVM, namely $\{|\lambda_i\rangle\}$, and for subsystem B we choose an arbitrary basis $\{|\alpha_i\rangle\}$. We can then decompose the state of subsystem AB as follows

$$\tilde{\rho}_s = \sum_i p_i^{(s)} |\lambda_i\rangle\langle\lambda_i| \otimes D_i + \rho'_s \tag{1.58}$$

where $\langle\lambda_i\alpha_j|\rho'_s|\lambda_i\alpha_{j'}\rangle = 0$. We now trace out subsystem A and obtain in the

arbitrary $\{|\alpha_i\rangle\}$ basis

$$\rho_s = \mathrm{Tr}_A \tilde{\rho}_s = \sum_i p_i^{(s)} D_i. \tag{1.59}$$

After having performed the optimal measurement on the entire system after broadcasting and the measurement outcome is λ_i, the marginal density matrix associated with subsystem B is D_i. If this marginal density matrix were to depend on s, then we could perform a second measurement, this time on subsystem B, enabling us to obtain more information about the entire system and accordingly distinguish more efficiently between Ω_0 and Ω_1. This is prohibited by quantum mechanics as noted above and hence the marginal density matrices for $s = 0$ and $s = 1$ of subsystem B after the measurement have to be identical. Thus the D_i's in eq. (1.59) do not depend on s.

I am now going to make use of eq. (1.57) to obtain an expression for the fidelity. In order to do that, we need to express ρ_s in the $\{|\lambda_i\rangle\}$ basis instead of the $\{|\alpha_i\rangle\}$ basis which is done by tracing out subsystem B from $\tilde{\rho}_s$ in eq. (1.58):

$$\rho_s = \sum_i p_i^{(s)} |\lambda_i\rangle\langle\lambda_i| + \text{off-diagonal elements} \tag{1.60}$$

and thus $\mathrm{Tr}(\rho_s E_{\lambda_i}) = \langle\lambda_i|\rho_s|\lambda_i\rangle = p_i^{(s)}$. So our final expression for the fidelity is

$$F[\,\rho_0, \rho_1\,] = \sum_i \sqrt{p_i^{(0)} p_i^{(1)}} \tag{1.61}$$

where $p_i^{(0)} = \mathrm{Tr}(\rho_0 E_{\lambda_i})$ and $p_i^{(1)} = \mathrm{Tr}(\rho_1 E_{\lambda_i})$. This expression must hold when broadcasting takes place.

From eq. (1.59) we have that the D_i's are density matrices themselves and so the strong concavity property of the fidelity [7] results in

$$F\Big[\sum_i p_i^{(0)} D_i, \sum_i p_i^{(1)} D_i\Big] \geq \sum_i \sqrt{p_i^{(0)} p_i^{(1)}}, \tag{1.62}$$

and since the fidelity remains the same in any basis, it holds that

$$F[\,\rho_0,\rho_1\,] \geq \sum_i \sqrt{p_i^{(0)} p_i^{(1)}}, \tag{1.63}$$

irrespective of broadcasting. Comparing eqs. (1.61) and (1.63) we see that eq. (1.61) implies that for broadcasting to take place there has to exist a constraint between ρ_0 and ρ_1 in (1.63). What we have to do is find the conditions that enforce strict equality in (1.63) and these are then the necessary conditions for broadcasting to take place.

In the following part which is a bit technical we show that equality in (1.62) or equivalently (1.63) is only achieved when the two linear combinations $\sum_i p_i^{(0)} D_i$ and $\sum_i p_i^{(1)} D_i$ commute and hence ρ_0 and ρ_1 commute. First, let us assume $\{E_i\}$ is the optimal POVM for distinguishing ρ_0 and ρ_1 which are expressed in the basis $\{|\alpha_i\rangle\}$ ($\{E_i\}$ and $\{E_{\lambda_i}\}$ are related by a unitary transformation) and let us introduce the following notation which enables us to write eq. (1.62) in a form that can be related to the Schwarz inequality for which we know the criterion for equality:

$$r_{ij} = \mathrm{Tr}(E_i D_j) \tag{1.64}$$

$$q_i^{(0)} = \sum_j r_{ij} p_j^{(0)}$$

$$q_i^{(1)} = \sum_j r_{ij} p_j^{(1)}. \tag{1.65}$$

Using eq. (1.55) and keeping in mind that $\{E_i\}$ is optimal, the left hand side of eq. (1.62) becomes

$$\begin{aligned} F\Big[\sum_i p_i^{(0)} D_i, \sum_i p_i^{(1)} D_i\Big] &= \sum_i \sqrt{\mathrm{Tr}\Big(\sum_j p_j^{(0)} D_j E_i\Big)} \sqrt{\mathrm{Tr}\Big(\sum_j p_j^{(1)} D_j E_i\Big)} \\ &= \sum_i \sqrt{\sum_j p_j^{(0)} \mathrm{Tr}(E_i D_j)} \sqrt{\sum_j p_j^{(1)} \mathrm{Tr}(E_i D_j)} \\ &= \sum_i \sqrt{\sum_j p_j^{(0)} r_{ij}} \sqrt{\sum_j p_j^{(1)} r_{ij}}. \end{aligned} \tag{1.66}$$

Thus eq. (1.62) turns out to be

$$\sum_i \sqrt{q_i^{(0)} q_i^{(1)}} \geq \sum_i \sqrt{p_i^{(0)} p_i^{(1)}}. \tag{1.67}$$

By relating the last inequality (1.67) with the Schwarz inequality

$$\sum_j \sqrt{a_j b_j} \leq \sqrt{\sum_j a_j} \sqrt{\sum_j b_j}, \tag{1.68}$$

we will show how one can deduce the criterion for equality in (1.67). Equality in the Schwarz inequality occurs when $\{a_j\}$ and $\{b_j\}$ (which are real and positive sets) are proportional. What we then get by performing the substitution $\{a_j\} \Rightarrow \{r_{ij} p_j^{(0)}\}$ and $\{b_j\} \Rightarrow \{r_{ij} p_j^{(1)}\}$ in eq. (1.68) is

$$\sum_j r_{ij} \sqrt{p_i^{(0)} p_i^{(1)}} \leq \sqrt{q_i^{(0)} q_i^{(1)}} \tag{1.69}$$

and subsequently summing both sides over i and taking into account that $\sum_j r_{ij} = 1$ we have

$$\sum_i \Big(\sum_j r_{ij} \Big) \sqrt{p_i^{(0)} q_i^{(1)}} = \sum_i \sqrt{p_i^{(0)} p_i^{(1)}} \leq \sum_i \sqrt{q_i^{(0)} q_i^{(1)}}. \tag{1.70}$$

This is exactly what we have in eq. (1.67). Equality in the last inequality (1.70) can only be obtained if we have equality in the previous inequality (1.69) for all i. This occurs only when $\{r_{ij} p_j^{(0)}\}$ and $\{r_{ij} p_j^{(1)}\}$ are proportional. Therefore the condition for equality is

$$r_{ij} p_j^{(0)} = r_{ij} p_j^{(1)} \cdot c_i \qquad \forall i, j \tag{1.71}$$

where c_i is a proportionality constant. In order to prove that this condition implies that ρ_0 and ρ_1 commute we need to get ρ_0 and ρ_1 in as compact a form as possible in terms of linear combinations of density matrices. This compactification is achieved by means of an iterative process as dictated by the optimal POVM. Once that most compactified form has been obtained we show that the density matrices in those final linear combinations commute. To that effect we introduce

the following notation:

$$\rho_s = \sum_{j_m} p^{(s)}_{j_m,m} D_{j_m,m} \tag{1.72}$$

$$r_{ij_m,m} = \mathrm{Tr}(E_i D_{j_m,m}) \tag{1.73}$$

$$r_{ij_m,m}\, p^{(0)}_{j_m,m} = r_{ij_m,m}\, p^{(1)}_{j_m,m} \cdot c_{i,m} \tag{1.74}$$

with the new index m referring to the mth iteration of the compactification process and $m = 0$ corresponds to the original expressions in eqs. (1.59), (1.64) and (1.71). We are successively going to consider each element of the POVM in order to compactify the original sums for ρ_0 and ρ_1. Let us demonstrate this for E_1. In order to cancel the $r_{1j_0,0}$'s from both sides in eq. (1.74) they have to be non-zero. So we need to consider the set of all j_0's such that $r_{1j_0,0}$ is non-zero, $J_{1,0} = \{j_0 | r_{1j_0,0} \neq 0\}$. For $j_0 \in J_{1,0}$ we have from eq. (1.74) that $p^{(0)}_{j_0,0} = p^{(1)}_{j_0,0} \cdot c_{1,0}$ and so

$$\sum_{j_0 \in J_{1,0}} p^{(0)}_{j_0,0} D_{j_0,0} = c_{1,0} \sum_{j_0 \in J_{1,0}} p^{(1)}_{j_0,0} D_{j_0,0}. \tag{1.75}$$

Since $c_{1,0}$ may possibly be zero and hence the above $p^{(0)}_{j_0,0}$'s are then also zero, we normalize the combined terms according to the $p^{(1)}_{j_0,0}$'s and give them a new label,

$$D_{1,1} = \frac{\sum_{j_0 \in J_{1,0}} p^{(1)}_{j_0,0} D_{j_0,0}}{\sum_{j_0 \in J_{1,0}} p^{(1)}_{j_0,0}}. \tag{1.76}$$

The new probabilities for $D_{1,1}$ in the cases $s = 0$ and $s = 1$ become

$$p^{(0)}_{1,1} = c_{1,0} \left(\sum_{j_0 \in J_{1,0}} p^{(1)}_{j_0,0} \right) \qquad p^{(1)}_{1,1} = \sum_{j_0 \in J_{1,0}} p^{(1)}_{j_0,0}. \tag{1.77}$$

Each $p^{(s)}_{j_0,0} D_{j_0,0}$ with $j_0 \notin J_{1,0}$ stays the same and is relabelled $p^{(s)}_{j_1,1} D_{j_1,1}$ ($j_1 \neq 1$). Thus

$$\rho_0 = \sum_{j_0} p^{(0)}_{j_0,0} D_{j_0,0} = \sum_{j_1} p^{(0)}_{j_1,1} D_{j_1,1} \qquad \rho_1 = \sum_{j_0} p^{(1)}_{j_0,0} D_{j_0,0} = \sum_{j_1} p^{(1)}_{j_1,1} D_{j_1,1} \tag{1.78}$$

with $dim\{j_1\} \leq dim\{j_0\}$. The dimensions are equal when only one $r_{1j_0,0} \neq 0$ and

so nothing changes. Apart from that case we have compactified the sum over the index j_0 to a sum over j_1 which consists of fewer terms. This procedure is then repeated for the next element of the POVM.

At the nth step (when we consider the POVM element E_n) we either have that nothing changes since only one $r_{nj_{n-1},n-1} \neq 0$ (for that particular j_{n-1}, $r_{nj_{n-1},n-1} = 1$) or we reduce the number of terms in the sum by combining the terms with $r_{nj_{n-1},n-1} \neq 0$ into one new term as shown explicitly for $n = 1$. Since the dimension N of our Hilbert space is finite, the number of E_i's and $D_{j_0,0}$'s is finite and so either we terminate the process with only one final term which would be identical for both ρ_0 and ρ_1 and hence ρ_0 and ρ_1 are the same, or we come to a point where we can collapse the sum no longer and so from that POVM element onwards, say E_{r+1}, only one $r_{ij_t,t} \neq 0$ ($t \geq r$, $\forall i$). The final sums subsequently have the following form,

$$\rho_0 = \sum_{j_0} p^{(0)}_{j_0,0} D_{j_0,0} = \sum_{j_r} p^{(0)}_{j_r,r} D_{j_r,r} \tag{1.79}$$

$$\rho_1 = \sum_{j_0} p^{(1)}_{j_0,0} D_{j_0,0} = \sum_{j_r} p^{(1)}_{j_r,r} D_{j_r,r}. \tag{1.80}$$

Now that ρ_0 and ρ_1 have been expressed in this compactified form where both are linear combinations of $D_{j_r,r}$'s we can easily demonstrate that they commute by providing an intuitive argument why the $D_{j_r,r}$'s have to commute. In order to show that the $D_{j_r,r}$ commute for all j_r, we now consider a different situation where we prepare a system in the state $\sum_{j_r} p^{(1)}_{j_r,r} D_{j_r,r}$ and perform the POVM measurements $\{E_i\}$ on that system. Since for each i we have one j_r, say j'_r, for which $r_{ij_r,r} = \mathrm{Tr}(E_i D_{j_r,r}) = 1$ we know with certainty the system is in the state $D_{j'_r,r}$ if we obtain outcome i . So we can perfectly distinguish between all the $D_{j_r,r}$'s which means they are orthogonal and hence commute. Coming back to the original situation, we thus have that eq. (1.79) and eq. (1.80) commute and hence ρ_0 and ρ_1 commute. Thus the equality (1.61) imposed upon a general property of the fidelity (1.63) when broadcasting is implemented, implies that ρ_0 and ρ_1 commute. This proves in an intuitive manner that broadcasting is only possible when ρ_0 and ρ_1 commute.

Chapter 2

Quantum Entanglement in Distinguishable and Indistinguishable Subsystems

Quantum entanglement is one of the most essential and fundamental aspects of quantum physics [7, 66, 67]. Entanglement constitutes a fundamental resource for the implementation of quantum information processes [7] which are of technological relevance, such as quantum teleportation [68], superdense coding [7, 69], entanglement-assisted communication [70], quantum cryptography [71] and quantum computation [7, 72]. Moreover, recent developments related to the study of quantum entanglement are leading to a deeper understanding of various fundamental features of quantum physics, such as, for example, the foundations of quantum statistical mechanics [73], quantum interference [74] and the origins of quantum-to-classical transitions via the decoherence process [75]. The entanglement properties of atomic and molecular systems have also been the focus of considerable research activity (see for instance [76] and references therein).

Einstein, Podolski and Rosen were the first to point out some of the counter-intuitive properties of entangled quantum states in their famous "EPR" article in 1935 [77]. They reasoned that the strange features exhibited by entangled states suggested that quantum mechanics does not provide a "complete" description of reality. Schrödinger's paper [78] in 1935 was a response to the EPR paper.

There Schrödinger coined the term entanglement in its German version, namely "Verschränkung", and discussed the concept of entanglement, emphasizing its responsibility for the strangeness of the world revealed by quantum mechanics. In his own words, quantum entanglement is "the characteristic trait of Quantum Mechanics, the one that enforces its entire departure from classical lines of thought".

The superposition principle in quantum mechanics gives rise to the property of entanglement between quantum mechanical systems. This is due to the Hilbert space structure of the quantum mechanical state space. Thus quantum entanglement is closely related to the tensor product structure of the Hilbert space used to describe quantum mechanical composite systems. This tensor product structure admits that pure states of composite systems exist which cannot be factorized as the product of states associated with each subsystem. Such pure states of a compound quantum system that admit no description in terms of pure states of the constituent parts, are dubbed entangled. The simplest quantum system admitting entangled states is the one composed of two particles, lets label them 1 and 2, each one described by a two-dimensional Hilbert space, that is, two qubits. Let $|0\rangle_{1,2}$ and $|1\rangle_{1,2}$ denote the respective orthonormal basis states for particles 1 and 2 and so the composite system is then described by a Hilbert space of dimension four, with basis $\{|0\rangle_1|0\rangle_2, |0\rangle_1|1\rangle_2, |1\rangle_1|0\rangle_2, |1\rangle_1|1\rangle_2\}$. The convention will be to drop the subscripts and so it is implicit that the first ket in the tensor product refers to particle 1 and the second ket to particle 2, where the symbol for the tensor product has been omitted already and is naturally implicit. A separable or non-entangled state would then for example be

$$|\psi_{sep}\rangle = |00\rangle \tag{2.1}$$

and an entangled or non-separable state would be given by a Bell state

$$|\psi_{ent}\rangle = \frac{1}{\sqrt{2}}\Big(|01\rangle + |10\rangle\Big). \tag{2.2}$$

An important event in the history of the study of the foundations of quantum mechanics was the development of the de Broglie-Bohm theory, also called the pilot-wave model of quantum mechanics. It is the simplest example of what is

often called a hidden variables model for quantum mechanics. In Bohmian mechanics a system of particles is partly described by its wave function, evolving as usual according to Schrödinger's equation. This description is completed by the specification of the actual positions of the particles. The latter evolve according to the "guiding equation" which expresses the velocities of the particles in terms of the wave function. Thus, in Bohmian mechanics the configuration of a system of particles evolves via a deterministic motion guided by the wave function. The Bohmian theory then postulates an appropriate statistical ensemble of systems, each one following this deterministic motion with different initial conditions. It is worthwhile to emphasize that the experimental predictions of Bohmian mechanics are exactly the same as those derived via the standard quantum mechanical formalism. In this sense the Bohmian model constitutes a powerful counter-example of some "no-go" theorems that "forbid" general hidden variable models for quantum mechanics [79]. An important feature of the Bohmian model is that it is strongly non-local. This leads to the natural question as to whether it is possible to find a local hidden variable model for quantum mechanics.

In 1964, Bell [80] formalized the ideas of EPR of a local hidden variable model and based it on the following assumptions known as local realism and free will:

- Realism: Physical properties have definite values which exist independent of observation. In other words, the outputs of measurements are determined by the properties of the system and not by the measurement process.
- Locality: The output of a local measurement is independent of any other event or action performed with a space-like separation from the local measurement.
- Free will: Any "observer" has the freedom, at all places and all times, to choose at will, what observables to observe and measure. That is, the measurement settings of a local apparatus are independent of the properties of the system which determine the local result.

With these assumptions Bell derived an inequality for the statistical correlations of measurements performed on a bipartite system. He proved that this inequality is violated by some states of two-qubit systems. The original Bell inequality was

the inspiration for the formulation by Clauser, Horne, Shimony and Holt (CHSH) [81] of an inequality which can be experimentally tested. The CHSH inequality is part of a larger set of inequalities known generally as Bell inequalities, since Bell found the first one.

Bell inequalities can be considered as the first procedure to distinguish entangled from separable states. All entangled pure states of bipartite systems exhibit non-local features which manifest themselves through the violation of Bell inequalities [7, 24]. However, there exist mixed states that comply with all Bell inequalities but that are nonetheless entangled [82].

2.1 Entanglement measures for composite systems with distinguishable subsystems

Consider a pure bipartite state $|\psi\rangle_{AB} \in \mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$, where the Hilbert space of the complete composite system $\mathcal{H}_{AB}$ is the tensor product of the Hilbert spaces of the two subsystems. This state is entangled if it cannot be expressed as a direct product,

$$|\psi\rangle_{AB} = |\phi\rangle_A \otimes |\varphi\rangle_B. \tag{2.3}$$

Pure states that can be factorized as (2.3) are called separable or non-entangled. This definition can be extended in a natural way to hold for any number of subsystems. In the case of three or more subsystems, when the global state cannot be factorized as direct products, it does not imply that every subsystem is entangled with the rest of the system. Some subsystems may be entangled amongst themselves and disentangled from the rest.

The marginal density matrices $\rho_A = \mathrm{Tr}_B(|\psi\rangle_{AB}\langle\psi|)$ and $\rho_B = \mathrm{Tr}_A(|\psi\rangle_{AB}\langle\psi|)$ associated with an entangled pure state correspond to mixed states. This means that the joint state can be completely known, yet the subsystems are in mixed states and hence we do not have maximal knowledge concerning them. Or, using Schrödinger's words "Maximal knowledge of a total system does not necessarily imply maximal knowledge of all its parts" [83, 84]. A classic example is the singlet state of two spin-$\frac{1}{2}$ particles, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, in which neither particle has a

definite spin direction, but when one is observed to be spin-up, the other one will always be observed to be spin-down and vice versa. This is the case despite the fact that it is impossible to predict (using quantum mechanics) which set of measurement results will be observed. As a consequence, measurements performed on one system seem to be instantaneously influencing other systems entangled with it. This "instantaneous effect" is not in conflict with special relativity theory because it cannot (on its own) be used to send a message. This is known as the "no-signalling" principle. If the state is separable then subsystems A and B are with certainty in the pure states $|\phi\rangle_A$ and $|\varphi\rangle_B$ respectively.

The general idea behind the most important entanglement measures of pure bipartite states is the following. The more "mixed" the marginal density matrices associated with the subsystems are, the more entangled is the global state of the bipartite system. Consequently, any appropriate measure of the degree of mixedness of a subsystem's marginal density matrix (such as entropic measures) provides a measure of the amount of entanglement exhibited by the global, bipartite pure state.

A bipartite mixed state of a composite quantum system is entangled if it cannot be represented as

$$\rho_{AB} = \sum_i \lambda_i \rho_i^{(A)} \otimes \rho_i^{(B)}, \tag{2.4}$$

where λ_i are positive weights satisfying $\sum_i \lambda_i = 1$ and $\{\rho_i^{(A)}\}$, $\{\rho_i^{(B)}\}$ are mixed states of the respective subsystems. We can assume without loss of generality in the above expression that $\{\rho_i^{(A)}\}$ and $\{\rho_i^{(B)}\}$ are all rank-1 projections, that is, they represent pure states of the subsystems. Thus, alternatively, an equivalent definition is that the state ρ_{AB} is entangled if it cannot be written as a mixture of factorizable pure states

$$\rho_{AB} = \sum_i p_i |\alpha_i\rangle\langle\alpha_i| \otimes |\beta_i\rangle\langle\beta_i|, \tag{2.5}$$

where the p_i are, again, positive weights adding up to one and $|\alpha_i\rangle$ and $|\beta_i\rangle$ are pure states of subsystems A and B respectively. It is clear from the definition

that the family of separable states is a convex set. Separable states can be characterized physically as those that can be prepared by distant agents that can only communicate classically and where each agent operates locally on their subsystem.

The problem of deciding whether a state is separable in general is often called the "separability problem" in quantum information theory. That is, the existence of non-separable states naturally leads to the following problem. Given a mixed state ρ of a bipartite system, we want to determine whether ρ represents a separable state or not. A simple example of a separability test would be to check if the state violates a Bell inequality. However, in 1989 Werner proved that some non-separable or entangled states satisfy all generalized Bell inequalities [82]. Thus this separability test is not fully reliable.

It is also of substantial interest to quantify the entanglement of general bipartite mixed states, but unfortunately mixed-state entanglement is often very difficult to characterize quantitatively. This is why the development of new entanglement criteria or entanglement indicators is still a very active research area. One reason for the relevance of mixed-state entanglement is a connection with the transmission of quantum information through noisy quantum channels [85].

Entanglement can be regarded as a physical resource which is associated with the peculiar non-classical correlations that are possible between separated quantum systems. Entanglement lies at the basis of important quantum information processes such as quantum cryptographic key distribution [71], quantum teleportation [68], superdense coding [69] and quantum computation [72]. The experimental implementation of these processes could lead to a deep revolution in both the communication and computational technologies. There are several valid measures of entanglement, some more useful and practical than others, depending on the type of analysis to be performed and on the specific application or system being analyzed.

Entangled states cannot be prepared locally by acting on each subsystem individually [86]. This property is directly related to entanglement being invariant under local unitary transformation: one can perform a unitary operation on a

subsystem without changing the entanglement of the global system. As an illustration consider a system consisting of two subsystems A and B. A local unitary operator is then defined to be $U = U_A \otimes U_B$ where the unitary operators U_A and U_B solely act on A and B respectively. A bipartite pure state can be expressed in a standard form (the Schmidt decomposition) that is often useful. That is, according to the Schmidt decomposition an arbitrary state $|\psi\rangle_{AB}$ in the Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ of the composite system can be expressed as follows

$$|\psi\rangle_{AB} = \sum_i \sqrt{\lambda_i} |\phi_i^{(A)}\rangle |\phi_i^{(B)}\rangle \tag{2.6}$$

in terms of particular orthonormal bases $\{|\phi_i^{(A)}\rangle\}$ and $\{|\phi_j^{(B)}\rangle\}$ in $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively. These bases are called the Schmidt bases for A and B respectively [7]. The summation over the index in the Schmidt decomposition goes to the smaller of the dimensionalities of the two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ [87]. The λ_i's are non-negative real numbers satisfying $\sum_i \lambda_i = 1$. It is important to note that the Schmidt decomposition of a given quantum state is not unique and that the Schmidt decomposition pertains to a specific state of the composite system, so for two different states we have two different Schmidt decompositions [87]. Also, the Schmidt decomposition can only be performed on pure states. The marginal density matrices for ρ_A and ρ_B are given by

$$\begin{aligned} \rho_A &= \mathrm{Tr}_B\big[|\psi\rangle_{AB}\langle\psi|\big] \\ &= \sum_i \lambda_i |\phi_i^{(A)}\rangle\langle\phi_i^{(A)}| \end{aligned} \tag{2.7}$$

$$\rho_B = \sum_i \lambda_i |\phi_i^{(B)}\rangle\langle\phi_i^{(B)}|. \tag{2.8}$$

From this it is clear that ρ_A and ρ_B have the same non-zero eigenvalues, which are precisely the non-vanishing Schmidt coefficients λ_i. If the subsystems A and B have different dimensions, then the number of zero eigenvalues of ρ_A and ρ_B differ. The number of non-zero eigenvalues in ρ_A (or ρ_B) and hence the number of terms in the Schmidt decomposition of $|\psi\rangle_{AB}$ is called the Schmidt number (or Schmidt rank) for the state $|\psi\rangle_{AB}$. The Schmidt number is preserved under unitary transformations on system A or system B alone and hence remains constant for a given state [7]. Many important properties of pure quantum states are

completely determined by the eigenvalues of the reduced density operator of the system and so for a pure state of a composite system such properties will be the same for both systems [7]. For example, in terms of this quantity one can define what it means for a bipartite pure state to be entangled: $|\psi\rangle_{AB}$ is entangled if its Schmidt number is greater than one, otherwise it is separable [7].

From equations (2.7) and (2.8), the von Neumann entropies of ρ_A and ρ_B are equal,

$$S_{vN}(\rho_A) = -\sum_i \lambda_i \log_2 \lambda_i = S_{vN}(\rho_B). \tag{2.9}$$

Acting on $|\psi\rangle_{AB}$ with the local unitary operator U results in the state $|\psi'\rangle_{AB}$,

$$\big[U_A \otimes U_B\big]|\psi\rangle_{AB} = \sum_i \sqrt{\lambda_i}\Big(U_A|\phi_i^{(A)}\rangle \otimes U_B|\phi_i^{(B)}\rangle\Big). \tag{2.10}$$

The marginal density matrix for subsystem A then becomes

$$\rho'_A = \mathrm{Tr}_B\Big(\big[U_A \otimes U_B\big]|\psi\rangle_{AB}\langle\psi|\big[U_A^\dagger \otimes U_B^\dagger\big]\Big) \tag{2.11}$$

and so the von Neumann entropy is

$$S_{vN}[\rho_A] = S_{vN}[\rho'_A] = -\sum_i \lambda_i \log_2 \lambda_i \tag{2.12}$$

which implies that the entanglement remains constant under local unitary operation. This means that the only way to entangle A and B is for the two subsystems to directly interact with one another, that is, one has to apply a collective or global unitary transformation to the state. It is a law of entanglement theory (which can be derived as a theorem of quantum mechanics [88]) that the entanglement between two spatially separated systems cannot, on average, be increased by carrying out local operations and classical communications (LOCC) protocols [89].

2.1.1 Entropy of entanglement or von Neumann entropy

The entropy of entanglement is given by the von Neumann entropy of the marginal density matrices. This is an operational measure: it gives the number of ebits

that are needed to create a pure entangled state in the laboratory. An "ebit" or entanglement bit is a unit of entanglement and is defined as the amount of entanglement in a Bell pair $|\beta_{00}\rangle, |\beta_{01}\rangle, |\beta_{10}\rangle$ or $|\beta_{11}\rangle$, see equations (2.30). These states and any related to them by local unitary operations are maximally entangled states of two qubits, and can be used to perform a variety of non-classical feats such as superdense coding and quantum teleportation and are thus a valuable resource [89].

For each pure state $|\psi\rangle_{AB}$, the entanglement is defined as the von Neumann entropy of either of the two subsystems A and B [90],

$$E(|\psi\rangle_{AB}) = -\mathrm{Tr}(\rho_A \log_2 \rho_A) = -\mathrm{Tr}(\rho_B \log_2 \rho_B), \tag{2.13}$$

where ρ_A and ρ_B are the marginal density matrices of the subsystems:

$$\begin{aligned} \rho_A &= \mathrm{Tr}_B(|\psi\rangle_{AB}\langle\psi|) \\ \rho_B &= \mathrm{Tr}_A(|\psi\rangle_{AB}\langle\psi|). \end{aligned} \tag{2.14}$$

These reduced density matrices correspond to mixed states when the pure state $|\psi\rangle_{AB}$ is entangled. The von Neumann entropy, which is the most fundamental of these entanglement measures, measures the degree of mixedness of these marginal density matrices and is thus a measure of the amount of entanglement of $|\psi\rangle_{AB}$.

2.1.2 Entanglement measure based upon the linear entropy

Another useful entanglement measure which gives the degree of mixedness of the density matrix ρ and which is easy to compute (since there is no need to diagonalize ρ) is given by the linear entropy,

$$S_L(\rho) = 1 - \mathrm{Tr}(\rho^2). \tag{2.15}$$

This entropic measure coincides (up to a constant multiplicative factor) with the quantum power-law entropy $S_q^{(T)}$ with Tsallis' parameter $q = 2$. Similar to the von Neumann entropy, for each pure state $|\psi\rangle_{AB}$ the entanglement is defined as

the linear entropy of either of the two subsystems A and B. The linear entropy does not stem from an operational point of view, but it gives a good idea of how much entanglement is present in quantum states when one is not interested in the detailed resources needed to create these states in a laboratory.

2.1.3 Entanglement of formation and concurrence

This is a physically motivated measure of entanglement for mixed states which is intended to quantify the resources needed to create a given entangled state [91]. That is, from an "engineering" point of view this measure gives the minimum number of ebits that are needed to create entangled states. Since entanglement is a valuable resource one wants to minimize the amount of ebits needed.

The entanglement of formation is defined as follows [91, 92]: given a density matrix ρ of a pair of quantum systems A and B, consider all possible pure-state decompositions of ρ, that is, all ensembles of states $|\psi_i\rangle$ with probabilities p_i such that

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|. \tag{2.16}$$

The non-unique character of the decomposition of ρ has been discussed in Subsection 1.1.6.

For each pure state, the entanglement E is defined as the von Neumann entropy of either of the two subsystems A or B (see (2.13)). The entanglement of formation of the mixed state ρ is then defined as the average entanglement of the pure states of the decomposition, minimized over all decompositions of ρ, that is, the minimum is taken over all statistical mixtures $\{p_i, |\psi_i\rangle\}$ that lead to the same state ρ:

$$\mathbf{E}(\rho) = \min_{\{p_i,|\psi_i\rangle\}} \sum_i p_i E[|\psi_i\rangle]. \tag{2.17}$$

In other words, the entanglement of formation of a mixed state ρ is defined as the minimum average entanglement of an ensemble of pure states that represents ρ. Of particular interest is the "entanglement of formation" (EOF) for mixed states of a two-qubit system. In that special case an explicit formula for the entanglement of formation has been discovered. For bipartite states of higher dimension

or for three and more qubits one has to resort to numerical optimization routines which are computationally expensive and often extremely hard to compute. In the latter instance one then has to use other measures such as the negativity discussed in Subsection 2.1.4. To obtain the EOF of an arbitrary state of two qubits, one has to follow the procedure by Wootters [91]. For a general state ρ of two qubits, the spin-flipped state is

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y), \tag{2.18}$$

where ρ^* is the complex conjugate of ρ taken in the standard basis and σ_y is the usual Pauli matrix. The EOF is then given by

$$\mathbf{E}(\rho) = \mathcal{E}(C(\rho)), \tag{2.19}$$

where the function $\mathcal{E}$ is

$$\begin{aligned} \mathcal{E}(C) &= h\left(\frac{1+\sqrt{1-C^2}}{2}\right), \\ h(x) &= -x\log_2 x - (1-x)\log_2(1-x) \end{aligned} \tag{2.20}$$

and the "concurrence" C is defined as

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{2.21}$$

with the λ_i's being the eigenvalues, in decreasing order, of the Hermitian matrix $R = \sqrt{\sqrt{\rho}\,\tilde{\rho}\,\sqrt{\rho}}$. This procedure clearly also holds for bipartite pure states $|\phi\rangle$ and in that case the EOF can be interpreted roughly as the number of qubits that must have been exchanged between two observers in order for them to share the state $|\phi\rangle$ [91].

2.1.4 The Peres separability criterion and the Negativity entanglement measure

In 1996 Peres [93] derived a separability criterion for density matrices which can detect entanglement better than the Bell inequalities. The Peres separability criterion is also known as the positive partial transpose (PPT) test. Peres realized

that the partial transpose of a density matrix ρ can be used to determine whether the mixed quantum state represented by ρ is separable [93] and can therefore also be used to detect entanglement in ρ [41, 94]. He proved that a necessary condition for separability is that the partial transpose of ρ has only non-negative eigenvalues. In other words, what it says for bipartite states is that if ρ_{AB} is separable, then the new matrix $\rho_{AB}^{T_B}$ with matrix elements defined in some fixed product basis as

$$\langle m|\langle\mu|\rho_{AB}^{T_B}|n\rangle|\nu\rangle = \langle m|\nu|\rho_{AB}|n\rangle|\mu\rangle \tag{2.22}$$

is a density operator, that is, it has a non-negative spectrum [67]. The partial transpose T_B, is an operation which corresponds to transposition of indices corresponding to the second subsystem. The Peres-Horodecki criterion states that PPT is a necessary and sufficient condition for bipartite states to be separable in the particular case of two-qubit systems and qubit-qutrit systems. In other cases PPT is only a necessary but not sufficient condition for separability [94]. An entanglement measure based on the PPT criterion is the negativity [41]. This entanglement measure is effective in numerical explorations of multipartite mixed states due to its relative simplicity and computability [95].

Consider an N-qubit state of the form

$$|\psi\rangle = \sum_{k=0}^{2^N-1} c_k|k\rangle, \tag{2.23}$$

where the c_k satisfy the normalization condition and each $|k\rangle$ is a basis state $|a_1a_2\ldots a_N\rangle$ with $a_1a_2\ldots a_N$ being the binary representation of the integer k, $a_i \in \{0,1\}$. A density operator of a mixed state ρ can be written in terms of pure states having the same form as $|\psi\rangle$:

$$\begin{aligned}\rho &= \sum_{j=1}^{n} p_j|\psi_j\rangle\langle\psi_j| \\ &= \sum_{j=1}^{n} p_j \sum_{a_1,a_2,\ldots,a_N=0}^{1} c^j_{a_1a_2\ldots a_N}|a_1a_2\ldots a_N\rangle \sum_{a'_1,a'_2,\ldots,a'_N=0}^{1} c^{j*}_{a'_1a'_2\ldots a'_N}\langle a'_1a'_2\ldots a'_N|\end{aligned}$$

$$= \sum_{j=1}^{n} p_j \sum_{\substack{a_1,a_2,\ldots,a_N=0 \\ a'_1,a'_2,\ldots,a'_N=0}}^{1} d^j_{a_1a_2\ldots a_N a'_1a'_2\ldots a'_N} |a_1a_2\ldots a_N\rangle\langle a'_1a'_2\ldots a'_N|, \tag{2.24}$$

$d^j_{a_1a_2\ldots a_N a'_1a'_2\ldots a'_N} = c^j_{a_1a_2\ldots a_N} c^{j*}_{a'_1a'_2\ldots a'_N}$. To construct the partial transpose of ρ with respect to the index i (corresponding to the cut set $\{i\}$), we have to transpose the bits a_i and a'_i in the basis states:

$$\begin{aligned}\rho^{T_{\{i\}}} &= \sum_{j=1}^{n} p_j \sum_{\substack{a_1,a_2,\ldots,a_N=0 \\ a'_1,a'_2,\ldots,a'_N=0}}^{1} d^j_{a_1\ldots a_i\ldots a_N a'_1\ldots a'_i\ldots a'_N} |a_1\ldots a'_i\ldots a_N\rangle\langle a'_1\ldots a_i\ldots a'_N| \\ &= \sum_{j=1}^{n} p_j \sum_{\substack{a_1,a_2,\ldots,a_N=0 \\ a'_1,a'_2,\ldots,a'_N=0}}^{1} d^j_{a_1\ldots a'_i\ldots a_N a'_1\ldots a_i\ldots a'_N} |a_1\ldots a_i\ldots a_N\rangle\langle a'_1\ldots a'_i\ldots a'_N|. \end{aligned} \tag{2.25}$$

The partial transpose with respect to a larger set of indices (larger cut set) is constructed in a similar way by transposing the bits corresponding to each index in the set. To obtain the entanglement of the mixed state (2.24) we need to consider all unique cut sets and then sum the negative eigenvalues of the corresponding partially transposed matrices. As entanglement measure one then takes the absolute value of the aforementioned sum. The number of unique cut sets is $2^{N-1}-1$, since the complementary cut sets result in partially transposed matrices which have the same eigenvalues and the trivial partial transpose with respect to the empty cut gives the original density matrix which has no negative eigenvalues [41, 94, 95].

2.1.5 Multipartite entanglement measures

Due to its great relevance, both from the fundamental and from the practical points of view, it is imperative to explore and characterize all aspects of the quantum entanglement of multipartite quantum systems [39, 96]. There are several possible N-qubit entanglement measures for pure states $|\phi\rangle$, one being the average of all the single-qubit linear entropies,

$$Q(|\phi\rangle) = 2\left(1 - \frac{1}{N}\sum_{k=1}^{N} \mathrm{Tr}(\rho_k^2)\right). \tag{2.26}$$

Here ρ_k, $k = 1, \ldots, N$, stands for the marginal density matrix describing the kth qubit of the system after tracing out the rest. This quantity, often referred to as "global entanglement" (GE), measures the average entanglement of each qubit of the system with the remaining $(N-1)$-qubits.

The GE measure can be generalized by using the average values of the linear entropies associated with more general partitions of the N-qubit system into two subsystems (and not only the partitions of the system into a 1-qubit subsystem and an $(N-1)$-qubit subsystem). A particular generalization is given by the following family of multi-qubit entanglement measures,

$$Q_m(|\phi\rangle) = \frac{2^m}{2^m - 1}\left(1 - \frac{m!(N-m)!}{N!}\sum_s \mathrm{Tr}(\rho_s^2)\right), \quad m = 1, \ldots, \lfloor N/2 \rfloor, \quad (2.27)$$

where the sum runs over all the subsystems s consisting of m qubits, ρ_s are the corresponding marginal density matrices and $\lfloor x \rfloor$ denotes the integer part of x. The quantities Q_m measure the average entanglement between all the subsystems consisting of m qubits and the remaining $(N-m)$ qubits. Another way of characterizing the global amount of entanglement exhibited by an N-qubit state is provided by the sum of the (bipartite) entanglement measures associated with all the possible bi-partitions of the N-qubits system [95]. These entanglement measures are given, essentially, by the degree of mixedness of the marginal density matrices associated with each bi-partition. These degrees of mixedness can be, in turn, evaluated in several ways. For instance, we can use the von Neumann entropy, the linear entropy or a Rényi entropy of index q [39, 96]. There has recently been great interest in the search for highly entangled multi-qubit states [95–97]. Multi-qubit entanglement measures have been applied to the study of several problems, such as, for instance, the entanglement dynamics of open multi-qubit systems [98].

2.1.6 Some examples of applications of entangled states

As mentioned before, two spectacular applications of entangled states are superdense coding and teleportation. Superdense coding combines all the basic ideas of elementary quantum mechanics and is a prime example of information processing

tasks that can be accomplished using quantum mechanics. Quantum teleportation is a technique for sending unknown quantum states without the need for a quantum communications channel connecting the sender of the quantum state to the recipient.

2.1.6.1 Superdense coding

For superdense coding we require two parties, conventionally known as 'Alice' and 'Bob', who are far from each other. Alice can send two classical bits of information to Bob by sending him a single qubit, if they initially share a pair of qubits in the entangled state:

$$|\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}. \tag{2.28}$$

The state $|\psi\rangle$ is fixed (no qubits need to be sent in order to prepare the state) with Alice and Bob being in possession of the first and second qubit respectively. The procedure Alice uses to send two bits of classical information via her qubit is as follows [7]: if she intends to send the bit string '00' to Bob then she does nothing to her qubit. To send '01' she applies the phase flip Z to her qubit. If she wishes to send '10' then she applies the quantum NOT gate, X, to her qubit and to send '11' she applies the iY gate. The X, Y and Z gates are given by

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.29}$$

The four resulting states are the Bell states:

$$\begin{aligned} 00 : |\psi\rangle &\rightarrow |\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \\ 01 : |\psi\rangle &\rightarrow |\beta_{01}\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}} \\ 10 : |\psi\rangle &\rightarrow |\beta_{10}\rangle = \frac{|10\rangle + |01\rangle}{\sqrt{2}} \\ 11 : |\psi\rangle &\rightarrow |\beta_{11}\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}, \end{aligned} \tag{2.30}$$

which are orthonormal and can thus be distinguished by an appropriate quantum measurement. Once Bob has received Alice's qubit he can perform a measurement in the Bell basis and determine which of the four possible bit strings Alice sent. Thus superdense coding is achieved by transmitting two bits of information through the interaction of a single qubit. This illustrates that information is indeed physical and that quantum mechanics can predict surprising information processing abilities [7].

2.1.6.2 Quantum teleportation

As for superdense coding, we need two separated parties Alice and Bob sharing the entangled EPR state $|\beta_{00}\rangle$. Alice wants to send Bob the unknown state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ (α and β are not known) by making use of the EPR pair and sending classical information to Bob. She accomplishes this by recourse to the following protocol. First she interacts the unknown qubit $|\psi\rangle$ with her half of the EPR pair, leading to the state $|\psi_0\rangle$

$$|\psi_0\rangle = |\psi\rangle|\beta_{00}\rangle = \frac{1}{\sqrt{2}}\Big[\alpha|0\rangle\Big(|00\rangle + |11\rangle\Big) + \beta|1\rangle\Big(|00\rangle + |11\rangle\Big)\Big], \tag{2.31}$$

where the first two qubits ($|\psi\rangle$ and the first qubit in the EPR pair) belong to Alice and the third qubit to Bob. She then sends her two qubits ($|\psi\rangle$ and her half of the EPR pair) of the resultant state $|\psi_0\rangle$ through a CNOT gate

$$U_{CN} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \tag{2.32}$$

obtaining the state

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\Big[\alpha|0\rangle\Big(|00\rangle + |11\rangle\Big) + \beta|1\rangle\Big(|10\rangle + |01\rangle\Big)\Big]. \tag{2.33}$$

She then sends her first qubit through a Hadamard gate

$$H_d = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{2.34}$$

obtaining

$$|\psi_2\rangle = \frac{1}{2}\Big[\alpha\Big(|0\rangle + |1\rangle\Big)\Big(|00\rangle + |11\rangle\Big) + \beta\Big(|0\rangle - |1\rangle\Big)\Big(|10\rangle + |01\rangle\Big)\Big]. \tag{2.35}$$

Rewriting this state by grouping Alice's qubits together, results in

$$\begin{aligned} |\psi_2\rangle \;=\; & \frac{1}{2}\Big[|00\rangle\Big(\alpha|0\rangle + \beta|1\rangle\Big) + |01\rangle\Big(\alpha|1\rangle + \beta|0\rangle\Big) \\ & + |10\rangle\Big(\alpha|0\rangle - \beta|1\rangle\Big) + |11\rangle\Big(\alpha|1\rangle - \beta|0\rangle\Big)\Big]. \end{aligned} \tag{2.36}$$

Then Alice performs on her two qubits a joint measurement of a (non-degenerate) observable with eigenbasis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. From the first term in (2.36) it can be seen that when Alice's qubits are in the state $|00\rangle$ then Bob's qubit is in the state $|\psi\rangle$. Thus when Alice performs the measurement and obtains the result 00, Bob's post-measurement state will be $|\psi\rangle$. In a similar way we can determine the state of Bob's system given Alice's measurement outcomes:

$$\begin{aligned} 00 &\longmapsto |\psi_3(00)\rangle = \alpha|0\rangle + \beta|1\rangle \\ 01 &\longmapsto |\psi_3(01)\rangle = \alpha|1\rangle + \beta|0\rangle \\ 10 &\longmapsto |\psi_3(10)\rangle = \alpha|0\rangle - \beta|1\rangle \\ 11 &\longmapsto |\psi_3(11)\rangle = \alpha|1\rangle - \beta|0\rangle. \end{aligned} \tag{2.37}$$

Alice now sends Bob the classical information of her outcome, thereby telling him in which one of the four possible states his qubit has ended up. This is tantamount to sending two classical bits. This classical information enables him to recover the state $|\psi\rangle$ by either doing nothing when the outcome is 00, applying the gate X when he receives 01, the Z gate when getting 10 or first applying an X and then a Z gate when the information 11 reaches him. Since classical information needs to be exchanged, quantum teleportation does not enable faster than light communication. Consequently, teleportation does not imply a conflict with special relativity. It is also interesting that the state $|\psi\rangle$ is completely erased

from the qubits in Alice's possession, in accordance with the no-cloning theorem. Quantum teleportation illustrates that different resources in quantum mechanics can be interchanged: one shared EPR pair together with two classical bits of communication is a resource at least the equal of one qubit of communication [7].

2.2 Quantum entanglement in a many-body system exhibiting multiple quantum phase transitions

This Section is based on the publication [99] "Quantum entanglement in a many-body system exhibiting multiple quantum phase transitions", C. Zander, A. Plastino and A.R. Plastino, *Braz. J. Phys.* **39** (2), (2009) pp. 464-467.

I investigate the quantum entanglement-related features of the many-body model of Plastino and Moszkowski [100]. This is an exactly solvable N-body, SU2 two-level model exhibiting several quantum phase transitions. We show that these transitions happen to be also entanglement-transitions associated with different many-body Dicke states. The main properties of the model considered here make it particularly well suited to study, by recourse to exact analytical computations, some connections between quantum phase transitions and quantum entanglement-theory.

2.2.1 Introduction

A quantum phase transition (QPT) is a phase transition between different quantum phases (phases of matter at zero temperature). The transition describes a structural change in the ground state of a many-body system.

Even at zero temperature a quantum-mechanical system can still support phase transitions. As a relevant physical quantity is varied (represented by a parameter in the system's Hamiltonian) it is possible to induce a phase transition into a different phase of matter. A paradigmatic example of a quantum phase transition is the well-studied superconductor/insulator transition in disor-

dered thin films which separates two quantum phases having different symmetries. Quantum magnets provide another example of QPT. Thus, in infinite as well as in finite systems a type of phase transition, often referred to as a quantum phase transition, may occur at $T = 0$. Such quantum phase transitions generally signal a change in the correlations present in the ground state of the system. For a system described by a Hamiltonian, $H(\xi) = H_0 + \xi H_1$, which varies as a function of the coupling constant ξ, the presence of a QPT can easily be understood in the following manner: *level crossing may come about and the ground state energy is no longer analytic nor monotonic*. Although there are other valid mathematical reasons that lead to the loss of analyticity, the above simple explanation will suffice for our purposes and provides a simple means for defining a QPT.

2.2.2 The Plastino-Moszkowski model

This is an exactly solvable N-body, SU2 two-level model [100]. Each level can accommodate an even number N of particles, i.e., is N-fold degenerate. There are two levels separated by an energy gap, say $\epsilon = 1$, and occupied by N particles. In the model the angular momentum-like operators $\hat{J}^2, \hat{J}_x, \hat{J}_y, \hat{J}_z$, with $J(J+1) = N(N+2)/4$ are used (see details below). The Hamiltonian is given by [100]

$$\hat{H} = \hat{J}_z - \xi\Big[\hat{J}^2 - \hat{J}_z^2 - \hat{N}/2\Big], \tag{2.38}$$

where $\hat{N}$ is the number operator. States belonging to the lowest lying multiplet, i.e., that with $J = N/2$, are usually referred to as Dicke-states $|J, M\rangle$ (M standing for the $\hat{J}_z$-eigenvalues) [101]. In building up our many-body Hamiltonian we use the second quantization form

$$\hat{J}_z = \frac{1}{2}\sum_{i=1}^{N}\sum_{\sigma=1}^{2}\hat{a}_{i,\sigma}^{\dagger}\,\hat{a}_{i,\sigma}, \tag{2.39}$$

with corresponding expressions for $\hat{J}_x$, $\hat{J}_y$. This is a simple yet non-trivial case of the Lipkin model [102–104]. Note that we deal here with a bonafide many-body system, since the number of states grows with N as 2^N. Here we will discuss only the model in the zero-temperature regime. The operators appearing in the model Hamiltonian form a commuting set of observables and are thus simultaneously

diagonalizable.

2.2.2.1 QPTs in the PM-model

The ground state of the unperturbed system ($\xi = 0$ and at $T = 0$) is $|J, M\rangle = \left|\frac{N}{2}, \text{-}\frac{N}{2}\right\rangle$ with the eigen-energy $E_0 = -\frac{1}{2}N$. When the interaction is turned on ($\xi \neq 0$) and gradually becomes stronger, the ground state energy will in general be different from the unperturbed system for some critical value of ξ that we will call ξ_c. This sudden change of the ground state energy signifies a quantum phase transition. It should be noted that for a given value of N, there could be more than one critical point, since there exist $2J+1$ possible values for M. If we denote by n the number of "holes" in the lowest of the two N-degenerate levels, then the critical value ξ_c of the nth transition point can be found from equation (2.40) below, provided that $\xi_c > 0$ and $\xi_c \neq \infty$ [100]

$$\xi_{c,n} = \frac{1}{N - (2n-1)}. \tag{2.40}$$

2.2.3 Dicke-states' two-qubit entanglement

Remember that for these states $J = N/2$ and $M = -J, \ldots, J$ [105, 106]. In the computational basis

$$|00\rangle, \quad |01\rangle, \quad |10\rangle, \quad |11\rangle,$$

one has a reduced two-body matrix [105, 106]

$$\rho_{12} = \begin{pmatrix} v_+ & 0 & 0 & 0 \\ 0 & y & y & 0 \\ 0 & y & y & 0 \\ 0 & 0 & 0 & v_- \end{pmatrix}, \tag{2.41}$$

with [105, 106]

$$\begin{aligned} v_\pm &= \frac{(N \pm 2M)(N - 2 \pm 2M)}{4N(N-1)} \\ y &= \frac{N^2 - 4M^2}{4N(N-1)} \end{aligned} \tag{2.42}$$

and concurrence,

$$C[\rho_{12}] \;=\; 2\,\mathrm{Max}\Big\{0, y - \sqrt{(v_- v_+)}\Big\}, \tag{2.43}$$

where, as stated, $C[\rho_{12}]$ stands for the all-important quantity that measures the entanglement-degree, namely, the concurrence. In Fig. 2.1 the concurrence of the ground states of the Plastino-Moszkowski model is depicted for $N = 10$. We immediately realize that at the extremal multiplet values $M = \pm J$ one has $y = 0$, $C[\rho_{12}] = 0$, so that these are two separable states, and, further,

$$\begin{aligned} v_+ \;&=\; 1;\; v_- \;=\; 0 \quad M = N/2 \\ v_+ \;&=\; 0;\; v_- \;=\; 1 \quad M = -N/2. \end{aligned} \tag{2.44}$$

Instead, for $M = 0$ we get a "minimal-finite" entanglement amount, i.e., that particular many-body state with this M-value is the least entangled non-separable Dicke state, for which

$$\begin{aligned} y \;&=\; \frac{N}{4(N-1)} \\ v_\pm \;&=\; \frac{N-2}{4(N-1)}, \end{aligned} \tag{2.45}$$

leading to

$$\begin{aligned} C[\rho_{12}] \;&=\; \frac{1}{N-1} \\ \lim_{N\to\infty} C[\rho_{12}] \;&=\; 0. \end{aligned} \tag{2.46}$$

Notice that $C[\rho_{12}] \leq 1$ for $N \geq 2$. For given N, the concurrence is always maximal for $M = \pm\frac{N}{2} \mp 1$, which is a so-called W-state [39, 96]. In terms of the number of holes n in the lowest lying of our two levels, the W-states are those with $n = 1$ or $n = N - 1$. The pertinent concurrence becomes $C_W = \frac{2}{N}$. These are known to be maximally entangled states in general. For an arbitrary Dicke-state the concurrence reads

$$C[\rho_{12}] = \frac{N^2 - 4M^2 - \sqrt{(N^2 - 4M^2)\,[(N-2)^2 - 4M^2]}}{2N(N-1)}, \tag{2.47}$$

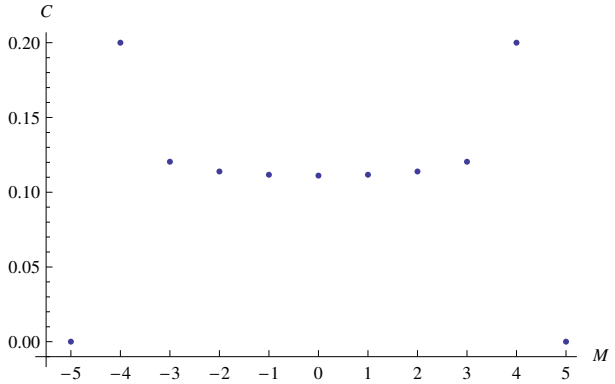


Figure 2.1: Concurrence of the ground states of the Plastino-Moszkowski model with $N = 10$ particles as a function of the quantum number M. All depicted quantities are dimensionless.

leading to the limit value

$$\lim_{N\to\infty} C[\rho_{12}] = 0. \tag{2.48}$$

2.2.3.1 QPT and entanglement

The ground state of the unperturbed system ($\xi = 0$ and at $T = 0$), i.e., $|J, M\rangle = \left|\frac{N}{2}, \text{-}\frac{N}{2}\right\rangle$ is a separable state. When the interaction is turned on ($\xi \neq 0$) and gradually becomes stronger, the ground state will in general be different from the unperturbed system for critical values ξ_c. Such sudden change of the ground state signifies *both* a quantum phase transition and *an entanglement transition*. As, for a given value of N, there exists more than one critical point (indeed $\frac{N}{2}$ ones) we have a matching set of sudden entanglement changes. The first transition is from a separable to a maximally entangled state. In our model Hamiltonian (2.38) the last transition occurs when the ground state becomes $\left|\frac{N}{2}, 0\right\rangle$, that is, when $M = 0$ is attained [100]. Thus, at the nth transition ξ_c, where the number of holes n grows by one, and $\xi_{c,n} = \frac{1}{N-(2n-1)}$, the ground state of the many-body system becomes a new kind of entangled state.

2.2.3.2 Thermodynamic limit

Notice that the very presence of other particles, even without interaction, diminishes the concurrence of ρ_{12}. What happens in the thermodynamic limit $N \to \infty$?

In answering, we can without loss of generality limit our considerations to

the W-states, whose concurrence steadily diminishes with N. Obviously, $C[\rho_{12}]$ vanishes then in the thermodynamic limit, which is, in a way, a classical one. This is consistent with other instances of quantum systems adopting classical-like properties in the limit cases corresponding to a large number of particles or a large number of degrees of freedom [39, 107]. An interesting example of this kind of behaviour concerns a typical feature of the dynamics of multipartite quantum systems: for some quantum states entanglement enhances the "speed" of quantum evolution, as measured by the time τ required to reach a state orthogonal to the initial one [39]. This evolution time τ has a lower bound $\tau_{\min}$ determined by the energy resources of the quantum state under consideration. When one has a system of N independent qubits, a certain amount of entanglement is always needed in order to saturate the aforementioned bound on the evolution time. However, when the number of qubits goes to infinity the entanglement required to reach this "quantum speed limit" goes to zero [39], which may be interpreted as a classical-like feature exhibited by the $N \to \infty$ limit.

2.2.4 Conclusion

We have in this Section obtained some significant new results:
1) The Plastino-Moszkowski model [100] exhibits a rich variety of entangled states. The transition between them takes place precisely at those critical values of the coupling constant for which a quantum phase transition occurs.
2) The above makes the Plastino-Moszkowski system a useful solvable model to study the link between entanglement and QPTs in many-body systems.
3) In the thermodynamic limit, which in a sense may be regarded as the classical limit, one analytically ascertains that the entanglement of the many-body system vanishes, at it should.
4) The PM model was advanced to exhibit inadequacies of the Hartree-Fock approach [100], which is unable to detect the QPTs. This fact is illuminated here on the basis of the QPT-entanglement link that we have investigated in the present contribution. The Hartree-Fock state is represented by one single Slater determinant and is, consequently, always a separable state. In fact, in modern quantum mechanical terminology, the Hartree-Fock approach can be described as a "zero entanglement" approximation.

2.3 Measures of quantum correlations: quantum discord

Characterizing and quantifying the information-processing capabilities exhibited by quantum phenomena such as entanglement and superposition has been the subject of intense research efforts [7, 66, 67, 108]. It is well established that entanglement is essential for certain types of quantum information tasks like superdense coding and teleportation (see Subsubsections 2.1.6.1 and 2.1.6.2). In both Shor's factoring algorithm [72] and Grover's search algorithm [7], the flow of entanglement plays a crucial role in the quantum evolution that implements these algorithms.

However, there are several instances where there is a quantum advantage in the absence or near absence of entanglement. One such case is quantum cryptography [7, 71], where several protocols involve quantum states that are not entangled. These quantum cryptography protocols have been proved to be more secure and thus better than the best known classical cryptographic techniques.

In the model referred to as "deterministic quantum computation with one qubit", introduced by Knill and Laflamme [109] in 1998, which is the first intrinsically mixed-state scheme of quantum computation, there are non-classical correlations present between the control qubit and the mixed qubits, despite there being no entanglement between these two parts [110]. These correlations are characterized by the quantum discord, which acts as a resource in this computational model [110].

Thus entanglement does not describe all aspects of the quantum correlations exhibited by multipartite physical systems. The quantum discord supplements the measures of entanglement which can be defined on the system under consideration and goes beyond them since it also includes quantum correlations different from those involved in entanglement. This concept has been receiving much attention lately and the reason for this is that the study of quantum discord is not only of intrinsic conceptual interest, but may also have technological implications [110–115].

Quantum discord has been related to the superposition principle and the vanishing of discord has been shown to be a criterion for the preferred, effectively classical state of a system, namely the pointer states [111]. It has been used in the investigation of the powers of a quantum Maxwell's demon [116].

Quantum discord tries to quantify all quantum correlations including entanglement. In the case of non-entangled mixed states there are correlations that cannot be captured by a probability distribution defined over the states of an equivalent classical system [110]. For pure states all non-classical correlations identified by the quantum discord coincide with the entanglement as measured by the von Neumann entropy of the reduced density matrix.

Quantum discord [111] is a quantitative measure of the non-classical correlations of a bipartite system. It arises from the discrepancy between the quantum analogues of two classically equivalent expressions for the mutual information given by equations (1.16) and (1.17). That is, quantum discord is defined as the difference between the two quantum mechanical expressions of the entropic quantifier, the mutual information. So let us identify the quantum mechanical counterpart of (1.16). In the quantum case, density matrices are used instead of probability distributions and the Shannon entropy is replaced by the von Neumann entropy. Let ρ_{AB} be the bipartite mixed state under consideration, ρ_A and ρ_B the reduced density matrices and let S stand for the von Neumann entropy. Then the quantum mutual information corresponding to (1.16) is

$$I_q(A:B) = I_q(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}). \tag{2.49}$$

To obtain the quantum analogue of (1.17) is not as straightforward as the above expression, since now we have to find the counterpart to $H(X|Y)$ which depends on a measurement of the second system. That is, $S(A|B)$ gives the uncertainty of the state of subsystem A, given a measurement on B, however, when A is a quantum system, the amount of information that can be extracted about it, depends on the choice of measurement. So one needs to define a measurement basis: let $\{\Pi_j^B\}$ be a complete set of orthogonal projectors, then the state after

outcome i is obtained is

$$\rho_{A|\Pi_i^B} = \frac{\Pi_i^B \rho_{AB} \Pi_i^B}{\mathrm{Tr}(\Pi_i^B \rho_{AB})}, \tag{2.50}$$

where outcome i occurs with probability

$$p_i = \mathrm{Tr}_{AB}(\Pi_i^B \rho_{AB}). \tag{2.51}$$

The uncertainty in A after measurement outcome i has been obtained is $S(\rho_{A|\Pi_i^B})$ and so if a complete projective measurement Π_j^B is performed on B, then the conditional entropy becomes

$$S(A|\{\Pi_j^B\}) = \sum_j p_j S(\rho_{A|\Pi_j^B}). \tag{2.52}$$

Now, we would like to maximize the amount of information gained from the measurement on B and hence minimize the uncertainty. This leads one to define a measurement-independent quantum conditional entropy,

$$S(\rho_A|\rho_B) = \min_{\{\Pi_j^B\}} \left\{ \sum_j p_j S(\rho_{A|\Pi_j^B}) \right\} \tag{2.53}$$

and thus the counterpart to (1.17) is measurement-independent and defined to be

$$J_q(A:B) = S(\rho_A) - S(\rho_A|\rho_B). \tag{2.54}$$

The quantum discord is then obtained,

$$\mathcal{D}(A:B) = I_q(A:B) - J_q(A:B) = S(\rho_B) - S(\rho_{AB}) + S(\rho_A|\rho_B), \tag{2.55}$$

which quantifies non-classical correlations in a quantum system, including those not captured by entanglement.

The discord is non-negative and is zero only for states that exhibit strictly classical correlations [111]. Such kind of states have negligible Hilbert space volume [114], which means that a randomly picked state from the Hilbert space

must have positive discord. As was mentioned before, for a pure state

$$\mathcal{D}(A:B) = S(\rho_B), \tag{2.56}$$

which uniquely quantifies bipartite entanglement. Thus all separable pure states have zero discord, however, the discord can be non-zero for certain separable mixed states involving mixtures of non-commuting product states [117].

To get some intuitive understanding of the quantum discord, we observe that $I_q(A:B)$ contains all information common to A and B, thus all correlations between them, whereas $J_q(A:B)$ contains the information gained about A as a result of a measurement $\{\Pi_j^B\}$ on B. Thus if $\mathcal{D} = 0$, then the measurement has extracted all information about correlations between A and B. Since $S(\rho_{AB}) - S(\rho_B)$ is the entropy of A before measurement and $S(\rho_A|\rho_B)$ is the entropy of A after measurement of B, $\mathcal{D} = 0$ also means that the system isn't perturbed by the measurement (no change in entropy of A), which it shouldn't be for purely classical correlations. So $\mathcal{D}$ measures the information that cannot be extracted by local measurements or alternatively, it can be viewed as the minimal correlations' loss due to measurement [118]. It should be noted that the discord is invariant under local unitary transformations, however, it is not symmetric under the exchange of the subsystems.

2.3.1 Perturbations under local measurements

For any bipartite state ρ_{AB} and complete local orthogonal projective measurements $\{\Pi_i^A\}$ and $\{\Pi_j^B\}$ on A and B respectively, one can associate with them a classical state $\Pi(\rho_{AB})$ after the measurement [119],

$$\Pi(\rho_{AB}) = \sum_{ij} \Pi_i^A \otimes \Pi_j^B \, \rho_{AB} \, \Pi_i^A \otimes \Pi_j^B. \tag{2.57}$$

In the case when $\Pi(\rho_{AB}) = \rho_{AB}$, it would mean that ρ_{AB} is not perturbed by a local measurement and hence it is classical with respect to the measurement $\{\Pi_i^A \otimes \Pi_j^B\}$. Any other state would be truly quantum. Since $\Pi(\Pi(\rho_{AB})) = \Pi(\rho_{AB})$, it means that any complete local projective measurement $\{\Pi_i^A \otimes \Pi_j^B\}$

will induce a classical state. The difference between the classical state $\Pi(\rho_{AB})$ and the original state ρ_{AB} captures the quantum correlations in ρ_{AB}.

Suppose that the eigenprojectors of the reduced states ρ_A and ρ_B are $\{\Pi_i^A\}$ and $\{\Pi_j^B\}$ respectively, that is, the spectral decompositions are

$$\rho_A = \sum_i p_i^A \Pi_i^A \qquad \rho_B = \sum_j p_j^B \Pi_j^B. \tag{2.58}$$

Luo [119] showed that ρ_{AB} is a classical state when $\{\Pi_i^A \otimes \Pi_j^B\}$ are the eigenprojectors of ρ_{AB}. He then argued that when taking as measurement Π the one induced by the spectral resolutions of the reduced states as given in eq. (2.58), this results in the closest classical state to the original quantum state, since this measurement leaves the reduced states ρ_A and ρ_B invariant. When ρ_{AB} is classical, the measurement $\Pi = \{\Pi_i^A \otimes \Pi_j^B\}$ will leave the state unchanged.

The quantum mutual information as given in eq. (2.49) quantifies the total correlations in a bipartite state ρ_{AB} and so $I_q(\Pi(\rho_{AB}))$ specifies the classical correlations in ρ_{AB}, as well as in $\Pi(\rho_{AB})$. Luo then proposed the following measure for quantum correlations,

$$\mathcal{Q}(\rho_{AB}) = I_q(\rho_{AB}) - I_q(\Pi(\rho_{AB})), \tag{2.59}$$

where $\Pi = \{\Pi_i^A \otimes \Pi_j^B\}$ and $\{\Pi_i^A\}$, $\{\Pi_j^B\}$ are as determined by eq. (2.58). When ρ_{AB} is a pure bipartite state, then $\mathcal{Q}(\rho_{AB}) = S(\rho_A)$ which agrees with (2.56) and $\mathcal{Q}(\rho_{AB}) = 0$ if ρ_{AB} is classical [119]. Also, $\mathcal{Q}(\rho_{AB})$ is invariant under local unitary transformations.

In Chapter 5 I introduce an approach for the characterization of quantum correlations in fermion systems based upon the state disturbances generated by the measurement of "local" observables (that is, quantum observables represented by one-body operators). This approach leads to a concept of quantum correlations in systems of identical fermions different from entanglement.

2.4 Distinguishable and indistinguishable particles

In this Section it will be explained what is meant by identical particles and by distinguishable and indistinguishable subsystems. A definition of identical particles can be given as follows: Two particles are said to be identical if all their intrinsic properties such as mass, electrical charge, spin, etc. are exactly the same [51]. Thus, we consider all electrons in the universe to be identical, as well as any other kind of quantum particles such as protons, positrons, photons, neutrons, muon neutrinos, up quarks, hydrogen atoms, etc. They each have exactly the same defining properties and behave the same way under interactions associated with those properties [120].

Another purely quantum effect is that of indistinguishable particles. To see that this is not a classical phenomenon, imagine we have two completely identical classical objects that we are unable to differentiate in any way. If we were to assign arbitrary labels to them, we could always, at least in principle, keep track of each object by following their respective trajectories. However, in quantum mechanics we have to abandon this classical concept since the best information we can obtain about the location of some particle without measuring it (and hence disturbing it) is that it has a certain probability of being in a particular position in space, at a given instant in time. This information is contained in the spatial state of the particle. The particle's wave function gives the probability of finding the particle at a certain position at time t and this wave function has a certain spread which determines how localized the particle is. Also bringing to mind Heisenberg's uncertainty relation, we cannot simultaneously measure the particle's position and its momentum with arbitrary precision.

The question arises how one can distinguish identical particles. Using their possibly different internal states as a criterion is not a good idea, since the dynamics can in general affect the internal degrees of freedom of the particles. The same holds for their momentum or other dynamical variables [120]. However, their spatial location can actually be used to distinguish them, if these particles are either kept distant enough or there is a sufficiently large enough energy bar-

rier separating them so that their wave functions in practice never overlap during the time interval of consideration. Then one can use the same method as in the classical case to keep track of them. If, however, the wave functions do overlap at some point, then we no longer know which particle is where. The particles then become completely indistinguishable and they are identified by completely arbitrary labels that have no physical meaning [120]. Note that swapping the fictitious labels of two identical particles is not the same as actually swapping their positions and other physical properties. In the former case we have a passive transformation whereas in the latter case we have an active transformation (objects are actually moved around) which may cause a phase shift, which is experimentally observable [24].

A consequence of the indistinguishability of particles is the exchange degeneracy [51]. Finding the unambiguous description for such systems requires the introduction of a new postulate for quantum mechanics, namely the Symmetrization Postulate [51, 120]: in a system containing indistinguishable particles, the only possible states of the system are the ones described by vectors that are, with respect to permutations of the fictitious labels that we arbitrarily attach to those particles, either

1. completely symmetrical - in which case the particles are called bosons
2. completely antisymmetrical - in which case the particles are called fermions.

The above postulate, which has been corroborated by extensive experimental observation, lifts the exchange degeneracy. The existence of fermions and bosons and their respective properties accounts for a series of fascinating new physical phenomena. To decide which particles belong to a particular symmetry is something that ultimately has to be determined by observation. Empirical knowledge of the collective behaviour of particles in indistinguishable situations tells us that there are two classes of particles in Nature, namely bosons and fermions. This could not have been deduced from the other postulates of quantum mechanics. The following empirical rule is obeyed by all currently known particles: particles with integer spin are bosons and particles with half-integer spin are fermions [51]. Within quantum field theory this rule can be derived as a theorem from

more fundamental principles. This is Pauli's celebrated "spin-statistics" theorem. Once this rule has been established for elementary particles, it then also holds for composite particles and is consistent with the fact that particles composed of an arbitrary number of bosons and/or of an even number of fermions are bosons, and that if particles are composed of an odd number of fermions they are fermions [120]. A prime example is given by the two isotopes of helium: ^{4}He is a boson (composed of 2 electrons, 2 protons and 2 neutrons) and ^{3}He is a fermion (composed of an odd number of fermions).

The Symmetrization Postulate needs to be applied only to indistinguishable particles, not to identical particles in general, since it can be shown that the (anti)symmetrization terms have a vanishing probability when one can distinguish the identical particles [51]. It should be noted that given a system, separate vectors are often considered to describe its spatial and its internal degrees of freedom. The symmetries of each vector are not independent since they have to consistently contribute to the symmetry requirement of the entire vector describing the state of the system [120].

Particles known to be fermions include electrons and in general all leptons as well as quarks, protons (made of three quarks), neutrons and in fact all baryons, ^{3}He, etc. Nuclei whose mass number A (total number of nucleons) is even are bosons and those whose mass number is odd are fermions [51].

2.5 Systems of identical fermions

Fermions are identical particles that, in a situation where they are indistinguishable, can only be found in completely antisymmetric states. That is, a fermionic state changes sign if any two labels (associated with the degrees of freedom of two particles) are swapped. This means their state vector is in the antisymmetric subspace of the system. To see what is meant by that, suppose we have a system of N indistinguishable fermions. Let us first consider the tensor product Hilbert space $\mathcal{H}_N = \mathcal{H}^{\otimes N}$, where each particle is described by the same single-particle Hilbert space $\mathcal{H}$. We have arbitrarily assigned labels 1 to N to the particles. The Hilbert space comprising all the antisymmetric vectors of $\mathcal{H}_N$ is $\mathcal{H}_A$, the

fully antisymmetric subspace of $\mathcal{H}_N$. Similarly $\mathcal{H}_S$ is the completely symmetric subspace of $\mathcal{H}_N$. We can then write

$$\mathcal{H}_N = \mathcal{H}_A \oplus \mathcal{H}_S \oplus \mathcal{H}_m \tag{2.60}$$

where $\mathcal{H}_m$ is the subspace of $\mathcal{H}_N$ with mixed symmetry [120]. The vectors in $\mathcal{H}_A$ represent all the possible (pure) quantum states of a system of N identical fermions.

If we have N states $|k_1\rangle, \ldots, |k_N\rangle$ belonging to an orthonormal basis of the single-particle Hilbert space $\{|1\rangle, |2\rangle, \ldots\}$, there is a natural way to construct a fully antisymmetric N-particle state via a structure known as a "Slater determinant". For instance, for $N = 3$, a Slater determinant has the form

$$\frac{1}{\sqrt{6}}\big\{|k_1k_2k_3\rangle - |k_1k_3k_2\rangle - |k_2k_1k_3\rangle + |k_2k_3k_1\rangle + |k_3k_1k_2\rangle - |k_3k_2k_1\rangle\big\}. \tag{2.61}$$

These Slater determinants describe legitimate pure states of N identical fermions. A Slater determinant like (2.61) describes a physical situation where we can say that "we have" one particle in state $|k_1\rangle$, one in state $|k_2\rangle$ and one in state $|k_3\rangle$ (of course, due to indistinguishability, it makes no sense to ask "which particle is in which state"). The Slater determinant is zero if two of the individual states of the particles coincide and so we obtain Pauli's exclusion principle: the same quantum mechanical state cannot be simultaneously occupied by several identical particles [51]. The set of Slater determinants constructed out of a single-particle orthonormal basis constitutes a basis of the state space describing the N-fermion system: any fully antisymmetric state of the N fermions can be written as a linear combination of these Slater determinants.

Throughout my Thesis, when discussing fermionic systems, I am going to use the first quantization formalism. The second quantization formalism [24] is not needed in this work, because I am going to investigate the entanglement between particles (as opposed to entanglement between modes [121, 122]) in non-relativistic fermion systems consisting of a constant number of particles.

The characterization of the entanglement features of systems of identical fermions constitutes a subject that is currently attracting the attention of several researchers. For example, the entanglement between pairs of electrons in a conduction band [123], the entanglement features exhibited by the eigenstates of soluble two-electrons atomic models [124, 125], the entanglement dynamics in scattering processes involving two electrons [126], the different families of entangled states in systems of three fermions [127], the role of entanglement in time-optimal evolutions of fermionic systems [128, 129] and the detection of entanglement in fermion systems through the violation of appropriate uncertainty relations [130, 131] have recently been investigated.

2.5.1 Separability criteria and entanglement measures

In a system composed of indistinguishable identical fermions, the definition of a separable system as given in eq. (2.3) is not valid since the Hilbert space of the system cannot be expressed as the tensor product of the single-particle Hilbert spaces. It therefore follows that a new definition of entanglement is required for those fermion systems. Note that from now on when the word fermions is used it is implied that they are indistinguishable and hence the fermionic character has to be taken into account.

To illustrate the problem of entanglement in fermion systems let us follow the discussion in reference [132]. A system consisting of two identical spin-$\frac{1}{2}$ particles separated by a potential barrier is analyzed, see Fig. 2.2. The particles are modelled by their spin degrees of freedom ($|\uparrow\rangle, |\downarrow\rangle$) and by their spatial single-particle wave functions ($|\phi_L\rangle, |\phi_R\rangle$) localized in the left and right potential well respectively. When the barrier is very high the overlap of the particles wave functions is negligible (they are spatially localized) and they can thus be regarded as effectively distinguishable particles.

We thus regard the system as being effectively described by a four-dimensional single-particle Hilbert space $\{|\phi_L\uparrow\rangle, |\phi_L\downarrow\rangle, |\phi_R\uparrow\rangle, |\phi_R\downarrow\rangle\}$. An initial state of the

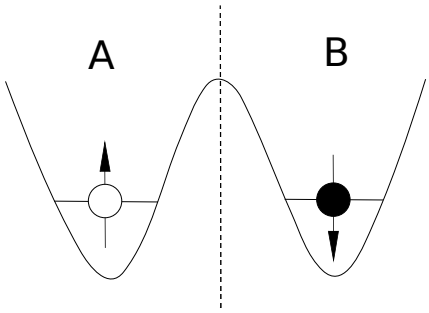


Figure 2.2: Illustration of the initial state $|\psi_{ini}\rangle_{AB}$ of two identical fermions, separated by a high potential barrier in order for them to be considered distinguishable.

system can then be represented as

$$|\psi_{ini}\rangle_{AB} = |\phi_L\uparrow\rangle_A \otimes |\phi_R\downarrow\rangle_B, \tag{2.62}$$

where A and B are physically meaningful labels for the particle in the left and right potential well respectively. This state is clearly separable with respect to the usual definition of separability as in eq. (2.3). In the situation shown in Fig. 2.3 where after a certain time t_1 the energy barrier between the particles is lowered, the antisymmetry of the wave function must be explicitly taken into account and so the state becomes

$$|\psi(t_1)\rangle = \frac{1}{\sqrt{2}}\Big\{|\phi_L\uparrow\rangle_1 \otimes |\phi_R\downarrow\rangle_2 - |\phi_R\downarrow\rangle_1 \otimes |\phi_L\uparrow\rangle_2\Big\}, \tag{2.63}$$

where the attached labels are now arbitrary and due to the spatial overlap of the wave functions the particles are not independently accessible anymore. Both particles are present in each one of the two states, as illustrated by Fig. 2.3. The antisymmetrized state $|\psi(t_1)\rangle$ formally resembles an entangled state although the correlations of this system are not accessible which means the system must be considered non-entangled. A state of the form of a single Slater determinant such as eq. (2.63) effectively behaves as the non-entangled (in the usual sense) state $|\phi_L\uparrow\rangle_A \otimes |\phi_R\downarrow\rangle_B$ describing two distinguishable objects A and B.

Suppose that the coupling between the electrons has been controlled in such

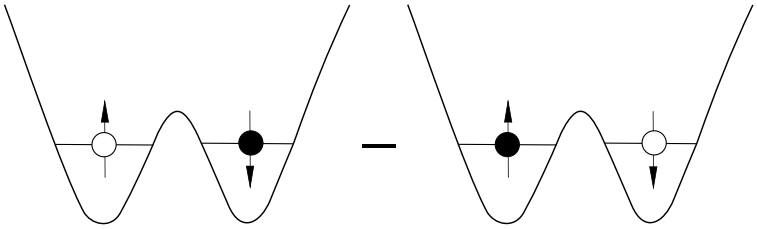


Figure 2.3: Representation of $|\psi(t_1)\rangle$, where the wave functions are no longer completely localized in one of the wells due to the tunnelling barrier being lowered.

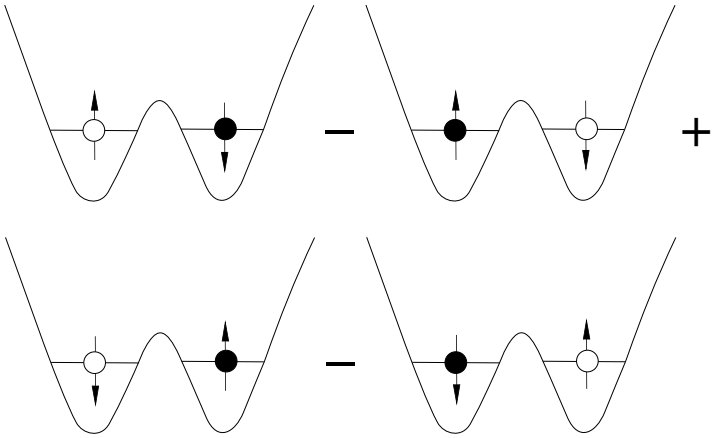


Figure 2.4: Illustration of $|\psi(t_2)\rangle$, which is an entangled state of the system of indistinguishable fermions.

a way that at time t_2 the system is described by

$$\begin{aligned} |\psi(t_2)\rangle \;=\; & \frac{1}{2}\Big\{|\phi_L\uparrow\rangle_1 \otimes |\phi_R\downarrow\rangle_2 - |\phi_R\downarrow\rangle_1 \otimes |\phi_L\uparrow\rangle_2 \\ & + |\phi_L\downarrow\rangle_1 \otimes |\phi_R\uparrow\rangle_2 - |\phi_R\uparrow\rangle_1 \otimes |\phi_L\downarrow\rangle_2\Big\}, \end{aligned} \tag{2.64}$$

which is represented in Fig. 2.4. In the given single-particle basis, $|\psi(t_2)\rangle$ is expressed in terms of two elementary Slater determinants and there is evidently no basis in which it can be written as a single one. Besides the required permutation symmetry, this state contains some useful correlations as can be seen through localizing the particles again by raising the potential barrier. This corresponds to a partition of the single-particle basis between A and B, $\{|\phi_L\uparrow\rangle, |\phi_L\downarrow\rangle\}$ forms the basis for A and the basis for B's space is $\{|\phi_R\uparrow\rangle, |\phi_R\downarrow\rangle\}$. Then the electrons

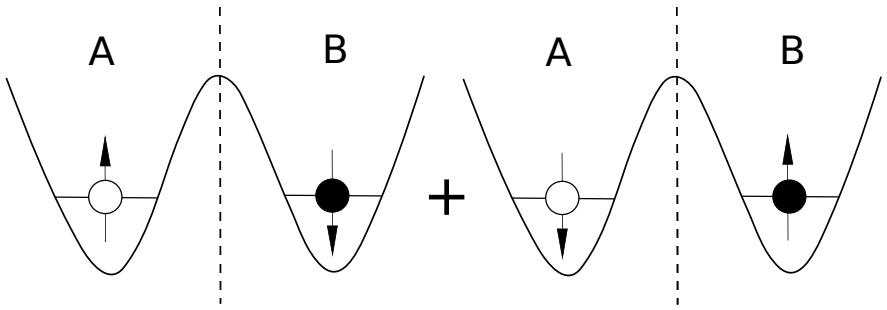


Figure 2.5: Representation of the final entangled state $|\psi_{fin}\rangle_{AB}$, obtained by raising the tunnel barrier which then localizes the wave functions again.

can again be regarded as effectively distinguishable and the final state of the system is

$$|\psi_{fin}\rangle_{AB} = \frac{1}{\sqrt{2}}\Big\{|\phi_L\uparrow\rangle_A \otimes |\phi_R\downarrow\rangle_B + |\phi_L\downarrow\rangle_A \otimes |\phi_R\uparrow\rangle_B\Big\}, \tag{2.65}$$

where new labels A and B are attributed to the electrons, corresponding to which potential well (left or right one respectively) they are found in after separation. The final state shown in Fig. 2.5 is a maximally entangled (in the usual sense) state. It is thus reasonable to call $|\psi(t_2)\rangle$ a maximally entangled state of two indistinguishable fermions in a four-dimensional single-particle space.

The above discussion makes it clear that a system composed of indistinguishable identical particles should be considered separable if and only if it can be expressed as a single Slater determinant [132]. Therefore entangled states are those that cannot be described by a single Slater determinant. Hence a pure state of identical fermions must be regarded as non-entangled (separable) if it is of the form of a single Slater determinant, that is, in the case of two fermions

$$|\psi_{sl}\rangle = \frac{1}{\sqrt{2}}\Big\{|\phi_1\rangle|\phi_2\rangle - |\phi_2\rangle|\phi_1\rangle\Big\}, \tag{2.66}$$

with $|\phi_1\rangle$ and $|\phi_2\rangle$ orthonormal, single-particle states. Elementary Slater determinants in two-fermion systems are thus the natural analogues of product states in systems of distinguishable particles.

When studying entanglement-related properties of pure states of bipartite distinguishable quantum systems it is sometimes convenient to use the Schmidt decomposition of the joint state, as described in Section 2.1. The Schmidt rank was shown to be a separability criterion and it is also an entanglement measure. The Schmidt decomposition admits a natural generalization in the case of a system composed of two identical fermions, namely the Slater decomposition which gives rise to the Slater rank, which is analogous to the Schmidt rank for the distinguishable case.

Given a pure state $|\psi\rangle$ of two fermions, it is possible in this case to find an orthonormal basis $\{|k\rangle, k = 0, 1, \ldots\}$ of the single-particle Hilbert space, such that $|\psi\rangle$ can be written as [125]

$$|\psi\rangle = \sum_k \sqrt{\frac{\lambda_k}{2}} \Big(|2k\rangle|2k+1\rangle - |2k+1\rangle|2k\rangle \Big), \tag{2.67}$$

where the Slater coefficients λ_k satisfy

$$0 \leq \lambda_k \leq 1 \quad \text{and} \quad \sum_k \lambda_k = 1. \tag{2.68}$$

If the single-particle Hilbert space has finite dimension N, then one assumes that N is even and so the summation over the index k goes from $k = 0$ to $k = N/2$. Thus, when expressed in such a basis, the state $|\psi\rangle$ is a sum of non-overlapping elementary Slater determinants where each single-particle basis state occurs at most in only one Slater term.

The concept of entanglement in systems of indistinguishable particles is more controversial than it is in the case of systems composed of distinguishable subsystems. However, there is by now a general agreement among researchers working in this field that in systems of two or more identical fermions quantum correlations between the particles that are solely due to the antisymmetric character of the fermionic state do not contribute to the state's amount of entanglement [108, 123, 132–134]. For instance, an M-fermion pure state of Slater rank equal

to one (that is, a state whose wave function can be represented as a single Slater determinant) has to be regarded as non-entangled [108, 134]. There are profound physical reasons for this. On the one hand, the correlations exhibited by such states cannot be used as a resource to implement non-classical information transmission or information processing tasks [132]. On the other hand, the non-entangled character of states represented by one Slater determinant is consistent with the possibility of associating complete sets of properties to both parts of the composite system [133]. Here, by entanglement in systems of identical fermions we mean entanglement between particles and not entanglement between modes, as was mentioned before (see reference [122] for a comprehensive discussion of entanglement between modes).

A convenient entanglement criterion for pure states $|\psi\rangle$ of systems of M identical fermions can be formulated in terms of the trace of the square of the single-particle reduced density matrix $\rho_1 = \mathrm{Tr}_{2,\ldots,M}(\rho)$, where $\rho = |\psi\rangle\langle\psi|$ [135]. The criterion is

$$\begin{cases} \mathrm{Tr}(\rho_1^2) = \frac{1}{M} & \text{non-entangled,} \\ \frac{1}{N} \leq \mathrm{Tr}(\rho_1^2) < \frac{1}{M} & \text{entangled,} \end{cases} \tag{2.69}$$

where N is the dimension of the single-particle state space and $M \leq N$. If $M > N$, then it is not possible to construct an antisymmetric M-fermion state [135].

The simplest fermionic system allowing a Slater rank greater than one and thus admitting entanglement is composed of two fermions with a four-dimensional single-particle Hilbert space, thus resulting in a six-dimensional two-particle Hilbert space. One of the implementations of such a system is exactly the system used for illustrative purposes in the example discussed in detail at the beginning of this Subsection. This system can be viewed as the fermionic version of the standard system composed of two distinguishable qubits. It allows for a fermionic analogue of the two-qubit concurrence (described in Subsection 2.1.3), both for pure and mixed states of two fermions. Thus a closed analytical expression for the amount of entanglement exhibited by a (mixed) state of two identical fermions (as measured by the concurrence) is known only for the fermionic case of smallest

dimensionality admitting the phenomenon of entanglement [132] (these systems can be mapped onto systems of spin-$\frac{3}{2}$ particles).

Mixed states of systems of M identical fermions are non-entangled when they can be written as a mixture of Slater determinants,

$$\rho_{sl} = \sum_i \lambda_i |\psi_{sl}^{(i)}\rangle\langle\psi_{sl}^{(i)}|, \tag{2.70}$$

where the states $|\psi_{sl}^{(i)}\rangle$ can be represented as single Slater determinants, and $0 \leq \lambda_i \leq 1$ with $\sum_i \lambda_i = 1$.

All multipartite fermionic systems consisting of fermions with a single-particle Hilbert space of dimension $2k$ (with $k \geq 2$) can be mapped onto systems consisting of spin-s particles, with $s = (2k-1)/2$. According to this mapping the members $\{|i\rangle,\ i = 1, \ldots, 2k\}$ of an orthonormal basis for the single-particle Hilbert space can be denoted $|s, m_s\rangle$, with $m_s = s - i + 1,\ i = 1, \ldots, 2k$. Since each particular case considered by us corresponds to a given value of k (and, consequently s), we are going to designate these states using the compact notation $\{|m_s\rangle,\ m_s = -s, \ldots, s\}$. Following this angular momentum representation, a basis for a system consisting of two identical fermions is given by the antisymmetric joint eigenstates $\{|j, m\rangle,\ -j \leq m \leq j,\ 0 \leq j \leq 2s\}$ of the total angular momentum operators J_z and J^2. The antisymmetric states $|j, m\rangle$ are those having an even value of the quantum number j. These states can be classified in multiplets according to the value of j. The notation we will use for the product basis is the following:

$$|s, m_1, m_2\rangle = |s, m_1\rangle|s, m_2\rangle = |m_1 m_2\rangle, \tag{2.71}$$

where m_1 and m_2 are always half-integral. The Clebsch-Gordan coefficients, which are the expansion coefficients of total angular momentum eigenstates in an uncoupled tensor product basis, are used to transform between the two bases [51]:

$$|j, m\rangle = \sum_{m_1 m_2} |m_1 m_2\rangle\langle m_1 m_2|j, m\rangle = \sum_{m_1 m_2} |m_1 m_2\rangle\, C_{jm}^{m_1 m_2}. \tag{2.72}$$

An exact, analytical formula for the amount of entanglement (as given by the

concurrence) of general (mixed) states of two identical fermions is known only for systems with single-particle Hilbert space of dimension four (that is, $s = \frac{3}{2}$) [132]. This concurrence can be written as

$$\mathcal{C}_{\mathcal{F}}(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 - \lambda_5 - \lambda_6\} \tag{2.73}$$

where the λ_i's are, in descending order of magnitude, the square roots of the eigenvalues of $\rho\tilde{\rho}$ with $\tilde{\rho} = \mathcal{D}\rho\mathcal{D}^{-1}$, where the operator $\mathcal{D}$ is given by

$$\mathcal{D} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \mathcal{K} \tag{2.74}$$

where $\mathcal{K}$ is the complex conjugation operator and $\mathcal{D}$ is expressed with respect to the aforementioned total angular momentum basis, ordered as $|2,2\rangle$, $|2,1\rangle$, $|2,0\rangle$, $|2,-1\rangle$, $|2,-2\rangle$ and $i|0,0\rangle$. Note that the phase of the last singlet state has been adjusted.

There is a need for separability criteria and entanglement indicators that are relatively easy to implement in practice and which can be extended to higher dimensional two-fermion systems or to situations involving more than two fermions [135]. In fact, the field of separability criteria and entanglement indicators for systems of identical fermions is a largely unexplored one.

2.6 Relevant properties and techniques related to uncertainty relations and entropic inequalities

The property required to move from entropic uncertainty relations involving pure states to uncertainty relations holding for mixed states, is the concavity property

of the entropy described in Subsection 1.1.7, eq. (1.32). This will be the tool used to establish uncertainty relations for mixed states of distinguishable subsystems (see Section 2.7) as well as mixed states of indistinguishable fermions (see Section 4.1).

For uncertainty relations involving the variances of observables M_k, one makes use of the fact that the uncertainty of a mixture is always greater or equal than the averaged uncertainties of the components, to move from uncertainty relations involving separable pure states to separable mixed states. This property is utilized in scenarios involving either distinguishable or indistinguishable subsystems. Thus in the case of two distinguishable subsystems, if $\sum_k \delta^2(M_k)_{|\alpha_i\rangle|\beta_i\rangle\langle\alpha_i|\langle\beta_i|} \geq C$, then this bound also holds for separable mixed states ρ_{sep} written in the form of eq. (2.5),

$$\sum_k \delta^2(M_k)_{\rho_{sep}} \geq \sum_i p_i \sum_k \delta^2(M_k)_{|\alpha_i\rangle|\beta_i\rangle\langle\alpha_i|\langle\beta_i|} \geq C, \tag{2.75}$$

since $\sum_i p_i = 1$. The physical meaning of this is, that one cannot decrease the uncertainty of an observable by mixing several states.

The unitary freedom in the ensemble for density matrices as described in Subsection 1.1.6, eq. (1.27) was utilized by Nielsen and Kempe [136] in their proof of the disorder criterion for separability (described in the next Subsection) and will be used in our proof of the entropic entanglement criteria based on the Rényi entropies (see Subsubsection 4.2.3.3).

2.6.1 Majorization

The theory of majorization is an area of mathematics that actually predates quantum mechanics. The powerful techniques related to the majorization concept were introduced to the field of quantum entanglement by Nielsen and Kempe [136].

Majorization is an ordering on d-dimensional real vectors, which is intended to capture the notion that one vector is more or less "mixed", that is, disordered than another [7]. To be more precise, suppose $x = (x_1, x_2, \ldots, x_d)$ and $y =$

$(y_1, y_2, \ldots, y_d)$ are two d-dimensional real vectors and suppose in addition that x and y are probability distributions, which means the components are non-negative and add up to one. Using the notation $x^{\downarrow}$ to signify x rearranged in such a way that its components are in decreasing order, for instance $x_1^{\downarrow}$ would denote the largest component of x. In other words, $x^{\downarrow} = (x_1^{\downarrow}, x_2^{\downarrow}, \ldots, x_d^{\downarrow})$, where $x_1^{\downarrow} \geq x_2^{\downarrow} \geq \ldots \geq x_d^{\downarrow}$. The following relation is intended to capture the notion that x is more disordered or mixed than y: $x \prec y$ (in words "x is majorized by y") if

$$\sum_{j=1}^{k} x_j^{\downarrow} \leq \sum_{j=1}^{k} y_j^{\downarrow}, \tag{2.76}$$

for $k = 1, 2, \ldots, d-1$ and with equality holding when $k = d$ (both vectors represent probability distributions).

The connection between majorization and disorder is clearly seen by means of the following result:

$$x \prec y \quad \text{if and only if} \quad x = Dy, \tag{2.77}$$

where D is a doubly stochastic matrix (that is, it has non-zero entries and each row and column add up to one). Thus, when $x \prec y$ one can think of y as being the input probability distribution to a noisy channel described by the doubly stochastic matrix D, resulting in a more disordered output probability distribution x [136]. Relating this to entropy, one has that if $x \prec y$ it follows that $H(x) \geq H(\mathrm{y})$. However, the converse does not necessarily hold in general and so majorization is a more stringent notion of disorder than entropy [136]. The connection between majorization and entropic functions is as follows: $x \prec y$ iff for all entropic functions $S(x) \geq S(y)$ holds [137]. It has been shown in [138] that there is a smaller set of concave entropic functions which is sufficient for implying $x \prec y$ in the above statement.

To have another intuitive meaning of the concept of majorization, one can make use of a result known as Birkhoff's theorem, which implies that the doubly stochastic matrices correspond exactly to the set of matrices which can be written as convex combinations of permutation matrices [7]. Then $x \prec y \iff x = Dy$

can be interpreted as x being more disordered than y since x can be obtained by, say first permuting the elements of y and then mixing the resulting vectors [7], thus resulting in greater disorder.

Given the known connections between separability and measures of disorder such as the von Neumann entropy, it makes sense to expect a relationship between separability and majorization involving the vectors of eigenvalues for ρ_{AB} and the reduced density matrices ρ_A and ρ_B. Nielsen and Kempe [136] proved the disorder criterion for separability: non-entangled states of quantum systems having distinguishable subsystems are such that the total density matrix ρ_{AB} is always majorized by the marginal density matrix associated with one of the subsystems, ρ_A or ρ_B. That is, the set of eigenvalues of separable mixed states ρ_{AB} is majorized by those of ρ_A and ρ_B (zeros are appended to the vectors of eigenvalues of ρ_A and ρ_B, in order to make their dimension equal to that of the vector of eigenvalues of ρ_{AB}). For mixed states the disorder criterion is only a necessary condition for separability since no sufficient condition for mixed states can be solely based on the knowledge of the eigenvalues of ρ_{AB}, ρ_A and ρ_B [136].

The proof by Nielsen and Kempe is as follows [136]. If ρ_{AB} is separable it can be written in the form eq. (2.5). Suppose the spectral decomposition for ρ_{AB} is $\rho_{AB} = \sum_k r_k |e_k\rangle\langle e_k|$. By making use of the unitary freedom eq. (1.27), there is a unitary matrix (u_{ki}) such that

$$\sqrt{r_k}|e_k\rangle = \sum_i u_{ki}\sqrt{p_i}|\alpha_i\rangle|\beta_i\rangle. \tag{2.78}$$

Tracing out system B in eq. (2.5) gives $\rho_A = \sum_i p_i|\alpha_i\rangle\langle\alpha_i|$, then letting $\rho_A = \sum_l a_l|f_l\rangle\langle f_l|$ be a spectral decomposition and once again using the unitary freedom, results in $\sqrt{p_i}|\alpha_i\rangle = \sum_l v_{il}\sqrt{a_l}|f_l\rangle$ with (v_{il}) being a unitary matrix. Substituting this into eq. (2.78) gives

$$\sqrt{r_k}|e_k\rangle = \sum_{il} \sqrt{a_l}\, u_{ki}\, v_{il}|f_l\rangle|\beta_i\rangle. \tag{2.79}$$

Multiplying this equation with its adjoint and then utilizing the orthonormality

of the vectors $|f_l\rangle$, one gets

$$r_k = \sum_l D_{kl} a_l, \tag{2.80}$$

where

$$D_{kl} = \sum_{i_1 i_2} u^*_{ki_1} u_{ki_2} v^*_{i_1 l} v_{i_2 l} \langle \beta_{i_1} | \beta_{i_2} \rangle. \tag{2.81}$$

To show that the eigenvalues of ρ_{AB}, namely $\{r_k\}$, are majorized by the eigenvalues of ρ_A, namely $\{a_l\}$, one has to show that D_{kl} is doubly stochastic. By defining $|\gamma_{kl}\rangle = \sum_i u_{ki}\, v_{il} |\beta_i\rangle$ one sees that $D_{kl} = \langle \gamma_{kl} | \gamma_{kl} \rangle \geq 0$. The next step is to demonstrate that the rows and columns sum to one by using the unitarity of (u_{ki}) and (v_{il}):

$$\begin{aligned} \sum_k D_{kl} &= \sum_{i_1 i_2} \Big(\sum_k u^*_{ki_1} u_{ki_2} \Big) v^*_{i_1 l}\, v_{i_2 l} \langle \beta_{i_1} | \beta_{i_2} \rangle \\ &= \sum_{i_1 i_2} \delta_{i_1 i_2}\, v^*_{i_1 l}\, v_{i_2 l} \langle \beta_{i_1} | \beta_{i_2} \rangle = \sum_i v^*_{il}\, v_{il} = 1, \end{aligned} \tag{2.82}$$

and similarly one has $\sum_l D_{kl} = 1$. Therefore (D_{kl}) is a doubly stochastic matrix.

In the case of non-entangled states of a system of identical fermions the total density matrix ρ is not necessarily majorized by the one-particle reduced density matrix ρ_r. In Section 4.2 I am going to derive entropic entanglement criteria for fermion systems by making use of majorization amongst others.

2.7 Uncertainty relations for distinguishable particles

The establishment of appropriate separability criteria is a fundamental first step in the study of the entanglement properties of a given class of quantum systems. This then enables us to tell whether a given quantum state is separable or entangled. However, a good separability criterion, in addition to being a tool for determining the absence or presence of entanglement, should also act as a basis for quantitative measures of entanglement. An estimation of the amount of entanglement exhibited by a given quantum state is provided by the deviation of

the actual properties of the state from those required by the separability criterion [135].

The approach for entanglement detection by means of local uncertainty relations advanced by Hofmann and Takeuchi [139] for systems with distinguishable subsystems is as follows. The idea is that the sum of the variances of local observables of a system admits a non-zero lower bound for separable states, and so any state violating this bound is necessarily entangled.

The statistical variance of measurement outcomes of an observable A_i gives the uncertainty of that Hermitian operator for any given quantum state $|\psi\rangle$ of the system:

$$\delta A_i(|\psi\rangle) = \langle (A_i - \langle A_i\rangle_{|\psi\rangle})^2\rangle_{|\psi\rangle} = \langle A_i^2\rangle_{|\psi\rangle} - \langle A_i\rangle^2_{|\psi\rangle}. \tag{2.83}$$

This uncertainty is positive for all relevant observables $\{A_i\}$ of the system and is zero only when the given quantum state is an eigenstate of A_i. However, the uncertainty principle in its general form states that it is never possible to simultaneously determine the measurement outcomes for all observables of the system. Thus, if there is no simultaneous eigenstate of all the operators in $\{A_i\}$, there must exist an absolute lower limit $U > 0$ for the sum of their uncertainties, holding for any quantum state $|\psi\rangle$,

$$\sum_i \delta A_i(|\psi\rangle) \geq U \quad \forall\, |\psi\rangle. \tag{2.84}$$

We now look at a bipartite quantum system composed of subsystems A and B, characterized by the operators A_i and B_i respectively. Using the previous argument, the sum uncertainty relations are then

$$\sum_i \delta A_i(|\phi^{(A)}\rangle) \geq U_A \quad \forall\, |\phi^{(A)}\rangle, \quad \sum_i \delta B_i(|\phi^{(B)}\rangle) \geq U_B \quad \forall\, |\phi^{(B)}\rangle. \tag{2.85}$$

The aim of the strategy was to find an uncertainty relation involving separable states. Recall that a mixed state was said to be separable if it can be written as a mixture of product states, see eq. (2.4) or eq. (2.5). So let us first look at

what happens with the sum of the local uncertainties for a joint measurement $A_i + B_i = A_i \otimes \mathbb{I} + \mathbb{I} \otimes B_i$ on any product state $\rho_m = \rho_m^{(A)} \otimes \rho_m^{(B)}$:

$$\delta[A_i + B_i](\rho_m) = \delta A_i(\rho_m^{(A)}) + \delta B_i(\rho_m^{(B)}) \qquad \forall\, \rho_m = \rho_m^{(A)} \otimes \rho_m^{(B)}. \tag{2.86}$$

Without loss of generality one can use as general separable state the form in eq. (2.5) and so we can take the product state ρ_m to be composed of the tensor product of two projectors, which gives rise to

$$\sum_i \delta[A_i + B_i](\rho_m) \geq U_A + U_B \qquad \forall\, \rho_m = |\phi_m^{(A)}\rangle\langle\phi_m^{(A)}| \otimes |\phi_m^{(B)}\rangle\langle\phi_m^{(B)}|. \tag{2.87}$$

Bringing to mind that the uncertainty of a mixture is always greater or equal than the averaged uncertainties of the components, one has that for a general separable mixed state $\rho_{sep} = \sum_m p_m \rho_m$ and an arbitrary observable R,

$$\delta R(\rho_{sep}) \geq \sum_m p_m \delta R(\rho_m). \tag{2.88}$$

It is thus clear that

$$\sum_i \delta[A_i + B_i](\rho_{sep}) \geq U_A + U_B \quad \forall\, \rho_{sep} = \sum_m p_m |\phi_m^{(A)}\rangle\langle\phi_m^{(A)}| \otimes |\phi_m^{(B)}\rangle\langle\phi_m^{(B)}|. \tag{2.89}$$

Hence any violation of this uncertainty relation indicates that the quantum state has to be entangled, since entanglement describes correlations that are more precise (hence the uncertainty is smaller than the lower bound) than the ones represented by mixtures of product states [139]. A quantitative measure of entanglement which can be implemented experimentally is provided by the relative violation of a local uncertainty [139], given by

$$C_{LUR}(\rho) = 1 - \frac{\sum_i \delta[A_i + B_i](\rho)}{U_A + U_B}. \tag{2.90}$$

For $0 < C_{LUR}(\rho) \leq 1$, the state ρ is entangled and the greater the value the more entangled is the state. Note that when $C_{LUR}(\rho) \leq 0$, we cannot draw any conclusion since the state ρ might be either separable or entangled as it complies with the uncertainty relation. To detect a given entangled state, one therefore

has to choose A_i and B_i in such a way that this given state actually violates the resulting uncertainty relation.

The approach described next was applied by Gühne [140] to composite quantum systems with distinguishable subsystems. Instead of formulating separability criteria based upon the uncertainties of observables of the form $A_i + B_i = A_i \otimes \mathbb{I} + \mathbb{I} \otimes B_i$, one considers families of non-local observables of the form $M_i = |\psi_i\rangle\langle\psi_i|$, where $|\psi_i\rangle$ are appropriate pure states of the system under consideration. The advantage of this method is that it can be generalized to multipartite systems.

Let us illustrate this scheme by considering a bipartite system composed of two qubits. The notation used for the variance or uncertainty of an observable M is

$$\delta^2(M)_\rho = \langle M^2\rangle_\rho - \langle M\rangle_\rho^2. \tag{2.91}$$

One starts with $|\psi_1\rangle = a|00\rangle + b|11\rangle$, an entangled state written in the Schmidt decomposition, with $a \geq b$. The idea is that there exist M_i such that, for $|\psi_1\rangle$, $\sum_i \delta^2(M_i)_{|\psi_1\rangle\langle\psi_1|} = 0$ holds, whereas separable states ρ_{sep} fulfil

$$\sum_{i=1}^{4} \delta^2(M_i)_{\rho_{sep}} \geq 2a^2b^2. \tag{2.92}$$

To achieve this one defines $|\psi_2\rangle = a|01\rangle + b|10\rangle$, $|\psi_3\rangle = b|01\rangle - a|10\rangle$, $|\psi_4\rangle = b|00\rangle - a|11\rangle$ and so $M_i = |\psi_i\rangle\langle\psi_i|$, $i = 1, 2, 3, 4$. This indeed gives

$$\sum_i \delta^2(M_i)_{|\psi_1\rangle\langle\psi_1|} = 0. \tag{2.93}$$

Making use of eq. (2.75), one only needs to prove the bound in eq. (2.92) for a pure product vector $|\phi_{sep}\rangle$. Writing

$$\sum_{i=1}^{4} \delta^2(M_i)_{|\phi_{sep}\rangle\langle\phi_{sep}|} = 1 - \sum_i (|\langle\phi_{sep}|\psi_i\rangle|^2)^2, \tag{2.94}$$

one can find the maximum of $\sum_i (|\langle\phi_{sep}|\psi_i\rangle|^2)^2$ instead of the minimum on the left

hand side. This one does by expanding the product vector $|\phi_{sep}\rangle$ in the product basis determined by the Schmidt basis of the $|\psi_i\rangle$'s,

$$|\phi_{sep}\rangle = (\alpha_0|0\rangle + \alpha_1|1\rangle)(\beta_0|0\rangle + \beta_1|1\rangle) = \alpha_0\beta_0|00\rangle + \alpha_0\beta_1|01\rangle + \alpha_1\beta_0|10\rangle + \alpha_1\beta_1|11\rangle. \tag{2.95}$$

So one should find the maximum of $|\langle\phi_{sep}|\psi_i\rangle|^2$ for each i, however, by making use of symmetry, it suffices to find the maximum for one i. Now

$$\begin{aligned} |\langle\phi_{sep}|\psi_1\rangle| &= |a\alpha_0^*\beta_0^* + b\alpha_1^*\beta_1^*| \\ &\leq |a||\alpha_0||\beta_0| + |b||\alpha_1||\beta_1| \qquad \text{(subadditivity of absolute value)} \\ &\leq |a|(|\alpha_0||\beta_0| + |\alpha_1||\beta_1|) \qquad (a \geq b) \\ &\leq |a|\sqrt{|\alpha_0|^2 + |\alpha_1|^2}\sqrt{|\beta_0|^2 + |\beta_1|^2} \qquad \text{(Schwarz inequality)} \\ &= |a| \qquad \text{(normalization).} \end{aligned} \tag{2.96}$$

Thus for all i, $|\langle\phi_{sep}|\psi_i\rangle|^2 \leq a^2$ and so $\sum_i(|\langle\phi_{sep}|\psi_i\rangle|^2)^2 \leq (a^2)^2 + (1-a^2)^2$, where the maximum is attained when $|\phi_{sep}\rangle$ is a Schmidt basis state. Then again using the normalization of the $|\psi_i\rangle$'s, this finally leads to

$$\sum_{i=1}^{4} \delta^2(M_i)_{|\phi_{sep}\rangle\langle\phi_{sep}|} \geq 2a^2b^2. \tag{2.97}$$

Since we want an uncertainty relation involving mixed separable states we make use of eq. (2.75) to arrive at

$$\sum_{i=1}^{4} \delta^2(M_i)_{\rho_{sep}} \geq 2a^2b^2. \tag{2.98}$$

Choosing $a = b = 1/\sqrt{2}$ gives the greatest value for the right hand side of the above expression and hence the best entanglement criterion, since any state violating the uncertainty relation is entangled.

Entropic uncertainty relations provide an alternative way to develop entanglement criteria based upon uncertainty relations. The idea of this approach is to replace the statistical variance or uncertainty with either the Shannon, Rényi or Tsallis entropy as a means of estimating the uncertainties associated with

the measurement process. The application of this procedure to the detection of entanglement in quantum systems consisting of distinguishable subsystems was investigated by Gühne and Lewenstein in [141] and by Giovannetti in [142].

The idea is to find entropic uncertainty relations which have to hold for separable states, but which might be violated by entangled states. Assume that one has a non-degenerate observable M with a spectral decomposition

$$M = \sum_{i=1}^{n} \mu_i |m_i\rangle\langle m_i|. \tag{2.99}$$

When the system is in a given quantum state ρ, a measurement of this observable gives rise to a probability distribution of the different outcomes (that is, the probabilities of obtaining the different eigenvalues of M),

$$\mathcal{P}(M)_\rho = (p_1, \ldots, p_n), \quad p_i = \mathrm{Tr}(|m_i\rangle\langle m_i|\rho) = \langle m_i|\rho|m_i\rangle. \tag{2.100}$$

One can now look at the entropy of this probability distribution, written as $S[\mathcal{P}(M)]_\rho = S[M]_\rho$. The scheme is to take one or several observables M_i and investigate the sum of the entropies $\sum_i S[M_i]_\rho$. Lower bounds for this sum can be derived for product states and then by concavity, these bounds also hold for separable mixed states. When a state violates this entropic uncertainty relation, it implies that the state must be entangled.

Gühne and Lewenstein [141] devised two methods for obtaining separability criteria from entropic uncertainty relations. For the first method one only looks at one observable M. The choice of M is such that the set $\{|m_i\rangle\}$ of eigenvectors of M does not contain any product vector and is non-degenerate, $M = \sum_i \mu_i |m_i\rangle\langle m_i|$. This means that there must exist a bound $C > 0$ such that for all separable pure states $|\phi_{sep}\rangle$,

$$S_q^{(T)}[\mathcal{P}(M)]_{|\phi_{sep}\rangle\langle\phi_{sep}|} \geq C \quad \forall\, |\phi_{sep}\rangle \tag{2.101}$$

since $p_i = |\langle m_i|\phi_{sep}\rangle|^2 \neq 1 \;\forall\, i$ and so the Tsallis entropy can never be zero. One can determine C from the Schmidt coefficients of the eigenvectors $|m_i\rangle$ of M.

Assume that $c < 1$ is an upper bound for all the squared Schmidt coefficients of all the $|m_i\rangle$. Since the maximal Schmidt coefficient of an entangled state $|m_i\rangle$ is just the maximal overlap between $|m_i\rangle$ and the product states [141], it means that all the probabilities p_i appearing in $\mathcal{P}(M)_{|\phi_{sep}\rangle\langle\phi_{sep}|}$ are bounded by c (all separable states are product states). Knowing this, one now has to minimize $S_q^{(T)}[\mathcal{P}(M)]_{|\phi_{sep}\rangle\langle\phi_{sep}|}$ in order to obtain C. Since the Tsallis entropy is concave, the minimum will be obtained when the probability distribution is as peaked as possible. For that we need to introduce the notation $\lfloor x \rfloor$ to denote the integer part of x. The minimum is reached when letting as many as possible, namely $\lfloor \frac{1}{c} \rfloor$ of the p_i satisfy the bound $p_i = c$ (the sum of their probabilities is then $\lfloor \frac{1}{c} \rfloor c$), while at most one other p_i does not satisfy the bound but is as big as possible, namely $1 - \lfloor \frac{1}{c} \rfloor c$ (remember $\sum_i p_i = 1$) and the remaining p_i are equal to zero. Then

$$S_q^{(T)}[M]_{|\phi_{sep}\rangle\langle\phi_{sep}|} \geq \frac{1 - \lfloor \frac{1}{c} \rfloor c^q - (1 - \lfloor \frac{1}{c} \rfloor c)^q}{q - 1}. \tag{2.102}$$

From the concavity of the entropy we have

$$S_q^{(T)}[M]_{\rho_{sep}} \geq \frac{1 - \lfloor \frac{1}{c} \rfloor c^q - (1 - \lfloor \frac{1}{c} \rfloor c)^q}{q - 1} \tag{2.103}$$

for all separable mixed states [141].

The second method for deriving separability criteria deals with product observables, which might be degenerate. Since the spectral decomposition of a degenerate observable M is not unique, the definition of $\mathcal{P}(M)$ is not unique. However, by combining eigenvectors with the same eigenvalue one obtains a unique decomposition of the form $M = \sum_i \eta_i X_i$ with $\eta_i \neq \eta_j$ for $i \neq j$ and the X_i are orthogonal projectors of maximal rank [141]. Hence one can define $p_i = \mathrm{Tr}(\rho X_i)$. Gühne and Lewenstein showed that for a bipartite Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and observables A_n and B_n (with non-zero eigenvalues) on $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively, we have that for all product states $\rho = \rho_A \otimes \rho_B$

$$\mathcal{P}(A_n \otimes B_n)_\rho \prec \mathcal{P}(A_n)_{\rho_A} \quad \forall\, \rho = \rho_A \otimes \rho_B \tag{2.104}$$

and also $\mathcal{P}(A_n \otimes B_n)_\rho \prec \mathcal{P}(B_n)_{\rho_B}$. This means

$$S[A_n \otimes B_n]_{\rho_A \otimes \rho_B} \geq S[A_n]_{\rho_A} \tag{2.105}$$

and also $S[A_n \otimes B_n]_{\rho_A \otimes \rho_B} \geq S[B_n]_{\rho_B}$. Now considering two observables (with non-zero eigenvalues) on each subsystem, namely A_1, A_2 and B_1, B_2, one has that if they obey an entropic uncertainty relation of the type

$$S[A_1]_{\rho^{(A)}} + S[A_2]_{\rho^{(A)}} \geq C \tag{2.106}$$

or the same bound for B_1, B_2, then

$$S[A_1 \otimes B_1]_\rho + S[A_2 \otimes B_2]_\rho \geq C \tag{2.107}$$

when $\rho = \sum_i q_i \rho_i^{(A)} \otimes \rho_i^{(B)}$ is a separable mixed state. This follows directly from the concavity property of entropy and eq. (2.105). This demonstrates how any entropic uncertainty relation on one subsystem can be transferred into a separability criterion. Also of interest is when one performs numerical calculations for separable states to determine the bounds on $S[A_1 \otimes B_1]_\rho + S[A_2 \otimes B_2]_\rho$ since then one only has to minimize the entropy for one subsystem [141].

In Section 4.1 I am going to extend the above approaches to fermionic systems.

Chapter 3

Extensions of Landauer's Principle and Conservation of Information in General Probabilistic Theories

3.1 Landauer's Principle and Divergenceless Dynamical Systems

Landauer's principle is one of the pillars of the physics of information as discussed in Subsection 1.2.3. It constitutes one of the foundations behind the idea that "information is physical". Landauer's principle establishes the smallest amount of energy that has to be dissipated when one bit of information is erased from a computing device. In this Section I explore an extended Landauer-like principle valid for general dynamical systems (not necessarily Hamiltonian) governed by divergenceless phase space flows.

This Section is based on the publication [57] "Landauer's Principle and Divergenceless Dynamical Systems", C. Zander, A.R. Plastino, A. Plastino, M. Casas and S. Curilef, *Entropy* **11** (4), (2009) pp. 586-597 and is organized as follows. In Subsection 3.1.1 a brief introduction is provided and in Subsection 3.1.2 we derive a generalized Landauer-like principle valid for divergenceless systems. Sub-

section 3.1.3 attempts to provide a further extension of this result utilizing the superstatistical formalism. Some conclusions are given in Subsection 3.1.4.

3.1.1 Introduction

The physics of information constitutes an active research field that has been the focus of considerable attention in recent times [1–6, 15, 16, 143, 144]. Due to seminal results generated by these research efforts the physical reality of information is by now generally acknowledged. In this regard, the ultimate performance limits imposed by the laws of physics on any real device that processes or transmits information are starting to be understood [6, 39]. On the other hand, several theoretical developments indicate that the concept of information is essential for understanding the basic fabric of the physical world [1–6]. Tools inspired by information-theoretical ideas, such as the maximum entropy (maxent) principle [145–147] have been successfully applied to the study of several physical scenarios. Last, but certainly not least, the ideas and methods from the physics of information lead to important points of contact between physics and biology. In fact, information processing is clearly at the very heart of biology and has been appropriately dubbed the "touchstone of life" [17].

Landauer's principle is one of the most fundamental results in the physics of information. It constituted a historical landmark in the development of the field by directly connecting information processing with conventional physical quantities [18]. Most remarkably, it played a prominent role in the final defeat of Maxwell's demon [6]. Landauer's principle states that there is a minimum amount of energy that has to be dissipated, on average, when erasing a bit of information in a computing device working at absolute temperature T. This minimum energy is equal to $kT \ln 2$, where k is Boltzmann's constant [19–21, 56]. Landauer's principle has profound implications as it allows for novel, physically motivated derivations of several important results in classical and quantum information theory [22]. Moreover, it proved to be a powerful heuristic tool for establishing new links between, or obtaining new derivations of, fundamental aspects of thermodynamics and other areas of physics [23].

3.1 Landauer's Principle and Divergenceless Dynamical Systems

It is fair to say that most derivations of Landauer's principle can be regarded as semi-phenomenological, since they are based on a direct application of the second law of thermodynamics. However, derivations based upon dynamical principles have also been advanced. They assume that the systems under consideration are governed by a Hamiltonian dynamics and are in thermal equilibrium, implying that they can be described by Gibbs' canonical distributions. In view of the fundamental character of Landauer's principle, however, it is highly desirable to explore extensions of it applicable to systems governed by more general kinds of dynamics. These developments are inscribed within the more general program of extending the methods of statistical mechanics to non-Hamiltonian systems [148, 149]. Of special relevance is the class of dynamical systems with divergenceless phase space flows, that include Hamiltonian systems as particular members. Divergenceless systems are characterized by the remarkable property that their dynamics preserves information. There are interesting divergenceless dynamical systems in physics, theoretical biology and other areas that are not Hamiltonian, or that have their most natural description in terms of a non-canonical set of variables. For example, the Lotka-Volterra predator-prey systems [150, 151] and the Nambu systems [152] share the vanishing divergence property. The Lotka-Volterra predator-prey systems constitute some of the most important dynamical systems considered in theoretical biology [150]. Nambu systems have been the focus of considerable research activity (see [153–157] and references therein). The main difference between Hamiltonian systems and Nambu systems is that, while the dynamics of a Hamiltonian system is governed by one single phase space function (the Hamiltonian function) the dynamics of a Nambu system is governed by a set of N ($N \geq 2$) such functions or "Hamiltonians" [152]. The dynamics of Nambu systems can be formulated in terms of Poisson-like brackets involving, in general, more than two functions. In the case of a Nambu system with N "Hamiltonians" the time derivative of a general phase space function A is given by an appropriate $(N+1)$-bracket depending on the function A and on the N Hamiltonians. Unlike Hamiltonian systems, Nambu systems can be defined on phase spaces with an odd number of dimensions. The Nambu dynamical structures arise in a natural way in several contexts. For instance, Nambu dynamics has been applied to the relativistic dynamics of charged spinning particles [156], and to some hydrodynamical type systems [157].

Information processing can be realized in various physical settings. Indeed, one of the main ideas behind the physics of information and computation is that every physical system (even the whole universe) can be construed as an information processing system. Consequently, it is of considerable interest to extend the fundamental principles of the physics of information to more general scenarios. These more general situations may encompass compelling examples of physical realizations of information processes such as, for instance, those related to biology. Indeed, biological systems process information at molecular, cellular, and higher levels [17].

The aim of the present work is to explore extensions of Landauer's principle to the aforementioned more general scenarios. We shall derive a Landauer-like principle for dynamical systems with divergenceless phase space flows. This result establishes a direct connection (within the alluded dynamical context) between an information-processing operation, on the one hand, and changes in the mean value of a relevant dynamical quantity, on the other hand. In the particular case of the usual Hamiltonian scenario our generalized result reduces to the standard Landauer principle. There is much to be gained from considering Landauer-like principles within the abovementioned general dynamical settings. Besides opening a range of possible new applications, this line of enquiry contributes to a deeper understanding of the main dynamical and information-theoretical ingredients at play behind Landauer's principle.

3.1.2 An extension of Landauer's principle to divergenceless dynamical systems

In this Subsection I am going to formulate a generalization of Landauer's principle appropriate for dynamical systems with vanishing divergence. We are going to consider a composite system $A + B$ compounded by an information "storing device" A and an "environment" B. The composite system will be described by an appropriate ensemble probability density describing the probability of finding the system in different regions of phase space. Generalizing the standard Hamiltonian scenario, the erasure of one bit of information from the storing device

A will be identified with a dynamical process (described by an appropriate Liouville equation) where the Gibbs-Shannon entropy of the marginal probability density corresponding to the device A decreases by $k \ln 2$ (here k is an appropriate constant defining the units in which the entropy is measured; in the standard Hamiltonian statistical mechanics setting k stands for Boltzmann's constant). In the Hamiltonian case the device A is modelled as a particle moving in a one-dimensional double-well potential, with the left and right wells representing the two possible states of the classical bit ("0" and "1"). Before erasure the marginal probability density describing the particle is such that the particle is equally likely to be in either well. This corresponds to a situation where the two states of the bit are equally probable. After erasure the bit is set to one of its possible states (say, state "0"), the particle's marginal probability density is concentrated in one well, and its entropy decreases by an amount $k \ln 2$. In the more general setting that we are going to explore we shall interpret the decrease in $k \ln 2$ of the entropy of subsystem A as the most fundamental characterization of a process corresponding to the erasure of one bit of information from A. This entropy reduction corresponds to a decrease of the "spread" of the phase space distribution of A and, consequently also to a decrease of the amount of information that can be encoded in the precise location of system A in phase space.

3.1.2.1 Divergenceless dynamical systems

Let us consider a dynamical system

$$\dot{\boldsymbol{z}} = \boldsymbol{w}(\boldsymbol{z}), \qquad \boldsymbol{z}, \boldsymbol{w} \in \mathcal{R}^N \tag{3.1}$$

where the vector $\boldsymbol{z}$ represents a point in the system's phase space. The phase space variables are separated in two subsets,

$$\boldsymbol{z} = (\boldsymbol{x}, \boldsymbol{y}) \tag{3.2}$$

with

$$\begin{aligned} \boldsymbol{x} &\in \mathcal{R}^{N_1}, \\ \boldsymbol{y} &\in \mathcal{R}^{N_2}, \qquad N_1 + N_2 = N \end{aligned} \tag{3.3}$$

where $\boldsymbol{x}$ stands for the phase space coordinates of the "information storage device" A and $\boldsymbol{y}$ denotes the phase space coordinates of the environment B.

The dynamical equations of motion of the composite $A+B$ can be written as

$$\begin{aligned} \dot{\boldsymbol{x}} &= \boldsymbol{u}(\boldsymbol{x},\boldsymbol{y}) \\ \dot{\boldsymbol{y}} &= \boldsymbol{v}(\boldsymbol{x},\boldsymbol{y}) \end{aligned} \tag{3.4}$$

where $\boldsymbol{w}=(\boldsymbol{u},\boldsymbol{v})$ is a divergence-free phase space flow. That is,

$$\nabla\cdot\boldsymbol{w} = \left(\sum_{i=1}^{N_1}\frac{\partial u_i}{\partial x_i}\right)+\left(\sum_{j=1}^{N_2}\frac{\partial v_j}{\partial y_j}\right) = 0 \tag{3.5}$$

where the N-dimensional ∇-operator is defined in the standard way,

$$\nabla = \left(\frac{\partial}{\partial x_1},\ldots,\frac{\partial}{\partial x_{N_1}},\frac{\partial}{\partial y_1},\ldots,\frac{\partial}{\partial y_{N_2}}\right). \tag{3.6}$$

We are going to consider divergenceless dynamical systems (3.4) admitting a constant of motion $I(\boldsymbol{x},\boldsymbol{y})$,

$$\frac{dI}{dt} = \left(\sum_{i=1}^{N_1}\frac{\partial I}{\partial x_i}\,u_i\right)+\left(\sum_{j=1}^{N_2}\frac{\partial I}{\partial y_j}\,v_j\right) = 0. \tag{3.7}$$

Hamiltonian systems fulfil condition (3.5) and admit the Hamiltonian itself as a constant of motion, but there are other interesting systems compliant with (3.5) and admitting an integral of motion I. Indeed, these two fundamental features allow for deriving many aspects of the canonical statistical mechanical formalism without recourse to the detailed structure of standard Hamiltonian dynamics [149, 158]. Among others, the Lotka-Volterra predator-prey systems [150, 151] and the Nambu systems [152–157] share the vanishing divergence property and admit an integral of motion.

If the system A is to behave as a proper "information storage device", it is reasonable to assume that before and after the information erasure process, the systems A and B are only weakly coupled. In fact, as far as the storage

of information is concerned, the effect of this "weak coupling" is assumed to be negligible before and after the erasure process (a system that "preserves" information should not interact too strongly with the environment). That is, we assume that in equation (3.4), $\boldsymbol{u}$ depends weakly on $\boldsymbol{y}$ and $\boldsymbol{v}$ depends weakly on $\boldsymbol{x}$. Consistent with the weak coupling between systems A and B, we are also going to assume that before and after the information erasure the integral of motion I adopts the additive form

$$I = D(\boldsymbol{x}) + C(\boldsymbol{y}). \tag{3.8}$$

The vector fields $\boldsymbol{u}$ and $\boldsymbol{v}$ are assumed to be time-independent before and after the erasure process (that is, the dynamical system (3.4) is autonomous), but $\boldsymbol{u}$ and $\boldsymbol{v}$ may depend explicitly on time during the erasure process. Consequently, during the erasure process the quantity I may not be conserved, but it is strictly conserved before and after that process. Notice, however, that the conservation of I does not imply that D and C are individually conserved. Even the weak coupling between the systems A and B allows for changes in C and D, but keeping their sum constant. (In the limit case of no interaction between systems A and B, the quantities D and C become individual integration constants of these two systems, respectively.) This situation is similar to the one considered (in connection with the energy) in standard statistical mechanics when discussing a system weakly coupled to a heat bath. The divergenceless property (3.5), which is the most important feature characterizing the dynamical systems that are considered here, and the main ingredient in the derivation of the extended Landauer's principle, is assumed to hold all the time.

A time-dependent statistical ensemble of systems evolving according to the equations of motion (3.4) is described by a phase space probability density $F(\boldsymbol{x}, \boldsymbol{y}, t)$ governed by Liouville's equation,

$$\frac{\partial F}{\partial t} + \nabla \cdot (F\, \boldsymbol{w}) = 0 \tag{3.9}$$

which, due to the divergenceless condition $\nabla \cdot \boldsymbol{w} = 0$ reduces to

$$\frac{\partial F}{\partial t} + \boldsymbol{w} \cdot \nabla F = 0. \tag{3.10}$$

As mentioned before, this includes Hamiltonian systems but encompasses more general situations as well, such as the Nambu systems and Lotka-Volterra predator-prey systems [155].

The Boltzmann-Gibbs-Shannon information measure is given by

$$S[F] = -k \int F \ln F d\Omega \tag{3.11}$$

where k is an appropriate constant determining the units in which S is measured and $d\Omega$ is the phase space volume element. The time dependence of the Boltzmann-Gibbs-Shannon measure evaluated on a time-dependent solution of Liouville's equation complies with (see [155] and references therein)

$$\begin{aligned} \frac{dS}{dt} = \frac{\partial S}{\partial t} &= -\int \frac{\partial F}{\partial t} \ln F d\Omega = \int \nabla \cdot (F\boldsymbol{w}) \ln F d\Omega \\ &= -\int \boldsymbol{w} \cdot \nabla F d\Omega = \int F \left(\nabla \cdot \boldsymbol{w}\right) d\Omega \\ &= \langle \nabla \cdot \boldsymbol{w} \rangle \end{aligned} \tag{3.12}$$

where the fact has been used that F is normalized to unity and then repeated integration by parts has been performed where one assumes that eventual boundary terms vanish. This relation holds for any autonomous dynamical system [155] and in the case of divergenceless systems this implies that we have

$$\frac{dS}{dt} = 0. \tag{3.13}$$

This equation summarizes one of the most important features of the behaviour of divergenceless dynamical systems: *the conservation of information*. If, following Jaynes, we interpret $S[F]$ as a measure of our lack of knowledge of the precise state of the system, then equation (3.13) means that the amount of "missing" knowledge is constant in time. This information-preserving character of dynamical evolution is one of the most important features of the basic laws of nature,

both in the classical and in the quantum regimes. Not only at the fundamental level is divergenceless dynamics relevant but also, in some cases, in connection with the phenomenological description of higher-level systems in physics, biology and other fields.

3.1.2.2 Extended Landauer-like principle

As part of the program of exploring some basic aspects of the physics of information within general dynamical settings, I here extend Landauer's principle to systems described by divergenceless phase space flows.

Prior to erasure the composite system is described by the ensemble distribution $F_{\text{initial}} = F_{\text{initial}}(\boldsymbol{x}, \boldsymbol{y})$ where, as already said, $\boldsymbol{x}$ and $\boldsymbol{y}$ represent the complete sets of phase space variables of the storage device A and the environment B, respectively. After erasure the composite $A + B$ is given by the final distribution $F_{\text{final}} = F_{\text{final}}(\boldsymbol{x}, \boldsymbol{y})$. The concomitant marginal distributions read $F^{(A)}_{\text{initial/final}} = F^{(A)}_{\text{initial/final}}(\boldsymbol{x}) = \int F_{\text{initial/final}}\, d\Omega^{(B)}$ and $F^{(B)}_{\text{initial/final}} = F^{(B)}_{\text{initial/final}}(\boldsymbol{y}) = \int F_{\text{initial/final}}\, d\Omega^{(A)}$, where $d\Omega^{(A)}$ and $d\Omega^{(B)}$ denote the phase space volume elements associated with the storing device and the environment, respectively. The total volume element of the composite system is $d\Omega^{(A+B)} = d\Omega^{(A)} d\Omega^{(B)}$. The erasure process starts with an initial distribution of the form

$$\begin{aligned} F_{\text{initial}}(\boldsymbol{x}, \boldsymbol{y}; \lambda) &= \frac{e^{-\frac{\lambda}{k}(D(\boldsymbol{x})+C(\boldsymbol{y}))}}{Z^{(A)}(\lambda)\, Z^{(B)}(\lambda)} = \frac{e^{-\frac{\lambda}{k}D(\boldsymbol{x})}}{Z^{(A)}(\lambda)} \cdot \frac{e^{-\frac{\lambda}{k}C(\boldsymbol{y})}}{Z^{(B)}(\lambda)} \\ &= F^{(A)}_{\text{initial}}(\boldsymbol{x}; \lambda) \cdot F^{(B)}_{\text{initial}}(\boldsymbol{y}; \lambda) \end{aligned} \tag{3.14}$$

where $I = D(\boldsymbol{x}) + C(\boldsymbol{y})$ denotes some appropriate, conserved dynamical quantity (see equation (3.8)). $Z^{(A)}(\lambda)$ and $Z^{(B)}(\lambda)$ are the accompanying partition functions of the bit-storage device (system A) and the "environment" (system B), respectively given by

$$\begin{aligned} Z^{(A)}(\lambda) &= \int e^{-\frac{\lambda}{k}D(\boldsymbol{x})} d\Omega^{(A)} \\ Z^{(B)}(\lambda) &= \int e^{-\frac{\lambda}{k}C(\boldsymbol{y})} d\Omega^{(B)}. \end{aligned} \tag{3.15}$$

We assume that both $D(\boldsymbol{x})$ and $C(\boldsymbol{y})$ comply with all the properties required for

the convergence of $Z^{(A)}(\lambda)$ and $Z^{(B)}(\lambda)$. In particular, we assume that $D(\boldsymbol{x})$ and $C(\boldsymbol{y})$ are bounded from below. In the standard Hamiltonian case we have that $D = H_A$ and $C = H_B$ are the Hamiltonians of the information storage device and the environment (heat bath), respectively, and the initial distribution (3.14) corresponds to the Gibbs canonical distribution describing thermal equilibrium at temperature $T = 1/\lambda$. The initial distribution is also a maximum entropy distribution that maximizes the entropy under the constraint given by the mean value of $\langle I \rangle = \langle D + C \rangle$. Before the erasure process (when the dynamics of the $A + B$ system is autonomous and the quantity I is conserved) this maxent distribution constitutes a stationary solution of Liouville's equation. This stationary maxent density can be regarded, according to information theoretical interpretation of equilibrium statistical mechanics, as the natural one for describing an equilibrium situation.

After erasure, the composite system, i.e., storage device plus heat bath, has evolved into a new state whose final distribution $F_{\text{final}} = F_{\text{final}}(\boldsymbol{x}, \boldsymbol{y}; \lambda)$ yields a marginal distribution of the storage device that verifies:

$$S\big[F^{(A)}_{\text{initial}}\big] = S\big[F^{(A)}_{\text{final}}\big] + k \ln 2. \tag{3.16}$$

In other words, the erasure of a single bit of memory implies a decrease of $k \ln 2$ in the entropy of the storage device.

The Lagrange multiplier λ describing the initial distribution can be seen as a parameter that characterizes a family of different realizations of the erasure process $F_{\text{initial}}(\boldsymbol{x}, \boldsymbol{y}; \lambda) \to F_{\text{final}}(\boldsymbol{x}, \boldsymbol{y}; \lambda)$. Each realization is associated with a particular time-dependent solution of Liouville's equation, $\frac{\partial F}{\partial t} + \nabla \cdot (F\, \boldsymbol{w}) = 0$. Notice, however, that the total ensemble distribution is not required to have the canonical form throughout the erasure process, particularly, not after the erasure process has finalized.

Before and after erasure the total entropies of the composite system are related

by

$$\begin{aligned} S\big[F_{\text{initial}}\big] &= S\big[F^{(A)}_{\text{initial}}\big] + S\big[F^{(B)}_{\text{initial}}\big] = S\big[F_{\text{final}}\big] \\ &\leq S\big[F^{(A)}_{\text{final}}\big] + S\big[F^{(B)}_{\text{final}}\big]. \end{aligned} \tag{3.17}$$

In (3.17) the first equality represents the additivity of Shannon's entropy for the initial canonical distribution (which is factorizable) and the second equality is the conservation of the total entropy in the course of Liouville's evolution. The inequality, in contrast, is due to the subadditivity of Shannon's entropy [137]. This inequality becomes an equality if the final joint probability density describing the composite $A + B$ is factorizable. In the general case, however, when the systems A and B are correlated after the erasure process, we have a strict inequality in (3.17).

Combining (3.16) with (3.17) leads to

$$S\big[F^{(B)}_{\text{final}}\big] - S\big[F^{(B)}_{\text{initial}}\big] \geq k \ln 2. \tag{3.18}$$

The maxent probability density can be characterized either as the probability density of maximum entropy S for a given value of $\langle C \rangle$ or, alternatively, as the probability density of minimum $\langle C \rangle$ for a given S. Therefore, the initial and final mean values of $C(\boldsymbol{y})$ verify

$$\langle C \rangle_{\text{final}} - \langle C \rangle_{\text{initial}} \geq \langle C \rangle^{(\text{canonical})}_{\text{final}} - \langle C \rangle_{\text{initial}} \tag{3.19}$$

where $\langle C \rangle^{(\text{canonical})}_{\text{final}}$ is the value of $\langle C \rangle$ associated with a maxent distribution having the same value of the entropy as $F^{(B)}_{\text{final}}$. The maxent probability distribution formally has the same structure as the canonical ensemble in standard statistical physics. The canonical distribution is a mono-parametric one, so that everything can be regarded as depending on one quantity. For instance, one can regard $\langle C \rangle$ as a function of the entropy S, where in the standard canonical ensemble $\langle C \rangle$ plays the role of the mean energy and λ plays the role of inverse temperature $1/T$.

Now, we have the following relations (which, replacing H for C, coincide with

well known relationships satisfied by Gibbs canonical distribution):

$$\begin{aligned} \frac{d\langle C\rangle}{dS} &= \frac{1}{\lambda} > 0 \\ \frac{d^2\langle C\rangle}{dS^2} &= -\left(\frac{1}{\lambda^2}\right)\left(\frac{d\lambda}{dS}\right) > 0, \end{aligned} \tag{3.20}$$

where in these derivatives $\langle C\rangle$ always refers to the canonical distribution. This means that $\langle C\rangle$ is an increasing function of S and the derivative $d\langle C\rangle/dS$ is also increasing with S. The latter statement is due to $d\lambda/dS < 0$, which in the standard sense arises from the entropy S being an increasing function of the temperature T and consequently S is a decreasing function of $1/T$. The first part of equation (3.20) can be seen from the expression of the entropy for the initial distribution which is canonical,

$$S[F_{\text{initial}}] = \lambda\langle D\rangle_{\text{initial}} + k\ln Z^{(A)} + \lambda\langle C\rangle_{\text{initial}} + k\ln Z^{(B)} = S\left[F^{(A)}_{\text{initial}}\right] + S\left[F^{(B)}_{\text{initial}}\right]. \tag{3.21}$$

The above two properties in (3.20) together with eq. (3.18) gives rise to the following inequality

$$\begin{aligned} \langle C\rangle^{(\text{canonical})}_{\text{final}} - \langle C\rangle_{\text{initial}} &= \int_{S^{(B)}_{\text{initial}}}^{S^{(B)}_{\text{final}}} \left(\frac{d\langle C\rangle}{dS}\right) dS \\ &\geq \int_{S^{(B)}_{\text{initial}}}^{S^{(B)}_{\text{final}}} \left(\frac{d\langle C\rangle}{dS}\right)_{\text{initial}} dS \\ &= \left[S^{(B)}_{\text{final}} - S^{(B)}_{\text{initial}}\right] \cdot \left(\frac{d\langle C\rangle}{dS}\right)_{\text{initial}} = \frac{1}{\lambda}\left[S^{(B)}_{\text{final}} - S^{(B)}_{\text{initial}}\right] \\ &\geq \frac{k}{\lambda}\ln 2. \end{aligned} \tag{3.22}$$

Combining now the inequalities (3.19) and (3.22), one readily obtains a generalized version of Landauer's principle:

$$\langle C\rangle_{\text{final}} - \langle C\rangle_{\text{initial}} = \Delta\langle C\rangle(\lambda) = \int\left\{F^{(B)}_{\text{final}} - F^{(B)}_{\text{initial}}\right\} C(\boldsymbol{y}) d\Omega^{(B)} \geq \frac{1}{\lambda} k\ln 2 \tag{3.23}$$

which relates the initial and final mean values of the dynamical quantity C associated with the environment B. Summing up, using (3.18) and basic features of the maxent probability density (which are basically those satisfied by Gibbs

canonical distribution) one can derive an extension of Landauer's principle valid in the context of general divergenceless dynamical systems. This result establishes a direct link between an information-processing operation (the erasure of one bit of information from system A) and the change in the mean value of a dynamical quantity that is relevant for characterizing the state of system B. In the standard Hamiltonian case, this means the minimum increase in energy of system B is $kT \ln 2$ (Landauer's principle in the standard sense).

3.1.2.3 Discussion on the derivation of the Landauer-like principle

It is worth noticing that some of the assumptions made in order to obtain a Landauer-like principle for general divergenceless dynamical systems were not explicitly used in the derivation of the main result (3.23). Specifically, the conservation of the dynamical quantity I (equation (3.8)) and the hypothesis of weak interaction between systems A and B were not, strictly speaking, used in order to derive equation (3.23). Even though these assumptions are physically very reasonable, they are not essential for obtaining (3.23). The precise form of the initial phase space probability density (3.14) is not required either. It can be verified that a more general initial probability density of the form:

$$F_{\text{initial}}\left(\boldsymbol{x}, \boldsymbol{y}; \lambda\right) \;=\; F^{(A)}_{\text{initial}}\left(\boldsymbol{x}\right) \frac{e^{-\frac{\lambda}{k} C(\boldsymbol{y})}}{Z^{(B)}(\lambda)} \tag{3.24}$$

with an arbitrary (normalizable) starting marginal probability density $F^{(A)}_{\text{initial}}$ for the system A still leads to the Landauer-like result (3.23).

It must be emphasized that, even if the previously mentioned assumptions are not mathematically indispensable for the derivation of (3.23), they are physically reasonable and, in particular, lend plausibility to the initial phase space probability density (3.14) as a maxent description of an equilibrium situation.

3.1.3 Systems described by non-exponential distributions

An interesting proposal for the description of non-equilibrium, meta-stable states has been advanced by Beck and Cohen (BC) [159–162]. The BC approach is based on the representation of statistical ensemble distributions as superpositions of

Gibbs distributions characterized by different temperatures. The corresponding formalism is usually referred to as "superstatistics" and proved to be successful in dealing with various physical scenarios, most notably turbulence [161]. We are now going to use the BC procedure to obtain an extended Landauer-like principle for divergenceless systems described by non-exponential distributions associated with out of equilibrium situations.

In order to develop the aforementioned extension of Landauer's principle one needs a proper representation of statistical ensembles that are more general than the standard, exponential maxent ensembles. One may consider maximum entropy representations of probability distributions based on generalized entropic measures. This approach has been adopted by several researchers in recent years, with remarkable success in the modelling of different systems in meta-stable states. Alas, this procedure does not seem to be appropriate for the generalization of Landauer's principle because the physically most relevant, generalized entropies are not subadditive. To overcome this difficulty we here apply the aforementioned alternative description of non-equilibrium ensembles, namely the one based on the BC formalism [159, 160]. This approach has the important advantage of being independent of specific properties of generalized entropic measures. Moreover, the BC formalism still allows for exploiting some of the nice and familiar features of the conventional Boltzmann-Gibbs-Shannon logarithmic entropy and of the associated canonical formalism. We introduce a normalized BC representation of the initial distribution of the composite system $A+B$ as

$$F_{\text{initial}}\left(\boldsymbol{x},\boldsymbol{y}\right)=\frac{\int_0^\infty f(\lambda)\left[\frac{e^{-\frac{\lambda}{k}\left(D(\boldsymbol{x})+C(\boldsymbol{y})\right)}}{Z^{(A)}(\lambda)\,Z^{(B)}(\lambda)}\right]d\lambda}{\int_0^\infty f(\lambda)d\lambda}. \tag{3.25}$$

A non-equilibrium phase space probability density of the form (3.25) is a linear superposition of a family of exponential maxent probability densities, in which the weight corresponding to each temperature is given by the function $f(\lambda)$ - the composite system 'bit-storing device A plus environment B' is in a non-equilibrium state characterized by a "superposition of different temperatures" or a "fluctuating temperature" described by $f(\lambda)$. The environment (both before and after the erasure process) "selects" a particular distribution of temperatures

$f(\lambda)$ for the bit-storing device. In the special case of $f(\lambda) = \delta(\lambda - \lambda_0)$, the usual equilibrium case ensues. Notice that, for any given weight function $f(\lambda)$, the initial probability density (3.25) constitutes a stationary solution of Liouville's equation if $I = D(\boldsymbol{x}) + C(\boldsymbol{y})$ is a constant of motion.

The starting probability density (3.25) is a linear combination of canonical exponential distributions $F_{\text{initial}}(\boldsymbol{x}, \boldsymbol{y}; \lambda)$. Due to the linearity of Liouville's equation this initial distribution (3.25) leads, after the erasure process is completed, to the final distribution

$$F_{\text{final}}(\boldsymbol{x}, \boldsymbol{y}) = \frac{\int_0^\infty f(\lambda) F_{\text{final}}(\boldsymbol{x}, \boldsymbol{y}; \lambda) d\lambda}{\int_0^\infty f(\lambda) d\lambda}. \tag{3.26}$$

By combining (3.23) with (3.25) and (3.26) we obtain a generalized Landauer-like principle providing a lower bound for the change in $\langle C \rangle$ during the erasure process,

$$\begin{aligned}
\Delta\langle C\rangle &= \int \left\{ F^{(B)}_{\text{final}} - F^{(B)}_{\text{initial}} \right\} C(\boldsymbol{y})\, d\Omega^{(B)} \\
&= \frac{1}{\int_0^\infty f(\lambda) d\lambda} \int_0^\infty f(\lambda) \left[\int \left(F_{\text{final}}(\boldsymbol{x}, \boldsymbol{y}; \lambda) - \frac{e^{-\frac{\lambda}{k}(D(\boldsymbol{x}) + C(\boldsymbol{y}))}}{Z^{(A)}(\lambda)\, Z^{(B)}(\lambda)} \right) C(\boldsymbol{y})\, d\Omega^{(B)} \right] d\lambda \\
&\geq \frac{\int_0^\infty f(\lambda) \frac{k}{\lambda} d\lambda}{\int_0^\infty f(\lambda) d\lambda} \ln 2,
\end{aligned} \tag{3.27}$$

where $F^{(B)}_{\text{initial}}$ and $F^{(B)}_{\text{final}}$ are, again, the bath's initial and final marginal probability distributions, respectively.

Remarks similar to those made in Subsubsection 3.1.2.3 apply here concerning the role played by the assumptions of weak coupling between the bit-storage system A and the environment B and the conservation of $C + D$. Furthermore, it can be verified that an initial phase space probability density of the form

$$F_{\text{initial}}(\boldsymbol{x}, \boldsymbol{y}) = F^{(A)}_{\text{initial}}(\boldsymbol{x}) \frac{\int_0^\infty f(\lambda) \frac{1}{Z(\lambda)} e^{-\frac{\lambda}{k} C(\boldsymbol{y})} d\lambda}{\int_0^\infty f(\lambda) d\lambda} \tag{3.28}$$

also leads to the Landauer-like result (3.27).

3.1.4 Summary and conclusions

In the present effort I have developed extended Landauer-like principles valid within scenarios involving general dynamical systems exhibiting divergenceless phase space flows.

Two fundamental features of Shannon's information measure $S[F]$ lead to these Landauer-like results:

- The conservation of S under the Liouville's ensemble dynamics associated with divergenceless systems.
- The subadditive character of S.

The profound links between Landauer's principle and the second law of thermodynamics [22] suggest that the present results may help to explore analogues of the second law in non-standard contexts, like the biological ones discussed in [150, 151].

The lack of subadditivity exhibited by some important non-logarithmic information or entropic functionals seems to be a serious difficulty for deriving generalizations of Landauer's principle in terms of the non-standard maxent formalisms that are nowadays popular for the study of non-equilibrium, meta-stable states. On the other hand, the Beck-Cohen approach allows for the extension of Landauer's principle to some of those scenarios. This important issue, however, needs further exploration and the idea would be to obtain a valid formulation of Landauer-like principles directly based upon generalized, non-standard entropic measures.

3.2 Fidelity Measure and Conservation of Information in General Probabilistic Theories

I investigate the main features of a measure of fidelity between states in a general family of probabilistic theories admitting classical probability theory and standard quantum theory as particular instances. We apply the aforementioned measure to investigate information-theoretical features of these theories related to the conservation of information during the evolution of closed physical systems. In particular, we derive a generalization of a fundamental result in quantum theory relevant for the measurement problem: Zurek's recent extension of the no-cloning theorem.

This Section is based on the publication [163] "Fidelity measure and conservation of information in general probabilistic theories", C. Zander and A.R. Plastino, *Europhys. Lett.* **86** (1), (2009) 18004 and is organized as follows. In Subsection 3.2.1 I provide a brief introduction and in Subsection 3.2.2 the BBLW operational framework is reviewed. The time evolution of closed systems and measurements as physical processes are considered in Subsection 3.2.3. In Subsection 3.2.4 the fidelity measure for states in general probabilistic theories is investigated. The conservation of the fidelity under the evolution of closed systems is explored in Subsection 3.2.5. Then, in Subsections 3.2.6 and 3.2.7 the generalized Zurek's information transfer theorem and the generalized no-deleting theorem are established. Finally, some conclusions are drawn in Subsection 3.2.8.

3.2.1 Introduction

The physics of information and computation [1–6] has been the focus of an intense and increasing research activity in recent years [5–7, 12, 144, 164–167]. Part of this research effort has been devoted to determine the ultimate limits imposed by the fundamental laws of physics on any device processing or transmitting information [6, 12, 164]. On the other hand, a growing body of theoretical developments indicate that the concept of information constitutes an essential ingredient for a deep understanding of physical systems and processes [1–6, 144, 165–167]. Ideas, techniques and models inspired on the theoretical analysis of information process-

ing devices proved to be relevant for the study of a variegated range of physical scenarios, including applications to subjects as diverse as quantum thermodynamical machines [165] or the fundamental limits on the accuracy of spacetime measurements [166]. Interesting attempts have been recently made to derive the basic formalism of quantum theory from information-theoretical concepts [167]. The advent of quantum information science, and the concomitant discovery of the novel, subtle, and counter-intuitive ways of processing and transmitting information allowed by quantum mechanics [6, 7] greatly stimulated the interest in these lines of enquiry. Work on quantum information theory is shedding new light on the foundations of quantum theory and on the relationships between the classical and quantum mechanical descriptions of Nature. An interesting and powerful new approach to these issues has been recently advanced by Barnum, Barrett, Leifer and Wilce [65] (from here on BBLW). These researchers proposed to investigate systematically the information-theoretical aspects of probabilistic descriptions of Nature, within a general operational framework that encompasses classical probabilities and quantum mechanical probabilities as two particular instances of a wide family of probabilistic theories. Similar or related ideas have been discussed previously in the literature (see [168, 169] and references in [65]) but BBLW provided the first systematic analysis of fundamental aspects of information physics, such as the no-broadcasting principle, within the general framework.

There is much to be gained from exploring generalizations of existing physical theories [170]. Historically this has been wonderfully illustrated by the great stimulus that research on general relativity got from the study of alternative theories of gravitation [171]. This kind of approach allows for the identification and investigation of important problems that otherwise might have gone unnoticed. For example, generalizations of the standard quantum theory are currently being used to study one of the most intriguing open questions on the foundations of quantum mechanics [172]: why doesn't Nature permit the maximum amount of nonlocality consistent with causality? Last, but certainly not least, these lines of research may shed new light on the epistemic vs. ontic debate on the basic meaning of the quantum mechanical formalism [173].

The aim of the present work is to investigate the main properties of a measure

of fidelity between states in general probabilistic theories described by the BBLW framework, and to explore its application to the study of basic information-related processes. We shall use the alluded fidelity measure to derive, within the aforementioned probabilistic theories, a generalization of a basic result in quantum theory with implications for the measurement problem: Zurek's recent extension of the no-cloning theorem.

3.2.2 The BBLW operational framework

The basic ingredients of the BBLW approach are the concepts of states, effects, measurements and transformations, as defined below (see [65] for details). These concepts generalize some well-known concepts of standard quantum mechanics.

States: The set Ω of all possible states of a physical system is a finite dimensional, compact and convex set. The extreme points of the set Ω are called "pure" states. In standard quantum mechanics the state set Ω corresponds to the set of all statistical operators ρ on the system's Hilbert space $\mathcal{H}$. In classical mechanics, the set of states is given by the set of all normalized probability distributions defined on an appropriate, classical phase space. A state determines the probabilities for different measurement outcomes. Let $e(\omega)$ denote the probability of obtaining outcome e when the system is in state ω.

Effects: Mathematically the probability $e(\omega)$ is given by an affine functional $e : \Omega \to [0, 1]$ which is referred to as an *effect*. In particular, we have the *unit effect* u verifying $u(\omega) = 1$ for all $\omega \in \Omega$. In quantum theory an effect is represented by a positive operator E bounded by 0 and the identity operator I. The probability of the concomitant outcome (if the system is in state ρ) is $\mathrm{Tr}(E\rho)$. The unit effect is given by the identity I. We are going to assume that a state ω is completely characterized by the probabilities $e(\omega)$. In other words, two states ω_1 and ω_2 yield the same probabilities for all effects e (that is $e(\omega_1) = e(\omega_2)$ for all e) iff $\omega_1 = \omega_2$.

Measurement: A measurement is identified with a set of effects $\{e_i\}$ such that $\sum_i e_i = u$, and, consequently, $\sum_i e_i(\omega) = 1$ for all $\omega \in \Omega$. This generalizes the

concept of a POVM in quantum theory.

Transformations: Physical transformations of a system are described by an appropriate set of affine mappings $T : \Omega \to \Omega'$, where Ω and Ω' stand, respectively, for the system's state space before and after the transformation. These transformations play the role of linear, trace-preserving, completely positive maps in the standard quantum formalism.

The rules for the description of bipartite systems constitutes another important component of the BBLW framework.

Bipartite Systems: Let us consider a bipartite system AB constituted by subsystems A and B. Lets denote the state spaces of subsystems A and B respectively by Ω_A and Ω_B. The state space of the composite system AB is denoted by Ω_{AB}. A joint state $\omega_{AB} \in \Omega_{AB}$ specifies completely the joint probabilities $\omega_{AB}(e_A, e_B)$ corresponding to pairs of effects (e_A, e_B) where $e_{A,B}$ are effects defined with respect to the individual subsystems A and B. Conversely, the joint probabilities for all pairs of effects (e_A, e_B) fully characterize the joint state ω_{AB}. The joint probabilities comply with the no-signaling constraint.

For each state ω_{AB} of the bipartite system there are reduced states $\omega_{A,B}$ characterized by $e_A(\omega_A) = \omega_{AB}(e_A, u_B)$ and $e_B(\omega_B) = \omega_{AB}(u_A, e_B)$. If either marginal state is pure, then the joint state is factorizable: $\omega_{AB} = \omega_A \otimes \omega_B$ and $\omega_{AB}(e_A, e_B) = e_A(\omega_A)e_B(\omega_B)$.

3.2.3 Time evolution of closed systems and measurements as physical processes

I am going to assume that there is a set of invertible transformations $\Gamma : \Omega \to \Omega$ representing the fundamental transformations that a closed physical system (with state space Ω) can experience. Each one of these transformations Γ admits an inverse $\Gamma^{(-1)}$ which is also a legitimate physical transformation for the system

under consideration. For all $\omega \in \Omega$ we have

$$\Gamma^{(-1)}(\Gamma(\omega)) = \Gamma\big(\Gamma^{(-1)}(\omega)\big) = \omega. \tag{3.29}$$

These invertible transformations are to be regarded as the truly fundamental ones. We assume that when one studies a given physical system it is always possible to extend it, and regard it as a subsystem of a larger, closed system. In this way, all possible transformations affecting the original system are manifestations of invertible transformations acting upon the extended closed system. This assumption is not part of the BBLW framework as exposed in [65]. However, both classical and quantum mechanics comply with it and it is therefore reasonable to regard it as a basic ingredient of our present understanding of the fundamental laws of physics.

Since measurement processes are themselves physical processes, there has to be a physical consistency relation between the set of all possible measurements and the set of all invertible operations acting upon a physical system. If we first apply a transformation Γ to our system, and then perform a measurement $\{e_i\}$ upon it, the overall process can always be regarded as performing a certain measurement $\{\tilde{e}_i\}$ on the initial state of the system. For instance, if we consider the state of a spin-$\frac{1}{2}$ particle in standard quantum mechanics, to first apply a $\pi/2$ rotation around the x-axis and then measure S_z is equivalent to measure S_y on the original state. In the context of a general probabilistic theory, given an effect e and an invertible operation Γ there exists an effect $\tilde{e}$ such that, for all states $\omega \in \Omega$, $\tilde{e}(\omega) = e(\Gamma(\omega))$. As a consequence, given a measurement $\{e_i\}$ and an invertible transformation Γ there is another measurement $\{\tilde{e}_i\}$ such that $\tilde{e}_i(\omega) = e_i(\Gamma(\omega))$ for all $\omega \in \Omega$.

3.2.4 Fidelity measure for states in general probabilistic theories

As a generalized fidelity measure between two states ω_1 and ω_2 we propose the infimum (that is, the largest lower bound) of the set of overlap values between the pairs of probability distributions $e_i(\omega_{1,2})$ associated with all the possible mea-

surements $\{e_i\}$,

$$\mathcal{F}[\omega_1, \omega_2] \;=\; \inf_{\{e_i\}} \sum_i \sqrt{e_i(\omega_1)\, e_i(\omega_2)}. \tag{3.30}$$

The alluded set of overlap values is bounded from below (all the overlaps are non-negative numbers) and, consequently, the aforementioned infimum always exists and we have

$$0 \;\leq\; \mathcal{F}[\omega_1, \omega_2] \;\leq\; 1, \tag{3.31}$$

with

$$\mathcal{F}[\omega_1, \omega_2] \;=\; 1 \;\;\text{iff}\;\; \omega_1 = \omega_2. \tag{3.32}$$

The fidelity $\mathcal{F}[\omega_1, \omega_2]$ measures how well the two states ω_1 and ω_2 can be distinguished by recourse to measurements. The extreme case $\mathcal{F}[\omega_1, \omega_2] = 0$ corresponds to a pair of states that can be distinguished with certainty by recourse to an appropriate measurement, while in the other limit case $\mathcal{F}[\omega_1, \omega_2] = 1$ the two states are identical and, consequently, indistinguishable. It is worth emphasizing that equation (3.30) provides an operational definition of the fidelity $\mathcal{F}[\omega_1, \omega_2]$ since the quantities appearing in the right hand side of (3.30) can be determined experimentally.

In the particular case of standard quantum mechanics the measure (3.30) reduces to the fidelity measure between density matrices [7]

$$\mathcal{F}[\rho, \sigma] \;=\; \mathrm{Tr}\sqrt{\rho^{1/2}\sigma\rho^{1/2}}, \tag{3.33}$$

see Subsection 1.1.8 for more detail.

Now I am going to study the main properties of the generalized fidelity functional (3.30). As we are going to see, most of the properties exhibited by the quantum mechanical fidelity (3.33) are shared by the measure (3.30), and can be proved in general, without using specific features of the quantum mechanical formalism.

Given a pair of states $\omega_{1,2}$ let us consider the two states $\omega_{1,2} \otimes \omega_0$ where ω_0 is a state of an ancilla system. Any measurement done on $\omega_i \otimes \omega_0$ can be construed

as a measurement on ω_i (the state ω_0 of the ancilla system can be regarded as characterizing the initial setting of (part of) the measurement apparatus). Indeed, the act of performing a measurement on $\omega_i \otimes \omega_0$ can be interpreted as follows: take the system to be measured (which is in the unknown state ω_i), "attach" to it an ancilla system in a standard initial state ω_0, and perform a measurement on the resulting composite (which is in state $\omega_i \otimes \omega_0$). Physically, it is clear that this procedure is tantamount to performing a measurement on ω_i. In point of fact, in any real measurement one always has to "attach" ancilla systems (in prescribed, standard initial states) to the system being measured. Now, since the set of possible measurements on $\omega_i \otimes \omega_0$ is a subset of all the possible measurements on ω_i, it follows from (3.30) that $\mathcal{F}[\omega_1 \otimes \omega_0, \omega_2 \otimes \omega_0] \geq \mathcal{F}[\omega_1, \omega_2]$. Conversely, a measurement on ω_i can also be regarded as a measurement performed on $\omega_i \otimes \omega_0$. Therefore, (3.30) implies that $\mathcal{F}[\omega_1 \otimes \omega_0, \omega_2 \otimes \omega_0] \leq \mathcal{F}[\omega_1, \omega_2]$ and, consequently,

$$\mathcal{F}[\omega_1 \otimes \omega_0, \omega_2 \otimes \omega_0] \;=\; \mathcal{F}[\omega_1, \omega_2]. \tag{3.34}$$

The argument leading to the inequality $\mathcal{F}[\omega_1 \otimes \omega_0, \omega_2 \otimes \omega_0] \geq \mathcal{F}[\omega_1, \omega_2]$ does not constitute a formal mathematical proof. In the strict mathematical sense this inequality has to be regarded as an assumption that we are making about the behaviour of the fidelity function. But it is an assumption based on a compelling physical argument. The second inequality leading to (3.34) can be obtained as a particular case of (3.37), which is proved below.

Given a pair of joint states $\omega_{1,2}^{(AB)}$ (of a bipartite system AB) with reduced states $\omega_{1,2}^{(A)}$ and $\omega_{1,2}^{(B)}$, we have

$$\mathcal{F}\big[\omega_1^{(A)}, \omega_2^{(A)}\big] \;\geq\; \mathcal{F}\big[\omega_1^{(AB)}, \omega_2^{(AB)}\big], \tag{3.35}$$

since any measurement performed on subsystem A can be construed as a measurement upon the composite system AB. Similarly,

$$\mathcal{F}\big[\omega_1^{(B)}, \omega_2^{(B)}\big] \;\geq\; \mathcal{F}\big[\omega_1^{(AB)}, \omega_2^{(AB)}\big]. \tag{3.36}$$

Let us consider now the fidelity $\mathcal{F}[\omega_1^{(A)} \otimes \omega_1^{(B)}, \omega_2^{(A)} \otimes \omega_2^{(B)}]$ between two factorizable states. If one uses equation (3.30) to compute $\mathcal{F}[\omega_1^{(A)} \otimes \omega_1^{(B)}, \omega_2^{(A)} \otimes \omega_2^{(B)}]$

it is clear that evaluating the infimum over the restricted family of product measurements $\{(e_{Ai}, e_{Bi})\}$ (which would yield $\mathcal{F}[\omega_1^{(A)}, \omega_2^{(A)}]\,\mathcal{F}[\omega_1^{(B)}, \omega_2^{(B)}]$) cannot lead to a smaller number than the one obtained by an unrestricted evaluation of the infimum. Consequently, we have

$$\mathcal{F}\big[\omega_1^{(A)} \otimes \omega_1^{(B)}, \omega_2^{(A)} \otimes \omega_2^{(B)}\big] \;\leq\; \mathcal{F}\big[\omega_1^{(A)}, \omega_2^{(A)}\big]\,\mathcal{F}\big[\omega_1^{(B)}, \omega_2^{(B)}\big]. \tag{3.37}$$

Given two sets of states $\{\omega_{1i},\ i = 1, \ldots, M\}$ and $\{\omega_{2i},\ i = 1, \ldots, M\}$ of a given system, and a measurement $\{e_j\}$, let us consider the fidelity measure between two convex linear combinations $\sum_i p_i\omega_{1i}$ and $\sum_i q_i\omega_{2i}$ of the alluded states, where $\{p_i,\ \ i = 1, \ldots, M\}$ and $\{q_i,\ \ i = 1, \ldots, M\}$ are two normalized probability distributions over the same index set. We have,

$$\begin{aligned}
\sum_j \Big\{ e_j \Big(\sum_i p_i\omega_{1i} \Big) e_j \Big(\sum_i q_i\omega_{2i} \Big) \Big\}^{\frac{1}{2}} \;&=\\
\sum_j \Big\{ \Big(\sum_i p_i e_j(\omega_{1i}) \Big) \Big(\sum_i q_i e_j(\omega_{2i}) \Big) \Big\}^{\frac{1}{2}} \;&\geq\\
\sum_j \sum_i \big\{ p_i q_i e_j(\omega_{1i}) e_j(\omega_{2i}) \big\}^{\frac{1}{2}} \;&=\\
\sum_i \sqrt{p_i q_i} \Big\{ \sum_j \Big[e_j(\omega_{1i}) e_j(\omega_{2i}) \Big]^{\frac{1}{2}} \Big\} \;&\geq\\
\sum_i \sqrt{p_i q_i}\ \mathcal{F}\big[\omega_{1i}, \omega_{2i}\big],&
\end{aligned} \tag{3.38}$$

where the first inequality follows from the Schwarz inequality ($\sqrt{\sum_i x_i \sum_i y_i} \geq \sum_i \sqrt{x_i y_i}$) and the second inequality is a consequence of the definition of the fidelity measure $\mathcal{F}$. Since equation (3.38) holds for any measurement $\{e_j\}$, including the one that gives rise to the infimum in the definition of $\mathcal{F}\big[\sum_i p_i\omega_{1i}, \sum_i q_i\omega_{2i}\big]$, it also implies that

$$\mathcal{F}\Big[\sum_i p_i\omega_{1i}, \sum_i q_i\omega_{2i} \Big] \geq \sum_i \sqrt{p_i q_i}\ \mathcal{F}\big[\omega_{1i}, \omega_{2i}\big], \tag{3.39}$$

meaning that the generalized fidelity measure complies with the *strong concavity* property.

Almost all the main properties of the quantum fidelity (3.33) (including invariance under unitary transformation, whose generalization we are going to discuss in the next Subsection) are shared by the general fidelity measure (3.30) defined in the BBLW family of probabilistic theories. An important property of the quantum fidelity that is not satisfied in the general scenario is given by Uhlmann's theorem, which says that,

$$\mathcal{F}[\rho,\sigma] \;=\; \max_{|\psi\rangle,|\phi\rangle} |\langle\psi|\phi\rangle|, \tag{3.40}$$

where the maximum is taken over all possible pairs of states $|\psi\rangle$ and $|\phi\rangle$ constituting purifications of the two density matrices ρ and σ, respectively [7]. A purification of a state ρ (not necessarily pure) of a system S is a pure state $|\psi\rangle$ of a larger system (of which S is a subsystem) such that the corresponding marginal state of S is given by ρ. Uhlmann's theorem is not generalizable within the BBLW framework because purification is not possible within arbitrary members of the BBLW family of theories. For instance, purification is not possible within classical probabilistic theories.

3.2.5 Conservation of the fidelity under the evolution of closed systems

The previously discussed consistency relation between measurements and invertible operations has the following consequence. Given a measurement $\{e_i\}$ to be performed on either of a pair of states $\omega_{1,2}$, and an invertible transformation Γ, there exists another measurement $\{\tilde{e}_i\}$ yielding the same probabilities when performed, respectively, upon either of the states $\Gamma(\omega_{1,2})$. Moreover, given any measurement $\{e_i\}$ to be performed on either of the states $\Gamma(\omega_{1,2})$ there is another measurement $\{e_i^*\}$ exhibiting the same probabilities when performed upon the states $\omega_{1,2} = \Gamma^{(-1)}(\Gamma(\omega_{1,2}))$. Consequently, it follows from the definition (3.30) of the generalized fidelity that

$$\mathcal{F}[\Gamma(\omega_1),\Gamma(\omega_2)] \;=\; \mathcal{F}[\omega_1,\omega_2]. \tag{3.41}$$

This constitutes a generalization of the invariance property of the quantum fidelity measure under unitary transformations [7]. A similar invariance property

is satisfied by the Liouville dynamics of classical ensemble probability densities [16, 174]. A relation like (3.41), stating the preservation of the distinguishability between states, can be regarded as meaning that *information is conserved by the time evolution of a closed physical system* [16].

3.2.6 Generalized Zurek's information transfer theorem

The quantum no-cloning theorem [58] is nowadays regarded as encapsulating one of the most distinctive features of quantum information, see Section 1.3 for more detail. The multiple and profound implications of this principle, and of its various extensions and generalizations, constitute an active research area [60, 64, 175–177].

A recent generalization of the no-cloning theorem advanced by Zurek sheds new light on the nature of the quantum mechanical measurement process [60]. During such a process information is transferred from the system being measured to the recording apparatus. An intuitive, basic feature of a physical measurement is that its immediate repetition always yields the same result. As a consequence, if the state of the system immediately after the measurement is ω, this state will be left unperturbed if the same measurement is performed a second time quickly after the first one. This uncontroversial assumption is referred to as the *predictability postulate* [60]. Zurek showed that two basic postulates of quantum mechanics, (i) the representation of quantum states by vectors in the system's Hilbert space and (ii) the unitarity of quantum evolutions, together with the predictability postulate, are enough to prove that the allowed outcome states of the system after a quantum measurement are restricted to an orthonormal subset of the system's possible states. This result holds true even for imperfect measurements: no matter how little information about the system's state is transferred to the apparatus (as long as this information is not strictly zero) the only allowed unperturbed outcome states for the system have to be orthonormal. This is a profound and intriguing result. It shows that a basic aspect of quantum measurements that is usually regarded as having or needing the status of an independent postulate can actually be derived from the most basic ingredients of quantum theory. Zurek's results have been deservedly hailed as "dissolving one

aspect of quantum weirdness" [177]. I am now going to show that a result similar to Zurek's holds true within the general family of probabilistic theories described by the BBLW framework.

Let us consider a special type of processes which are an extension to general probabilistic theories of the processes studied by Zurek [60]. Suppose that we have a composite system $\mathcal{SA}$ consisting of a system $\mathcal{S}$ and an "apparatus" $\mathcal{A}$. We shall consider the possibility of implementing transformations that transfer information from the system $\mathcal{S}$ to the "recording apparatus" $\mathcal{A}$. In particular, we want to determine under what circumstances this can occur without altering the initial state of $\mathcal{S}$. We assume that $\mathcal{S}$ starts in a pure state ω_i and the apparatus in an initial reference state Σ_0. The process is represented by an invertible transformation Γ. This does not imply a loss of generality since, as we already said, we assume that the invertible transformations constitute the fundamental ones for closed systems. We can always consider the system $\mathcal{A}$ to be large enough so that the composite system $\mathcal{SA}$ can be regarded as closed, and all the transformations affecting it can be regarded as invertible. The main question that we want to address is the following: For which initial pure states ω_i of $\mathcal{S}$ is it possible to perform this operation without altering the state ω_i? Let us consider two initial states $\omega_{1,2}$ for which the aforementioned information transfer is doable. We then have,

$$\begin{aligned} \Gamma(\omega_1 \otimes \Sigma_0) &= \omega_1 \otimes \Sigma_1, \\ \Gamma(\omega_2 \otimes \Sigma_0) &= \omega_2 \otimes \Sigma_2. \end{aligned} \tag{3.42}$$

Therefore,

$$\begin{aligned} \mathcal{F}[\omega_1, \omega_2] &= \mathcal{F}[\omega_1 \otimes \Sigma_0, \omega_2 \otimes \Sigma_0] && \text{from eq. (3.34)} \\ &= \mathcal{F}[\Gamma(\omega_1 \otimes \Sigma_0), \Gamma(\omega_2 \otimes \Sigma_0)] && \text{from eq. (3.41)} \\ &= \mathcal{F}[\omega_1 \otimes \Sigma_1, \omega_2 \otimes \Sigma_2] && \text{from eq. (3.42)} \\ &\leq \mathcal{F}[\omega_1, \omega_2]\, \mathcal{F}[\Sigma_1, \Sigma_2] && \text{from eq. (3.37).} \end{aligned} \tag{3.43}$$

Now, it follows from the last equation that it is not possible to have $\mathcal{F}[\Sigma_1, \Sigma_2] < 1$

when $\mathcal{F}[\omega_1, \omega_2] \neq 0$. Consequently,

$$\Sigma_1 \neq \Sigma_2 \implies \mathcal{F}[\omega_1, \omega_2] = 0. \tag{3.44}$$

That is, if the final states of $\mathcal{A}$ are even partially distinguishable we necessarily have $\mathcal{F}[\omega_1, \omega_2] = 0$. This means that information can be transferred from system $\mathcal{S}$ to system $\mathcal{A}$ without altering the initial (pure) state of $\mathcal{S}$ only for states of $\mathcal{S}$ that have zero mutual fidelity. That is, if Zurek's process can be implemented for a family ω_i of initial pure states of $\mathcal{S}$, these states must be perfectly distinguishable. This constitutes a generalization of the fundamental theorem recently proved by Zurek [60, 177]. In terms of the measurement problem our present result can be stated as follows: *if a probabilistic theory contained within the BBLW framework complies with the predictability postulate, then the only possible output states of a measurement (even an imperfect one) are restricted to a set of states with mutual zero fidelity.* Our generalization of Zurek's theorem constitutes a general principle constraining the transfer of information between physical systems that admits as a particular case the BBLW-no-cloning theorem discussed in [178]. Our approach is different from the one adopted in [178], which is not based on the generalized fidelity measure. Note that in classical probabilistic theories all "pure" states are perfectly distinguishable from each other so that, in such a context, the present result imposes no restrictions on the possible outcomes of measurements.

3.2.7 Generalized no-deleting theorem

Let us consider now a counterpart of the quantum no-deleting theorem [179] holding within general BBLW probabilistic theories. We are going to study processes whose aim is to delete information from a given system against that of a second system (both initially in the same, unknown state ω) bringing the state of one of these systems to a blank state ω_0 without altering the state of the other one,

$$\omega \otimes \omega \longrightarrow \omega \otimes \omega_0. \tag{3.45}$$

In order to investigate the possible implementation of such a process in a universal way (that is, for any state ω) let us consider a tripartite system comprising a source system, a target system, and a "deleting machine". We assume that this

tripartite system can be treated as closed and, consequently, evolves in a reversible way. We shall also assume that initially the source and the target systems are both described by the same state ω while the deleting machine starts in an initial standard state Σ_0. During the deleting process the information stored in the target system is deleted against that of the source system. Hence, the joint evolution of the tripartite system (which, as said, we assume to be a closed one) is

$$\Gamma(\omega \otimes \omega \otimes \Sigma_0) \; = \; \omega \otimes \omega_0 \otimes \Sigma_\omega. \tag{3.46}$$

As already said, we are interested in a *universal* deleting process. That is, equation (3.46) must hold for an arbitrary state ω. In particular, let us assume that (3.46) is verified for two particular states $\omega_{1,2}$. Then, the conservation of the fidelity measure during the transformation (3.46) leads to

$$\begin{aligned} \mathcal{F}\left[\omega_1 \otimes \omega_1, \omega_2 \otimes \omega_2\right] \; &= \\ \mathcal{F}\left[\omega_1 \otimes \omega_1 \otimes \Sigma_0, \omega_2 \otimes \omega_2 \otimes \Sigma_0\right] \; &= \\ \mathcal{F}\left[\Gamma(\omega_1 \otimes \omega_1 \otimes \Sigma_0)\,, \Gamma(\omega_2 \otimes \omega_2 \otimes \Sigma_0)\right] \; &= \\ \mathcal{F}\left[\omega_1 \otimes \omega_0 \otimes \Sigma_{\omega_1}, \omega_2 \otimes \omega_0 \otimes \Sigma_{\omega_2}\right]. \end{aligned} \tag{3.47}$$

Applying now property (3.34) of the fidelity measure we obtain,

$$\mathcal{F}\left[\omega_1 \otimes \omega_1, \omega_2 \otimes \omega_2\right] = \mathcal{F}\left[\omega_1 \otimes \Sigma_{\omega_1}, \omega_2 \otimes \Sigma_{\omega_2}\right], \tag{3.48}$$

meaning that the initial degree of distinguishability of the source-target composite coincides with the final degree of distinguishability between the source-deleting machine composite. This implies that the information deleted from the target system is not "destroyed", but is entirely transferred into the final state of the deleting machine. This constitutes a generalization of the quantum no-deleting theorem. It is worth mentioning that, strictly speaking, what we have shown is the impossibility of deleting information in a reversible way. The same observation applies to the standard quantum derivation of the no-deleting theorem [179].

3.2.8 Conclusions

In the present contribution I have explored some information-related aspects of the BBLW framework for probabilistic physical theories. We have investigated,

within this general setting, the main features of a fidelity measure between pairs of states that reduces, in the case of quantum theory, to the standard fidelity measure between statistical operators. We showed that our generalized fidelity measure complies with all the basic properties (excepting Uhlmann's theorem) satisfied by the quantum fidelity measure for density matrices. All the alluded properties admit direct derivations not involving specific features of standard quantum theory, such as the Hilbert space formalism or the properties of density matrices.

I have used the aforementioned fidelity measure to obtain a generalization to the BBLW family of probabilistic theories of Zurek's recent extension of the quantum no-cloning theorem. We considered two systems $\mathcal{S}$ and $\mathcal{A}$ interacting in such a way that a finite amount of information is transferred from $\mathcal{S}$ to $\mathcal{A}$. No matter how little information about the state of $\mathcal{S}$ is finally stored in $\mathcal{A}$ (as long as it is not strictly zero) the only initial states of $\mathcal{S}$ that are left unchanged by this process are restricted to a set of states with vanishing mutual fidelity.

It would be interesting to apply the present results to other specific theories (besides classical probabilistic ones or standard quantum mechanics). An interesting candidate is the recent proposal by Hall [180] of a theory incorporating a consistent classical and quantum mixed dynamics. According to Hall's formalism mixed classical-quantum physical systems are characterized by joint classical-quantum configurations, and states are described by mixed classical-quantum ensembles. Hall provides specific prescriptions for evaluating the expectation values of classical phase space functions, on the one hand, and of quantum Hermitian operators, on the other one. It then seems possible to identify "classical effects" with phase space functions f adopting the value 1 inside a given region $\mathcal{R}$ of the classical phase space and vanishing outside $\mathcal{R}$. The expectation value $\langle f \rangle$ then represents the probability of finding the classical part of the system's configuration within the region $\mathcal{R}$. In a similar fashion, "quantum effects" can be associated with Hermitian operators having eigenvalue 1 for some of their eigenstates and eigenvalue zero for the rest (that is, these operators are projectors on a subspace of the full Hilbert space associated with the possible quantum configurations of the system).

Some of the ideas advanced here may also be useful for analyzing even theories not belonging to the BBLW framework, such as the toy model proposed by Spekkens [173] to explore the ontic vs. epistemic controversy concerning the meaning of the quantum formalism. Spekkens' model is a probabilistic one where a physical state determines the probabilities of getting different outcomes when measuring physical observables. Therefore, it is then possible the define a fidelity measure between states. It would be interesting to explore which of the properties exhibited by fidelity measures in BBLW theories are also satisfied within Spekkens' model.

Chapter 4

Separability Criteria for Fermions

Entanglement is one of the most fundamental features of quantum systems [7, 66]. In addition to its revolutionary technological implications, current research in quantum entanglement is providing deep new insights in connection with fundamental issues such as the justification of the basic tenets of equilibrium quantum statistical mechanics [73], the origins of the quantum-to-classical transition [75] and the thermodynamic arrow of time [181] (some aspects of this last point are, however, the subject of controversy).

The entanglement features exhibited by systems consisting of identical fermions have attracted the attention of several researchers in recent years [108, 123, 124, 126–130, 132, 133, 135, 182–185]. Entanglement in fermion systems has been studied in connection with different problems, such as the entanglement between electrons in a conduction band [123], the entanglement dynamics associated with scattering processes involving two electrons [126], the role played by entanglement in the time-optimal evolution of fermionic systems [128, 129], the classification of three-fermion states based on their entanglement features [127], the detection of entanglement in fermion systems through the violation of appropriate uncertainty relations [130, 131], the entanglement features of fractional quantum Hall liquids [185] and the entanglement properties of the eigenstates of soluble two-electrons atomic models [124, 125].

The concept of entanglement in systems of indistinguishable particles exhibits

some differences from the corresponding concept as applied to systems consisting of distinguishable parts. There is general consensus among researchers that in systems of identical fermions the minimum quantum correlations between the particles that are required by the antisymmetric character of the fermionic state do not contribute to the state's amount of entanglement [108, 123, 124, 126–130, 132, 133, 135, 182–185]. There are profound physical reasons for this. First, the correlations exhibited by such states cannot be used as a resource to implement non-classical information transmission or information processing tasks [132]. Second, the non-entangled character of states represented by one Slater determinant is consistent with the possibility of associating complete sets of properties to both parts of the composite system [133]. This means that the separable (that is, non-entangled) pure states of N fermions are those having Slater rank 1. These are the states whose wave function can be expressed (with respect to an appropriate single-particle basis) as a single Slater determinant [108]. On the other hand, the set of mixed non-entangled states comprises those states that can be written as a statistical mixture of pure states of Slater rank 1. So the amount of entanglement associated with an N-fermion state corresponds in essence to the quantum correlations exhibited by the state on top of the minimum correlations needed to comply with the constraint of antisymmetry on the fermionic wave function [135]. Here, when discussing systems of identical fermions, we are considering entanglement between particles and not entanglement between modes.

The problem of determining whether a given quantum state ρ is separable or entangled is known as "the separability problem". It constitutes one of the most fundamental problems in the theory of quantum entanglement and is the subject of a sustained and intense research activity (see [67, 142, 186–191] and references therein). Besides its intrinsic interest, the development of separability criteria also leads to useful quantitative entanglement indicators: the degree to which a separability criterion is violated constitutes in itself a valuable quantitative indicator of entanglement. For instance, the well-known negativity measure of entanglement (which is one of the most used practical measures of entanglement for mixed states of systems with distinguishable subsystems) is based upon the celebrated Peres' separability criterion [67], see Subsection 2.1.4.

In the case of pure states of two identical fermions, necessary and sufficient separability criteria can be formulated in terms of the entropy of the single-particle reduced density matrix [133, 135, 184]. Alas, no such criteria are known for general, mixed states of two fermions, except for the case of two fermions with a single-particle Hilbert space of dimension four, for which a closed analytical expression for the concurrence (akin to the celebrated Wootters' formula for two qubits [91]) is known. In general, to determine whether a given density matrix of a two-fermion system represents a separable state or not is a notoriously difficult (and largely unexplored) problem. Consequently, there is a clear need for practical separability criteria, or entanglement indicators, which can be extended to systems of higher dimensionality or to scenarios involving more than two fermions [135].

An overview of distinguishable and indistinguishable particles was provided in Section 2.4 and a review of the entanglement between particles in systems of identical fermions has been given in Section 2.5.

4.1 Uncertainty Relations and Entanglement in Fermion Systems

The violation of uncertainty relations is used as a signature of entanglement for both pure and mixed states of two identical fermions. In the case of fermions with a four-dimensional single-particle Hilbert space we obtain several different types of uncertainty-related entanglement criteria based on local uncertainty relations, on the sum of variances of projectors, and on various entropic measures. Within the latter approach we consider either entropic uncertainty relations involving a single observable or relations based upon the sum of entropies associated with more than one observable. We extend the projector-based entanglement criterion to the case of two-fermion and three-fermion systems with a six-dimensional single-particle Hilbert space.

This Section is based on the publication [130] "Uncertainty relations and entanglement in fermion systems", C. Zander and A.R. Plastino, *Phys. Rev. A* **81**,

(2010) 062128 and is organized as follows. In Subsection 4.1.1 the use of uncertainty relations as entanglement detection criteria is placed into context. Subsection 4.1.2 deals with the connection between entanglement and local uncertainty relations for pure and mixed states of two fermions with a four-dimensional single-particle Hilbert space. In Subsection 4.1.3 the violation of variance-based uncertainty relations of projectors is used as a signature of entanglement for systems of two fermions, for both four-dimensional and six-dimensional single-particle Hilbert spaces, and also for systems of three fermions with a six-dimensional Hilbert space. In Subsection 4.1.4 we investigate entanglement detection through uncertainty relations based on q-entropies (of which the Shannon entropy is a special, limit case). Finally, in Subsection 4.1.5 some conclusions are given.

4.1.1 Introduction

The development of criteria for the detection of entanglement based on the violation of appropriate uncertainty relations has been the focus of some interesting recent investigations [139–141, 192–195]. One can establish uncertainty relations that are satisfied by all separable (pure or mixed) states and, consequently, any violation of these relations indicates that the quantum state under consideration is entangled. Since these uncertainty-based entanglement criteria are directly formulated in terms of the expectation values of quantum mechanical observables, they provide potentially valuable tools for the experimental detection of entanglement, complementing other ways of detection. The use of uncertainty relations for entanglement characterization has so far only been established for systems consisting of distinguishable subsystems. The aim of this Section is the application of various uncertainty relations to the study of entanglement in fermionic systems. Besides its practical usefulness for the identification of families of entangled states, the characterization of entanglement via uncertainty relations is also of considerable conceptual interest because it establishes a connection between two fundamental ingredients of quantum mechanics, namely the uncertainty relations and entanglement.

In the present work we are going to investigate entanglement-related properties of systems consisting of a given, fixed number of identical fermions. Con-

sequently, all our present developments can be formulated in terms of the first quantization formalism.

4.1.2 Local uncertainty relations for systems of two identical fermions with a four-dimensional single-particle Hilbert space

I am going to use the violation of uncertainty relations as a signature of entanglement for pure and mixed states of systems consisting of two identical fermions. In this way we are going to extend to fermionic systems the approach advanced by Hofmann and Takeuchi in [139] for systems with distinguishable subsystems. We are going to identify appropriate sets of observables such that the sum δ of their uncertainties admits a non-zero lower bound $\delta_{\min}$ for separable states. Therefore, a state violating this uncertainty relation (that is, a state exhibiting a δ-value smaller than $\delta_{\min}$) is necessarily entangled. This violation of the uncertainty relation is not only a means of entanglement detection but can also be regarded as a rough indicator of the amount of entanglement exhibited by the state under consideration, since the general tendency when entanglement is detected is that the smaller the value of δ (i.e. the greater the violation of the uncertainty relation) the more entangled the state is. In fact, in the case of composite quantum systems consisting of distinguishable subsystems, lower bounds for the concurrence have been recently established based upon the violation of appropriate uncertainty relations [193–195].

In order to appreciate and highlight the difference between the uncertainty relations for distinguishable particles and for identical fermions, we look at the behaviour of the uncertainty δ when evaluated for arbitrary observables of the form $A^{(1)} + A^{(2)} = A \otimes \mathbb{I} + \mathbb{I} \otimes A$, where A is an observable corresponding to one fermion and $\mathbb{I}$ is the identity operator acting in the single-particle Hilbert space. We are going to refer to this kind of observables as "local". Since we are interested in finding lower bounds for separable states, let us consider a separable pure state. Let $|\psi\rangle$ be as in eq. (2.66), then

$$\delta(|\psi\rangle) \quad = \quad \langle (A^{(1)} + A^{(2)})^2 \rangle_{|\psi\rangle} - \langle A^{(1)} + A^{(2)} \rangle^2_{|\psi\rangle}$$

$$= \langle A^2\rangle_{|\phi_1\rangle} - \langle A\rangle^2_{|\phi_1\rangle} + \langle A^2\rangle_{|\phi_2\rangle} - \langle A\rangle^2_{|\phi_2\rangle} - 2|\langle\phi_2|A|\phi_1\rangle|^2. \quad (4.1)$$

When comparing the above expression with the corresponding one for factorizable states $|\phi_1\rangle|\phi_2\rangle$ of bipartite systems with distinguishable subsystems, it is clear that the uncertainty evaluated on separable states of fermionic systems has the additional term $-2|\langle\phi_2|A|\phi_1\rangle|^2$, which makes the study of uncertainty relations more complicated in the fermion case. Since the additional term is negative, it means that the uncertainty for identical fermions is always smaller than that for distinguishable particles. Thus we can have a state which gives a non-zero value for the two individual uncertainties $\langle A^2\rangle_{|\phi_{1,2}\rangle} - \langle A\rangle^2_{|\phi_{1,2}\rangle}$ in eq. (4.1), but the resultant uncertainty $\delta(|\psi\rangle)$ is zero. As an illustration let $A = S_z$ ($s = 3/2$) and $|\phi_1\rangle = \frac{1}{\sqrt{2}}\left[\left|\text{-}\frac{1}{2}\right\rangle - \left|\frac{1}{2}\right\rangle\right]$, $|\phi_2\rangle = \frac{1}{\sqrt{2}}\left[\left|\text{-}\frac{1}{2}\right\rangle + \left|\frac{1}{2}\right\rangle\right]$. Then we have $\langle S_z^2\rangle_{|\phi_1\rangle} - \langle S_z\rangle^2_{|\phi_1\rangle} = \frac{1}{4} = \langle S_z^2\rangle_{|\phi_2\rangle} - \langle S_z\rangle^2_{|\phi_2\rangle}$, however, the variance of the Slater state is $\delta = 0$. This is due to the correlations between the two particles which arise from the antisymmetric character of the state. A similar situation may occur if, instead of looking at just one observable, we evaluate the sum of the uncertainties associated with a given set of observables. For example, let us consider the sum

$$\delta(|\psi\rangle) = \sum_{i=1}^{3}\left\{\langle(A_i^{(1)} + A_i^{(2)})^2\rangle_{|\psi\rangle} - \langle A_i^{(1)} + A_i^{(2)}\rangle^2_{|\psi\rangle}\right\}, \quad (4.2)$$

where the observables $A_i^{(1)} + A_i^{(2)} = A_i \otimes \mathbb{I} + \mathbb{I} \otimes A_i$, $i = 1, 2, 3$, corresponding to the composite system, are given in terms of the non-commuting (one fermion) observables A_1, A_2 and A_3 represented (in the single-particle basis $\left\{\left|\text{-}\frac{3}{2}\right\rangle, \left|\text{-}\frac{1}{2}\right\rangle, \left|\frac{1}{2}\right\rangle, \left|\frac{3}{2}\right\rangle\right\}$) by the matrices

$$A_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad A_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \quad A_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (4.3)$$

We have that $\delta(|\psi\rangle) = 0$ for the state,

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left[\left|\text{-}\frac{3}{2}\right\rangle\left|\text{-}\frac{1}{2}\right\rangle - \left|\text{-}\frac{1}{2}\right\rangle\left|\text{-}\frac{3}{2}\right\rangle\right]. \quad (4.4)$$

Therefore, there are separable two-fermion states with vanishing $\delta(|\psi\rangle)$ even though the three (one-fermion) non-commuting operators A_1, A_2, and A_3 don't share a common eigenvector and, consequently, the uncertainty sum $\sum_{i=1}^{3}(\langle A_i^2\rangle - \langle A_i\rangle^2)$ has a non-trivial (that is, non-zero) lower bound over the single-particle states. We are going to show that, in spite of this difficulty, it is possible to find sets of non-commuting local observables for two-fermion systems such that the corresponding sum of variances admits a non-trivial, finite lower bound over the set of separable fermion states.

Regarding, as already mentioned, our two-fermion system as a system of two spin-s particles, we are now going to focus on the uncertainties associated with the three components J_x, J_y, J_z of the total angular momentum of the system. The sum of the corresponding uncertainties evaluated on a pure state $|\psi\rangle$ of the two fermions is then

$$\delta(|\psi\rangle) = \langle\psi|J^2|\psi\rangle - \langle\psi|J_x|\psi\rangle^2 - \langle\psi|J_y|\psi\rangle^2 - \langle\psi|J_z|\psi\rangle^2 \tag{4.5}$$

where

$$\begin{aligned} J^2 &= J_x^2 + J_y^2 + J_z^2 \\ J_x &= S_x \otimes \mathbb{I} + \mathbb{I} \otimes S_x \\ J_y &= S_y \otimes \mathbb{I} + \mathbb{I} \otimes S_y \\ J_z &= S_z \otimes \mathbb{I} + \mathbb{I} \otimes S_z, \end{aligned} \tag{4.6}$$

S_x, S_y, S_z are the angular momentum operators corresponding to one fermion and $\mathbb{I}$ denotes the identity operator for the single-particle Hilbert space. From here on we are going to assume that $\hbar = 1$.

The sum of uncertainties δ corresponding to a general mixed state ρ of the two-fermion system reads

$$\delta(\rho) = \mathrm{Tr}(\rho J_x^2) - [\mathrm{Tr}(\rho J_x)]^2 + \mathrm{Tr}(\rho J_y^2) - [\mathrm{Tr}(\rho J_y)]^2 + \mathrm{Tr}(\rho J_z^2) - [\mathrm{Tr}(\rho J_z)]^2. \tag{4.7}$$

Our aim is to determine an uncertainty relation for separable mixed states ρ_{sl} of two-fermion systems based on the quantity (4.7). In order to achieve this end it

is enough to establish a lower bound for (4.7) valid for pure states $|\psi_{sl}\rangle$ having Slater rank 1. To see that the uncertainty limit for separable pure states also applies to mixed separable states, we note that the uncertainty of a mixture is always equal to or greater than the averaged uncertainties of the components. Thus for a general mixture of pure states of Slater rank 1 as in eq. (2.70), we have

$$\delta(\rho_{sl}) \geq \sum_i \lambda_i \delta(|\psi_{sl}^{(i)}\rangle). \tag{4.8}$$

In the $s = 3/2$ case (corresponding to a single-particle Hilbert space of dimension four) we are going to establish that for any pure state $|\psi_{sl}\rangle$ of the Slater form,

$$\delta(|\psi_{sl}\rangle) \geq 2s - 1. \tag{4.9}$$

Consequently, we also have

$$\delta(\rho_{sl}) \geq 2s - 1, \tag{4.10}$$

for general non-entangled mixed states ρ_{sl} of the two-fermion system.

The following is a list of the antisymmetric total angular momentum eigenstates for $s = 3/2$ (which, according to the angular momentum representation, constitute a basis of the Hilbert space describing the two-fermion system) with the value for the uncertainty δ indicated on the right:

	δ
$\|2,2\rangle = -\frac{1}{\sqrt{2}}\|\frac{1}{2}\frac{3}{2}\rangle + \frac{1}{\sqrt{2}}\|\frac{3}{2}\frac{1}{2}\rangle$	2
$\|2,1\rangle = -\frac{1}{\sqrt{2}}\|\text{-}\frac{1}{2}\frac{3}{2}\rangle + \frac{1}{\sqrt{2}}\|\frac{3}{2}\text{-}\frac{1}{2}\rangle$	5
$\|2,0\rangle = -\frac{1}{2}\|\text{-}\frac{3}{2}\frac{3}{2}\rangle - \frac{1}{2}\|\text{-}\frac{1}{2}\frac{1}{2}\rangle + \frac{1}{2}\|\frac{1}{2}\text{-}\frac{1}{2}\rangle + \frac{1}{2}\|\frac{3}{2}\text{-}\frac{3}{2}\rangle$	6
$\|2,-1\rangle = -\frac{1}{\sqrt{2}}\|\text{-}\frac{3}{2}\frac{1}{2}\rangle + \frac{1}{\sqrt{2}}\|\frac{1}{2}\text{-}\frac{3}{2}\rangle$	5
$\|2,-2\rangle = -\frac{1}{\sqrt{2}}\|\text{-}\frac{3}{2}\text{-}\frac{1}{2}\rangle + \frac{1}{\sqrt{2}}\|\text{-}\frac{1}{2}\text{-}\frac{3}{2}\rangle$	2
$\|0,0\rangle = -\frac{1}{2}\|\text{-}\frac{3}{2}\frac{3}{2}\rangle + \frac{1}{2}\|\text{-}\frac{1}{2}\frac{1}{2}\rangle - \frac{1}{2}\|\frac{1}{2}\text{-}\frac{1}{2}\rangle + \frac{1}{2}\|\frac{3}{2}\text{-}\frac{3}{2}\rangle.$	0

The singlet state $|0,0\rangle$ has $\delta = 0$ and is maximally entangled, $\mathrm{Tr}(\rho_1^2) = 1/4$. What we want to find is the minimum δ_{min} for $\delta(|\psi_{sl}\rangle)$ among all separable pure states $|\psi_{sl}\rangle$, such that for $0 \leq \delta < \delta_{min}$ the state is certainly entangled (not separable)

and for $\delta_{min} \leq \delta \leq 6$ the state is either entangled or separable. This bound is

$$\min_{\{|\psi_{sl}\rangle\}} \delta(|\psi_{sl}\rangle) = 2. \tag{4.11}$$

In order to prove this we first establish the maximum of $|\langle\psi_{sl}|0,0\rangle|$ among separable states, which turns out to be $1/\sqrt{2}$. When expressing a general state $|\psi\rangle$ in the total angular momentum basis (which comprises the $j=0$ singlet and the $j=2$ multiplet) we see that the maximum of $|c_0|^2$ is $1/2$, where c_0 is the coefficient of the singlet state. After an uncertainty inequality (4.24) holding for general two-fermion states is established, we then use the previous result to obtain the uncertainty relation (4.26) for separable states. To see the first part, let

$$|\psi_{sl}\rangle = \frac{1}{\sqrt{2}}\Big\{|\phi_1\rangle|\phi_2\rangle - |\phi_2\rangle|\phi_1\rangle\Big\} \tag{4.12}$$

with normalized, orthogonal single-particle states

$$|\phi_1\rangle = \alpha_1\Big|\frac{3}{2}\Big\rangle + \alpha_2\Big|\frac{1}{2}\Big\rangle + \alpha_3\Big|\text{-}\frac{1}{2}\Big\rangle + \alpha_4\Big|\text{-}\frac{3}{2}\Big\rangle \tag{4.13}$$

$$|\phi_2\rangle = \beta_1\Big|\frac{3}{2}\Big\rangle + \beta_2\Big|\frac{1}{2}\Big\rangle + \beta_3\Big|\text{-}\frac{1}{2}\Big\rangle + \beta_4\Big|\text{-}\frac{3}{2}\Big\rangle. \tag{4.14}$$

Then

$$\langle 0,0|\psi_{sl}\rangle = \frac{1}{\sqrt{2}}\Big[\alpha_3\beta_2 - \alpha_2\beta_3 + \alpha_1\beta_4 - \alpha_4\beta_1\Big]. \tag{4.15}$$

Using first the subadditivity property, then the Schwarz inequality and finally the normalization condition of the states $|\phi_1\rangle$ and $|\phi_2\rangle$, we obtain

$$\begin{aligned} |\langle 0,0|\psi_{sl}\rangle| &\leq \frac{1}{\sqrt{2}}\Big[|\alpha_3||\beta_2| + |\alpha_2||\beta_3| + |\alpha_1||\beta_4| + |\alpha_4||\beta_1|\Big] \\ &\leq \frac{1}{\sqrt{2}}\sqrt{|\alpha_1|^2+|\alpha_2|^2+|\alpha_3|^2+|\alpha_4|^2}\sqrt{|\beta_1|^2+|\beta_2|^2+|\beta_3|^2+|\beta_4|^2} \\ &= \frac{1}{\sqrt{2}}. \end{aligned} \tag{4.16}$$

Equality can be achieved by $|\psi_{sl}\rangle = \frac{1}{\sqrt{2}}\left[\left|\frac{3}{2}\right\rangle\left|\text{-}\frac{3}{2}\right\rangle - \left|\text{-}\frac{3}{2}\right\rangle\left|\frac{3}{2}\right\rangle\right]$ and thus

$$\max|\langle 0,0|\psi_{sl}\rangle| = \frac{1}{\sqrt{2}}. \tag{4.17}$$

Now any two-fermion state $|\psi\rangle$ (whether separable or not and with a four-dimensional single-particle state space) can be expressed as

$$|\psi\rangle = c_0|0,0\rangle + c_1|\tilde{\psi}\rangle \tag{4.18}$$

with $\langle\tilde{\psi}|\tilde{\psi}\rangle = 1$ (normalized) and $|\tilde{\psi}\rangle$ being a linear combination of the five members of the $j = 2$ multiplet. Therefore we have

$$\begin{aligned} \langle\tilde{\psi}|0,0\rangle &= 0 \\ |c_0|^2 + |c_1|^2 &= 1. \end{aligned} \tag{4.19}$$

Obviously we have $c_0 = \langle 0,0|\psi\rangle$ and therefore we know that for separable states the maximum possible value for $|c_0|^2$, is

$$\max|c_0|^2 = \frac{1}{2}. \tag{4.20}$$

The allowed values for $|c_0|^2$ for separable states $|\psi\rangle$ are then

$$0 \leq |c_0|^2 \leq \frac{1}{2}. \tag{4.21}$$

Now we have to find an expression for the variance (4.5) from which we can then obtain an uncertainty relation for general bipartite states with $s = 3/2$ and then using the previous information we establish an uncertainty relation for separable states. This means we have to simplify eq. (4.5). By observing that J_x, J_y, J_z and J^2 have vanishing matrix elements (in the basis $|j,m\rangle$) connecting states with different values of j,

$$j \neq j' \rightarrow \begin{cases} \langle j,m|J_x|j',m'\rangle = 0 \\ \langle j,m|J_y|j',m'\rangle = 0 \\ \langle j,m|J_z|j',m'\rangle = 0 \\ \langle j,m|J^2|j',m'\rangle = 0 \end{cases} \tag{4.22}$$

and by making use of the normalization condition,

$$\begin{aligned}\langle\psi|J^2|\psi\rangle &= |c_0|^2 \overbrace{\langle 0,0|J^2|0,0\rangle}^{=0(0+1)} + |c_1|^2 \overbrace{\langle\tilde{\psi}|J^2|\tilde{\psi}\rangle}^{=2(2+1)} = 6|c_1|^2 = 6(1-|c_0|^2) \\ \langle\psi|J_x|\psi\rangle &= |c_0|^2 \underbrace{\langle 0,0|J_x|0,0\rangle}_{=0} + |c_1|^2\langle\tilde{\psi}|J_x|\tilde{\psi}\rangle = (1-|c_0|^2)\langle\tilde{\psi}|J_x|\tilde{\psi}\rangle \end{aligned} \quad (4.23)$$

and similarly for J_y and J_z. So eq. (4.5) becomes

$$\begin{aligned}\delta(|\psi\rangle) &= 6(1-|c_0|^2) - (1-|c_0|^2)^2\left[\langle\tilde{\psi}|J_x|\tilde{\psi}\rangle^2 + \langle\tilde{\psi}|J_y|\tilde{\psi}\rangle^2 + \langle\tilde{\psi}|J_z|\tilde{\psi}\rangle^2\right] \\ &\geq 6(1-|c_0|^2) - 4(1-|c_0|^2)^2. \end{aligned} \quad (4.24)$$

This last inequality holds because the maximum possible value of $\langle\tilde{\psi}|J_x|\tilde{\psi}\rangle^2 + \langle\tilde{\psi}|J_y|\tilde{\psi}\rangle^2 + \langle\tilde{\psi}|J_z|\tilde{\psi}\rangle^2$ is 4. This can be seen by rotating the axes such that $\langle J_x\rangle$ and $\langle J_y\rangle$ are zero and so the maximum of the above is the square of $j = 2$. For example the state $|2,2\rangle$ achieves this. Expanding eq. (4.24) results in

$$\delta(|\psi\rangle) \geq 2(1 + |c_0|^2 - 2|c_0|^4). \quad (4.25)$$

This inequality holds for any two-fermion state with $s = 3/2$, regardless of it being separable or not. Now for separable states we have that $|c_0|^2$ lies in the interval $[0, 1/2]$. Within this interval we have $(1 + |c_0|^2 - 2|c_0|^4) \geq 2$. This expression achieves the value 2 only in the extremes of the interval, $|c_0|^2 = 0$ or $|c_0|^2 = 1/2$. Therefore, for separable states we have that

$$\delta(|\psi\rangle) \geq 2 \qquad (|\psi\rangle \text{ separable}). \quad (4.26)$$

The equality case can be achieved, for instance, by the state $|2,2\rangle$.

In order to illustrate this method of entanglement detection we consider three examples of two-fermion states (with $s = 3/2$). In each case we compute the concurrence of the states and the relative violation of the local uncertainty relation, which is defined as [139]

$$\delta' = 1 - \frac{\delta}{\delta_{min}}, \quad (4.27)$$

where δ_{min} is the uncertainty limit for separable states, in this case $\delta_{min} = 2$.

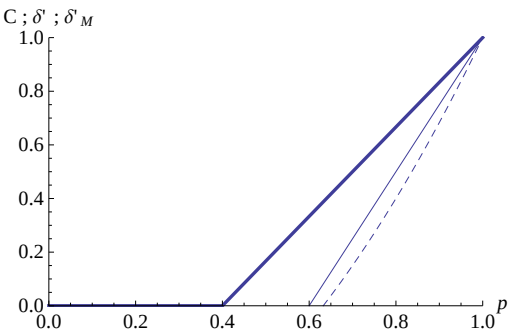


Figure 4.1: Concurrence (thick line), δ' and δ'_M (dashed line) for the state in eq. (4.28).

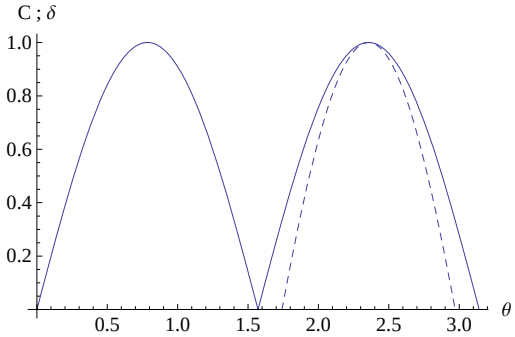


Figure 4.2: Concurrence and δ' (dashed line) for the state in eq. (4.31).

For the first example, let ρ be a mixture of a maximally entangled state and a maximally mixed state of the fermion system,

$$\rho = p|0,0\rangle\langle 0,0| + \frac{1-p}{6}\,\mathbb{I}, \tag{4.28}$$

where

$$\mathbb{I} = |0,0\rangle\langle 0,0| + \sum_{m=-2}^{2} |2,m\rangle\langle 2,m| \tag{4.29}$$

is the identity operator acting on the six-dimensional Hilbert space corresponding to the two-fermion system. The plot of the concurrence as a function of p depicted in Figure 4.1 indicates that all states with p larger than $p^* = 0.4$ are entangled. In comparison, we have $\delta(p) = 5 - 5p$ and so the uncertainty based criterion detects entanglement for $3/5 < p \leq 1$. Thus, the interval of p-values where entanglement is detected is $2/3$ of the total range of p-values corresponding to entangled states.

As a second illustration of the criterion we now consider the family of states

$$\rho = p|0,0\rangle\langle 0,0| + \frac{1-p}{2}\Big(|2,-2\rangle\langle 2,-2| + |2,2\rangle\langle 2,2|\Big). \tag{4.30}$$

The expression for $\delta(p) = 6 - 6p$ and thus the minimal p for which entanglement is detected is $p_{min} = 2/3$. Evaluating the concurrence for these states shows that

they are entangled from $p^* = 0.5$ and hence $^2/_3$ of entangled states are detected.

As third example we take

$$|\psi\rangle = \frac{\sin\theta}{\sqrt{2}}\left[\left|-\frac{3}{2}\right\rangle\left|\frac{3}{2}\right\rangle - \left|\frac{3}{2}\right\rangle\left|-\frac{3}{2}\right\rangle\right] + \frac{\cos\theta}{\sqrt{2}}\left[\left|-\frac{1}{2}\right\rangle\left|\frac{1}{2}\right\rangle - \left|\frac{1}{2}\right\rangle\left|-\frac{1}{2}\right\rangle\right]. \tag{4.31}$$

From Figure 4.2 we can see that for $\theta \in (0,\pi), \theta \neq \frac{\pi}{2}$ all states are entangled. In comparison, the uncertainty measure detects entanglement for $1.74071 < \theta \leq 2.97167$, thus about 0.392 of the entangled states are detected.

4.1.2.1 Bipartite states with higher-dimensional single-particle systems

Performing numerical searches for six-dimensional ($s = \frac{5}{2}$) up to 16-dimensional ($s = \frac{15}{2}$) single-particle Hilbert spaces, I conjecture that the general uncertainty relation for separable pure bipartite states is $\delta(|\psi\rangle) \geq 2s - 1$, where s is the dimension of the single-particle Hilbert space. The searches converged to $2s - 1$ with a precision of nine digits. Thus we conjecture that both pure and mixed bipartite states are entangled with certainty when

$$\delta(|\psi\rangle \text{ or } \rho) < 2s - 1 \implies |\psi\rangle \text{ or } \rho \text{ entangled.} \tag{4.32}$$

As an illustration for a bipartite mixed state with single-particle Hilbert space of dimension six ($s = \frac{5}{2}$), we choose

$$\rho = p|0,0\rangle\langle 0,0| + \frac{1-p}{15}\mathbb{I}, \tag{4.33}$$

where $0 \leq p \leq 1$, $|0,0\rangle$ is given in the Table below and $\mathbb{I}$ is the identity operator acting on the Hilbert space associated with the two-fermion system. For this state we have $\delta(p) = 14(1-p)$ and thus for $^5/_7 < p \leq 1$ states are entangled. The degree of violation of the uncertainty relation is then also used as a measure of entanglement for those states.

The following is a list of the antisymmetric total angular momentum eigenstates for $s = {}^5/_2$ (which, according to the angular momentum representation,

constitute a basis of the Hilbert space describing the two-fermion system) with the value for the uncertainty δ indicated on the right:

	δ
$\|4,4\rangle = -\frac{1}{\sqrt{2}}\|\frac{3}{2}\frac{5}{2}\rangle + \frac{1}{\sqrt{2}}\|\frac{5}{2}\frac{3}{2}\rangle$	4
$\|4,3\rangle = -\frac{1}{\sqrt{2}}\|\frac{1}{2}\frac{5}{2}\rangle + \frac{1}{\sqrt{2}}\|\frac{5}{2}\frac{1}{2}\rangle$	11
$\|4,2\rangle = -\frac{3}{2\sqrt{7}}\|\text{-}\frac{1}{2}\frac{5}{2}\rangle - \frac{1}{2}\sqrt{\frac{5}{7}}\|\frac{1}{2}\frac{3}{2}\rangle + \frac{1}{2}\sqrt{\frac{5}{7}}\|\frac{3}{2}\frac{1}{2}\rangle + \frac{3}{2\sqrt{7}}\|\frac{5}{2}\text{-}\frac{1}{2}\rangle$	16
$\|4,1\rangle = -\frac{1}{\sqrt{7}}\|\text{-}\frac{3}{2}\frac{5}{2}\rangle - \sqrt{\frac{5}{14}}\|\text{-}\frac{1}{2}\frac{3}{2}\rangle + \sqrt{\frac{5}{14}}\|\frac{3}{2}\text{-}\frac{1}{2}\rangle + \frac{1}{\sqrt{7}}\|\frac{5}{2}\text{-}\frac{3}{2}\rangle$	19
$\|4,0\rangle = -\frac{1}{2\sqrt{7}}\|\text{-}\frac{5}{2}\frac{5}{2}\rangle - \frac{3}{2\sqrt{7}}\|\text{-}\frac{3}{2}\frac{3}{2}\rangle - \frac{1}{\sqrt{7}}\|\text{-}\frac{1}{2}\frac{1}{2}\rangle + \frac{1}{\sqrt{7}}\|\frac{1}{2}\text{-}\frac{1}{2}\rangle + \frac{3}{2\sqrt{7}}\|\frac{3}{2}\text{-}\frac{3}{2}\rangle + \frac{1}{2\sqrt{7}}\|\frac{5}{2}\text{-}\frac{5}{2}\rangle$	20
$\|4,-1\rangle = -\frac{1}{\sqrt{7}}\|\text{-}\frac{5}{2}\frac{3}{2}\rangle - \sqrt{\frac{5}{14}}\|\text{-}\frac{3}{2}\frac{1}{2}\rangle + \sqrt{\frac{5}{14}}\|\frac{1}{2}\text{-}\frac{3}{2}\rangle + \frac{1}{\sqrt{7}}\|\frac{3}{2}\text{-}\frac{5}{2}\rangle$	19
$\|4,-2\rangle = -\frac{3}{2\sqrt{7}}\|\text{-}\frac{5}{2}\frac{1}{2}\rangle - \frac{1}{2}\sqrt{\frac{5}{7}}\|\text{-}\frac{3}{2}\text{-}\frac{1}{2}\rangle + \frac{1}{2}\sqrt{\frac{5}{7}}\|\text{-}\frac{1}{2}\text{-}\frac{3}{2}\rangle + \frac{3}{2\sqrt{7}}\|\frac{1}{2}\text{-}\frac{5}{2}\rangle$	16
$\|4,-3\rangle = -\frac{1}{\sqrt{2}}\|\text{-}\frac{5}{2}\text{-}\frac{1}{2}\rangle + \frac{1}{\sqrt{2}}\|\text{-}\frac{1}{2}\text{-}\frac{5}{2}\rangle$	11
$\|4,-4\rangle = -\frac{1}{\sqrt{2}}\|\text{-}\frac{5}{2}\text{-}\frac{3}{2}\rangle + \frac{1}{\sqrt{2}}\|\text{-}\frac{3}{2}\text{-}\frac{5}{2}\rangle$	4
$\|2,2\rangle = -\frac{1}{2}\sqrt{\frac{5}{7}}\|\text{-}\frac{1}{2}\frac{5}{2}\rangle + \frac{3}{2\sqrt{7}}\|\frac{1}{2}\frac{3}{2}\rangle - \frac{3}{2\sqrt{7}}\|\frac{3}{2}\frac{1}{2}\rangle + \frac{1}{2}\sqrt{\frac{5}{7}}\|\frac{5}{2}\text{-}\frac{1}{2}\rangle$	2
$\|2,1\rangle = -\sqrt{\frac{5}{14}}\|\text{-}\frac{3}{2}\frac{5}{2}\rangle + \frac{1}{\sqrt{7}}\|\text{-}\frac{1}{2}\frac{3}{2}\rangle - \frac{1}{\sqrt{7}}\|\frac{3}{2}\text{-}\frac{1}{2}\rangle + \sqrt{\frac{5}{14}}\|\frac{5}{2}\text{-}\frac{3}{2}\rangle$	5
$\|2,0\rangle = -\frac{5}{2\sqrt{21}}\|\text{-}\frac{5}{2}\frac{5}{2}\rangle - \frac{1}{2\sqrt{21}}\|\text{-}\frac{3}{2}\frac{3}{2}\rangle + \frac{2}{\sqrt{21}}\|\text{-}\frac{1}{2}\frac{1}{2}\rangle - \frac{2}{\sqrt{21}}\|\frac{1}{2}\text{-}\frac{1}{2}\rangle + \frac{1}{2\sqrt{21}}\|\frac{3}{2}\text{-}\frac{3}{2}\rangle + \frac{5}{2\sqrt{21}}\|\frac{5}{2}\text{-}\frac{5}{2}\rangle$	6
$\|2,-1\rangle = -\frac{5}{\sqrt{14}}\|\text{-}\frac{5}{2}\frac{3}{2}\rangle + \frac{1}{\sqrt{7}}\|\text{-}\frac{3}{2}\frac{1}{2}\rangle - \frac{1}{\sqrt{7}}\|\frac{1}{2}\text{-}\frac{3}{2}\rangle + \frac{5}{\sqrt{14}}\|\frac{3}{2}\text{-}\frac{5}{2}\rangle$	5
$\|2,-2\rangle = -\frac{1}{2}\frac{5}{\sqrt{7}}\|\text{-}\frac{5}{2}\frac{1}{2}\rangle + \frac{3}{2\sqrt{7}}\|\text{-}\frac{3}{2}\text{-}\frac{1}{2}\rangle - \frac{3}{2\sqrt{7}}\|\text{-}\frac{1}{2}\text{-}\frac{3}{2}\rangle + \frac{1}{2}\frac{5}{\sqrt{7}}\|\frac{1}{2}\text{-}\frac{5}{2}\rangle$	2
$\|0,0\rangle = -\frac{1}{6}\|\text{-}\frac{5}{2}\frac{5}{2}\rangle + \frac{1}{\sqrt{6}}\|\text{-}\frac{3}{2}\frac{3}{2}\rangle - \frac{1}{\sqrt{6}}\|\text{-}\frac{1}{2}\frac{1}{2}\rangle + \frac{1}{\sqrt{6}}\|\frac{1}{2}\text{-}\frac{1}{2}\rangle - \frac{1}{\sqrt{6}}\|\frac{3}{2}\text{-}\frac{3}{2}\rangle + \frac{1}{\sqrt{6}}\|\frac{5}{2}\text{-}\frac{5}{2}\rangle.$	0

Any state for which $\delta(\rho) < 4$ is necessarily entangled. Thus in the above list of states, three of the eleven entangled states are detected.

4.1.3 Characterization of entanglement via the variances of projector operators

Here I am going to formulate separability criteria for systems of identical fermions based upon the uncertainties of observables that are not of the form $A^{(1)} + A^{(2)} = A \otimes \mathbb{I} + \mathbb{I} \otimes A$. Instead, we are going to consider families of observables of the form $M_i = |\psi_i\rangle\langle\psi_i|$, where $|\psi_i\rangle$ are appropriate pure states of the N-fermion system under consideration. This kind of approach was recently applied by Gühne [140] to composite quantum systems with distinguishable subsystems.

4.1.3.1 Bipartite states of two fermions with a four-dimensional single-particle Hilbert space

We are interested in finding an entanglement detection criterion involving the sum $\delta_M = \sum_i \delta^2(M_i)$ of the variances of an appropriate set of projector operators $\{M_i\}$. First, let's introduce the following notation:

$$|m_1 m_2| = \frac{1}{\sqrt{2}}\Big[|m_1\rangle|m_2\rangle - |m_2\rangle|m_1\rangle\Big]. \tag{4.34}$$

We now define six orthogonal basis states each exhibiting the same amount of entanglement and all consisting of a linear combination of two Slater determinants which are orthogonal as well,

$$\begin{aligned}
|\psi_1\rangle &= a\left|\tfrac{3}{2}\tfrac{1}{2}\right| + b\left|\text{-}\tfrac{1}{2}\text{-}\tfrac{3}{2}\right| \\
|\psi_2\rangle &= b\left|\tfrac{3}{2}\tfrac{1}{2}\right| - a\left|\text{-}\tfrac{1}{2}\text{-}\tfrac{3}{2}\right| \\
|\psi_3\rangle &= a\left|\tfrac{1}{2}\text{-}\tfrac{1}{2}\right| + b\left|\tfrac{3}{2}\text{-}\tfrac{3}{2}\right| \\
|\psi_4\rangle &= b\left|\tfrac{1}{2}\text{-}\tfrac{1}{2}\right| - a\left|\tfrac{3}{2}\text{-}\tfrac{3}{2}\right| \\
|\psi_5\rangle &= a\left|\tfrac{3}{2}\text{-}\tfrac{1}{2}\right| + b\left|\tfrac{1}{2}\text{-}\tfrac{3}{2}\right| \\
|\psi_6\rangle &= b\left|\tfrac{3}{2}\text{-}\tfrac{1}{2}\right| - a\left|\tfrac{1}{2}\text{-}\tfrac{3}{2}\right|,
\end{aligned} \tag{4.35}$$

where a and b are assumed to be real and $|a| \geq |b|$. Then we let $M_i = |\psi_i\rangle\langle\psi_i|, i = 1, \ldots, 6$. The proof of the uncertainty relation (4.40) is as follows. We let $|\phi_{sl}\rangle$, $|\phi_1\rangle$ and $|\phi_2\rangle$ be the same as in eqs. (4.12), (4.13) and (4.14). The idea is to find the minimum of

$$\sum_{i=1}^{6} \delta^2(M_i)_{|\phi_{sl}\rangle\langle\phi_{sl}|} = 1 - \sum_{i=1}^{6} \left(|\langle\phi_{sl}|\psi_i\rangle|^2\right)^2 \tag{4.36}$$

for all separable states $|\phi_{sl}\rangle$, so that when $\sum_{i=1}^{6} \delta^2(M_i)_{|\psi\rangle\langle\psi|}$ is less than that minimum, we know with certainty that the state $|\psi\rangle$ is entangled. This amounts to finding the maximum for $\sum_{i=1}^{6} \left(|\langle\phi_{sl}|\psi_i\rangle|^2\right)^2$. This can be determined by finding

first the maximum of $|\langle\phi_{sl}|\psi_i\rangle|^2$ for each i (here we follow a procedure similar to the one used in [140] for systems of two distinguishable qubits). Due to symmetry, it is only necessary to find the maximum for one i. Now,

$$\begin{aligned}
|\langle\phi_{sl}|\psi_1\rangle| &= \left|a\alpha_1\beta_2 - a\alpha_2\beta_1 + b\alpha_3\beta_4 - b\alpha_4\beta_3\right| \\
&\leq |a|\Big[|\alpha_1||\beta_2| + |\alpha_2||\beta_1|\Big] + |b|\Big[|\alpha_3||\beta_4| + |\alpha_4||\beta_3|\Big] \\
&\leq |a|\Big[|\alpha_1||\beta_2| + |\alpha_2||\beta_1| + |\alpha_3||\beta_4| + |\alpha_4||\beta_3|\Big] \\
&\leq |a|\sqrt{|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 + |\alpha_4|^2}\sqrt{|\beta_1|^2 + |\beta_2|^2 + |\beta_3|^2 + |\beta_4|^2} \\
&= |a|, \qquad (4.37)
\end{aligned}$$

where the inequalities follow from subadditivity, then from $|a| \geq |b|$ and the last inequality comes from the Schwarz inequality and the equality follows from the normalization of $|\phi_1\rangle$ and $|\phi_2\rangle$. As mentioned, due to symmetry, this last inequality will hold for all $|\psi_i\rangle$,

$$|\langle\phi_{sl}|\psi_i\rangle|^2 \leq a^2 \quad \forall i. \qquad (4.38)$$

The inequality (4.38) together with the normalization of $|\phi_{sl}\rangle$, leads to the inequality

$$\sum_{i=1}^{6} \left(|\langle\phi_{sl}|\psi_i\rangle|^2\right)^2 \leq a^4 + (1-a^2)^2. \qquad (4.39)$$

This upper bound is achieved, for instance, by the state $|\phi'_{sl}\rangle = \left|\frac{3}{2}\frac{1}{2}\right|$.
From (4.39) and using the normalization of the $|\psi_i\rangle$'s ($a^2 + b^2 = 1$), we finally obtain,

$$\sum_{i=1}^{6} \delta^2(M_i)_{|\phi_{sl}\rangle\langle\phi_{sl}|} \geq 2a^2b^2. \qquad (4.40)$$

At least one entangled state violates this inequality, namely $|\psi_1\rangle$ which gives zero for the left hand side of equation (4.40). To compare the efficiency of this entanglement criterion with the previous one we use the same families of mixed states ρ as in equations (4.28) and (4.30). When applying the criterion to those states we consider the case $a = b = 1/\sqrt{2}$, which is the one maximizing the right hand side of equation (4.40). The results corresponding to the first illustration are shown in Figure 4.1 where we again use the relative violation (4.27) with

$\delta_{min} = 1/2$,

$$\delta'_M = 1 - 2\delta_M, \tag{4.41}$$

and since $\delta_M(p) = -\frac{5}{6}(-1 + p^2)$, entanglement is detected for $\sqrt{\frac{2}{5}} < p \leq 1$. Thus the range of entanglement detection in this case is very close to the one of the first uncertainty relation established. For the second density matrix (4.30), $\delta_M(p) = \frac{1}{2} + p - \frac{3p^2}{2}$ and so entanglement is detected from $p_{min} = 2/3$, which is exactly the same as for the local uncertainty relation.

4.1.3.2 Two-fermion systems with a six-dimensional single-particle Hilbert space

As mentioned before, the particular case of systems of two identical fermions with a four-dimensional single-particle Hilbert space (the simplest fermion system admitting entanglement) is the only one for which we have a closed, analytical expression for the concurrence. No such expression is known for fermion systems of higher dimensionality, nor any necessary and sufficient separability criteria for general mixed states of those systems. It is thus of considerable interest to explore the application of separability criteria based upon uncertainty relations of a two-fermion system with single-particle Hilbert space of dimension larger than four. Here we are going to consider fermions with single-particle Hilbert space of dimension six. The dimension of the concomitant two-fermion system is then 15 and, again, we have to choose a basis of orthogonal states $\{|\psi_i\rangle,\ \ i = 1, \ldots, 15\}$, all exhibiting the same amount of entanglement. We are going to use an orthonormal basis comprising five "triplets" of states of the form

$$\begin{aligned} a\,|m_1 m_2| \ &+\ a\,|m_3 m_4| - \frac{a}{2}\,|m_5 m_6|\,, \\ a\,|m_1 m_2| \ &-\ \frac{a}{2}\,|m_3 m_4| + a\,|m_5 m_6|\,, \\ -\frac{a}{2}\,|m_1 m_2| \ &+\ a\,|m_3 m_4| + a\,|m_5 m_6|\,, \end{aligned} \tag{4.42}$$

where the six m_i's appearing in (4.42) are all different and $a = 2/3$. The three Slater determinants $|m_i m_j|$ appearing in each of the "triplets" are different from

the Slater determinants appearing in the other four triplets. Thus the basis reads

$$\begin{aligned}
|\psi_1\rangle &= \frac{2}{3}\left|\tfrac{5}{2}\tfrac{3}{2}\right| + \frac{2}{3}\left|\tfrac{1}{2}\text{-}\tfrac{1}{2}\right| - \frac{1}{3}\left|\text{-}\tfrac{3}{2}\text{-}\tfrac{5}{2}\right| \\
|\psi_2\rangle &= \frac{2}{3}\left|\tfrac{5}{2}\tfrac{3}{2}\right| - \frac{1}{3}\left|\tfrac{1}{2}\text{-}\tfrac{1}{2}\right| + \frac{2}{3}\left|\text{-}\tfrac{3}{2}\text{-}\tfrac{5}{2}\right| \\
|\psi_3\rangle &= -\frac{1}{3}\left|\tfrac{5}{2}\tfrac{3}{2}\right| + \frac{2}{3}\left|\tfrac{1}{2}\text{-}\tfrac{1}{2}\right| + \frac{2}{3}\left|\text{-}\tfrac{3}{2}\text{-}\tfrac{5}{2}\right| \\
|\psi_4\rangle &= \frac{2}{3}\left|\tfrac{5}{2}\tfrac{1}{2}\right| + \frac{2}{3}\left|\text{-}\tfrac{1}{2}\text{-}\tfrac{3}{2}\right| - \frac{1}{3}\left|\tfrac{3}{2}\text{-}\tfrac{5}{2}\right| \\
|\psi_5\rangle &= \frac{2}{3}\left|\tfrac{5}{2}\tfrac{1}{2}\right| - \frac{1}{3}\left|\text{-}\tfrac{1}{2}\text{-}\tfrac{3}{2}\right| + \frac{2}{3}\left|\tfrac{3}{2}\text{-}\tfrac{5}{2}\right| \\
|\psi_6\rangle &= -\frac{1}{3}\left|\tfrac{5}{2}\tfrac{1}{2}\right| + \frac{2}{3}\left|\text{-}\tfrac{1}{2}\text{-}\tfrac{3}{2}\right| + \frac{2}{3}\left|\tfrac{3}{2}\text{-}\tfrac{5}{2}\right| \\
&\vdots \\
|\psi_{13}\rangle &= \frac{2}{3}\left|\tfrac{5}{2}\text{-}\tfrac{5}{2}\right| + \frac{2}{3}\left|\tfrac{3}{2}\text{-}\tfrac{1}{2}\right| - \frac{1}{3}\left|\tfrac{1}{2}\text{-}\tfrac{3}{2}\right| \\
|\psi_{14}\rangle &= \frac{2}{3}\left|\tfrac{5}{2}\text{-}\tfrac{5}{2}\right| - \frac{1}{3}\left|\tfrac{3}{2}\text{-}\tfrac{1}{2}\right| + \frac{2}{3}\left|\tfrac{1}{2}\text{-}\tfrac{3}{2}\right| \\
|\psi_{15}\rangle &= -\frac{1}{3}\left|\tfrac{5}{2}\text{-}\tfrac{5}{2}\right| + \frac{2}{3}\left|\tfrac{3}{2}\text{-}\tfrac{1}{2}\right| + \frac{2}{3}\left|\tfrac{1}{2}\text{-}\tfrac{3}{2}\right| .
\end{aligned} \tag{4.43}$$

The derivation of the uncertainty relation (4.45) follows along similar lines as the one in the previous Subsubsection. The general separable state is as in eq. (4.12), however, the two orthogonal single-particle states are of dimension six. The overlap between a member $|\psi_i\rangle$ of the above basis and any separable state $|\phi_{sl}\rangle$ is always less or equal to a. Making use of the normalization of the $|\psi_i\rangle$'s, $2a^2 + (\frac{a}{2})^2 = 1$, this leads to the inequality

$$\sum_{i=1}^{15}(|\langle\phi_{sl}|\psi_i\rangle|^2)^2 \leq 2a^4 + (1-2a^2)^2 = \frac{33}{81} \tag{4.44}$$

which, in turn, implies the following lower bound for the sum of the uncertainties evaluated on a separable state,

$$\sum_{i=1}^{15}\delta^2(M_i)_{|\phi_{sl}\rangle\langle\phi_{sl}|} \geq \frac{48}{81}. \tag{4.45}$$

The separable state $|\phi'_{sl}\rangle = \left|\frac{5}{2}\frac{3}{2}\right|$ attains this lower bound and at least one entangled state violates this inequality, namely $|\psi_1\rangle$ gives $\sum_{i=1}^{15}\delta^2(M_i)_{|\psi_1\rangle\langle\psi_1|} = 0$.

As an illustration of this separability criterion let us look at the following family of states having Slater rank equal to 2,

$$|\phi\rangle = \frac{1}{\sqrt{2}}\Big[|\phi_1\phi_2| + |\phi_3\phi_4|\Big], \tag{4.46}$$

with the $|\phi_i\rangle$'s being four normalized, orthogonal single-particle states. The overlap between this family of states and $|\psi_1\rangle$ is less or equal to $\frac{4}{3\sqrt{2}}$. The minimum value adopted by the quantity $\sum_{i=1}^{15}\delta^2(M_i)$ when evaluated on states belonging to the family (4.46) is $\frac{33}{162}$ and it is achieved by the state $|\phi'\rangle = \frac{1}{\sqrt{2}}\left[\left|\frac{5}{2}\frac{3}{2}\right| + \left|\frac{1}{2}\text{-}\frac{1}{2}\right|\right]$. Thus we obtain

$$\sum_{i=1}^{15}\delta^2(M_i)_{|\phi\rangle\langle\phi|} \geq \frac{33}{162}. \tag{4.47}$$

So all the states within the family (4.46) whose sum of uncertainties lies between $\frac{33}{162}$ and $\frac{48}{81}$ are identified as entangled.

As a second example we apply the criterion to mixed states of the form

$$\rho = p|\varphi_i\rangle\langle\varphi_i| + \frac{1-p}{15}\,\mathbb{I}, \tag{4.48}$$

where $0 \leq p \leq 1$, $|\varphi_i\rangle$ is an entangled pure state, and $\mathbb{I} = \sum_{i=1}^{15}|\psi_i\rangle\langle\psi_i|$ is the identity operator acting on the Hilbert space associated with the two-fermion system, the $|\psi_i\rangle$'s being the members of an orthonormal basis of this space (for instance, the basis (4.43)). We are going to consider the following three different cases for the state $|\varphi_i\rangle$:

1) $|\varphi_1\rangle = \frac{1}{\sqrt{3}}\left[\left|\frac{5}{2}\frac{3}{2}\right| + \left|\frac{1}{2}\text{-}\frac{1}{2}\right| - \left|\text{-}\frac{3}{2}\text{-}\frac{5}{2}\right|\right]$, in which case entanglement is detected in the interval $1 \geq p > \sqrt{\frac{207}{482}} \approx 0.655$, since $\delta_M = \frac{14}{15} - \frac{964}{1215}p^2$.

2) $|\varphi_2\rangle = |\psi_1\rangle$, then $\delta_M = -\frac{14}{15}(-1+p^2)$ and entanglement is detected for $1 \geq p > \sqrt{\frac{23}{63}} \approx 0.604$.

3) $|\varphi_3\rangle = \frac{1}{\sqrt{2}}\left[\left|\frac{5}{2}\frac{3}{2}\right| + \left|\frac{1}{2}\text{-}\frac{1}{2}\right|\right]$, with $\delta_M = \frac{1}{270}(252 - 197p^2)$ and entangled states are detected for $1 \geq p > \sqrt{\frac{92}{197}} \approx 0.683$.

4.1.3.3 Systems of three fermions with a six-dimensional single-particle Hilbert space

In the case of three fermions with $s = 5/2$, a general separable state (Slater determinant) is of the form

$$\begin{aligned}|\phi_{sl}\rangle = |\phi_1\phi_2\phi_3| &= \frac{1}{\sqrt{6}}\Big[|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle - |\phi_1\rangle|\phi_3\rangle|\phi_2\rangle - |\phi_2\rangle|\phi_1\rangle|\phi_3\rangle + |\phi_2\rangle|\phi_3\rangle|\phi_1\rangle \\ &\quad + |\phi_3\rangle|\phi_1\rangle|\phi_2\rangle - |\phi_3\rangle|\phi_2\rangle|\phi_1\rangle\Big], \end{aligned} \tag{4.49}$$

with the three orthonormal single-particle states being

$$\begin{aligned}|\phi_1\rangle &= \alpha_1\left|\frac{5}{2}\right\rangle + \alpha_2\left|\frac{3}{2}\right\rangle + \alpha_3\left|\frac{1}{2}\right\rangle + \alpha_4\left|\text{-}\frac{1}{2}\right\rangle + \alpha_5\left|\text{-}\frac{3}{2}\right\rangle + \alpha_6\left|\text{-}\frac{5}{2}\right\rangle \\ |\phi_2\rangle &= \beta_1\left|\frac{5}{2}\right\rangle + \beta_2\left|\frac{3}{2}\right\rangle + \beta_3\left|\frac{1}{2}\right\rangle + \beta_4\left|\text{-}\frac{1}{2}\right\rangle + \beta_5\left|\text{-}\frac{3}{2}\right\rangle + \beta_6\left|\text{-}\frac{5}{2}\right\rangle \\ |\phi_3\rangle &= \gamma_1\left|\frac{5}{2}\right\rangle + \gamma_2\left|\frac{3}{2}\right\rangle + \gamma_3\left|\frac{1}{2}\right\rangle + \gamma_4\left|\text{-}\frac{1}{2}\right\rangle + \gamma_5\left|\text{-}\frac{3}{2}\right\rangle + \gamma_6\left|\text{-}\frac{5}{2}\right\rangle. \end{aligned} \tag{4.50}$$

In this Subsubsection we are extending the previous one to three fermions. Since the dimension of the system is 20, we need to construct 20 orthogonal states whose entanglement is the same and where there is no overlap between the two Slater determinants that each state consists of. So the basis consists of ten pairs of states which are unique combinations of non-overlapping Slater determinants and where the members of each pair are permutations of each other:

$$\begin{aligned}|\psi_1\rangle &= \frac{1}{\sqrt{2}}\left(\left|\frac{5}{2}\frac{3}{2}\frac{1}{2}\right| + \left|\text{-}\frac{1}{2}\text{-}\frac{3}{2}\text{-}\frac{5}{2}\right|\right) \\ |\psi_2\rangle &= \frac{1}{\sqrt{2}}\left(\left|\frac{5}{2}\frac{3}{2}\frac{1}{2}\right| - \left|\text{-}\frac{1}{2}\text{-}\frac{3}{2}\text{-}\frac{5}{2}\right|\right) \\ |\psi_3\rangle &= \frac{1}{\sqrt{2}}\left(\left|\frac{3}{2}\text{-}\frac{1}{2}\text{-}\frac{5}{2}\right| + \left|\frac{5}{2}\frac{1}{2}\text{-}\frac{3}{2}\right|\right) \\ |\psi_4\rangle &= \frac{1}{\sqrt{2}}\left(\left|\frac{3}{2}\text{-}\frac{1}{2}\text{-}\frac{5}{2}\right| - \left|\frac{5}{2}\frac{1}{2}\text{-}\frac{3}{2}\right|\right) \end{aligned}$$

$$\begin{aligned} &\vdots \\ |\psi_{19}\rangle &= \frac{1}{\sqrt{2}}\left(\left|\tfrac{5}{2}\tfrac{1}{2}\tfrac{5}{2}\right| + \left|\tfrac{1}{2}\tfrac{3}{2}\tfrac{3}{2}\right|\right) \\ |\psi_{20}\rangle &= \frac{1}{\sqrt{2}}\left(\left|\tfrac{5}{2}\tfrac{1}{2}\tfrac{5}{2}\right| - \left|\tfrac{1}{2}\tfrac{3}{2}\tfrac{3}{2}\right|\right). \end{aligned} \tag{4.51}$$

Once again, let $M_i = |\psi_i\rangle\langle\psi_i|, i = 1, \ldots, 20$ and so we obtain exactly the same equation as in (4.36), except that the summation goes to 20. A bound on the maximum overlap of $|\psi_i\rangle$ and $|\phi_{sl}\rangle$ is

$$\begin{aligned} |\langle\phi_{sl}|\psi_i\rangle| &= \frac{1}{\sqrt{2}}\big|\alpha_1\beta_2\gamma_3 - \alpha_1\beta_3\gamma_2 - \alpha_2\beta_1\gamma_3 + \alpha_2\beta_3\gamma_1 + \alpha_3\beta_1\gamma_2 - \alpha_3\beta_2\gamma_1 \\ &\qquad +\alpha_4\beta_5\gamma_6 - \alpha_4\beta_6\gamma_5 - \alpha_5\beta_4\gamma_6 + \alpha_5\beta_6\gamma_4 + \alpha_6\beta_4\gamma_5 - \alpha_6\beta_5\gamma_4\big| \\ &\leq \frac{1}{\sqrt{2}}, \end{aligned} \tag{4.52}$$

where the last inequality follows from the Schwarz inequality and normalization. A state that realizes the maximum is $|\phi'_{sl}\rangle = \left|\frac{5}{2}\frac{3}{2}\frac{1}{2}\right|$ and so together with normalization

$$\sum_{i=1}^{20}\left(|\langle\phi_{sl}|\psi_i\rangle|^2\right)^2 \leq \frac{1}{2} \tag{4.53}$$

and hence

$$\sum_{i=1}^{20}\delta^2(M_i)_{|\phi_{sl}\rangle\langle\phi_{sl}|} \geq \frac{1}{2} \quad \forall\,|\phi_{sl}\rangle. \tag{4.54}$$

At least one entangled state violates this inequality, namely $|\psi_1\rangle$ gives zero for the sum on the left hand side of eq. (4.54).

As an example of entanglement detection, let us consider the following family of states

$$|\Phi\rangle = a|\phi_1\phi_2\phi_3| + b|\phi_4\phi_5\phi_6| \tag{4.55}$$

with the $|\phi_i\rangle$'s being six orthogonal single-particle states. The above procedure is repeated, this time for the family given in eq. (4.55). Then

$$\sum_{i=1}^{20}\delta^2(M_i)_{|\Phi\rangle\langle\Phi|} \geq 1 - \frac{1}{4}\left[|a+b|^4 + |a-b|^4\right] \tag{4.56}$$

and the specific case $a = \sqrt{\frac{2}{3}}$, $b = \frac{1}{\sqrt{3}}$ [127, 134] (which is a state with genuine tripartite entanglement) gives the value $\frac{1}{18}$ for the right hand side. Thus all the states whose sum of uncertainties lies between $\frac{1}{18}$ and $\frac{1}{2}$ are identified as entangled.

4.1.4 Separability criteria for two-fermion systems with a four-dimensional single-particle Hilbert space based on entropic uncertainty relations

Entropic uncertainty relations provide an alternative way to develop entanglement criteria based upon uncertainty relations. The application of this procedure to the detection of entanglement in quantum systems consisting of distinguishable subsystems was investigated by Gühne and Lewenstein in [141] and by Giovannetti in [142]. Here we are going to explore the use of entropic uncertainty relations to identify entangled states of systems constituted by identical fermions. Within this approach the statistical variances are replaced by entropic measures as a means of estimating the uncertainties associated with the measurement of observables. If $\{p_i\}$ denotes the probabilities of obtaining the different eigenvalues of an observable A when measuring it on a system prepared in a given state ρ, one can use the concomitant Shannon entropy,

$$H[A]_\rho \; = \; -\sum_i p_i \ln p_i, \tag{4.57}$$

to characterize the uncertainty associated with the measurement. Alternatively, one can consider the Rényi or the Tsallis families of q-entropies [142, 191, 196], respectively given by

$$H_q^{(R)}[A]_\rho \; = \; \frac{1}{1-q} \, \ln \left(\sum_i p_i^q \right), \tag{4.58}$$

and

$$H_q^{(T)}[A]_\rho \; = \; \frac{1 - \sum_i p_i^q}{q-1}. \tag{4.59}$$

The Shannon measure is a particular member of the above two entropic families, corresponding to the limit case $q \to 1$. The above entropic measures have been discussed in Subsections 1.1.1, 1.1.2, 1.1.3 and 1.1.7.

Given a suitable set of observables $\{A_k\}$ we want to establish the minimum value

$$H_{\min} = \min_{\{|\psi_{sl}\rangle\}} \sum_k H[A_k]_{|\psi_{sl}\rangle}, \tag{4.60}$$

over all separable pure states $|\psi_{sl}\rangle$, adopted by the sum of the entropies $H[A_k]$ associated with the measurement of the observables A_k. If the entropic measure H used in (4.60) is concave, then

$$\sum_k H[A_k]_\rho \geq \sum_{k,i} \lambda_i H[A_k]_{|\psi_{sl}^{(i)}\rangle} \geq \sum_i \lambda_i H_{\min} = H_{\min}, \tag{4.61}$$

for any separable mixed state ρ of the form (2.70).

We are going to consider the set of observables

$$\hat{X} = S_x \otimes S_x, \qquad \hat{Y} = S_y \otimes S_y, \qquad \hat{Z} = S_z \otimes S_z, \tag{4.62}$$

associated with a system of two identical fermions, where S_x, S_y and S_z are the single-fermion angular momentum operators in the x, y and z direction respectively. Once again, we are going to assume that $\hbar = 1$. In order to determine the minimum value of the corresponding entropic sum (4.60), it is convenient to represent the general separable state $|\psi_{sl}\rangle$ as

$$|\psi_{sl}\rangle = \frac{|\chi\rangle}{\sqrt{\langle\chi|\chi\rangle}}, \tag{4.63}$$

where

$$|\chi\rangle = |\phi_1\rangle|\phi_2\rangle - |\phi_2\rangle|\phi_1\rangle, \tag{4.64}$$

and the single-particle states $|\phi_1\rangle$ and $|\phi_2\rangle$ are parameterized as [197]

$$\begin{aligned}
|\phi_1\rangle &= \cos\alpha_3 \left|-\frac{3}{2}\right\rangle + \sin\alpha_3 \cos\alpha_2\, e^{i\gamma_3} \left|-\frac{1}{2}\right\rangle + \sin\alpha_3 \sin\alpha_2 \cos\alpha_1\, e^{i\gamma_2} \left|\frac{1}{2}\right\rangle \\
&\quad + \sin\alpha_3 \sin\alpha_2 \sin\alpha_1\, e^{i\gamma_1} \left|\frac{3}{2}\right\rangle \\
|\phi_2\rangle &= \cos\beta_3 \left|-\frac{3}{2}\right\rangle + \sin\beta_3 \cos\beta_2\, e^{i\delta_3} \left|-\frac{1}{2}\right\rangle + \sin\beta_3 \sin\beta_2 \cos\beta_1\, e^{i\delta_2} \left|\frac{1}{2}\right\rangle
\end{aligned}$$

$$+\sin\beta_3 \sin\beta_2 \sin\beta_1\, e^{i\delta_1} \left|\frac{3}{2}\right\rangle. \tag{4.65}$$

The six parameters $\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3 \in [0, \frac{\pi}{2}]$, whereas the phase-parameters lie in the interval $[0, 2\pi]$. Note that here we don't require that $|\phi_1\rangle$ and $|\phi_2\rangle$ are orthogonal. Thus the state (4.63) has Slater rank 1 even if the states $|\phi_1\rangle$ and $|\phi_2\rangle$ are non-orthogonal. This means $\langle\phi_1|\phi_2\rangle = c$, however, as long as $c \neq 1$ we have $|\phi_1\rangle$ and $|\phi_2\rangle$ linearly independent and so $|\psi_{sl}\rangle$ is proportional to a Slater determinant. The entropic uncertainties (Shannon entropy) corresponding to the measurement of the observables $\hat{X}$, $\hat{Y}$ and $\hat{Z}$ on the state (4.63) are calculated and added together. This procedure leads to two functions, $H[\hat{X}] + H[\hat{Y}]$ and $H[\hat{X}] + H[\hat{Y}] + H[\hat{Z}]$, of the 12 parameters characterizing the state (4.63), that have to be minimized in order to obtain the separability criteria. Since the states are expressed in the product basis, one first has to obtain the eigenvectors of $\hat{X}$, $\hat{Y}$ and $\hat{Z}$ in the product basis, then take linear combinations of the degenerate eigenvectors to get six antisymmetric eigenvectors for each observable. These are then used to obtain the probabilities

$$p_k = |\langle\psi_{sl}|e_v^k\rangle|^2 \quad k = 1, 2, \ldots, 6. \tag{4.66}$$

In all three cases $\hat{X}$, $\hat{Y}$, $\hat{Z}$, two of the eigenvalues are two-fold degenerate and so one respectively adds the two probabilities corresponding to the same eigenvalue. When measuring either $\hat{X}$, $\hat{Y}$ or $\hat{Z}$, we thus have the probabilities for obtaining the four eigenvalues when the system is in the state $|\psi_{sl}\rangle$. It is these probabilities that are used in the Shannon entropy in eq. (4.60). Since the resultant expressions $H[\hat{X}] + H[\hat{Y}]$ and $H[\hat{X}] + H[\hat{Y}] + H[\hat{Z}]$ are much too complicated to establish the corresponding minima H_{xy} and H_{xyz} analytically, we implemented instead a numerical minimization using the Metropolis algorithm. The idea behind the Metropolis algorithm is to try and prevent ending up with a local minimum by doing the following. Starting from a random configuration $\mathcal{A}$, one calculates the entropy $H_{\mathcal{A}} = H[\hat{X}]_{\mathcal{A}} + H[\hat{Y}]_{\mathcal{A}}$ and then makes a change in the configuration to obtain a new (nearby) configuration $\mathcal{B}$ which is also normalized. The entropy $H_{\mathcal{B}}$ is then computed and if $H_{\mathcal{B}} < H_{\mathcal{A}}$ the new configuration is assumed since it has lower entropy. However, if $H_{\mathcal{B}} > H_{\mathcal{A}}$, the new higher entropy configuration is accepted with probability $p = e^{-(H_{\mathcal{B}} - H_{\mathcal{A}})/T}$, where T is a parameter that is decreased

as the algorithm proceeds in order to settle into the lowest entropy configuration one can find in the neighbourhood. That is, when T is larger there is a greater probability of moving out of local minima regions and hence exploring the configuration space in order to find the global minimum. As T is decreased it forces the algorithm to narrow its search and one can simultaneously then also decrease the amount by which one perturbs the parameters in order to narrow the search even further. The Metropolis algorithm was run numerous times with different random initial states to ensure that it always converges to the same global minimum. The result of this numerical optimization is $H_{xy} = 0.693147$ and $H_{xyz} = 1.38629$. This means that states for which $H[\hat{X}] + H[\hat{Y}]$ or $H[\hat{X}] + H[\hat{Y}] + H[\hat{Z}]$ is smaller than their respective minimal values, are necessarily entangled.

In what follows we are going to consider separability criteria for systems of two identical fermions based, instead of on the Shannon entropy, on Tsallis' q-entropy. The separability bounds associated with the q-entropies are obtained by recourse to a procedure similar to the previously discussed one corresponding to Shannon's measure. In fact, the Shannon-based criteria can be regarded as special instances of the Tsallis-based ones, corresponding to $q \to 1$. So for a range of values of q we numerically determine the minima

$$\begin{aligned} H_{xy}(q) &= \min_{|\psi_{sl}\rangle} \left\{ H_q^{(T)}[S_x \otimes S_x]_{|\psi_{sl}\rangle} + H_q^{(T)}[S_y \otimes S_y]_{|\psi_{sl}\rangle} \right\} \\ H_{xyz}(q) &= \min_{|\psi_{sl}\rangle} \left\{ H_q^{(T)}[S_x \otimes S_x]_{|\psi_{sl}\rangle} + H_q^{(T)}[S_y \otimes S_y]_{|\psi_{sl}\rangle} + \right. \\ &\qquad \left. H_q^{(T)}[S_z \otimes S_z]_{|\psi_{sl}\rangle} \right\}, \end{aligned} \tag{4.67}$$

where $|\psi_{sl}\rangle$ is a pure state of Slater rank 1 (expressed as in (4.63)) with $|\phi_1\rangle$, $|\phi_2\rangle$ being the same as in eq. (4.65). Then we have

$$\begin{aligned} H_q^{(T)}[S_x \otimes S_x]_{|\psi_{sl}\rangle} + H_q^{(T)}[S_y \otimes S_y]_{|\psi_{sl}\rangle} &\geq H_{xy}(q) \\ H_q^{(T)}[S_x \otimes S_x]_{|\psi_{sl}\rangle} + H_q^{(T)}[S_y \otimes S_y]_{|\psi_{sl}\rangle} + H_q^{(T)}[S_z \otimes S_z]_{|\psi_{sl}\rangle} &\geq H_{xyz}(q), \end{aligned} \tag{4.68}$$

for all separable pure states $|\psi_{sl}\rangle$. Since the entropic measure $H_q^{(T)}$ is concave, the inequality (4.68) actually holds for any separable state ρ, pure or mixed. The results corresponding to the numerical minimization (4.67) are shown in Figure 4.3. The Metropolis algorithm was used to obtain the minimum for each q, with

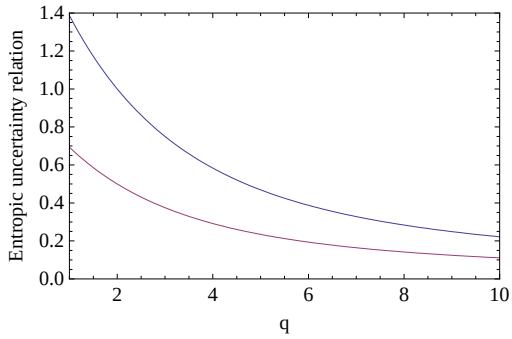


Figure 4.3: Numerical lower bounds in eq. (4.68). The upper curve is $H_{xyz}(q)$ and the lower one $H_{xy}(q)$.

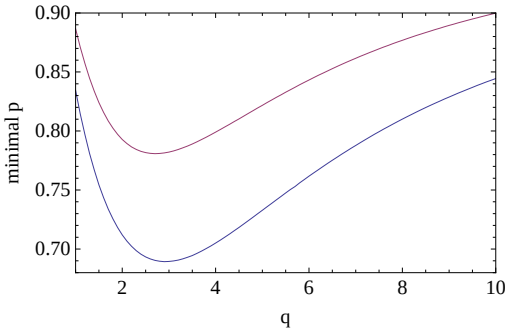


Figure 4.4: Minimal values p_{min} depending on q such that for $p > p_{min}$ entanglement in (4.69) is detected. These states are entangled for $p > 0.4$. The upper curve is $p_{xy}(q)$ and the lower one $p_{xyz}(q)$.

q increasing in intervals of 0.1. The starting point for each minimization were the values of the 12 parameters which minimized the sum of the Tsallis entropies for the previous value for q, and for $q = 1.1$ the initial values taken were the result from the Metropolis algorithm for the sum of the Shannon entropies (remember that the Shannon entropy is recovered from the Tsallis entropy in the limit $q \to 1$). To make sure that this perturbation-based minimization approach works, cross-checks were performed for a select number of values of q by running the Metropolis algorithm directly with random initial input values. These results did indeed correspond to the minima obtained by the perturbation method.

As illustrations of the efficiency of these criteria we can consider the same families of states (4.28) and (4.30) as in Subsection 4.1.2. The six antisymmetric eigenvectors of $\hat{X}$ are utilized to obtain the probabilities $p_k = \langle e_v^k|\rho|e_v^k\rangle$, $k = 1, 2, \ldots, 6$ and probabilities arising from eigenvectors corresponding to degenerate eigenvalues are added together. So one ends up with four resultant probabilities which are used in the Tsallis or Shannon entropies. Similarly for $\hat{Y}$ and $\hat{Z}$ two of the eigenvalues are two-fold degenerate. However, neither the Shannon nor the Tsallis entropic criteria detect entanglement for these states. Another family of states was thus constructed

$$\rho = p \cdot \frac{1}{2}\Big(|2,2\rangle - |2,-2\rangle\Big)\Big(\langle 2,2| - \langle 2,-2|\Big) + \frac{1-p}{6}\,\mathbb{I}, \tag{4.69}$$

where $\frac{1}{\sqrt{2}}(|2,2\rangle - |2,-2\rangle)$ is maximally entangled and is a common eigenvector of $\hat{X}$, $\hat{Y}$ and $\hat{Z}$. Evaluating the concurrence shows that the state is entangled for $0.4 < p \leq 1$. The values of p from which onward the criteria detect entanglement are given in Figure 4.4. These values are obtained by setting

$$\begin{aligned} H_q^{(T)}[S_x \otimes S_x]_\rho + H_q^{(T)}[S_y \otimes S_y]_\rho &= H_{xy}(q) \\ H_q^{(T)}[S_x \otimes S_x]_\rho + H_q^{(T)}[S_y \otimes S_y]_\rho + H_q^{(T)}[S_z \otimes S_z]_\rho &= H_{xyz}(q) \end{aligned} \tag{4.70}$$

for the values of q for which the minima $H_{xy}(q)$, $H_{xyz}(q)$ were obtained, and solving for p. This gives the minimal value of p for which entanglement is detected. Thus for q between 2.5 and 2.9 the greatest range of entanglement is detected.

Next we are going to formulate another family of separability criteria for systems of two fermions. These criteria are based upon either Tsallis or Rényi entropies, and are similar to the ones proposed by Gühne and Lewenstein [141] for bipartite systems comprising distinguishable subsystems.

Lets consider the non-degenerate observable M

$$M = \sum_{i=1}^{6} \mu_i |\psi_i\rangle\langle\psi_i|, \tag{4.71}$$

with the $|\psi_i\rangle$'s being the states in eq. (4.35) with $a = 1/\sqrt{2}$. When measuring M on a separable state $|\psi_{sl}\rangle$ (that is, a state of Slater rank 1) the maximum possible value of the probability $|\langle\psi_{sl}|\psi_i\rangle|^2$ of obtaining a given eigenvalue of M is $\frac{1}{2}$. Due to concavity of the Tsallis entropy, the minimum possible value of $H_q^{(T)}(M)_{|\psi_{sl}\rangle}$ is then attained when two of these probabilities are equal to $\frac{1}{2}$ and the other four probabilities are zero, since then the probability distribution is as peaked as possible. Therefore (for $q > 1$) we have that any separable state ρ (pure or mixed) complies with

$$H_q^{(T)}(M)_\rho \geq \frac{1 - 2^{1-q}}{q-1}. \tag{4.72}$$

This inequality provides an entanglement criterion since any state violating this inequality is necessarily entangled. For $q = 2$ this criterion turns out to be equivalent to the one considered in Subsection 4.1.3, which is formulated in terms of

the variances of projector operators (an equivalent situation occurs in the case of distinguishable subsystems [141]).

Since the Rényi entropy is a monotonic function of the Tsallis entropy, see eq. (1.11), this bound reads

$$H_q^{(R)}(M)_\rho \geq \ln 2 \tag{4.73}$$

and the criterion gets stronger as q increases. For $q \to \infty$ the Rényi entropy becomes very simple, namely $H_\infty^{(R)}(M)_\rho = -\ln(\max\{p \in \mathcal{P}(M)_\rho\})$, where $\mathcal{P}(M)_\rho$ is the probability distribution associated with the measurement of the observable M.

To have an idea of the power of this criterion, we apply it to the states given by (4.28). The expression for the Tsallis entropy is then

$$H_q^{(T)}(M)_\rho = \frac{6^{-q}\Big(6^q - 5(1-p)^q - (1+5p)^q\Big)}{q-1}. \tag{4.74}$$

However, it is more useful to use the Rényi entropy as the violations of (4.72) become smaller and smaller as q increases until it becomes impossible to say clearly whether the inequality (4.72) is violated or not due to finite accuracy. Table 4.1 shows the minimal p from which onwards entanglement is detected for various values of q. The limit $q \to \infty$ gives the best result, namely entanglement detection for $p > 0.4$ (thus all the entangled states in the family (4.28) are detected) and the violation of the inequality (4.73) as a function of p is very clear.

Table 4.1: Minimal values of p for which entanglement is detected in eq. (4.28).

q	2	4	6	8	10	20	50	∞
min p	0.632	0.513	0.473	0.454	0.443	0.421	0.408	0.4

For the family of states (4.30) the limit $q \to \infty$ gives entanglement detection for $p > 0.5$, so entanglement is detected within the total range of p-values

corresponding to entangled states.

4.1.5 Conclusions

I derived a separability criterion for states (pure or mixed) of two fermions with a single-particle Hilbert space of dimension four ($s = \frac{3}{2}$) based on the violation of local uncertainty relations. The violation of these relations provides a means of entanglement detection and also a quantitative indicator of entanglement. Then we developed separability criteria for fermion systems using sums of variances of appropriate projector operators. We implemented this type of criterion for two-fermions systems with four-dimensional ($s = \frac{3}{2}$) and six-dimensional ($s = \frac{5}{2}$) single-particle Hilbert spaces, and for systems of three identical fermions with a six-dimensional single-particle Hilbert space. In the latter two instances no analytical, closed expression for the concurrence, nor a necessary and sufficient separability criterion exists. Therefore, the present criteria for entanglement detection provide in these cases a valuable tool for the identification of families of entangled mixed states. The violation of entropic uncertainty relations was then investigated as a means of entanglement detection. Criteria were established using the Shannon, Tsallis and Rényi entropies. I also provided illustrations of families of entangled states that are detected by our separability criteria.

4.2 Entropic Entanglement Criteria for Fermion Systems

Entanglement criteria for general (pure or mixed) states of systems consisting of two identical fermions are introduced. These criteria are based on appropriate inequalities involving the entropy of the global density matrix describing the total system, on the one hand, and the entropy of the one-particle reduced density matrix, on the other hand. A majorization-related relation between these two density matrices is obtained, leading to a family of entanglement criteria based on Rényi's entropic measure. These criteria are applied to various illustrative examples of parameterized families of mixed states. The dependence of the entanglement detection efficiency on Rényi's entropic parameter is investigated. The extension of these criteria to systems of N identical fermions is also considered.

This Section is based on the publication [131] "Entropic Entanglement Criteria for Fermion Systems", C. Zander, A.R. Plastino, M. Casas and A. Plastino, *Eur. Phys. J. D* **66**, (2012) 14 and is organized as follows. The development of entropic separability criteria is placed into context in Subsection 4.2.1. A brief review of entanglement between particles in systems of identical fermions is given in Subsection 4.2.2. Entropic entanglement criteria for systems of two identical fermions based on the von Neumann, the linear, and the Rényi entropies are derived in Subsection 4.2.3. These entropic criteria are applied to particular families of states of two-fermion systems in Subsections 4.2.4 and 4.2.5. The extension to systems of N fermions of the entanglement criteria based upon the Rényi entropies is considered in Subsection 4.2.6. Finally, some conclusions are drawn in Subsection 4.2.7.

4.2.1 Entropic criteria and the separability problem

The problem of determining whether a given quantum state ρ is separable or entangled is known as "the separability problem". It constitutes one of the most fundamental problems in the theory of quantum entanglement and is the subject of a sustained and intense research activity (see [67, 142, 186–191] and references

therein). Besides its intrinsic interest, the development of separability criteria also leads to useful quantitative entanglement indicators: the degree to which a separability criterion is violated constitutes in itself a valuable quantitative indicator of entanglement. For instance, the well-known negativity measure of entanglement (which is one of the most used practical measures of entanglement for mixed states of systems with distinguishable subsystems) is based upon the celebrated Peres' separability criterion [67], see Subsection 2.1.4.

Entropic separability criteria have played a distinguished role in the study of the entanglement-related features of mixed states of multipartite systems constituted by distinguishable subsystems [67, 186–191]. For this kind of composite quantum system, non-entangled states behave classically in the sense that the entropy of a subsystem is always less or equal than the entropy of the whole system. If the entropy of a subsystem happens to be larger than the entropy of the whole system, then we know for sure that the state is entangled (that is, this constitutes a sufficient entanglement criterion). This statement can be formulated mathematically in terms of the Rényi entropic measures,

$$S_q^{(R)}[\rho] = \frac{1}{1-q} \ln(\mathrm{Tr}[\rho^q]), \tag{4.75}$$

leading to the following family of inequalities satisfied by separable states [67, 186–191],

$$\begin{aligned} S_q^{(R)}[\rho_A] &\leq S_q^{(R)}[\rho_{AB}] \\ S_q^{(R)}[\rho_B] &\leq S_q^{(R)}[\rho_{AB}]. \end{aligned} \tag{4.76}$$

In the above equations ρ_{AB} is the joint density matrix describing a bipartite system consisting of the subsystems A and B, and $\rho_{A,B}$ are the marginal density matrices describing the subsystems. The entropic parameter in (4.75) and (4.76) adopts values $q \geq 1$. In the limit $q \to 1$ the Rényi entropy reduces to the von Neumann entropy. Note that the entropic criteria considered in [67, 186–191] and in the present work, which depend on the entropies of the total and reduced density matrices, are different from those studied in [141, 142], which involve entropic uncertainty relations associated with the measurement of particular observables.

The study of entropic entanglement criteria based upon the above considerations has been the focus of a considerable amount of research over the years [67, 186–191]. It would be interesting to extend this approach to systems consisting of identical fermions. The aim of the present work is to investigate entanglement criteria for general (mixed) states of systems of two identical fermions based upon the comparison of the entropy of the global density matrix describing the total system and the entropy of the one-particle reduced density matrix.

4.2.2 Entanglement between particles in fermionic systems

As already explained in Section 2.5, the concept of entanglement between particles in a system of identical fermions is associated with the quantum correlations exhibited by quantum states on top of the minimal correlations due to the indistinguishability of the particles and the antisymmetric character of fermionic states. A pure state of N identical fermions that has Slater rank 1 (that is, a state that can be described by one single Slater determinant) must be regarded as separable (non-entangled) [108, 132]. The correlations exhibited by such states do not provide a resource for implementing non-classical information transmission or information processing tasks. Moreover, the non-entangled character of states of Slater rank 1 is consistent with the possibility of assigning complete sets of properties to the parts of the composite system [133]. Consequently, a pure state of two identical fermions of the form

$$|\psi_{sl}\rangle = \frac{1}{\sqrt{2}}\Big\{|\phi_1\rangle|\phi_2\rangle - |\phi_2\rangle|\phi_1\rangle\Big\}, \tag{4.77}$$

where $|\phi_1\rangle$ and $|\phi_2\rangle$ are orthonormal single-particle states, is regarded as separable.

A pure state $|\psi\rangle$ of a system of N identical fermions has Slater rank 1, and is therefore separable, if and only if

$$\mathrm{Tr}(\rho_1^2) = \frac{1}{N}, \tag{4.78}$$

where $\rho_1 = \mathrm{Tr}_{2,\ldots,N}(\rho)$ is the single-particle reduced density matrix, $\rho = |\psi\rangle\langle\psi|$, n is the dimension of the single-particle state space and $N \leq n$ [135]. On the other hand, entangled pure states satisfy

$$\frac{1}{n} \leq \mathrm{Tr}(\rho_1^2) < \frac{1}{N}. \tag{4.79}$$

It is interesting that this relation can be re-cast under the guise of an entropic inequality involving the linear entropy (2.15),

$$\frac{n-1}{n} \geq S_L(\rho_1) > \frac{N-1}{N}. \tag{4.80}$$

In fact, the quantity $S_L(\rho_1) - \frac{N-1}{N}$ constitutes a useful measure of entanglement, especially in the case of systems of two fermions [124–126]. This suggests that entropic inequalities may lead to useful entanglement criteria (and entanglement indicators) also in the case of mixed fermionic states. As we are going to see in this Section, this is indeed the case.

Non-entangled mixed states of systems of N identical fermions are those that can be written as a mixture of Slater determinants,

$$\rho_{sl} = \sum_i \lambda_i |\psi_{sl}^{(i)}\rangle\langle\psi_{sl}^{(i)}|, \tag{4.81}$$

where the states $|\psi_{sl}^{(i)}\rangle$ can be expressed as single Slater determinants, and $0 \leq \lambda_i \leq 1$ with $\sum_i \lambda_i = 1$.

As has been discussed in Subsection 2.5.1, systems of identical fermions with a single-particle Hilbert space of dimension $2k$ (with $k \geq 2$) can be formally regarded as systems consisting of spin-s particles, with $s = (2k-1)/2$. The members $\{|i\rangle,\ i = 1, \ldots, 2k\}$ of an orthonormal basis of the single-particle Hilbert space can be identified with the states $|s, m_s\rangle$, with $m_s = s - i + 1,\ i = 1, \ldots, 2k$. We can use for these states the shorthand notation $\{|m_s\rangle,\ m_s = -s, \ldots, s\}$, because each particular example discussed here will correspond to a given value of k (and s). According to this angular momentum representation, the antisymmetric joint eigenstates $\{|j, m\rangle,\ -j \leq m \leq j,\ 0 \leq j \leq 2s\}$ of the total angular momentum

operators J^2 and J_z constitute a basis for the Hilbert space associated with a system of two identical fermions. The antisymmetric states $|j, m\rangle$ are those with an even value of the quantum number j.

A closed analytical expression for the concurrence of general (pure or mixed) states of two identical fermions sharing a single-particle Hilbert space of dimension four (corresponding to $s = 3/2$) was discovered by Eckert, Schliemann, Bruss, and Lewenstein (ESBL) in [132]. The ESBL concurrence formula is given in Subsection 2.5.1, eq. (2.73).

In what follows we are going to consider systems comprising a given, fixed number of identical fermions. Therefore, we are going to work within the first quantization formalism.

4.2.3 Entropic entanglement criteria for systems of two identical fermions

In this Subsection I am going to derive the main results of the present Section. We shall advance new entropic criteria for mixed states of systems constituted by identical fermions. In Subsubsection 4.2.3.1 we derive entropic criteria for mixed states of two fermions (based on inequality (4.84)) and N fermions (based on inequality (4.86)) formulated in terms of the von Neumann entropy, and an entropic criterion for two fermions based upon the linear entropy. In Subsubsection 4.2.3.2 we introduce a full family of entropic criteria based on the Rényi entropy.

4.2.3.1 Entanglement criteria based on the von Neumann and the linear entropies

Let ρ be a density matrix describing a quantum state of two identical fermions and ρ_r be the corresponding single-particle reduced density matrix, obtained by computing the partial trace over one of the two particles.

If $\rho = |\psi_{sl}\rangle\langle\psi_{sl}|$, where $|\psi_{sl}\rangle$ represents a separable pure state of the form (4.77), and

$$S_{\mathrm{vN}}[\rho] = -\mathrm{Tr}(\rho \ln \rho) \tag{4.82}$$

is the von Neumann entropy of ρ, we have that $S_{\rm vN}[\rho] = 0$ and $S_{\rm vN}[\rho_r] = \ln 2$, since $\rho_r = \frac{1}{2}(|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|)$. That is, for separable pure states we have $S_{\rm vN}[\rho] - S_{\rm vN}[\rho_r] = -\ln 2$. It then follows from the concavity property of the quantum conditional entropy [137] that, for a separable mixed state ρ_{sl} of the form (4.81), $S_{\rm vN}[\rho_{sl}] - S_{\rm vN}[\rho_r] \geq -\ln 2$. To see this, let $\rho^{(i)} = |\psi_{sl}^{(i)}\rangle\langle\psi_{sl}^{(i)}|$ and $\rho_r^{(i)}$ be the corresponding reduced density matrix. Then $S_{\rm vN}[\rho^{(i)}] - S_{\rm vN}[\rho_r^{(i)}] = -\ln 2$ and the reduced density matrix of ρ_{sl} in eq. (4.81) is $\rho_r = \sum_i p_i \rho_r^{(i)}$. The quantum conditional entropy is then

$$\begin{aligned} S_{\rm vN}[\rho_r|\rho_r] &= S_{\rm vN}[\rho_{sl}] - S_{\rm vN}[\rho_r] \\ &\geq \sum_i p_i \left\{ S_{\rm vN}[\rho^{(i)}] - S_{\rm vN}[\rho_r^{(i)}] \right\} \\ &= \sum_i p_i(-\ln 2) = -\ln 2, \end{aligned} \tag{4.83}$$

where the inequality follows from the conditional entropy being concave in ρ_{sl} [137]. Consequently, all separable states (pure or mixed) of a system of two identical fermions satisfy the inequality

$$S_{\rm vN}[\rho_r] \leq S_{\rm vN}[\rho_{sl}] + \ln 2, \tag{4.84}$$

where ρ_r is the single-particle reduced density matrix.

Hence, if the quantity

$$D_{\rm vN} = S_{\rm vN}[\rho_r] - S_{\rm vN}[\rho] - \ln 2 \tag{4.85}$$

is positive the state ρ is necessarily entangled. Indeed, in the particular case of pure states this quantity has been used as a measure of entanglement in some applications (see, for instance, [185] and references therein).

The argument leading to inequality (4.84) can be extended to the more general case of systems of N identical fermions. A separable pure state $\rho = |\psi_{sl}\rangle\langle\psi_{sl}|$ of N identical fermions (that is, a pure state expressible as a single Slater determinant) satisfies $S_{\rm vN}[\rho] = 0$ and $S_{\rm vN}[\rho_r] = \ln N$. To see the latter, we notice that the Slater determinant $|\psi_{sl}\rangle$ consists of $N!$ permutation terms and so the single-particle

reduced density matrix is then $\rho_r = \frac{1}{N}(|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2| + \ldots + |\phi_N\rangle\langle\phi_N|)$. Hence $S_{\rm vN}[\rho_r] = -N[\frac{1}{N}\ln(\frac{1}{N})] = \ln N$. Therefore, for this kind of state we have $S_{\rm vN}[\rho] - S_{\rm vN}[\rho_r] = -\ln N$. The concavity property of the quantum conditional entropy then implies that for a separable mixed state ρ of N fermions having the form (4.81) we have $S_{\rm vN}[\rho] - S_{\rm vN}[\rho_r] \geq -\ln N$. Consequently, a separable mixed state of N fermions (that is, a state that can be written as a statistical mixture of pure states each having the form of a single Slater determinant) satisfies the inequality

$$S_{\rm vN}[\rho_r] \leq S_{\rm vN}[\rho] + \ln N. \tag{4.86}$$

Consequently, a state of N fermions violating inequality (4.86) is necessarily entangled. In the case of pure states of N fermions this entanglement criterion reduces to one of the entanglement criteria previously discussed in [135]. The special case of this criterion corresponding to pure states of two fermions was first analyzed in [133]. That is, our present result (4.86) constitutes a generalization to arbitrary mixed states of an inequality that has been previously known and shown to be useful for the study of fermionic entanglement in the special case of pure states. When deriving the inequalities (4.84) and (4.86) we have used the concavity of the quantum conditional entropy. This property is usually discussed in connection with composite systems comprising distinguishable subsystems. However, within the first quantization formalism, any density matrix of two identical fermions has mathematically also the form of a density matrix describing distinguishable subsystems (in fact, it is just a density matrix that happens to be expressible as a statistical mixture of antisymmetric pure states). Consequently, any mathematical property that is satisfied by general density matrices describing distinguishable subsystems is also satisfied by the special subset of density matrices that can describe a system of identical fermions.

An entanglement criterion for states of two fermions which is similar to the previous one involving the von Neumann entropy, can be formulated in terms of the linear entropy (2.15),

$$S_L[\rho] = 1 - {\rm Tr}(\rho^2). \tag{4.87}$$

Given a quantum state ρ of two fermions, lets consider the concurrence-like quan-

tity

$$c[\rho] \;=\; \inf \sum_i p_i c[|\phi_i\rangle], \tag{4.88}$$

where $c[|\phi_i\rangle] = \sqrt{2\left[1 - \mathrm{Tr}\left[(\rho_r^{(i)})^2\right]\right]}$, $\rho_r^{(i)}$ is the one-particle reduced density matrix corresponding to $|\phi_i\rangle$, $\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i|$, and the infimum is taken over all the possible decompositions of ρ as a statistical mixture $\{p_i, |\phi_i\rangle\}$ of pure states (note that $c[\rho]$ adopts values in the range $[0, \sqrt{2}]$). The quantity defined in (4.88) satisfies the inequality [198]

$$c[\rho]^2 \;\geq\; 2\left[\mathrm{Tr}(\rho^2) - \mathrm{Tr}\left(\rho_r^2\right)\right]. \tag{4.89}$$

If ρ corresponds to a separable state of the two fermions, we have that $\rho = \sum_i p_i |\psi_{sl}^{(i)}\rangle\langle\psi_{sl}^{(i)}|$ with $c[|\psi_{sl}^{(i)}\rangle] = 1$ for all i, since $(\rho_r^{(i)})^2 = \frac{1}{4}(|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|)$ and so $\mathrm{Tr}[(\rho_r^{(i)})^2] = \frac{1}{2}$. Therefore, for a separable state we have from (4.88) that $c[\rho] \leq 1$ and combining this with (4.89), gives $1 \geq c\,[\rho]^2 \geq 2\,[\mathrm{Tr}(\rho^2) - \mathrm{Tr}\,(\rho_r^2)]$. Hence

$$\begin{aligned} \tfrac{1}{2} \;&\geq\; \left\{1 - \mathrm{Tr}\left(\rho_r^2\right)\right\} - \left\{1 - \mathrm{Tr}\left(\rho^2\right)\right\} \\ \Rightarrow \quad \tfrac{1}{2} \;&\geq\; S_L[\rho_r] - S_L[\rho]. \end{aligned} \tag{4.90}$$

Consequently, separable states (pure or mixed) of a system of two identical fermions comply with the inequality,

$$S_L[\rho_r] \leq S_L[\rho] + \frac{1}{2}. \tag{4.91}$$

In other words, states for which the quantity

$$D_L = S_L[\rho_r] - S_L[\rho] - \frac{1}{2} \tag{4.92}$$

is positive are necessarily entangled. In the particular case of pure states of two identical fermions, the positivity of (4.92) becomes both a necessary and sufficient entanglement criterion (see [135] and references therein). That is, for a pure state $\mathrm{Tr}(\rho^2) = 1$ and so the pure state is entangled when $\mathrm{Tr}(\rho_r^2) < \frac{1}{2}$, which corresponds to eq. (4.79) for $N = 2$. Moreover, a quantity basically equal to (4.92) has been

proposed as an entanglement measure for pure states of two fermions and indeed constitutes one of the most useful entanglement measures for these states [126].

4.2.3.2 Entropic entanglement criteria based on the Rényi entropies

On the basis of the Rényi family of entropies we are going to derive now a generalization of the separability criterion associated with inequality (4.84). We are going to prove that a (possibly mixed) quantum state ρ of a system of two identical fermions satisfying the inequality

$$S_q^{(R)}[\rho] + \ln 2 < S_q^{(R)}[\rho_r], \tag{4.93}$$

for some $q \geq 1$, is necessarily entangled. Here $S_q^{(R)}$ stands for the Rényi entropy,

$$S_q^{(R)}[\rho] = \frac{1}{1-q} \ln(\mathrm{Tr}[\rho^q]). \tag{4.94}$$

The inequality (4.93) leads to an entropic entanglement criterion that detects entanglement whenever the quantity

$$R_q = S_q^{(R)}[\rho_r] - S_q^{(R)}[\rho] - \ln 2 \tag{4.95}$$

is strictly positive. In the limit $q \to 1$ the Rényi measure reduces to the von Neumann entropy and we recover the entanglement criterion given by inequality (4.84). When $q \to \infty$ the Rényi entropy becomes

$$S_\infty^{(R)}[\rho] = -\ln\left(\lambda_{\max}^{(\rho)}\right), \tag{4.96}$$

where $\lambda_{\max}^{(\rho)}$ is the largest eigenvalue of ρ. In this limit case, the entropic criterion says that any state satisfying

$$\begin{aligned} -\ln\left(\lambda_{\max}^{(\rho_r)}\right) + \ln\left(\lambda_{\max}^{(\rho)}\right) - \ln 2 > 0 \\ \Rightarrow \quad \ln\left(\lambda_{\max}^{(\rho)}\right) > \ln\left(2\lambda_{\max}^{(\rho_r)}\right) \\ \Rightarrow \quad 2\,\lambda_{\max}^{(\rho_r)} < \lambda_{\max}^{(\rho)} \end{aligned} \tag{4.97}$$

is entangled, where $\lambda_{\max}^{(\rho)}$ and $\lambda_{\max}^{(\rho_r)}$ are, respectively, the largest eigenvalues of ρ and ρ_r.

4.2.3.3 Proof of the entropic criteria based on the Rényi entropies

The following proof is based on the powerful techniques related to the majorization concept [136, 138] that were introduced to the field of quantum entanglement by Nielsen and Kempe in [136]. These authors proved that non-entangled states of quantum systems having distinguishable subsystems are such that the total density matrix is always majorized by the marginal density matrix associated with one of the subsystems, see Subsection 2.6.1 for details of their proof. In the case of non-entangled states of a system of identical fermions the total density matrix ρ is not necessarily majorized by the one-particle reduced density matrix ρ_r. However, as we are going to prove, *there is still a definite majorization-related relation between ρ and ρ_r that yields a family of inequalities between the Rényi entropies of these two matrices, which leads in turn to a family of entropic entanglement criteria.*

In our proof of the entropic criterion associated with the inequality (4.93) we are going to use the fundamental property of quantum statistical mixtures discussed in Subsection 1.1.6, eq. (1.27). If $\rho = \sum_i p_i |a_i\rangle\langle a_i| = \sum_j q_j |b_j\rangle\langle b_j|$ are two statistical mixtures representing the same density matrix ρ, then there exists a unitary matrix $\{U_{ij}\}$ such that [7, 136]

$$\sqrt{p_i}|a_i\rangle = \sum_j U_{ij}\sqrt{q_j}|b_j\rangle. \tag{4.98}$$

The other property utilized is majorization, which is reviewed in Subsection 2.6.1. Given two probability distributions $\{p_i\}$ and $\{q_k\}$ such that $p_i = \sum_k M_{ik} q_k$, where the matrix $\{M_{ik}\}$ is doubly stochastic: $\sum_i M_{ik} = \sum_k M_{ik} = 1$ and each element is real and $M_{ik} \geq 0$. Then the probability $\{p_i\}$ is said to be more "mixed" than the probability $\{q_k\}$. Alternatively $\{q_k\}$ is said to "majorize" $\{p_i\}$ and

$$S_q^{(R)}[p_i] \geq S_q^{(R)}[q_k]. \tag{4.99}$$

The two probability distributions need not have the same number of events and

consequently the matrix M_{ik} does not have to be a square matrix [7, 199].

Let us now consider a separable state of two identical fermions,

$$\rho = \sum_j \frac{p_j}{2}\Big(|\psi_1^{(j)}\rangle|\psi_2^{(j)}\rangle - |\psi_2^{(j)}\rangle|\psi_1^{(j)}\rangle\Big)\Big(\langle\psi_1^{(j)}|\langle\psi_2^{(j)}| - \langle\psi_2^{(j)}|\langle\psi_1^{(j)}|\Big) \tag{4.100}$$

where $0 \leq p_j \leq 1$, $\sum_j p_j = 1$ and $|\psi_1^{(j)}\rangle$, $|\psi_2^{(j)}\rangle$ are normalized single-particle states with $\langle\psi_1^{(j)}|\psi_2^{(j)}\rangle = 0$. Equation (4.100) represents the standard definition of a non-entangled mixed state of two identical fermions. Notice that in (4.100) no special relation between states $|\psi_i^{(j)}\rangle$ with different values of the label j is assumed. In particular, the overlap between two states with different labels j is not necessarily equal to 0 or 1. This, in turn, means that the overlap between two different members of the family of (separable) two-fermion pure states participating in the statistical mixture leading to (4.100) may be non-zero.

Let us consider now a spectral representation

$$\rho = \sum_k \lambda_k |e_k\rangle\langle e_k| \tag{4.101}$$

of ρ. That is, the $|e_k\rangle$ constitute an orthonormal basis of eigenvectors of ρ and the λ_k are the corresponding eigenvalues. Then, (4.100) and (4.101) are two different representations of ρ as a mixture of pure states. Therefore, there is a unitary matrix U with matrix elements $\{U_{kj}\}$ such that

$$\sqrt{\lambda_k}|e_k\rangle = \sum_j U_{kj}\sqrt{\frac{p_j}{2}}\Big(|\psi_1^{(j)}\rangle|\psi_2^{(j)}\rangle - |\psi_2^{(j)}\rangle|\psi_1^{(j)}\rangle\Big). \tag{4.102}$$

The single-particle reduced density matrix corresponding to the two-fermion density matrix (4.100) is

$$\rho_r = \sum_j \frac{p_j}{2}\Big(|\psi_1^{(j)}\rangle\langle\psi_1^{(j)}| + |\psi_2^{(j)}\rangle\langle\psi_2^{(j)}|\Big), \tag{4.103}$$

admitting a spectral representation

$$\rho_r = \sum_l \alpha_l |f_l\rangle\langle f_l|. \tag{4.104}$$

We now define,

$$q_{2j} = q_{2j-1} = \frac{1}{2}p_j \qquad (j = 1, 2, 3, \ldots) \tag{4.105}$$

$$|\phi_{2j-1}\rangle = |\psi_1^{(j)}\rangle$$

$$|\phi_{2j}\rangle = |\psi_2^{(j)}\rangle \qquad (j = 1, 2, 3, \ldots). \tag{4.106}$$

Now, since (4.103) and (4.104) correspond to two statistical mixtures yielding the same density matrix, there must exist a unitary matrix W with matrix elements $\{W_{il}\}$ such that,

$$\sqrt{q_i}|\phi_i\rangle = \sum_l W_{il}\sqrt{\alpha_l}|f_l\rangle \qquad (i = 1, 2, 3, \ldots). \tag{4.107}$$

Now, eq. (4.102) can be rewritten as

$$\sqrt{\lambda_k}|e_k\rangle = \sum_j U_{kj}\Big(\sqrt{q_{2j-1}}|\phi_{2j-1}\rangle|\phi_{2j}\rangle - \sqrt{q_{2j}}|\phi_{2j}\rangle|\phi_{2j-1}\rangle\Big). \tag{4.108}$$

Combining (4.107) and (4.108) gives

$$\begin{aligned}\sqrt{\lambda_k}|e_k\rangle &= \sum_j U_{kj}\left[\sum_l \Big(W_{2j-1,l}|\phi_{2j}\rangle - W_{2j,l}|\phi_{2j-1}\rangle\Big)\sqrt{\alpha_l}|f_l\rangle\right] \\ &= \sum_l \left[\sum_j U_{kj}\Big(W_{2j-1,l}|\phi_{2j}\rangle - W_{2j,l}|\phi_{2j-1}\rangle\Big)\right]\sqrt{\alpha_l}|f_l\rangle. \end{aligned} \tag{4.109}$$

Therefore, since $\langle e_k|e_{k'}\rangle = \delta_{kk'}$ and $\langle f_l|f_{l'}\rangle = \delta_{ll'}$, we have that

$$\begin{aligned}\lambda_k = \sum_l \Bigg[&\left(\sum_{j'} U^*_{kj'}\Big\{W^*_{2j'-1,l}\langle\phi_{2j'}| - W^*_{2j',l}\langle\phi_{2j'-1}|\Big\}\right)\times \\ &\left(\sum_{j''} U_{kj''}\Big\{W_{2j''-1,l}|\phi_{2j''}\rangle - W_{2j'',l}|\phi_{2j''-1}\rangle\Big\}\right)\Bigg]\alpha_l. \end{aligned} \tag{4.110}$$

From (4.110) it follows that we can write

$$\lambda_k = \sum_l M_{kl}\alpha_l, \tag{4.111}$$

where

$$\begin{aligned} M_{kl} \;=\; & \left(\sum_{j'} U^*_{kj'}\Big\{W^*_{2j'-1,l}\langle\phi_{2j'}| - W^*_{2j',l}\langle\phi_{2j'-1}|\Big\}\right)\times \\ & \left(\sum_{j''} U_{kj''}\Big\{W_{2j''-1,l}|\phi_{2j''}\rangle - W_{2j'',l}|\phi_{2j''-1}\rangle\Big\}\right). \end{aligned} \tag{4.112}$$

We now investigate the properties of the matrix M with matrix elements $\{M_{kl}\}$. First of all, we have

$$M_{kl} \geq 0, \tag{4.113}$$

since the matrix elements of M are of the form $M_{kl} = \langle\Sigma|\Sigma\rangle$, with

$$|\Sigma\rangle = \sum_j U_{kj}\Big(W_{2j-1,l}|\phi_{2j}\rangle - W_{2j,l}|\phi_{2j-1}\rangle\Big). \tag{4.114}$$

We now consider the sum of the elements within a given row or column of M. The sum of a row yields,

$$\begin{aligned} \sum_k M_{kl} &= \sum_{j'j''}\left[\sum_k U^*_{kj'}U_{kj''}\right]\begin{pmatrix}\text{depends on}\\ j'\end{pmatrix}\begin{pmatrix}\text{depends on}\\ j''\end{pmatrix} \\ &= \sum_{j'j''}\left[\sum_k U^\dagger_{j'k}U_{kj''}\right]\begin{pmatrix}\text{depends on}\\ j'\end{pmatrix}\begin{pmatrix}\text{depends on}\\ j''\end{pmatrix} \\ &= \sum_{j'j''}\delta_{j'j''}\Big(W^*_{2j'-1,l}\langle\phi_{2j'}| - W^*_{2j',l}\langle\phi_{2j'-1}|\Big)\Big(W_{2j''-1,l}|\phi_{2j''}\rangle - W_{2j'',l}|\phi_{2j''-1}\rangle\Big) \\ &= \sum_j\Big(W^*_{2j-1,l}W_{2j-1,l} + W^*_{2j,l}W_{2j,l}\Big) = \sum_i \left(W^\dagger\right)_{li}W_{il} = 1, \end{aligned} \tag{4.115}$$

while the sum of a column is,

$$\sum_l M_{kl} \;=\; \sum_{j'j''} U^*_{kj'}U_{kj''}\left(\langle\phi_{2j'}|\phi_{2j''}\rangle\left[\sum_l W^*_{2j'-1,l}W_{2j''-1,l}\right] + \right.$$

$$\begin{aligned}
&\langle\phi_{2j'-1}|\phi_{2j''-1}\rangle\left[\sum_l W^*_{2j',l}W_{2j'',l}\right] - \langle\phi_{2j'}|\phi_{2j''-1}\rangle\left[\sum_l W^*_{2j'-1,l}W_{2j'',l}\right] - \\
&\langle\phi_{2j'-1}|\phi_{2j''}\rangle\left[\sum_l W^*_{2j',l}W_{2j''-1,l}\right]\Bigg) \\
&= \sum_{j'j''} U^*_{kj'}U_{kj''}\Big(\langle\phi_{2j'}|\phi_{2j''}\rangle\delta_{j'j''} + \langle\phi_{2j'-1}|\phi_{2j''-1}\rangle\delta_{j'j''}\Big) \\
&= 2\sum_j U^*_{kj}U_{kj} = 2\sum_j \left(U^\dagger\right)_{jk} U_{kj} = 2. \qquad (4.116)
\end{aligned}$$

When deriving the above two equations (4.115) and (4.116) we made use of the unitarity of the matrices $\{U_{kj}\}$ and $\{W_{il}\}$. Summing up, we have,

$$\begin{aligned}
\sum_k M_{kl} &= 1 \\
\sum_l M_{kl} &= 2. \qquad (4.117)
\end{aligned}$$

We now define a new set of variables $\{\lambda'_n\}$ and a new matrix M' with elements M'_{nl}, respectively given by,

$$\lambda'_{2k-1} = \lambda'_{2k} = \frac{1}{2}\lambda_k \qquad (k = 1, 2, 3, \ldots) \qquad (4.118)$$

$$M'_{2k-1,l} = M'_{2k,l} = \frac{1}{2}M_{kl} \qquad (k = 1, 2, 3, \ldots), \qquad (4.119)$$

and so we have that eq. (4.111) can be expressed as

$$\lambda'_n = \sum_l M'_{nl}\alpha_l. \qquad (4.120)$$

By construction, then, we have

$$\begin{aligned}
\{\lambda_k\} &= \{\lambda_1, \lambda_2, \lambda_3, \ldots\} \\
\{\lambda'_n\} &= \left\{\frac{\lambda_1}{2}, \frac{\lambda_1}{2}, \frac{\lambda_2}{2}, \frac{\lambda_2}{2}, \frac{\lambda_3}{2}, \frac{\lambda_3}{2}, \ldots\right\}. \qquad (4.121)
\end{aligned}$$

Let us now compare the matrices $\{M_{kl}\}$ and $\{M'_{nl}\}$. The matrix $\{M'_{nl}\}$ has twice as many rows as $\{M_{kl}\}$, but the rows of $\{M'_{nl}\}$ can be grouped in pairs of consecutive rows such that within each pair the rows are equal to $1/2$ a row of

$\{M_{kl}\}$. It follows that

$$\begin{aligned} \sum_k M_{kl} = 1 \quad &\Longrightarrow \quad \sum_n M'_{nl} = 1 \\ \sum_l M_{kl} = 2 \quad &\Longrightarrow \quad \sum_l M'_{nl} = 1. \end{aligned} \tag{4.122}$$

Thus,

$$\sum_n M'_{nl} = \sum_l M'_{nl} = 1 \tag{4.123}$$

and, therefore, $\{M'_{nl}\}$ is a doubly stochastic matrix. Interpreting the λ'_n's and the α_l's as probabilities, it follows from (4.120) and (4.123) that the probability distribution $\{\lambda'_n\}$ is more "mixed" than the probability distribution $\{\alpha_l\}$ [137] (or, alternatively that $\{\alpha_l\}$ majorizes $\{\lambda'_n\}$ [136]). This, in turn, implies that for any Rényi entropy $S_q^{(R)}$ with $q \geq 1$, we have

$$S_q^{(R)}[\lambda'_n] \geq S_q^{(R)}[\alpha_l]. \tag{4.124}$$

Thus,

$$\begin{aligned} S_q^{(R)}[\lambda'_n] &= \frac{1}{1-q} \ln\left(2 \sum_k \left(\frac{\lambda_k}{2}\right)^q\right) = \frac{1}{1-q} \ln\left(2^{1-q} \sum_k \lambda_k^q\right) \\ &= \frac{1}{1-q} \left\{\ln\left(2^{1-q}\right) + \ln\left(\sum_k \lambda_k^q\right)\right\} \\ &= \ln 2 + \frac{1}{1-q} \ln\left(\sum_k \lambda_k^q\right) \\ &= \ln 2 + S_q^{(R)}[\lambda_k]. \end{aligned} \tag{4.125}$$

Therefore, all separable states of the two-fermion system comply with the inequality $S_q^{(R)}[\lambda_k] + \ln 2 \geq S_q^{(R)}[\alpha_l]$ and since $\{\lambda_k\}$ and $\{\alpha_l\}$ are the eigenvalues of ρ and ρ_r respectively,

$$S_q^{(R)}[\rho] + \ln 2 \geq S_q^{(R)}[\rho_r]. \tag{4.126}$$

The above inequality leads to an entanglement criterion that detects entanglement when the indicator R_q defined in equation (4.95) is strictly positive.

4.2.3.4 Connection with a quantitative measure of entanglement

As already mentioned in Subsection 4.2.1, the development of separability criteria often leads to useful entanglement indicators. In particular, when the separability criterion takes the form of an inequality, such that entanglement is detected when the inequality is not verified, the degree of violation of the inequality constitutes an entanglement indicator. In the case of the entropic indicators advanced in the present work, it is indeed a reasonable expectation that states with larger values of the indicators $D_{\rm vN}$ and R_q tend to be more entangled. In the next Subsection we shall illustrate this behaviour in the case of two-fermion systems with a single-particle Hilbert space of dimension four, where the exact amount of entanglement can be evaluated analytically.

Now we shall discuss two general aspects of the connection between the above-mentioned entanglement indicators and a quantitative measure of entanglement. First of all, it is worth emphasizing that in the case of pure states, the indicators $D_{\rm vN}$ and D_L themselves coincide (up to unessential multiplicative constants) with useful quantitative measures of entanglement for fermion systems that have already been applied to the study of fermionic entanglement. In particular, let us focus on the indicator $D_{\rm vN}$ of a two-fermion system, which is based on the von Neumann entropies of the total and single-particle density matrices, ρ and ρ_r. For a pure state $|\Phi\rangle$ of the two-fermion system we have $\rho = |\Phi\rangle\langle\Phi|$ and $S_{\rm vN}[\rho] = 0$. Consequently, in this case we have $D_{\rm vN} = S_{\rm vN}[\rho_r] - \ln 2$. As already mentioned, this quantity constitutes a quantitative entanglement measure for pure states,

$$\varepsilon[|\Phi\rangle] \;=\; S_{\rm vN}[\rho_r] - \ln 2. \tag{4.127}$$

The extension of this quantitative entanglement measure to mixed two-fermion states ρ is obtained via the standard convex roof construction,

$$\varepsilon[\rho] \;=\; \inf \sum_i p_i \, \varepsilon[|\Phi_i\rangle], \tag{4.128}$$

where the infimum is taken over all the possible mixtures $\{p_i, |\Phi_i\rangle\}$ of pure states $|\Phi_i\rangle$ (with weights p_i, $0 \leq p_i \leq 1$, $\sum_i p_i = 1$) generating the mixed state under consideration, $\rho = \sum_i p_i |\Phi_i\rangle\langle\Phi_i|$. Now, given a particular decomposition

$\rho = \sum_i p_i |\Phi_i\rangle\langle\Phi_i|$ of the two-fermion state ρ, let $\rho^{(i)} = |\Phi_i\rangle\langle\Phi_i|$ be the total density matrix corresponding to the pure state $|\Phi_i\rangle$ and $\rho_r^{(i)}$ be the corresponding single-particle reduced density matrix. Then, using the concavity property of the quantum conditional entropy (see Subsubsection 4.2.3.1) one obtains,

$$\begin{aligned} D_{\mathrm{vN}}[\rho] &= S_{\mathrm{vN}}[\rho_r] - S_{\mathrm{vN}}[\rho] - \ln 2 \\ &\leq \sum_i p_i \Big[S_{\mathrm{vN}}[\rho_r^{(i)}] - S_{\mathrm{vN}}[\rho^{(i)}] - \ln 2 \Big] \end{aligned} \tag{4.129}$$

which implies that

$$D_{\mathrm{vN}}[\rho] \leq \inf \sum_i p_i \Big[S_{\mathrm{vN}}[\rho_r^{(i)}] - S_{\mathrm{vN}}[\rho^{(i)}] - \ln 2 \Big] = \varepsilon[\rho], \tag{4.130}$$

which leads to an inequality directly linking the entropic indicator $D_{\mathrm{vN}}[\rho]$ with the quantitative entanglement measure $\varepsilon[\rho]$,

$$\varepsilon[\rho] \geq D_{\mathrm{vN}}[\rho]. \tag{4.131}$$

Summing up, the entropic indicator $D_{\mathrm{vN}}[\rho]$ provides a lower bound for the quantitative entanglement measure $\varepsilon[\rho]$. In the case of pure states of a systems of two fermions this lower bound is saturated and the inequality (4.131) becomes an equality.

4.2.4 Two-fermion systems with a single-particle Hilbert space of dimension four

In this Subsection and the next one we are going to illustrate our entanglement criteria by recourse to examples of fermion systems with a single-particle Hilbert space of low dimensionality. In this Subsection we are going to focus on systems of two fermions with a single-particle Hilbert space of dimension four. This case is of considerable relevance both from the conceptual and the practical points of view, and has been the subject of various recent research efforts [130, 132, 184]. It is the fermionic system of lowest dimensionality admitting the phenomenon of entanglement and it has profound physical and mathematical relationships with the celebrated two-qubit system of paramount importance in quantum informa-

tion science [132]. It is worth mentioning that, in spite of its low dimensionality, this system is of considerable complexity, its generic (mixed) state depending on 35 (real) parameters. This system can be realized when one has spin-$\frac{1}{2}$ particles confined by an external potential well such that, within the range of energies available in the experimental setting, there are only two relevant eigenfunctions, $\Psi_a(\mathbf{x})$ and $\Psi_b(\mathbf{x})$ [132] corresponding, for instance, to the ground and first excited states of the confining potential. In such a scenario, the relevant single-particle Hilbert space is spanned by the single-particle states $|\Psi_a, +\rangle$, $|\Psi_a, -\rangle$, $|\Psi_b, +\rangle$, $|\Psi_b, -\rangle$ (here we use standard, self-explanatory notation, the $\pm$ signs corresponding to the spin degree of freedom).

Now we are going to apply our entropic entanglement criteria derived in the previous Subsection to some parameterized families of states of two fermions with a single-particle Hilbert space of dimension four. In this case there is an exact, analytical expression for the state's concurrence C, see eq. (2.73). It is then possible to compare the range of parameters for which entanglement is detected by the criteria with the exact range of parameters for which the states under consideration are entangled. We also illustrate the fact that the quantities D_{vN}, D_L and R_q involved in the entanglement criteria advanced here can also be regarded as entanglement indicators, in the sense that states exhibiting large values of these quantities tend to have higher entanglement. Two-fermion states with a single-particle Hilbert space of dimension four allow for the illustration of this, because in the case of these systems we have a closed analytical expression for the amount of entanglement of mixed states,

$$\begin{aligned} E[\rho] &= h\left(\frac{1+\sqrt{1-C[\rho]^2}}{2}\right), \\ h(x) &= -x\log_2 x - (1-x)\log_2(1-x). \end{aligned} \tag{4.132}$$

As mentioned in Subsection 4.2.2, in this case the two-fermion states can be formally mapped onto the states of two $s = \frac{2}{3}$ spins. The antisymmetric eigenstates $|j, m\rangle$ of the total angular momentum operators J^2 and J_z constitute then a basis of the system's Hilbert space. These states are $|0, 0\rangle$, $|2, -2\rangle$, $|2, -1\rangle$, $|2, 0\rangle$, $|2, 1\rangle$ and $|2, 2\rangle$.

To have an idea of the efficiency of the criteria discussed in Subsubsections 4.2.3.1 and 4.2.3.2, we are going to analyze three families of states. The one family consists solely of pure states, whereas the other two comprise mixed states. In the case of distinguishable subsystems, the latter two families would be the Werner state [82] and a mixed state introduced by Gisin [200], which are different representative ways of mixing a maximally entangled state and separable states. The Werner state can be viewed as an impure singlet state, consisting of a mixture of a maximally entangled state and a maximally mixed state. The Gisin state mixes a maximally entangled state with a mixture of product states, which enables one to investigate the role of classical correlations of the product states. These two classes of states are then translated into their fermionic counterpart.

4.2.4.1 Werner-like states

First we are going to consider a family of states consisting of a mixture of the maximally entangled state $|0,0\rangle$ and a totally mixed state. These states are of the form

$$\rho_W = p|0,0\rangle\langle 0,0| + \frac{1-p}{6}\,\mathbb{I}, \tag{4.133}$$

where $0 \leq p \leq 1$, and

$$\mathbb{I} \;=\; |0,0\rangle\langle 0,0| + \sum_{m=-2}^{2} |2,m\rangle\langle 2,m| \tag{4.134}$$

is the identity operator acting on the six-dimensional Hilbert space corresponding to the two-fermion system. Evaluation of the concurrence shows that these states are entangled when $p > 0.4$. For these states, we have

$$\begin{aligned}
D_{\mathrm{vN}}[\rho_W] &= \ln 2 + \frac{5}{6}(1-p)\ln\left(\frac{1-p}{6}\right) + \frac{1}{6}(1+5p)\ln\left(\frac{1}{6}(1+5p)\right) \\
D_L[\rho_W] &= -\frac{7}{12} + \frac{5p^2}{6} \\
R_2[\rho_W] &= \ln\left(\frac{1+5p^2}{3}\right) \\
R_\infty[\rho_W] &= \ln\left(\frac{1+5p}{3}\right)
\end{aligned}$$

$$C[\rho_W] \;=\; \begin{cases} 0 & 0 \leq p \leq 0.4 \\ -\frac{2}{3} + \frac{5p}{3} & 0.4 \leq p \leq 1. \end{cases} \tag{4.135}$$

Figure 4.5(a) shows the entanglement measure (eq. (4.132)) and depicts when the entanglement indicators given in eq. (4.135) detect entanglement. The logarithms in the entanglement indicators are taken to the base 2 for comparison purposes.

The minimum values p_{min} of the parameter p such that for $p > p_{min}$ the entanglement indicators D_{vN}, D_L, R_2 and R_∞ are positive (and thus entanglement is detected by the corresponding criteria) are given in the following Table (that is, in each case, entanglement is detected when p is larger than the listed value):

	$D_{\text{vN}} > 0$	$D_L > 0$	$R_{q=2} > 0$	$R_{q\to\infty} > 0$
p_{min}	≈ 0.809	$\sqrt{0.7} \approx 0.837$	≈ 0.632	0.4

.

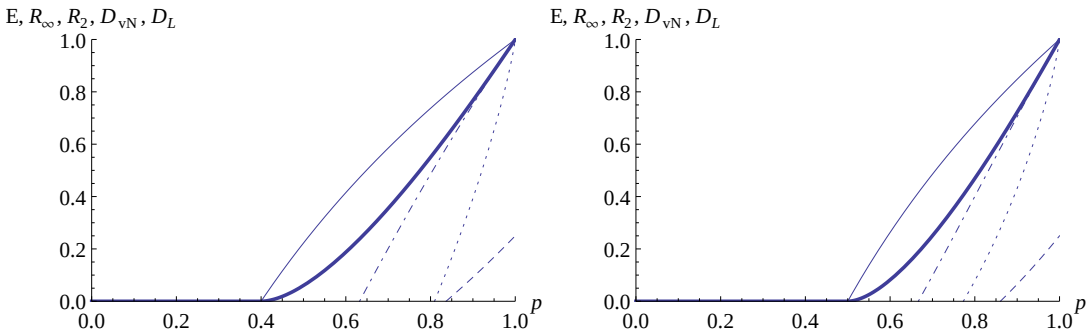


Figure 4.5: Entanglement measure (thick line) and entanglement indicators R_∞ (solid line), R_2 (dash-dotted line), D_{vN} (dotted line) and D_L (dashed line) for the states (a) ρ_W defined in eq. (4.133) and (b) ρ_G given by eq. (4.138). The logarithms in the entanglement indicators are taken to the base 2.

The entanglement detection efficiency of the entropic criterion based upon Rényi entropy increases with q. Indeed, in the limit $q \to \infty$ the Rényi entropic criterion detects all the entangled states within the family of states (4.133). The behaviour of the minimum value of p for which entanglement is detected as a function of the entropic parameter q is depicted in Figure 4.6.

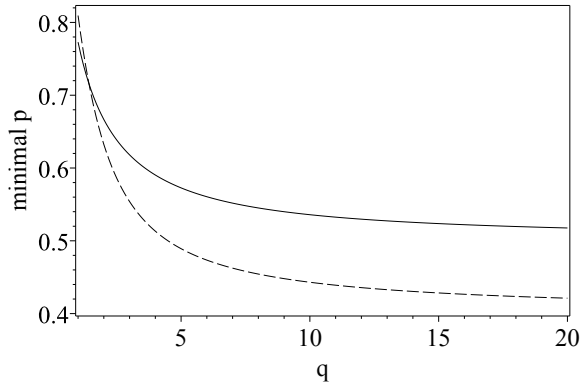


Figure 4.6: Minimum p-value for which entanglement is detected in the case of ρ_W defined in eq. (4.133) (dashed line) and ρ_G given by eq. (4.138) (solid line).

4.2.4.2 θ-state

As second illustration we consider the following pure state,

$$|\psi\rangle = \frac{\sin\theta}{\sqrt{2}}\left[\left|-\frac{3}{2}\frac{3}{2}\right\rangle - \left|\frac{3}{2}\text{-}\frac{3}{2}\right\rangle\right] + \frac{\cos\theta}{\sqrt{2}}\left[\left|-\frac{1}{2}\frac{1}{2}\right\rangle - \left|\frac{1}{2}\text{-}\frac{1}{2}\right\rangle\right], \tag{4.136}$$

for which

$$\begin{aligned} D_{\text{vN}}[|\psi\rangle\langle\psi|] &= -\ln 2 - \cos^2\theta \ln\left(\frac{\cos^2\theta}{2}\right) - \sin^2\theta \ln\left(\frac{\sin^2\theta}{2}\right) \\ D_L[|\psi\rangle\langle\psi|] &= \cos^2\theta \sin^2\theta. \end{aligned} \tag{4.137}$$

Thus, both D_{vN} and $D_L = 0$ for $\theta = 0, \frac{\pi}{2}, \pi$ and both quantities are positive for all other values of θ in the interval $[0, \pi]$. We also have $S_q^{(R)}[\rho] + \ln 2 < S_q^{(R)}[\rho_r]$ for all $\theta \in (0, \pi), \theta \neq \frac{\pi}{2}$. Therefore, comparing this with the concurrence, one sees that all entangled states are detected.

4.2.4.3 Gisin-like states

As a final example let us consider the parameterized family of mixed states given by,

$$\rho_G = p|0,0\rangle\langle 0,0| + \frac{1-p}{2}\Big(|2,-2\rangle\langle 2,-2| + |2,2\rangle\langle 2,2|\Big), \tag{4.138}$$

with $0 \leq p \leq 1$. In this case, we have

$$\begin{aligned} D_{\mathrm{vN}}[\rho_G] &= (1-p)\ln(1-p) + p\ln(2p) \\ D_L[\rho_G] &= \frac{1}{4}\left(-1-4p+6p^2\right) \\ R_2[\rho_G] &= \ln(1-2p+3p^2) \\ R_\infty[\rho_G] &= \begin{cases} \ln(1-p) & 0 \leq p \leq \frac{1}{3} \\ \ln(2p) & \frac{1}{3} \leq p \leq 1 \end{cases} \\ C[\rho_G] &= \begin{cases} 0 & 0 \leq p \leq 0.5 \\ 2p-1 & 0.5 \leq p \leq 1. \end{cases} \end{aligned} \tag{4.139}$$

Figure 4.5(b) shows the entanglement measure (eq. (4.132)) and depicts when the entanglement indicators given in eq. (4.139) detect entanglement. The logarithms in the entanglement indicators are taken to the base 2 for comparison purposes.

The critical p values at which the entropic criteria based on the indicators D_{vN}, D_L, R_2 and R_∞ begin to detect entanglement are listed in the Table below:

	$D_{\mathrm{vN}} > 0$	$D_L > 0$	$R_{q=2} > 0$	$R_{q\to\infty} > 0$
p_{min}	≈ 0.773	$\frac{2+\sqrt{10}}{6} \approx 0.860$	≈ 0.667	0.5

.

From the evaluation of the concurrence it follows that the Gisin-like states are entangled for $p > 0.5$. Thus, once again, the Rényi-based entropic criterion based on the indicator R_∞ detects all the entangled states in the family (4.138). The behaviour of the minimum value of p for which entanglement is detected as a function of the entropic parameter q is depicted in Figure 4.6.

We shall now illustrate the fact that the quantities D_{vN}, D_L and R_q involved in the entanglement criteria advanced here can also be regarded as entanglement indicators, in the sense that states exhibiting large values of these quantities tend to have higher entanglement. Two-fermion states with a single-particle Hilbert space of dimension four allow for the illustration of this, because in the case of these systems we have a closed analytical expression for the amount of entanglement of mixed states, see eq. (4.132).

In Figures 4.5(a) and 4.5(b) we compare, for two parameterized families of mixed states, the behaviour of the entanglement measure with the behaviour of the abovementioned quantities. Note that in order to compare the entanglement measure with our entanglement indicators, the logarithms in the entanglement indicators are taken to the base 2 in Figures 4.5(a) and 4.5(b). It transpires from Figures 4.5(a) and 4.5(b) that for these families of states the indicators associated with our entropic entanglement criteria do indeed tend to increase with the amount of entanglement exhibited by these states.

4.2.5 Two-fermion systems with a single-particle Hilbert space of dimension six

Two identical fermions with a four-dimensional single-particle Hilbert space (the simplest fermionic system admitting the phenomenon of entanglement) constitutes the only fermion system for which an exact analytical formula for the concurrence has been obtained. It is thus of interest to apply the entropic entanglement criteria to systems of higher dimensionality, for which such an expression for the concurrence is not known. Here we are going to consider a system consisting of two identical fermions with a single-particle Hilbert space of dimension six. The Hilbert space of this system is 15-dimensional. The generic (mixed) state of this system depends on 224 (real) parameters. The entanglement features of mixed states of this system are (up to now) basically "terra incognita". Here we are going to identify, for some parameterized families of mixed states, the range of values of the relevant parameters for which the states are entangled.

Using the angular momentum representation, the two-fermion system considered in this Subsection can be mapped onto a system of two spins with $s = \frac{5}{2}$. It is useful to introduce the following notation,

$$|m_1 m_2| = \frac{1}{\sqrt{2}}\Big[|m_1\rangle|m_2\rangle - |m_2\rangle|m_1\rangle\Big]. \tag{4.140}$$

I am going to study three particular families of mixed states of the form

$$\rho_i = p|\varphi_i\rangle\langle\varphi_i| + \frac{1-p}{15}\,\mathbb{I}, \tag{4.141}$$

where $0 \leq p \leq 1$ and

$$\mathbb{I} = |0,0\rangle\langle 0,0| + \sum_{m=-2}^{2} |2,m\rangle\langle 2,m| + \sum_{m=-4}^{4} |4,m\rangle\langle 4,m| \tag{4.142}$$

is the identity operator acting on the 15-dimensional Hilbert space describing the two-fermion system, and $|\varphi_i\rangle$ is an entangled two-fermion pure state. We consider three particular instances of $|\varphi_i\rangle$. In each case we provide the expressions for the indicators D_{vN}, D_L, R_2 and R_∞, and give the minimum values p_{min} of the parameter p such that for $p > p_{min}$ entanglement is detected by the criteria based on the positivity of the entanglement indicators.

The first illustration corresponds to

$$|\varphi_1\rangle = \frac{1}{\sqrt{3}}\left[\left|\frac{5}{2}\frac{3}{2}\right| + \left|\frac{1}{2}\text{-}\frac{1}{2}\right| - \left|\text{-}\frac{3}{2}\text{-}\frac{5}{2}\right|\right], \tag{4.143}$$

for which

$$\begin{aligned} D_{\text{vN}}[\rho_1] &= \ln 3 + \frac{14}{15}(1-p)\ln\left(\frac{1-p}{15}\right) + \frac{1}{15}(1+14p)\ln\left(\frac{1}{15}(1+14p)\right) \\ D_L[\rho_1] &= \frac{1}{15}\left(-9+14p^2\right) \\ R_2[\rho_1] &= \ln\left(\frac{1}{5}(1+14p^2)\right) \\ R_\infty[\rho_1] &= \ln\left(\frac{1}{15}(1+14p)\right) + \ln 3, \end{aligned} \tag{4.144}$$

resulting in

	$D_{\text{vN}} > 0$	$D_L > 0$	$R_{q=2} > 0$	$R_{q\to\infty} > 0$
p_{min}	≈ 0.767	$\frac{3}{\sqrt{14}} \approx 0.802$	≈ 0.535	$\frac{2}{7} \approx 0.286$

.

The second example is given by

$$|\varphi_2\rangle = -\frac{2}{3}\left|\frac{5}{2}\frac{3}{2}\right| - \frac{2}{3}\left|\frac{1}{2}\text{-}\frac{1}{2}\right| + \frac{1}{3}\left|\text{-}\frac{3}{2}\text{-}\frac{5}{2}\right|, \tag{4.145}$$

with

$$\begin{aligned} D_{\mathrm{vN}}[\rho_2] &= \frac{1}{45}\left(-45\ln 2 + 42(1-p)\ln\left(\frac{1-p}{15}\right) - 5(3-2p)\ln\left(\frac{3-2p}{18}\right)\right. \\ &\qquad \left. -10(3+p)\ln\left(\frac{3+p}{18}\right) + 3(1+14p)\ln\left(\frac{1}{15}(1+14p)\right)\right) \\ D_L[\rho_2] &= -\frac{3}{5} + \frac{121p^2}{135} \\ R_2[\rho_2] &= -\ln(9+2p^2) + \ln\left(\frac{9}{5}(1+14p^2)\right) \\ R_\infty[\rho_2] &= -\ln\left(\frac{1-p}{6} + \frac{2p}{9}\right) + \ln\left(\frac{1}{15}(1+14p)\right) - \ln 2, \end{aligned} \tag{4.146}$$

and

	$D_{\mathrm{vN}} > 0$	$D_L > 0$	$R_{q=2} > 0$	$R_{q\to\infty} > 0$
p_{min}	≈ 0.788	$\frac{9}{11} \approx 0.818$	≈ 0.557	$\frac{12}{37} \approx 0.324$

.

As a third instance we tackle

$$|\varphi_3\rangle = \frac{1}{\sqrt{2}}\left[\left|\frac{5}{2}\frac{3}{2}\right| + \left|\frac{1}{2}\text{-}\frac{1}{2}\right|\right], \tag{4.147}$$

leading to

$$\begin{aligned} D_{\mathrm{vN}}[\rho_3] &= -\ln 2 - \frac{1-p}{3}\ln\left(\frac{1-p}{6}\right) - \frac{2+p}{3}\ln\left(\frac{2+p}{12}\right) \\ &\qquad + \frac{14}{15}(1-p)\ln\left(\frac{1-p}{15}\right) + \frac{1+14p}{15}\ln\left(\frac{1}{15}(1+14p)\right) \\ D_L[\rho_3] &= -\frac{3}{5} + \frac{17p^2}{20} \\ R_2[\rho_3] &= -\ln(2+p^2) + \ln\left(\frac{2}{5}(1+14p^2)\right) \\ R_\infty[\rho_3] &= -\ln\left(\frac{1-p}{6} + \frac{p}{4}\right) + \ln\left(\frac{1}{15}(1+14p)\right) - \ln 2, \end{aligned} \tag{4.148}$$

and

	$D_{\mathrm{vN}} > 0$	$D_L > 0$	$R_{q=2} > 0$	$R_{q\to\infty} > 0$
p_{min}	≈ 0.825	$2\sqrt{\frac{3}{17}} \approx 0.840$	≈ 0.590	$\frac{8}{23} \approx 0.348$

.

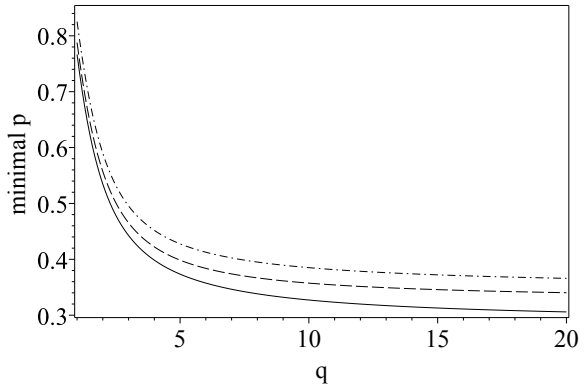


Figure 4.7: Minimum value of p, as a function of the entropic parameter q, for entanglement detection in the states (4.141) with $|\varphi_1\rangle$ (solid line), $|\varphi_2\rangle$ (dashed line) and $|\varphi_3\rangle$ (dash-dotted line).

For the above three cases, the behaviour of the minimum value of p for which entanglement is detected, as a function of the entropic parameter q, is depicted in Figure 4.7.

4.2.6 Systems of N identical fermions

Let us consider the general case of N fermions with single-particle Hilbert space of general (even) dimension $n > N$. The dimension of the Hilbert space associated with the N-fermion system is then $d = \frac{n!}{(n-N)!N!}$. The Rényi-based entropic criterion for two fermions that we derived in Subsection 4.2.3 can be extended to the case of N fermions. According to the extended criterion a state ρ of N identical fermions satisfying the inequality

$$S_q^{(R)}[\rho_r] > S_q^{(R)}[\rho] + \ln N \tag{4.149}$$

for some $q \geq 1$, is necessarily entangled, where ρ_r is the single-particle reduced density matrix. This criterion can be derived following a procedure that is a straightforward generalization to the case of N fermions of the one detailed in Subsubsection 4.2.3.2 for the case of two fermions. One starts with a state of the N fermions that is a statistical mixture of pure states, each one represented by a single Slater determinant which contains $N!$ terms. Then one considers two

equivalent representations for the total density matrix ρ: the spectral one, and the abovementioned one as a mixture of separable pure states. On the other hand, one considers two equivalent representations for the single-particle reduced density matrix ρ_r: again, the spectral one, and the one derived from the representation of the total state as a mixture of separable states. The two representations for ρ and the two ones for ρ_r are then related via appropriate unitary transformations according to equation (4.98). Following the same steps as in Subsubsection 4.2.3.3 it is then possible to obtain a majorization relation connecting ρ and ρ_r, which finally leads to the inequality (4.149). The generalized proof is as follows.

First, a separable pure state of N identical fermions is given by a single Slater determinant

$$\left|\psi_1^{(j)}\psi_2^{(j)}\ldots\psi_N^{(j)}\right| = \frac{1}{\sqrt{N!}}\sum_{m_1,m_2,\ldots,m_N=1}^{N}\varepsilon_{m_1m_2\ldots m_N}|\psi_{m_1}^{(j)}\rangle|\psi_{m_2}^{(j)}\rangle\ldots|\psi_{m_N}^{(j)}\rangle, \tag{4.150}$$

where the single-particle states are all orthonormal and $\varepsilon_{m_1m_2\ldots m_N}$ is the generalized Levi-Civita symbol,

$$\varepsilon_{ijkl\ldots} = \begin{cases} +1 & \text{if } (i,j,k,l,\ldots) \text{ is an even permutation of } (1,2,3,4,\ldots) \\ -1 & \text{if } (i,j,k,l,\ldots) \text{ is an odd permutation of } (1,2,3,4,\ldots) \\ 0 & \text{otherwise.} \end{cases} \tag{4.151}$$

Let us consider a separable mixed state of N identical fermions,

$$\begin{aligned}\rho \;=\; \sum_j \frac{p_j}{N!}\Big(\sum_{m_1,m_2,\ldots,m_N=1}^{N}\varepsilon_{m_1m_2\ldots m_N}|\psi_{m_1}^{(j)}\rangle|\psi_{m_2}^{(j)}\rangle\ldots|\psi_{m_N}^{(j)}\rangle\Big)\times \\ \Big(\sum_{m_1,m_2,\ldots,m_N=1}^{N}\varepsilon_{m_1m_2\ldots m_N}\langle\psi_{m_1}^{(j)}|\langle\psi_{m_2}^{(j)}|\ldots\langle\psi_{m_N}^{(j)}|\Big)\end{aligned} \tag{4.152}$$

where $0 \leq p_j \leq 1$, $\sum_j p_j = 1$ and $|\psi_1^{(j)}\rangle, |\psi_2^{(j)}\rangle, \ldots, |\psi_N^{(j)}\rangle$ are normalized single-particle states with $\langle\psi_n^{(j)}|\psi_{n'}^{(j)}\rangle = \delta_{nn'}$ $(n, n' = 1, 2, \ldots, N)$, for all j. Equation (4.152) represents the standard definition of a non-entangled mixed state of N identical fermions. Notice that in (4.152) no special relation between states $|\psi_i^{(j)}\rangle$

with different values of the label j is assumed. In particular, the overlap between two states with different labels j is not necessarily equal to 0 or 1. This, in turn, means that the overlap between two different members of the family of (separable) two-fermion pure states participating in the statistical mixture leading to (4.152) may be non-zero.

Let us consider now a spectral representation

$$\rho = \sum_k \lambda_k |e_k\rangle\langle e_k| \tag{4.153}$$

of ρ. That is, the $|e_k\rangle$ constitute an orthonormal basis of eigenvectors of ρ and the λ_k are the corresponding eigenvalues. Then, (4.152) and (4.153) are two different representations of ρ as a mixture of pure states. Therefore, there is a unitary matrix U with matrix elements $\{U_{kj}\}$ such that

$$\sqrt{\lambda_k}|e_k\rangle = \sum_j U_{kj}\sqrt{\frac{p_j}{N!}}\sum_{m_1,m_2,\ldots,m_N=1}^{N}\varepsilon_{m_1 m_2 \ldots m_N}|\psi_{m_1}^{(j)}\rangle|\psi_{m_2}^{(j)}\rangle\ldots|\psi_{m_N}^{(j)}\rangle. \tag{4.154}$$

The single-particle reduced density matrix corresponding to the N-fermion density matrix (4.152) is

$$\rho_r = \sum_j \frac{p_j}{N}\Big(|\psi_1^{(j)}\rangle\langle\psi_1^{(j)}| + |\psi_2^{(j)}\rangle\langle\psi_2^{(j)}| + \cdots + |\psi_N^{(j)}\rangle\langle\psi_N^{(j)}|\Big), \tag{4.155}$$

admitting a spectral representation

$$\rho_r = \sum_l \alpha_l |f_l\rangle\langle f_l|. \tag{4.156}$$

We now define,

$$q_{Nj-(N-1)} = q_{Nj-(N-2)} = \ldots = q_{Nj-2} = q_{Nj-1} = q_{Nj} = \frac{1}{N}p_j \qquad (j = 1, 2, 3, \ldots) \tag{4.157}$$

$$\begin{aligned} |\phi_{Nj-(N-1)}\rangle &= |\psi_1^{(j)}\rangle \\ |\phi_{Nj-(N-2)}\rangle &= |\psi_2^{(j)}\rangle \\ &\vdots \end{aligned}$$

$$\begin{aligned} |\phi_{Nj-2}\rangle &= |\psi^{(j)}_{N-2}\rangle \\ |\phi_{Nj-1}\rangle &= |\psi^{(j)}_{N-1}\rangle \\ |\phi_{Nj}\rangle &= |\psi^{(j)}_{N}\rangle \qquad (j=1,2,3,\ldots). \end{aligned} \tag{4.158}$$

Now, since (4.155) and (4.156) correspond to two statistical mixtures yielding the same density matrix, there must exist a unitary matrix W with matrix elements $\{W_{il}\}$ such that,

$$\sqrt{q_i}|\phi_i\rangle = \sum_l W_{il}\sqrt{\alpha_l}|f_l\rangle \qquad (i=1,2,3,\ldots). \tag{4.159}$$

Now, eq. (4.154) can be rewritten as

$$\begin{aligned} &\sqrt{\lambda_k}|e_k\rangle \\ &= \sum_j \frac{U_{kj}}{\sqrt{(N-1)!}}\sqrt{\frac{p_j}{N}} \sum_{m_1,m_2,\ldots,m_N=1}^{N} \varepsilon_{m_1 m_2 \ldots m_N}|\psi^{(j)}_{m_1}\rangle|\psi^{(j)}_{m_2}\rangle\ldots|\psi^{(j)}_{m_N}\rangle = \sum_j \frac{U_{kj}}{\sqrt{(N-1)!}}\Big\{ \\ &\sqrt{q_{Nj-(N-1)}}|\phi_{Nj-(N-1)}\rangle \sum_{s_2,s_3,\ldots,s_N=2}^{N} \varepsilon_{s_2 s_3 \ldots s_N}|\phi_{Nj-(N-s_2)}\rangle|\phi_{Nj-(N-s_3)}\rangle\ldots|\phi_{Nj-(N-s_N)}\rangle \\ &-\sqrt{q_{Nj-(N-2)}}|\phi_{Nj-(N-2)}\rangle \sum_{s_1,s_3,\ldots,s_N=1,3}^{N} \varepsilon_{s_1 s_3 \ldots s_N}|\phi_{Nj-(N-s_1)}\rangle|\phi_{Nj-(N-s_3)}\rangle\ldots|\phi_{Nj-(N-s_N)}\rangle \\ &+\ldots+ \\ &-\sqrt{q_{Nj-1}}|\phi_{Nj-1}\rangle \sum_{s_1,s_2,\ldots,s_{N-2},s_N=1}^{N-2,N} \varepsilon_{s_1 s_2 \ldots s_{N-2} s_N}|\phi_{Nj-(N-s_1)}\rangle\ldots|\phi_{Nj-(N-s_{N-2})}\rangle|\phi_{Nj-(N-s_N)}\rangle \\ &+\sqrt{q_{Nj}}|\phi_{Nj}\rangle \sum_{s_1,s_2,\ldots,s_{N-1}=1}^{N-1} \varepsilon_{s_1 s_2 \ldots s_{N-1}}|\phi_{Nj-(N-s_1)}\rangle|\phi_{Nj-(N-s_2)}\rangle\ldots|\phi_{Nj-(N-s_{N-1})}\rangle\Big\}. \end{aligned} \tag{4.160}$$

Combining (4.159) and (4.160) gives

$$\begin{aligned} \sqrt{\lambda_k}|e_k\rangle \;=\; \sum_j \frac{U_{kj}}{\sqrt{(N-1)!}}\Bigg[\sum_l\Big(& \\ W_{Nj-(N-1),l} \sum_{s_2,s_3,\ldots,s_N=2}^{N} & \varepsilon_{s_2 s_3 \ldots s_N}|\phi_{Nj-(N-s_2)}\rangle|\phi_{Nj-(N-s_3)}\rangle\ldots|\phi_{Nj-(N-s_N)}\rangle \\ -W_{Nj-(N-2),l} \sum_{s_1,s_3,\ldots,s_N=1,3}^{N} & \varepsilon_{s_1 s_3 \ldots s_N}|\phi_{Nj-(N-s_1)}\rangle|\phi_{Nj-(N-s_3)}\rangle\ldots|\phi_{Nj-(N-s_N)}\rangle \end{aligned}$$

$$
\begin{aligned}
&+\ldots+\\
&-W_{Nj-1,l}\sum_{s_1,s_2,\ldots,s_{N-2},s_N=1}^{N-2,N}\varepsilon_{s_1s_2\ldots s_{N-2}s_N}|\phi_{Nj-(N-s_1)}\rangle\ldots|\phi_{Nj-(N-s_{N-2})}\rangle|\phi_{Nj-(N-s_N)}\rangle\\
&+W_{Nj,l}\sum_{s_1,s_2,\ldots,s_{N-1}=1}^{N-1}\varepsilon_{s_1s_2\ldots s_{N-1}}|\phi_{Nj-(N-s_1)}\rangle|\phi_{Nj-(N-s_2)}\rangle\ldots|\phi_{Nj-(N-s_{N-1})}\rangle\Big)\sqrt{\alpha_l}|f_l\rangle\Big].
\end{aligned}
\tag{4.161}
$$

Therefore, since $\langle e_k|e_{k'}\rangle=\delta_{kk'}$ and $\langle f_l|f_{l'}\rangle=\delta_{ll'}$, we have that

$$
\begin{aligned}
\lambda_k \;=\; \sum_l\Bigg[\frac{1}{(N-1)!}\Bigg(\sum_{j'}U^*_{kj'}\Big\{&\\
&W^*_{Nj'-(N-1),l}\sum_{s_2,s_3,\ldots,s_N=2}^{N}\varepsilon_{s_2s_3\ldots s_N}\langle\phi_{Nj'-(N-s_2)}|\langle\phi_{Nj'-(N-s_3)}|\ldots\langle\phi_{Nj'-(N-s_N)}|\\
&-W^*_{Nj'-(N-2),l}\sum_{s_1,s_3,\ldots,s_N=1,3}^{N}\varepsilon_{s_1s_3\ldots s_N}\langle\phi_{Nj'-(N-s_1)}|\langle\phi_{Nj'-(N-s_3)}|\ldots\langle\phi_{Nj'-(N-s_N)}|\\
&+\ldots+\\
&-W^*_{Nj'-1,l}\sum_{s_1,s_2,\ldots,s_{N-2},s_N=1}^{N-2,N}\varepsilon_{s_1s_2\ldots s_{N-2}s_N}\langle\phi_{Nj'-(N-s_1)}|\ldots\langle\phi_{Nj'-(N-s_{N-2})}|\langle\phi_{Nj'-(N-s_N)}|\\
&+W^*_{Nj',l}\sum_{s_1,s_2,\ldots,s_{N-1}=1}^{N-1}\varepsilon_{s_1s_2\ldots s_{N-1}}\langle\phi_{Nj'-(N-s_1)}|\langle\phi_{Nj'-(N-s_2)}|\ldots\langle\phi_{Nj'-(N-s_{N-1})}|\Big\}\Bigg)\times\\
\Bigg(\sum_{j''}U_{kj''}\Big\{&W_{Nj''-(N-1),l}\sum_{s_2,s_3,\ldots,s_N=2}^{N}\varepsilon_{s_2s_3\ldots s_N}|\phi_{Nj''-(N-s_2)}\rangle|\phi_{Nj''-(N-s_3)}\rangle\ldots|\phi_{Nj''-(N-s_N)}\rangle\\
&-W_{Nj''-(N-2),l}\sum_{s_1,s_3,\ldots,s_N=1,3}^{N}\varepsilon_{s_1s_3\ldots s_N}|\phi_{Nj''-(N-s_1)}\rangle|\phi_{Nj''-(N-s_3)}\rangle\ldots|\phi_{Nj''-(N-s_N)}\rangle\\
&+\ldots+\\
&-W_{Nj''-1,l}\sum_{s_1,s_2,\ldots,s_{N-2},s_N=1}^{N-2,N}\varepsilon_{s_1s_2\ldots s_{N-2}s_N}|\phi_{Nj''-(N-s_1)}\rangle\ldots|\phi_{Nj''-(N-s_{N-2})}\rangle|\phi_{Nj''-(N-s_N)}\rangle\\
&+W_{Nj'',l}\sum_{s_1,s_2,\ldots,s_{N-1}=1}^{N-1}\varepsilon_{s_1s_2\ldots s_{N-1}}|\phi_{Nj''-(N-s_1)}\rangle|\phi_{Nj''-(N-s_2)}\rangle\ldots|\phi_{Nj''-(N-s_{N-1})}\rangle\Big\}\Bigg)\Bigg]\alpha_l.
\end{aligned}
\tag{4.162}
$$

From (4.162) it follows that we can write

$$\lambda_k = \sum_l M_{kl}\alpha_l, \tag{4.163}$$

where M_{kl} is the expression in the square brackets in equation (4.162).

We now investigate the properties of the matrix M with matrix elements $\{M_{kl}\}$. First of all, we have

$$M_{kl} \geq 0, \tag{4.164}$$

since the matrix elements of M are of the form $M_{kl} = \langle \Sigma | \Sigma \rangle$ as can be seen directly from equation (4.162). We now consider the sum of the elements within a given row or column of M. The sum of a row yields,

$$\begin{aligned}
\sum_k M_{kl} &= \frac{1}{(N-1)!}\sum_{j'j''}\left[\sum_k U^*_{kj'}U_{kj''}\right]\begin{pmatrix}\text{depends on}\\ j'\end{pmatrix}\begin{pmatrix}\text{depends on}\\ j''\end{pmatrix} \\
&= \frac{1}{(N-1)!}\sum_{j'j''}\left[\sum_k (U^\dagger)_{j'k}U_{kj''}\right]\begin{pmatrix}\text{depends on}\\ j'\end{pmatrix}\begin{pmatrix}\text{depends on}\\ j''\end{pmatrix} \\
&= \frac{1}{(N-1)!}\sum_{j'j''}\delta_{j'j''}\begin{pmatrix}\text{depends on}\\ j'\end{pmatrix}\begin{pmatrix}\text{depends on}\\ j''\end{pmatrix} \\
&= \sum_j \frac{1}{(N-1)!}\Big(W^*_{Nj-(N-1),l}W_{Nj-(N-1),l}\,(N-1)! \\
&\qquad + W^*_{Nj-(N-2),l}W_{Nj-(N-2),l}\,(N-1)! + \ldots \\
&\qquad + W^*_{Nj-1,l}W_{Nj-1,l}\,(N-1)! \\
&\qquad + W^*_{Nj,l}W_{Nj,l}\,(N-1)!\Big) \\
&= \sum_i \left(W^\dagger\right)_{li}W_{il} = 1,
\end{aligned} \tag{4.165}$$

while the sum of a column is,

$$\begin{aligned}
\sum_l M_{kl} = \frac{1}{(N-1)!}\sum_{j'j''}U^*_{kj'}U_{kj''}\Big(&\sum_l W^*_{Nj'-(N-1),l}W_{Nj''-(N-1),l}\,(N-1)!\,\delta_{j'j''} \\
&+ \sum_l W^*_{Nj'-(N-2),l}W_{Nj''-(N-2),l}\,(N-1)!\,\delta_{j'j''} + \ldots \\
&+ \sum_l W^*_{Nj'-1,l}W_{Nj''-1,l}\,(N-1)!\,\delta_{j'j''}
\end{aligned}$$

$$
\begin{aligned}
&\quad + \sum_l W^*_{Nj',l} W_{Nj'',l}\,(N-1)!\,\delta_{j'j''}\Big) \\
&= \frac{1}{(N-1)!}\sum_j U^*_{kj}U_{kj}\,(N-1)!\,\Big(\sum_l (W^\dagger)_{l,Nj-(N-1)} W_{Nj-(N-1),l} \\
&\qquad + \sum_l (W^\dagger)_{l,Nj-(N-2)} W_{Nj-(N-2),l} + \ldots \\
&\qquad + \sum_l (W^\dagger)_{l,Nj-1} W_{Nj-1,l} \\
&\qquad + \sum_l (W^\dagger)_{l,Nj} W_{Nj,l}\Big) \\
&= N\sum_j U^*_{kj}U_{kj} = N\sum_j \left(U^\dagger\right)_{jk} U_{kj} = N. \qquad (4.166)
\end{aligned}
$$

When deriving the above two equations (4.165) and (4.166) we made use of the unitarity of the matrices $\{U_{kj}\}$ and $\{W_{il}\}$. Summing up, we have,

$$
\begin{aligned}
\sum_k M_{kl} &= 1 \\
\sum_l M_{kl} &= N. \qquad (4.167)
\end{aligned}
$$

We now define a new set of variables $\{\lambda'_n\}$ and a new matrix M' with elements M'_{nl}, respectively given by,

$$\lambda'_{Nk-(N-1)} = \lambda'_{Nk-(N-2)} = \ldots = \lambda'_{Nk-1} = \lambda'_{Nk} = \frac{\lambda_k}{N}\ (k = 1, 2, \ldots) \qquad (4.168)$$

$$M'_{Nk-(N-1),l} = M'_{Nk-(N-2),l} = \ldots = M'_{Nk-1,l} = M'_{Nk,l} = \frac{M_{kl}}{N}\ (k = 1, 2, \ldots), \qquad (4.169)$$

and so we have that eq. (4.163) can be expressed as

$$\lambda'_n = \sum_l M'_{nl}\alpha_l. \qquad (4.170)$$

By construction, then, we have

$$
\begin{aligned}
\{\lambda_k\} &= \{\lambda_1, \lambda_2, \lambda_3, \ldots\} \\
\{\lambda'_n\} &= \Big\{\underbrace{\frac{\lambda_1}{N}, \frac{\lambda_1}{N}, \ldots, \frac{\lambda_1}{N}}_{N \text{ terms}}, \underbrace{\frac{\lambda_2}{N}, \frac{\lambda_2}{N}, \ldots, \frac{\lambda_2}{N}}_{N \text{ terms}}, \ldots\Big\}. \qquad (4.171)
\end{aligned}
$$

Let us now compare the matrices $\{M_{kl}\}$ and $\{M'_{nl}\}$. The matrix $\{M'_{nl}\}$ has N times as many rows as $\{M_{kl}\}$, but the rows of $\{M'_{nl}\}$ can be divided into groups of N consecutive rows such that within each group of N rows, these rows are equal to N times the corresponding row of $\{M_{kl}\}$. The number of columns of M'_{nl} and M_{kl} are clearly the same and so the sum of the entries of any row of $\{M'_{nl}\}$ is $\frac{1}{N}$ of the corresponding one for M_{kl}. It follows that

$$\begin{aligned} \sum_k M_{kl} = 1 \quad &\Longrightarrow \quad \sum_n M'_{nl} = 1 \\ \sum_l M_{kl} = N \quad &\Longrightarrow \quad \sum_l M'_{nl} = 1. \end{aligned} \tag{4.172}$$

Thus,

$$\sum_n M'_{nl} = \sum_l M'_{nl} = 1 \tag{4.173}$$

and, therefore, $\{M'_{nl}\}$ is a doubly stochastic matrix. Interpreting the λ'_n's and the α_l's as probabilities, it follows from (4.170) and (4.173) that the probability distribution $\{\lambda'_n\}$ is more "mixed" than the probability distribution $\{\alpha_l\}$ [137] (or, alternatively that $\{\alpha_l\}$ majorizes $\{\lambda'_n\}$ [136]). This, in turn, implies that for any Rényi entropy $S_q^{(R)}$ with $q \geq 1$, we have

$$S_q^{(R)}[\lambda'_n] \geq S_q^{(R)}[\alpha_l]. \tag{4.174}$$

Thus,

$$\begin{aligned} S_q^{(R)}[\lambda'_n] &= \frac{1}{1-q} \ln \left(N \sum_k \left(\frac{\lambda_k}{N} \right)^q \right) = \frac{1}{1-q} \ln \left(N^{1-q} \sum_k \lambda_k^q \right) \\ &= \frac{1}{1-q} \left\{ \ln \left(N^{1-q} \right) + \ln \left(\sum_k \lambda_k^q \right) \right\} \\ &= \ln N + \frac{1}{1-q} \ln \left(\sum_k \lambda_k^q \right) \\ &= \ln N + S_q^{(R)}[\lambda_k]. \end{aligned} \tag{4.175}$$

Therefore, all separable states of the N-fermion system comply with the inequality $S_q^{(R)}[\lambda_k] + \ln N \geq S_q^{(R)}[\alpha_l]$ and since $\{\lambda_k\}$ and $\{\alpha_l\}$ are the eigenvalues of ρ and

ρ_r respectively,

$$S_q^{(R)}[\rho] + \ln N \geq S_q^{(R)}[\rho_r]. \tag{4.176}$$

The above inequality leads to an entanglement criterion that detects entanglement when the indicator R_q is strictly positive,

$$R_q = S_q^{(R)}[\rho_r] - S_q^{(R)}[\rho] - \ln N. \tag{4.177}$$

As an illustration of the entanglement criterion based on the inequality (4.149) let us consider a family of states of a system of N fermions having the form

$$p\,|\Phi\rangle\langle\Phi| + \frac{(1-p)}{d}\,\mathbb{I}_d, \tag{4.178}$$

where $0 \leq p \leq 1$, $\mathbb{I}_d$ is the identity operator acting on the N-fermion Hilbert space (the dimension associated with the N-fermion system is $d = \frac{n!}{(n-N)!N!}, n > N$), and the single-particle Hilbert space has dimension $n = kN$, with $k \geq 2$ integer when N is even and for N odd $k \geq 2t$ ($t \geq 1$ integer). We also assume that the (pure) N-fermion state $|\Phi\rangle$ is of the form

$$\begin{aligned} |\Phi\rangle \;=\; & \frac{1}{\sqrt{k}}\Big(|1,2,\ldots,N| + |N+1,N+2,\ldots,2N| + \ldots \\ & + |(k-1)N+1,(k-1)N+2,\ldots,kN|\Big), \end{aligned} \tag{4.179}$$

where $|i_1,i_2,\ldots,i_N|$ denotes the Slater determinant (as in equation (4.140)) constructed with N different members $\{|i_1\rangle,\ldots,|i_N\rangle\}$ of an orthonormal basis $\{|1\rangle,\ldots,|n\rangle\}$ of the single-particle Hilbert space. The state $|\Phi\rangle$ is constructed in such a way that the Slater determinants it consists of do not overlap. The single-particle reduced density matrix associated with the (pure) state $|\Phi\rangle$ corresponds to the totally mixed (single-particle) state $\frac{1}{k}\frac{1}{N!}(N-1)!(|1\rangle\langle 1|+\ldots+|n\rangle\langle n|) = \frac{1}{n}\mathbb{I}_n$, where $\mathbb{I}_n$ is the identity operator corresponding to the single-particle Hilbert space. On the basis of the Rényi entropic criterion corresponding to $q \to \infty$ we identify as entangled the states of the form (4.178) satisfying the inequality,

$$\ln n + \ln\left(p + \frac{(1-p)}{d}\right) - \ln N > 0 \tag{4.180}$$

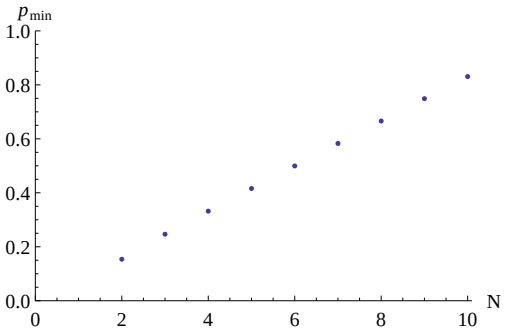


Figure 4.8: p_{min} vs. N for eq. (4.178) with $n = 12$.

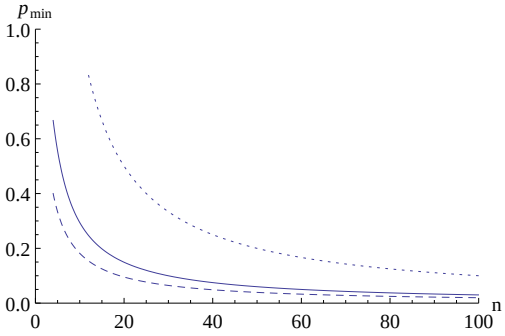


Figure 4.9: p_{min} vs. n for eq. (4.178) with $N = 2$ (dashed line), $N = 3$ (solid line) and $N = 10$ (dotted line).

and hence entanglement is detected for

$$p > \frac{\frac{N}{n} - \frac{(n-N)!N!}{n!}}{1 - \frac{(n-N)!N!}{n!}} = \frac{N\,(n-1)! - (n-N)!\,N!}{n! - (n-N)!\,N!}. \tag{4.181}$$

With N fixed, we find that the efficiency of the entanglement criterion grows as the dimension of the single-particle states, n, increases (that is, p_{min} decreases with n). The behaviour of p_{min} vs. N or n is illustrated in Figures 4.8 and 4.9 respectively.

4.2.6.1 Full multi-particle entanglement: the case of systems of three fermions

When studying entanglement criteria for composite systems with more than two distinguishable subsystems a new problem arises: how to distinguish states exhibiting full multipartite entanglement from those that, although being entangled, are such that a subset of the parts constituting the system is disentangled from the rest of the system. A problem somewhat similar to this one also arises in the case of systems of N identical fermions with $N > 2$, although in the fermionic case this problem is much more subtle than in the case of distinguishable subsystems [183]. Although the analysis of this problem is beyond the scope of the present work, we shall now discuss it (in connection with our entropic entanglement criteria) for the case of systems of three identical fermions.

In the case of three fermions, a general separable state (Slater determinant) is of the form

$$|\phi_{sl}\rangle = |\phi_1, \phi_2, \phi_3| = \frac{1}{\sqrt{6}}\Big[|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle - |\phi_1\rangle|\phi_3\rangle|\phi_2\rangle - |\phi_2\rangle|\phi_1\rangle|\phi_3\rangle + |\phi_2\rangle|\phi_3\rangle|\phi_1\rangle + |\phi_3\rangle|\phi_1\rangle|\phi_2\rangle - |\phi_3\rangle|\phi_2\rangle|\phi_1\rangle\Big], \tag{4.182}$$

with $|\phi_1\rangle, |\phi_2\rangle, \phi_3\rangle$ being three orthonormal single-particle states. A general, separable mixed state is a state that can be expressed as a statistical mixture of states like (4.182). Now, let us consider a pure state of three fermions of the form,

$$|\Psi\rangle = \sum_{1<i<j} c_{ij} \, |1, i, j| \, , \tag{4.183}$$

where $|1, i, j|$ stands for the Slater determinant constructed with the three normalized and orthogonal single-particle states $|1\rangle, |i\rangle, |j\rangle$, and $\{|k\rangle, \ k = 1, 2, \ldots\}$ is a single-particle orthonormal basis. Now, in general, pure states of the above form are entangled in the sense that they cannot be written as one, single Slater determinant (that is, they are not "fully separable"). However, these states are special because they are a superposition of Slater determinants each of them involving the single-particle state $|1\rangle$. This means that it is physically sensible to say that when the system is in a state like (4.183) one of the particles is in the state $|1\rangle$ (although it does not make sense to ask which particle is in the state $|1\rangle$). Consequently, according to the analysis made in [133], where separability is associated to the possibility of assigning complete set of properties to the constituting particles, the state (4.183) can be regarded as describing a physical situation where one of the particles is disentangled from the other two. The same considerations apply to mixed states that are a mixture of states like (4.183) (each one involving the same "privileged" single-particle state $|1\rangle$).

The above discussion raises the following question: can the entropic entanglement criteria advanced here be used to discriminate between entangled states that are mixtures of states of the form (4.183) (having one "disentangled" particle in a given, single-particle state $|1\rangle$), on the one hand, and entangled states that cannot be expressed as (4.183) (or cannot be written as statistical mixtures of states

like (4.183)) on the other hand? To address this problem let us first notice that, as can be verified after some algebra, the single-particle, reduced density matrix ρ_r corresponding to states of the form (4.183) (or to mixtures of such states) always has its largest eigenvalue equal to $\frac{1}{3}$. This implies that $S_\infty^{(R)}(\rho_r) = \ln 3$. Consequently, if a three-fermion state satisfies the (strict) inequality

$$R_\infty \;=\; S_\infty^{(R)}(\rho_r) \;-\; S_\infty^{(R)}(\rho) \;-\; \ln 3 \;>\; 0, \tag{4.184}$$

which implies $S_\infty^{(R)}(\rho_r) - \ln 3 > S_\infty^{(R)}(\rho) \geq 0$, one then knows for sure that this state is entangled and that it cannot be written as a statistical mixture of states like (4.183) (all with the same "privileged" single-particle state $|1\rangle$). In other words, for three-fermion systems, the entropic entanglement criterion based on the Rényi entropy with $q \to \infty$ is not just a sufficient entanglement criterion, but also a sufficient criterion for full, three-particle entanglement.

To illustrate the above discussion we choose the minimum single-particle dimension compatible with three-fermion entanglement, namely the single-particle Hilbert space of dimension six. As examples of entangled three-fermion states that do not exhibit full three-particle entanglement, let us consider the following family of states,

$$\rho = p|\phi\rangle\langle\phi| + (1-p)\rho_{mix}, \tag{4.185}$$

where

$$|\phi\rangle = \cos\theta|1,2,3| + \sin\theta|1,4,5|, \tag{4.186}$$

ρ_{mix} is a mixture (with equal weights) of the projectors corresponding to the ten Slater states containing a "1", that is, $|1,2,3|, |1,2,4|, |1,2,5|, |1,2,6|, |1,3,4|, \ldots,$ $|1,5,6|$, where $|1\rangle, |2\rangle, \ldots, |6\rangle$ are normalized and mutually orthogonal single-particle states that form a basis for the single-particle state space. It is clear that one particle is in the state $|1\rangle$ whereas the other two particles are entangled (although, as mentioned before, it does not make sense to ask which particle is in the state $|1\rangle$), which means this is a multipartite system that is neither fully separable, nor fully entangled in the sense that all three particles are entangled. In order to evaluate the entanglement indicators D_{vN}, R_2 and R_∞, one has to find the eigenvalues of ρ and ρ_r. These are, $\{0, \ldots, 0, \frac{1-p}{10}, \ldots, \frac{1-p}{10}, \frac{1+9p}{10}\}$ and

$\{\frac{1}{3}, \frac{p\cos^2\theta}{3}+\frac{2}{15}(1-p), \frac{p\cos^2\theta}{3}+\frac{2}{15}(1-p), \frac{p\sin^2\theta}{3}+\frac{2}{15}(1-p), \frac{p\sin^2\theta}{3}+\frac{2}{15}(1-p), \frac{2}{15}(1-p)\}$ respectively. In this case $R_\infty = \ln(\frac{1+9p}{10}) \leq 0$ and consequently full three-particle entanglement is (correctly) not detected. However, the entanglement indicators D_{vN} and R_2 do detect entanglement and Figures 4.10(a) and 4.10(b) show the results. Hence entanglement is detected for this multipartite state where not all particles are entangled with each other. However, full multi-particle entanglement is (correctly) not detected.

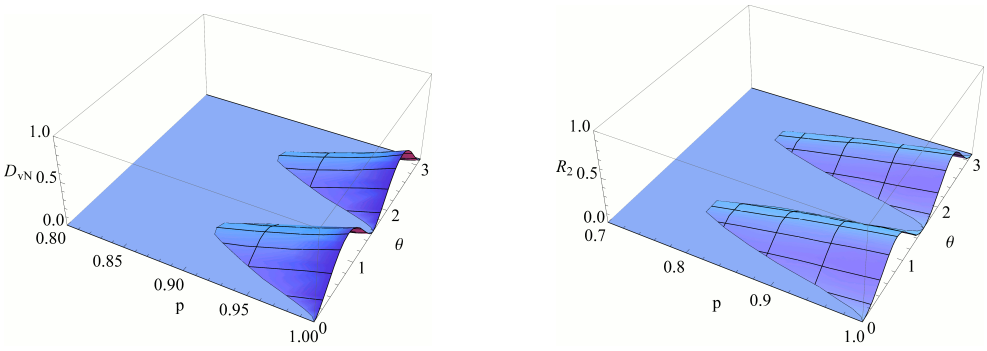


Figure 4.10: Entanglement indicators (a) D_{vN} and (b) R_2 for the state (4.185).

Summing up, we have seen that the entropic criterion based on the Rényi entropy $S_\infty^{(R)}$ is, in the three-fermion case, also a sufficient criterion for full three-particle entanglement. Incidentally, this is another manifestation of the fact that the most powerful entropic entanglement criterion based upon the Rényi entropy corresponds to the limit $q \to \infty$. The case of N-fermion systems with $N \geq 4$ is much more complex and certainly deserves further research. Previous experience with composite quantum systems with distinguishable subsystems (see [96] and references therein) suggests that in this case, besides the entropies of the single-particle reduced density matrix, the entropies of M-particle reduced density matrices (with $2 \leq M < N$) are going to be necessary to tackle this problem.

4.2.7 Summary

In the present Section new entropic entanglement criteria for systems of two identical fermions have been advanced. These criteria have the form of appropriate inequalities involving the entropy of the density matrix associated with the total

system, on the one hand, and the entropy of the single-particle reduced density matrix, on the other hand. I obtained entanglement criteria based upon the von Neumann, the linear, and the Rényi entropies. The criterion associated with the von Neumann entropy constitutes a special instance, corresponding to the particular value $q \to 1$ of the Rényi entropic parameter, of the more general criteria associated with the Rényi family of entropies. Extensions of these criteria to systems constituted by N identical fermions were also considered.

I applied our entanglement criteria to various illustrative examples of parameterized families of mixed states, and studied the dependence of the entanglement detection efficiency on the entropic parameter q. For the two-fermion states we considered, the entanglement criterion improves as q increases and is the most efficient in the limit $q \to \infty$.

For the two-fermion states with single-particle Hilbert space of dimension four, we illustrated the fact that the quantities D_{vN}, D_L and R_q involved in the entanglement criteria advanced here can also be regarded as entanglement indicators, in the sense that states exhibiting large values of these quantities have higher entanglement.

In the three-fermion case we have seen that the entropic criterion based on the Rényi entropy $S_{\infty}^{(R)}$ is also a sufficient criterion for full three-particle entanglement. Incidentally, this is another manifestation of the fact that the most powerful entropic entanglement criterion based upon the Rényi entropy corresponds to the limit $q \to \infty$.

Chapter 5

Characterization of Correlations in Fermion Systems Based on Measurement Induced Disturbances

I introduce an approach for the characterization of quantum correlations in fermion systems based upon the state disturbances generated by the measurement of "local" observables (that is, quantum observables represented by one-body operators). This approach leads to a concept of quantum correlations in systems of identical fermions different from entanglement.

5.1 Introduction

Considerable attention has been devoted recently to the applications of tools and concepts from quantum information theory to the study of correlations in systems of identical fermions [123, 124, 127, 129, 130, 132, 133, 135, 182]. Most of these developments have focused on the analysis of quantum entanglement in fermion systems. However, it is well-known that the concept of entanglement does not capture all the relevant, information-theoretical aspects of the quantum correlations exhibited by composite systems. Indeed, as was established in a pioneering work by Zurek and Ollivier [111], even separable mixed states can be

endowed with correlations exhibiting non-trivial quantum features. In the case of systems consisting of distinguishable parts various measures have been advanced to characterize quantitatively the different ways (besides entanglement) in which quantum correlations can manifest themselves [111, 119, 201–207]. Prominent among these are quantum discord (discussed in Section 2.3) and the measures of correlations based upon the disturbances of quantum states due to local measurements proposed by Luo [119, 202, 203] (discussed in Subsection 2.3.1) and by SaiToh and collaborators [204, 205]. In the case of pure states these measures reduce to quantum entanglement. In the case of mixed states, however, these measures describe physical properties of quantum states that are different from entanglement.

The purpose of the present work is to investigate manifestations of the quantum correlations in fermion systems that do not correspond to quantum entanglement, focusing on the measurement induced disturbance approach. Quantum discord does not seem to admit a counterpart in the case of systems of identical fermions, because its definition involves a strong asymmetry between the constituting parts of the composite system under consideration. On the other hand, as we shall see, the measures of correlations based upon measurement induced disturbances do admit a natural generalization to the fermion systems.

5.2 Correlations in fermion systems and measurement induced disturbance

As already mentioned, a pure state of a system of two identical fermions is non-entangled if and only if it can be written as a single Slater determinant,

$$|\psi(1,2)\rangle = \frac{1}{\sqrt{2}}\big[|\alpha_1\rangle \otimes |\alpha_2\rangle - |\alpha_2\rangle \otimes |\alpha_1\rangle\big], \tag{5.1}$$

where the single-particle states $|\alpha_1\rangle$, $|\alpha_2\rangle$ are two orthogonal and normalized states. A state like (5.1) exhibits the "classical-like" feature that both constituents of the composite system possess a complete set of properties [133]. That is, one can objectively say that one particle possesses the complete set of prop-

erties associated with the single-particle pure state $|\alpha_1\rangle$ and the other particle possesses the set of properties corresponding to $|\alpha_2\rangle$ (of course, it makes no sense to ask "which particle possesses which set of properties"). States having the form (5.1) are the only pure states of two fermions exhibiting this classical property. Indeed, the possibility of assigning a definite set of properties to each of the two fermions constitutes one of the strong conceptual reasons for regarding the state (5.1) as non-entangled.

The above discussion naturally leads to the question of how to characterize the set of mixed states that share the "classical-like" features of (5.1). There are at least two possible ways of extending the above discussion to the case of mixed states of systems of two identical fermions. On the one hand, we can consider the set of mixed states that are expressible as a statistical mixture of a family of pure states, each one being of the form (5.1). That is, we may consider states of the form,

$$\rho_{sep} = \sum_k \frac{p_k}{2}\left[|\phi_1^{(k)}\rangle\otimes|\phi_2^{(k)}\rangle - |\phi_2^{(k)}\rangle\otimes|\phi_1^{(k)}\rangle\right]\left[\langle\phi_1^{(k)}|\otimes\langle\phi_2^{(k)}| - \langle\phi_2^{(k)}|\otimes\langle\phi_1^{(k)}|\right], \quad (5.2)$$

where $0 \leq p_k \leq 1$, $\sum_k p_k = 1$, and the single-particle pure states $|\phi_i^{(k)}\rangle$ verify,

$$\langle\phi_i^{(k)}|\phi_j^{(k)}\rangle = \delta_{ij}. \quad (5.3)$$

Equation (5.2) represents the standard definition of a non-entangled, or separable, mixed state of two identical fermions. Notice that in (5.2) no special relation between states $|\phi_i^{(k)}\rangle$ with different values of the label k is assumed. In particular, the overlap between two states with different labels k is not necessarily equal to 0 or 1. This, in turn, means that the overlap between two different members of the family of (separable) two-fermion pure states participating in the statistical mixture leading to (5.2) may be non-zero.

The above considerations suggest an alternative, and complementary, way of extending to mixed states the "classical-like" features exhibited by pure states of the form (5.1). One can consider statistical mixtures of states like (5.1) such that for all these states the two (complete) sets of properties associated with the pair

of particles belong to the same family $\mathcal{F}$ of mutually exclusive sets of (complete) single-particle properties. This family $\mathcal{F}$ corresponds to an orthonormal basis $\{|\alpha_i\rangle, i = 1, 2, 3, \ldots\}$ of the single-particle Hilbert space. Such a state then has the form

$$\rho_{class} = \sum_{i<j} \frac{p_{ij}}{2} \big[|\alpha_i\rangle \otimes |\alpha_j\rangle - |\alpha_j\rangle \otimes |\alpha_i\rangle\big] \big[\langle\alpha_i| \otimes \langle\alpha_j| - \langle\alpha_j| \otimes \langle\alpha_i|\big], \tag{5.4}$$

with $0 \leq p_{ij} \leq 1$, $\sum_{i<j} p_{ij} = 1$. The density operator (5.4) is diagonal in an orthonormal basis of the two-fermion state space consisting of all the states of the Slater determinant form, $\frac{1}{\sqrt{2}}(|\alpha_i\rangle \otimes |\alpha_j\rangle - |\alpha_j\rangle \otimes |\alpha_i\rangle)$, $i < j$, that can be constructed with states belonging to the single-particle basis $\{|\alpha_i\rangle\}$. Such a basis of the two-fermion system will be called a "Slater basis". We shall say that this Slater basis is constructed from, or induced or generated by the single-particle orthonormal basis $\{|\alpha_i\rangle\}$. Let us now consider a single-particle non-degenerate observable A_{sp} with eigenbasis $\{|\alpha_i\rangle\}$ and corresponding eigenvalues $\{a_i\}$, $A_{sp} = \sum_i a_i |\alpha_i\rangle\langle\alpha_i|$, and also the two-fermion observable (which we also assume to be non-degenerate)

$$A = A_{sp}^{(1)} \otimes \mathbb{I}^{(2)} + \mathbb{I}^{(1)} \otimes A_{sp}^{(2)}. \tag{5.5}$$

The two-fermion observable A has as its eigenbasis the Slater basis constructed from the single-particle basis $\{|\alpha_i\rangle\}$, the eigenvalue corresponding to the eigenvector $\frac{1}{\sqrt{2}}(|\alpha_i\rangle \otimes |\alpha_j\rangle - |\alpha_j\rangle \otimes |\alpha_i\rangle)$ being $a_i + a_j$. We shall call the measurement of an observable of the form (5.5) a "local" measurement. In other words, a local measurement is a measurement in a Slater basis. To each possible outcome of the measurement of A we can associate the projector

$$P_{ij} = \frac{1}{2}\big(|\alpha_i\rangle \otimes |\alpha_j\rangle - |\alpha_j\rangle \otimes |\alpha_i\rangle\big)\big(\langle\alpha_i| \otimes \langle\alpha_j| - \langle\alpha_j| \otimes \langle\alpha_i|\big), \quad i < j. \tag{5.6}$$

These projectors satisfy,

$$\begin{aligned} P_{ij}P_{i'j'} &= P_{ij}\delta_{ii'}\delta_{jj'}, \quad i < j,\ i' < j' \\ \sum_{i<j} P_{ij} &= \mathbb{I}. \end{aligned} \tag{5.7}$$

Now, the process of measurement in quantum mechanics is associated with an alteration of the state. If the two-fermion system is initially in the state ρ, the state immediately after the measurement (and before the observation) is given by

$$\Pi(\rho) = \sum_{i<j} P_{ij}\rho P_{ij}. \tag{5.8}$$

If the initial state ρ is of the form (5.4) then one has $\Pi(\rho) = \rho$. In other words, for a state of the form (5.4) there always exists a local measurement that leaves the state undisturbed. As a particular instance of two-fermion states with this property we have the pure, separable states (5.1). We then propose to adopt this property as the criterion characterizing two-fermion states (pure or mixed) with "minimal quantum correlations". In summary, *a two-fermion state has minimal quantum correlations if there exists a local measurement that leaves the state undisturbed (in the sense that* $\Pi(\rho) = \rho$*).* To denote these two-fermion states with minimal quantum correlations we shall also use the expressions "classically correlated states" or "classical states".

It follows from the above definition of classically correlated two-fermion states that the following statements are equivalent (see Appendix A, Section 5.7),

1. The state ρ is classical.
2. There exists a local measurement, with associated projectors P_{ij} (of the form (5.6)) such that ρ commutes with each P_{ij}.
3. The state ρ can be represented as

$$\rho = \sum_{i<j} \frac{p_{ij}}{2}\big(|\alpha_i\rangle \otimes |\alpha_j\rangle - |\alpha_j\rangle \otimes |\alpha_i\rangle\big)\big(\langle\alpha_i| \otimes \langle\alpha_j| - \langle\alpha_j| \otimes \langle\alpha_i|\big) \tag{5.9}$$

for some single-particle orthonormal basis $\{|\alpha_i\rangle\}$ and some probability distribution $\{p_{ij}\}$ (normalized as $\sum_{i<j} p_{ij} = 1$).

The single-particle reduced density matrix $\rho_r = \mathrm{Tr}_2\rho = \mathrm{Tr}_1\rho$ associated with a two-fermion state of the form (5.9) is given by,

$$\rho_r = \sum_{i<j} \frac{p_{ij}}{2}\big(|\alpha_i\rangle\langle\alpha_i| + |\alpha_j\rangle\langle\alpha_j|\big). \tag{5.10}$$

5.3 Measure of quantum correlations for two-fermion systems

The above definition of classically correlated two-fermion states (or of states with minimal quantum correlations) suggests to one to adopt as a quantitative measure of quantum correlations of a two-fermion state ρ the minimum possible "distance" between ρ and the disturbed state $\Pi(\rho)$ resulting from a local measurement. That is, a measure of the form

$$\xi_D(\rho) = \inf_{\Pi} D(\rho, \Pi(\rho)), \tag{5.11}$$

where the infimum is taken over all complete local projective measurements and D may be almost any distance or divergence measure for quantum states (a similar proposal was advanced by Luo for treating systems with distinguishable subsystems [119]). To calculate ξ_D from the above definition it is necessary to implement an optimization procedure to determine the local measurement leading to the minimal disturbance, which is in general a very difficult problem. A more tractable approach is given by the expression

$$\xi_D^{sp}(\rho) = D(\rho, \Pi_{sp}(\rho)), \tag{5.12}$$

where the measurement Π_{sp} is the one induced by the spectral resolution of the single-particle reduced state ρ_r. That is, in (5.12) we consider a local measurement in the Slater basis constructed from the (single-particle) eigenbasis of ρ_r. The main problem with the measure (5.12) is that it is not unique when ρ_r has degenerate eigenvalues. This problem obviously disappears if one introduces in (5.12) a minimization over all the Slater bases induced by an eigenbasis of ρ_r. If we call these bases "local bases", we can then adopt the measure

$$\xi_D^{local}(\rho) = \inf_{\text{local bases}} D(\rho, \Pi_{sp}(\rho)). \tag{5.13}$$

It is clear that a measurement associated with a local basis leaves the single-particle reduced density matrix ρ_r undisturbed.

A convenient way of implementing the above ideas is the one advanced by

SaiToh *et al.* [204] in the case of distinguishable subsystems: we can define as a measure of correlations,

$$\xi(\rho) = \min_{\text{local bases}} S[\Pi(\rho)] - S[\rho]. \tag{5.14}$$

This is the measure we are going to use in order to characterize the quantum correlations in systems of two identical fermions. Notice that we always have $S[\Pi(\rho)] \geq S[\rho]$ and, consequently, the measure (5.14) is always a non-negative quantity. In fact, it vanishes if and only if ρ is a classically correlated state.

In order to evaluate (5.14) we have to determine the local measurement that minimizes $S[\Pi(\rho)]$ under the constraint that ρ_r remains undisturbed (from here on, unless the contrary is explicitly stated, this constraint is always assumed when we discuss optimization processes over the set of local measures or, equivalently, over the set of Slater bases). As we are going to see in the following Sections, in many cases this optimization problem can be conveniently tackled using the concept of majorization. Let us consider a local measurement associated with the Slater basis $\{|sl_1\rangle, |sl_2\rangle, \ldots\}$. We denote by $\lambda^{(\Pi(\rho))} = \{\langle sl_1|\rho|sl_1\rangle, \ldots\}$ the eigenvalues of $\Pi(\rho)$. If we now compare two local measurements, we have that

$$\lambda^{(\Pi(\rho))} \prec \lambda^{(\Pi^*(\rho))} \rightarrow S[\Pi^*(\rho)] \leq S[\Pi(\rho)]. \tag{5.15}$$

Consequently, if we find a local measurement associated with a Slater basis $\{|sl_i^*\rangle\}$ such that the eigenvalues $\lambda^{(\Pi^*(\rho))}$ satisfy $\lambda^{(\Pi(\rho))} \prec \lambda^{(\Pi^*(\rho))}$ for any other local measurement, then we have that

$$\xi(\rho) \;=\; S[\Pi^*(\rho)] - S[\rho]. \tag{5.16}$$

Summing up, the optimization problem is solved if one finds a local measurement such that the set of eigenvalues $\lambda^{(\Pi^*(\rho))}$ majorizes the set of eigenvalues $\lambda^{(\Pi(\rho))}$ associated with any other local measurement.

5.4 Pure states of two identical fermions

First I am going to analyze the quantum correlations exhibited by pure states of a two-fermion system. So I am going to evaluate the measure $\xi(\rho)$ defined in eq. (5.14) on a pure state $\rho = |\psi\rangle\langle\psi|$ of a two-fermion system with a single-particle Hilbert space of dimension $2k$, $k \geq 2$. In order to evaluate $\xi(\rho)$ in this case it will prove convenient to use the fermionic Schmidt decomposition of the state $|\psi\rangle$. It is always possible to find an orthonormal basis $\{|1\rangle, |2\rangle, ..., |2k\rangle\}$ of the single-particle Hilbert space (the "Schmidt basis") such that the state $|\psi\rangle$ can be cast as,

$$|\psi\rangle = \sum_{i=1}^{k} \sqrt{\frac{\lambda_i}{2}} \big(|2i-1\rangle|2i\rangle - |2i\rangle|2i-1\rangle\big), \tag{5.17}$$

with the Schmidt coefficients λ_i satisfying $0 \leq \lambda_i \leq 1$ and $\sum_{i=1}^{k} \lambda_i = 1$. The single-particle reduced density operator is,

$$\rho_r = \sum_{i=1}^{k} \frac{\lambda_i}{2} \big(|2i-1\rangle\langle 2i-1| + |2i\rangle\langle 2i|\big), \tag{5.18}$$

so that the Schmidt basis is an eigenbasis of ρ_r, and the halved Schmidt coefficients, $\lambda_i/2$, are the eigenvalues of ρ_r. Notice that each of these eigenvalues is (at least) two-fold degenerate. Since in this case we have $S[\rho] = 0$, the correlations measure (5.14) reduces to the infimum of $S[\Pi(\rho)]$ over all the possible local measurements.

Let us first discuss the case where the k Schmidt coefficients are all different. Each eigenvalue of ρ_r is then two-fold degenerate: the eigenvectors $|2i-1\rangle$ and $|2i\rangle$ of ρ_r share the same eigenvalue $\lambda_i/2$. Consequently, we have to minimize $S[\Pi(\rho)]$ over all possible local bases consisting of Slater determinants constructed from single-particle bases of the form,

$$\begin{aligned} |\varepsilon_i\rangle &= c_{11}^{(i)}|2i-1\rangle + c_{12}^{(i)}|2i\rangle, \\ |\varepsilon_i^{\perp}\rangle &= c_{21}^{(i)}|2i-1\rangle + c_{22}^{(i)}|2i\rangle, \quad i = 1, \ldots, k, \end{aligned} \tag{5.19}$$

with appropriate coefficients $c_{jl}^{(i)}$ such that $|\varepsilon_i\rangle$ and $|\varepsilon_i^{\perp}\rangle$ are normalized and orthogonal. However, it can be verified that, for any of these local bases we have

$$\Pi(\rho) = \sum_{i=1}^{k} \frac{\lambda_i}{2} \big(|2i-1\rangle|2i\rangle - |2i\rangle|2i-1\rangle\big)\big(\langle 2i-1|\langle 2i| - \langle 2i|\langle 2i-1|\big). \tag{5.20}$$

That is, in this case the disturbed two-fermion density operator $\Pi(\rho)$ is the same for all the possible local bases. Consequently, $S[\Pi(\rho)]$ is constant over all the associated local measurements, and so we have that the quantum correlations measure is,

$$\xi(\rho) \;=\; -\sum_{i=1}^{k} \lambda_i \log_2 \lambda_i. \tag{5.21}$$

Now, suppose that two or more λ_i's are equal. Assume, for instance, that t Schmidt coefficients have the same value, $\lambda_{j_i} = \lambda$, $i = 1, 2, \ldots, t$. In such a case we have within the Schmidt expansion of $|\psi\rangle$ a term of the form,

$$\sqrt{\frac{\lambda}{2}} \sum_{i=1}^{t} \Big(|2j_i-1\rangle|2j_i\rangle - |2j_i\rangle|2j_i-1\rangle\Big), \tag{5.22}$$

with $t \leq k$. The eigenvalue $\lambda/2$ of ρ_r is then $2t$-fold degenerate. Consequently, within the single-particle orthonormal basis inducing the local (Slater) two-fermion basis we can substitute the set $\{|2j_i-1\rangle, |2j_i\rangle,\, i = 1, 2, \ldots, t\}$ by any other set of $2t$ orthonormal linear combinations of these vectors. The corresponding two-fermion local basis (characterizing a local measurement) will then include the $t(2t-1)$ Slater determinants constructed with these new $2t$ single-particle vectors. Let us now compare the set of eigenvalues $\lambda^{(\Pi(\rho))}$ of the disturbed density matrix $\Pi(\rho)$ associated with this new local basis (resulting from the above substitution) with the set $\lambda^{(\mathrm{Sch})} = \{\lambda_1, \lambda_2, \ldots, \lambda_k, 0, \ldots\}$ of eigenvalues of the disturbed density matrix $\Pi^{(\mathrm{Sch})}(\rho)$ associated with the local (Slater) basis induced by the Schmidt basis $\{|1\rangle, |2\rangle, \ldots, |2k\rangle\}$. Let $|\zeta\rangle$ be one of the Slater determinants constructed with two of the abovementioned orthonormal linear combinations of the states $\{|2j_i-1\rangle, |2j_i\rangle,\, i = 1, 2, \ldots, t\}$. It can be shown, after some algebra (see

Appendix B, Section 5.8), that

$$\left|\langle\zeta|\frac{1}{\sqrt{2}}\sum_{i=1}^{t}\Big(|2j_i-1\rangle|2j_i\rangle-|2j_i\rangle|2j_i-1\rangle\Big)\right|\leq 1. \tag{5.23}$$

This means that, as a result of the abovementioned substitution, the eigenvalue λ, which appears t times in $\lambda^{(\mathrm{Sch})}$, is substituted in $\lambda^{(\Pi(\rho))}$ by a new set of eigenvalues, each one of them less or equal to λ, and adding up to $t\lambda$. This substitution leads to a $\lambda^{(\Pi(\rho))}$ that is majorized by $\lambda^{(\mathrm{Sch})}$. That is, we have

$$\lambda^{(\Pi(\rho))}\prec\lambda^{(\mathrm{Sch})}, \tag{5.24}$$

and thus

$$-\sum_{i=1}^{k}\lambda_i\log_2\lambda_i\leq S[\Pi(\rho)], \tag{5.25}$$

meaning that the quantum correlation measure for the pure two-fermion state is again given by (5.21).

The expression on the right hand side of equation (5.21) coincides with the amount of entanglement of the two-fermion pure state $|\psi\rangle$. This means that, in the case of pure states the concept of quantum correlation for two-fermion systems introduced here by us coincides with entanglement. In particular, our measure vanishes for a pure state if and only if this state has Slater rank equal to one (that is, if we have one Schmidt coefficient $\lambda_l=1$ and $\lambda_i=0\;\forall\, i\neq l$).

5.5 Mixed states of two identical fermions

In this Section I shall compute analytically the above-introduced measure of quantum correlations for some relevant instances of mixed states of two-fermion systems. Here we shall use the angular momentum representation for two-fermion states, as described in Subsection 2.5.1. Within this representation, the states $|j,m\rangle$ constitute a natural basis for the two-fermion state space. We use a compact notation according to which, for instance, the ket $|0,0\rangle$ stands for $|j=0,m=0\rangle$.

I first consider fermions with a single-particle Hilbert space of dimension four. We shall evaluate the correlation measure for the state,

$$\rho = p|0,0\rangle\langle 0,0| + (1-p)\rho_{mix}, \tag{5.26}$$

where

$$\rho_{mix} = \frac{1}{6}\big(|0,0\rangle\langle 0,0| + \sum_{m=-2}^{2} |2,m\rangle\langle 2,m|\big) \tag{5.27}$$

is the totally mixed state of the two-fermion system. The state (5.26) is entangled if $p > 0.4$. The single-particle reduced density matrix ρ_r corresponding to this state is proportional to the identity matrix. Then, the choice of the local measurement (in a Slater basis constructed from an eigenbasis of ρ_r) is not uniquely defined. Using the majorization technique we can optimize this local measurement, finding the one leading to the disturbed matrix $\Pi^*(\rho)$ of minimum entropy.

When performing a local measurement on ρ the eigenvalues of the resulting $\Pi(\rho)$ are of the form,

$$\langle Sl|\rho|Sl\rangle = p|\langle Sl|0,0\rangle|^2 + \frac{1-p}{6}, \tag{5.28}$$

where $|Sl\rangle$ is a two-fermion state of Slater rank 1. For these states one always has $|\langle Sl|0,0\rangle|^2 \leq \frac{1}{2}$, see eq. (4.16). Equality here can be achieved by $|Sl\rangle = \frac{1}{\sqrt{2}}[|\frac{3}{2}\rangle|\text{-}\frac{3}{2}\rangle - |\text{-}\frac{3}{2}\rangle|\frac{3}{2}\rangle]$ [130].

Let us first consider the local measurement performed in the Slater basis generated from the single-particle basis $\{|\frac{3}{2}\rangle, |\frac{1}{2}\rangle, |\text{-}\frac{1}{2}\rangle, |\text{-}\frac{3}{2}\rangle\}$ (we shall sometimes refer to this basis as $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$). Let $\Pi^*(\rho)$ denote the density matrix resulting from this local measurement, and $\lambda^{(\Pi^*(\rho))} = \{\lambda_1^*, \ldots, \lambda_6^*\}$ the corresponding set of eigenvalues. We now prove that that this set majorizes the eigenvalues $\lambda^{(\Pi(\rho))} = \{\lambda_1, \ldots, \lambda_6\}$ corresponding to any other local measurement. The members of $\lambda^{(\Pi^*(\rho))}$ are $\lambda_1^* = \lambda_2^* = \frac{p}{2} + \frac{1-p}{6}$ and $\lambda_3^* = \cdots = \lambda_6^* = \frac{1-p}{6}$. The eigenvalues of the operator $\Pi(\rho)$ corresponding to a general local measurement are of the form,

$$\langle Sl_i|\rho|Sl_i\rangle = p\epsilon_i + \frac{1-p}{6}, \qquad 0 \leq \epsilon_i \leq \frac{1}{2}; \ \sum_{i=1}^{6} \epsilon_i = 1. \tag{5.29}$$

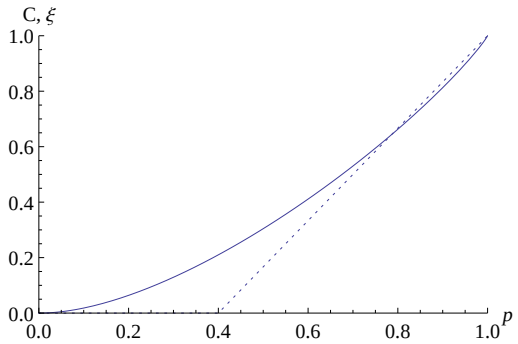


Figure 5.1: $\xi(\rho)$ (solid line) and concurrence (dotted line) for the state given by eq. (5.26).

The majorization inequalities $\sum_{i=1}^{t} \lambda_i^* \geq \sum_{i=1}^{t} \lambda_i$, $1 \leq t \leq 6$ are then satisfied, and consequently we have that $\lambda^{(\Pi(\rho))} \prec \lambda^{(\Pi^*(\rho))}$, meaning that the quantum correlations measure is equal to $S[\Pi^*(\rho)] - S[\rho]$. Thus, for the state (5.26) we have,

$$\xi(\rho) = \frac{1-p}{6} \log_2 \frac{1-p}{6} + \frac{1+5p}{6} \log_2 \frac{1+5p}{6} - \frac{1+2p}{3} \log_2 \frac{1+2p}{6}. \tag{5.30}$$

The concurrence of this state is given by

$$C(\rho) = \begin{cases} 0, & \text{if } 0 \leq p \leq 0.4 \\ \frac{5p-2}{3}, & \text{if } 0.4 < p \leq 1. \end{cases} \tag{5.31}$$

When $p = 1$, the state (5.26) is a pure, maximally entangled state of two fermions, and the quantum correlations measure adopts its maximum value, $\xi(\rho) = 1$. On the other hand, when $p = 0$ the state is equal to the maximally mixed one, ρ_{mix} and in this case $\xi(\rho) = 0$. However, we have non-vanishing quantum correlations, i.e. $\xi(\rho) \neq 0$, for non-entangled states. $\xi(\rho)$ can be larger than the concurrence for some states and it can be smaller for other states, see Fig. 5.1. In this respect, the behaviour of the fermionic quantum correlations measure exhibits some similarities with the behaviour of the quantum correlations measure corresponding to distinguishable systems [202].

The previous example admits a generalization to systems of two identical

fermions with a d-dimensional single-particle Hilbert space. Let $d^* = \frac{d(d-1)}{2}$ denote the dimension of the corresponding two-fermion state space. We consider states consisting of a mixture of a maximally entangled state $|\psi\rangle$ and the maximally mixed one,

$$\rho = p|\psi\rangle\langle\psi| + (1-p)\frac{2}{d(d-1)}\mathbb{I}. \tag{5.32}$$

Here $\mathbb{I}$ is the $d^* \times d^*$ identity matrix, and $|\psi\rangle$ can be written as a superposition of non-overlapping Slater terms

$$|\psi\rangle = \frac{1}{\sqrt{d}}\big[|2\rangle|1\rangle - |1\rangle|2\rangle + |4\rangle|3\rangle - |3\rangle|4\rangle + ... + |d\rangle|d-1\rangle - |d-1\rangle|d\rangle\big], \tag{5.33}$$

where $\{|1\rangle, |2\rangle, \ldots, |d\rangle\}$ is a single-particle orthonormal basis. Let

$$|Sl\rangle = \frac{1}{\sqrt{2}}\big[|\phi_1\rangle|\phi_2\rangle - |\phi_2\rangle|\phi_1\rangle\big], \tag{5.34}$$

be an arbitrary pure state of Slater rank one, constructed from the pair of orthonormalized single-particle states, $|\phi_1\rangle$ and $|\phi_2\rangle$. Then

$$|\langle\psi|Sl\rangle| \leq \sqrt{\frac{2}{d}}, \tag{5.35}$$

with equality obtained for states of the form $\frac{1}{\sqrt{2}}(|l+1\rangle|l\rangle - |l\rangle|l+1\rangle)$, see Appendix B (Section 5.8). The eigenvalues of ρ are $\frac{(1-p)}{d^*}$ with multiplicity $d^* - 1$ and $p + \frac{1-p}{d^*}$ with multiplicity 1, and the single-particle reduced density operator is $\rho_r = \mathbb{I}/d$.

Let $\Pi^*(\rho)$ denote the density matrix resulting from the local measurement associated with the Slater basis generated by the single-particle basis $\{|1\rangle, \ldots, |d\rangle\}$, and $\lambda^{(\Pi^*(\rho))} = \{\lambda_1^*, \ldots, \lambda_{d^*}^*\}$ the corresponding set of eigenvalues. Let $\lambda^{(\Pi(\rho))} = \{\lambda_1, \ldots, \lambda_{d^*}\}$ be the eigenvalues of the $\Pi(\rho)$ corresponding to any other local measurement. The members of $\lambda^{(\Pi^*(\rho))}$ are $\frac{p(d-2)+1}{d^*}$ with multiplicity $\frac{d}{2}$ and $\frac{1-p}{d^*}$ with multiplicity $\frac{d(d-2)}{2}$. On the other hand, due to (5.35), the members of $\lambda^{(\Pi(\rho))}$ are of the form $p\epsilon_i + \frac{1-p}{d^*}$, with $\epsilon_i \leq \frac{2}{d}$ and $\sum_{i=1}^{d^*} \epsilon_i = 1$. It follows that $\lambda^{(\Pi(\rho))} \prec \lambda^{(\Pi^*(\rho))}$,

and therefore we have,

$$\begin{aligned}\xi(\rho) &= S[\Pi^*(\rho)] - S[\rho] \\ &= (d^*-1)\frac{(1-p)}{d^*}\log_2\frac{(1-p)}{d^*} + \left(p+\frac{1-p}{d^*}\right)\log_2\left(p+\frac{1-p}{d^*}\right) \\ &\quad -\frac{d(d-2)}{2}\frac{(1-p)}{d^*}\log_2\frac{(1-p)}{d^*} - \frac{d}{2}\frac{p(d-2)+1}{d^*}\log_2\frac{p(d-2)+1}{d^*}. \quad (5.36)\end{aligned}$$

We shall now compute the quantum correlations measure of the state

$$\rho = p|0,0\rangle\langle 0,0| + (1-p)\big[q|2,-2\rangle\langle 2,-2| + (1-q)|2,2\rangle\langle 2,2|\big], \quad (5.37)$$

with $0 \leq p, q \leq 1$. It will prove convenient to rewrite this state under the guise $\rho = p\rho_1 + (1-p)\rho_2$, where $\rho_1 = |0,0\rangle\langle 0,0|$ and $\rho_2 = q|2,-2\rangle\langle 2,-2| + (1-q)|2,2\rangle\langle 2,2|$. Then, it is possible to prove that the set of eigenvalues $\lambda^{(\Pi^*(\rho))}$ of the density matrix $\Pi^*(\rho)$ resulting from the local measurement in the Slater basis generated by the single-particle states $\{|\frac{3}{2}\rangle, |\frac{1}{2}\rangle, |\text{-}\frac{1}{2}\rangle, |\text{-}\frac{3}{2}\rangle\}$ is the one that majorizes the set of eigenvalues $\lambda^{(\Pi(\rho))}$ associated with any other local measurement. The single-particle reduced states corresponding to the three states ρ, ρ_1 and ρ_2 are all diagonal in the same single-particle basis. Consequently, these three states share the same family of admissible local measurements. Our strategy will be to show that the local measurement in the Slater basis associated with the single-particle basis $\{|\frac{3}{2}\rangle, |\frac{1}{2}\rangle, |\text{-}\frac{1}{2}\rangle, |\text{-}\frac{3}{2}\rangle\}$ is the optimal one both for ρ_1 and ρ_2, and then conclude that it is optimal for ρ as well. To that effect first note that, if one has four probability distributions $\lambda^{(1)}$, $\lambda^{(1*)}$, $\lambda^{(2)}$, $\lambda^{(2*)}$, such that $\lambda^{(1)} \prec \lambda^{(1*)}$ and $\lambda^{(2)} \prec \lambda^{(2*)}$ then for any p $(0 \leq p \leq 1)$ we have that

$$p\lambda^{(1)} + (1-p)\lambda^{(2)} \prec p\lambda^{(1*)} + (1-p)\lambda^{(2*)}. \quad (5.38)$$

Now, it is clear that for any local measurement we have $\lambda^{(\Pi(\rho_1))} \prec \lambda^{(\Pi^*(\rho_1))}$, since this is a particular instance of the previously considered case corresponding to the state (5.26). Now, the state ρ_2 is a convex linear combination of the states $\rho_{2a} = |2,-2\rangle\langle 2,-2|$ and $\rho_{2b} = |2,2\rangle\langle 2,2|$. It is clear that $\lambda^{(\Pi(\rho_{2a}))} \prec \lambda^{(\Pi^*(\rho_{2a}))}$ and $\lambda^{(\Pi(\rho_{2b}))} \prec \lambda^{(\Pi^*(\rho_{2b}))}$, since for both $\lambda^{(\Pi^*(\rho_{2a}))}$ and $\lambda^{(\Pi^*(\rho_{2b}))}$ we have one eigenvalue equal to 1 and the rest equal to zero (remember that the states $|2,-2\rangle$ and $|2,2\rangle$ are themselves members of the Slater basis induced by the single-particle

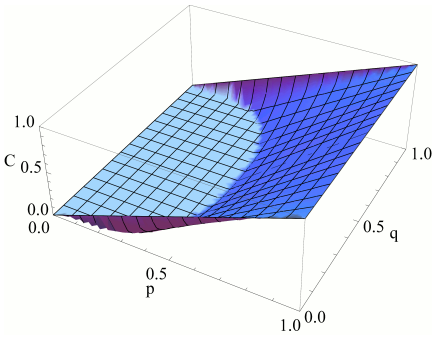


Figure 5.2: Concurrence for the state given by (5.37).

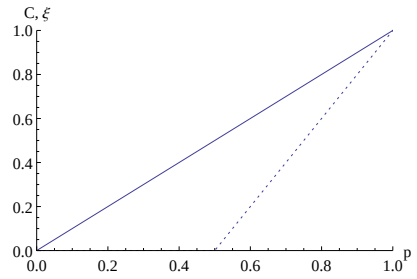


Figure 5.3: $\xi(\rho)$ (solid line) and concurrence (dotted line) for the state given by eq. (5.37). For this state $\xi(\rho)$ does not depend on q. The concurrence is evaluated by setting $q = \frac{1}{2}$.

basis $\{|\frac{3}{2}\rangle, |\frac{1}{2}\rangle, |\text{-}\frac{1}{2}\rangle, |\text{-}\frac{3}{2}\rangle\}$). Then, since $\lambda^{(\Pi(\rho_2))} = q\lambda^{(\Pi(\rho_{2a}))} + (1-q)\lambda^{(\Pi(\rho_{2b}))}$ and $\lambda^{(\Pi^*(\rho_2))} = q\lambda^{(\Pi^*(\rho_{2a}))} + (1-q)\lambda^{(\Pi^*(\rho_{2b}))}$ it follows from (5.38) that $\lambda^{(\Pi(\rho_2))} \prec \lambda^{(\Pi^*(\rho_2))}$. Then, taking into account that for any local measurement we have $\lambda^{(\Pi(\rho))} = p\lambda^{(\Pi(\rho_1))} + (1-p)\lambda^{(\Pi(\rho_2))}$, and applying once more the relation (5.38), we obtain that $\lambda^{(\Pi(\rho))} \prec \lambda^{(\Pi^*(\rho))}$.
So finally we find that

$$\xi(\rho) = p. \tag{5.39}$$

We also compute the concurrence $C(\rho) = C(p,q)$, see Figure 5.2. For $q = \frac{1}{2}$ we obtain

$$C(\rho) = \begin{cases} 0, & \text{if } 0 \le p \le 0.5 \\ 2p-1, & \text{if } 0.5 < p \le 1. \end{cases} \tag{5.40}$$

Note that in this case ρ is entangled for $p > 0.5$. We plot the concurrence and $\xi(\rho)$ in Fig. 5.3 for this state, with $q = \frac{1}{2}$.

I now consider the following state,

$$\rho = p|\Psi\rangle\langle\Psi| + (1-p)\rho_{mix}, \tag{5.41}$$

with ρ_{mix} as in eq. (5.27) and

$$|\Psi\rangle = \frac{\sin\theta}{\sqrt{2}}\left[\left|\text{-}\frac{3}{2}\right\rangle\left|\frac{3}{2}\right\rangle - \left|\frac{3}{2}\right\rangle\left|\text{-}\frac{3}{2}\right\rangle\right] + \frac{\cos\theta}{\sqrt{2}}\left[\left|\text{-}\frac{1}{2}\right\rangle\left|\frac{1}{2}\right\rangle - \left|\frac{1}{2}\right\rangle\left|\text{-}\frac{1}{2}\right\rangle\right]. \tag{5.42}$$

The eigenvalues of ρ are $\{\frac{1-p}{6},...,\frac{1-p}{6},\frac{1+5p}{6}\}$ and the eigenvalues of the single-particle reduced density matrix ρ_r are $\frac{p\sin^2\theta}{2}+\frac{(1-p)}{4}$ (corresponding to the eigenvectors $|\text{-}\frac{3}{2}\rangle$ and $|\frac{3}{2}\rangle$) and $\frac{p\cos^2\theta}{2}+\frac{(1-p)}{4}$ (corresponding to the eigenvectors $|\text{-}\frac{1}{2}\rangle$ and $|\frac{1}{2}\rangle$). The admissible local measurements are thus those done in the Slater basis generated by a single-particle orthonormal basis $\{|\alpha_l\rangle\}$ consisting of four states of the form,

$$\begin{aligned}
|\alpha_1\rangle &= d_{11}\Big|\text{-}\frac{3}{2}\Big\rangle + d_{12}\Big|\frac{3}{2}\Big\rangle,\\
|\alpha_2\rangle &= d_{21}\Big|\text{-}\frac{3}{2}\Big\rangle + d_{22}\Big|\frac{3}{2}\Big\rangle,\\
|\alpha_3\rangle &= d_{31}\Big|\text{-}\frac{1}{2}\Big\rangle + d_{32}\Big|\frac{1}{2}\Big\rangle,\\
|\alpha_4\rangle &= d_{41}\Big|\text{-}\frac{1}{2}\Big\rangle + d_{42}\Big|\frac{1}{2}\Big\rangle,
\end{aligned} \tag{5.43}$$

with complex coefficients d_{ij} such that the vectors $\{|\alpha_l\rangle\}$ are orthonormal. Now, it can be verified after some algebra that the eigenvalues of the statistical operator $\Pi(\rho)$ resulting from any of these local measurements are always the same (that is, they do not depend on the particular values adopted by the coefficients d_{ij}). These eigenvalues are $\{\frac{1-p}{6},...,\frac{1-p}{6},\frac{1-p}{6}+p\cos^2\theta,\frac{1-p}{6}+p\sin^2\theta\}$. Consequently, we have $\xi(\rho)=S[\Pi(\rho)]-S[\rho]$, yielding

$$\begin{aligned}
\xi(\rho) &= \frac{1-p}{6}\log_2\frac{1-p}{6}+\frac{1+5p}{6}\log_2\frac{1+5p}{6}\\
&\quad -\left[\frac{1-p}{6}+p\cos^2\theta\right]\log_2\left[\frac{1-p}{6}+p\cos^2\theta\right]\\
&\quad -\left[\frac{1-p}{6}+p\sin^2\theta\right]\log_2\left[\frac{1-p}{6}+p\sin^2\theta\right].
\end{aligned} \tag{5.44}$$

The concurrence of the state (5.41) is,

$$C=\frac{1}{6}\Big(\sqrt{c_1+c_2}-\sqrt{c_1-c_2}\Big)-4\frac{1-p}{6}, \tag{5.45}$$

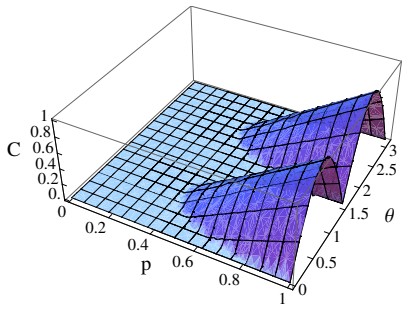
where c_1 and c_2 are given by the following expressions,

$$\begin{aligned}
c_1 &= 1+4p+4p^2-9p^2\cos(4\theta)\\
c_2 &= 3p\sqrt{2\big[2+8p-p^2(1+9\cos(4\theta))\big]}\,\big|\sin(2\theta)\big|.
\end{aligned} \tag{5.46}$$

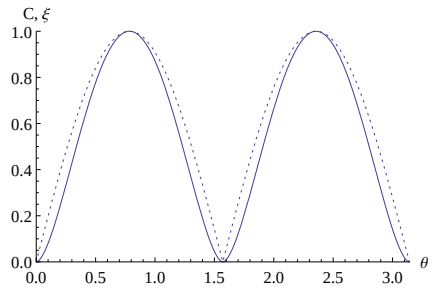
I plot the concurrence and ξ for this state in Figures 5.4(a) and 5.4(b) respectively. Setting $p = 1$ gives $\rho = |\Psi\rangle\langle\Psi|$ and so we obtain

$$\xi(\rho, p = 1) = -\sin^2\theta \log_2(\sin^2\theta) - \cos^2\theta \log_2(\cos^2\theta). \tag{5.47}$$

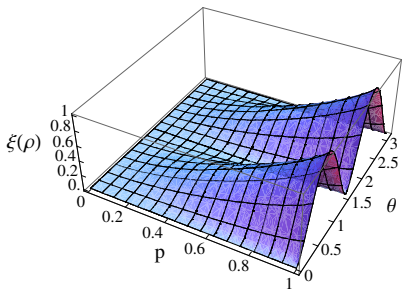
We plot the slice $p = 1$ in Fig. 5.4(c) and the difference $C(\rho) - \xi(\rho)$ in Fig. 5.4(d).



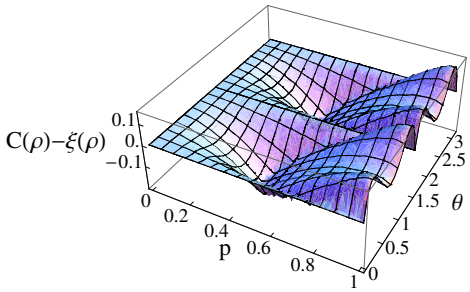
(a) Concurrence as a function of p and θ.



(c) $\xi(\rho)$ (solid line) and concurrence (dotted line) for $p = 1$.



(b) $\xi(\rho)$ as a function of p and θ.



(d) Difference between concurrence and $\xi(\rho)$, C is not always larger than ξ.

Figure 5.4: The graphs pertain to the state given by eq. (5.41).

We consider now a mixture of two orthogonal, maximally entangled states,

$$\begin{aligned} |\phi_1\rangle &= \frac{1}{\sqrt{2}}\big(|12| + |34|\big) \\ |\phi_2\rangle &= \frac{1}{\sqrt{2}}\big(|12| - |34|\big), \end{aligned} \tag{5.48}$$

where $|ij| = (|ij\rangle - |ji\rangle)/\sqrt{2}$. That is, we shall now study the state,

$$\rho = p|\phi_1\rangle\langle\phi_1| + (1-p)|\phi_2\rangle\langle\phi_2|. \tag{5.49}$$

The concurrence of (5.49) is given by $C = |2p-1|$. The eigenvalues of the state $\Pi^*(\rho)$ resulting from a local measurement in the Slater basis induced by the single-particle basis $\{|1\rangle = |\frac{3}{2}\rangle, |2\rangle = |\text{-}\frac{3}{2}\rangle, |3\rangle = |\frac{1}{2}\rangle, |4\rangle = |\text{-}\frac{1}{2}\rangle\}$, are $\lambda^{(\Pi^*(\rho))} = \left\{\frac{1}{2}, \frac{1}{2}, 0, 0, 0, 0\right\}$. Now, for any two-fermion state $|Sl\rangle$ of Slater rank 1 we have

$$\begin{aligned} \langle Sl|\rho|Sl\rangle &= p|\langle\phi_1|Sl\rangle|^2 + (1-p)|\langle\phi_2|Sl\rangle|^2 \\ &\leq \frac{1}{2}. \end{aligned} \tag{5.50}$$

Thus, the two non-vanishing eigenvalues of $\Pi^*(\rho)$ adopt the maximum possible value, equal to $\frac{1}{2}$. It is plain then that $\lambda^{(\Pi^*(\rho))}$ majorizes the set of eigenvalues $\lambda^{(\Pi(\rho))}$ corresponding to any other possible local measurement. This leads to a quantum correlations measure for (5.49) equal to,

$$\xi(\rho) = 1 + p\log_2 p + (1-p)\log_2(1-p). \tag{5.51}$$

5.6 Conclusions

I introduced an approach for the analysis of quantum correlations in fermion systems based upon the state disturbances generated by the measurement of "local" observables (that is, quantum observables represented by one-body operators). The concomitant concept of quantum correlations in systems of identical fermions differs from entanglement. According to this approach the quantum states of two identical fermions exhibiting the minimum amount of quantum correlations ("classical" states) are those that are diagonal in a Slater basis (induced by a single-particle basis). We proposed a quantitative measure for the quantum correlations of two-fermion systems, and computed it analytically for some relevant states. In the case of pure states of two identical fermions the present concept of quantum correlations coincides with entanglement, and the measure of quantum correlations reduces to the amount of entanglement exhibited by the fermionic state.

5.7 Appendix A: Quantum states undisturbed by a projective measurement

Let $\{|k\rangle\}$ be an orthonormal basis of a quantum system's Hilbert space and $\{P_k = |k\rangle\langle k|\}$ the corresponding complete set of one-dimensional projectors, so that $P_k P_{k'} = \delta_{kk'} P_k$ and $\mathbb{I} = \sum_k P_k$ is the identity operator. Then, given a quantum state ρ, the following three statements are equivalent:

- (i) The state ρ is undisturbed by a measurement in the basis $\{|k\rangle\}$. That is, $\rho = \sum_k P_k \rho P_k$.
- (ii) The density operator ρ commutes with all the projectors: $P_k \rho = \rho P_k$.
- (iii) The state ρ is of the form $\rho = \sum_k \lambda_k P_k$, with $0 \leq \lambda_k \leq 1$ and $\sum_k \lambda_k = 1$.

It follows from (i) that $P_k \rho = \sum_{k'} P_k P_{k'} \rho P_{k'} = \sum_{k'} P_{k'} \rho P_{k'} P_k = \rho P_k$. Therefore (i) $\rightarrow$ (ii). Now, if ρ verifies (ii) we have $\rho = \rho \mathbb{I} = \sum_k \rho P_k = \sum_k \rho P_k P_k = \sum_k P_k \rho P_k = \sum_k \lambda_k P_k$, with $\lambda_k = \langle k|\rho|k\rangle$. Therefore, (ii) $\rightarrow$ (iii). Finally, it is clear that (iii) $\rightarrow$ (i).

The equivalence between the three statements concerning classical states of two fermions, discussed in Section 5.2, follows immediately from the above considerations if we identify the projectors $\{P_k\}$ with the projectors associated with a local measurement of the system (that is, with the projectors corresponding to a Slater basis of the two-fermion system).

5.8 Appendix B: Upper bound for the overlap between a maximally entangled state and a state of Slater rank one

A maximally entangled state of two fermions with single-particle Hilbert space of dimension d can be written as a superposition of non-overlapping Slater determinants,

$$|\psi\rangle = \frac{1}{\sqrt{d}}\big[|2\rangle|1\rangle - |1\rangle|2\rangle + |4\rangle|3\rangle - |3\rangle|4\rangle + ... + |d\rangle|d-1\rangle - |d-1\rangle|d\rangle\big], \quad (5.52)$$

5.8 Appendix B: Upper bound for the overlap between a maximally entangled state and a state of Slater rank one

where $\{|1\rangle, |2\rangle, \ldots, |d\rangle\}$ is a single-particle orthonormal basis. Let

$$|Sl\rangle = \frac{1}{\sqrt{2}}\big[|\phi_1\rangle|\phi_2\rangle - |\phi_2\rangle|\phi_1\rangle\big], \tag{5.53}$$

be an arbitrary pure state of Slater rank one, constructed from the pair of orthonormalized single-particle states, $|\phi_1\rangle = \sum_{i=1}^{d} \alpha_i|i\rangle$ and $|\phi_2\rangle = \sum_{i=1}^{d} \beta_i|i\rangle$. Then

$$\langle\psi|Sl\rangle = \sqrt{\frac{2}{d}}\big[\alpha_2\beta_1 - \alpha_1\beta_2 + \alpha_4\beta_3 - \alpha_3\beta_4 + ... + \alpha_d\beta_{d-1} - \alpha_{d-1}\beta_d\big] \tag{5.54}$$

$$\begin{aligned} |\langle\psi|Sl\rangle| &= \sqrt{\frac{2}{d}}\big|\alpha_2\beta_1 - \alpha_1\beta_2 + \alpha_4\beta_3 - \alpha_3\beta_4 + ... + \alpha_d\beta_{d-1} - \alpha_{d-1}\beta_d\big| \\ &\leq \sqrt{\frac{2}{d}}\big[|\alpha_2||\beta_1| + |\alpha_1||\beta_2| + |\alpha_4||\beta_3| + |\alpha_3||\beta_4| + ... \\ &\qquad + |\alpha_d||\beta_{d-1}| + |\alpha_{d-1}||\beta_d|\big] \end{aligned} \tag{5.55}$$

and using the Schwarz inequality we obtain

$$|\langle\psi|Sl\rangle| \leq \sqrt{\frac{2}{d}}. \tag{5.56}$$

The equality is obtained for states of the form

$$|Sl\rangle = \frac{1}{\sqrt{2}}\big(|l+1\rangle|l\rangle - |l\rangle|l+1\rangle\big). \tag{5.57}$$

Chapter 6

Conclusions

The first theme of the present work was to explore some aspects of the dynamics of information in both classical and quantum mechanical systems. The relevant background was provided in Chapter 1, while the new work done in this direction was presented in Chapter 3.

The second topic concerned entanglement in fermion systems and this was analyzed by means of the classification and quantification of entanglement in fermionic systems. The necessary background material was given in Chapter 2, followed by several new entanglement indicators and entanglement measures being advanced in Chapter 4. In Chapter 5 an approach for the characterization of quantum correlations going beyond entanglement was investigated for fermionic systems.

Besides background material, Chapters 1 and 2 also contained some new results. In Chapter 1 I presented an alternative and more intuitive proof of the no-broadcasting theorem. In Chapter 2 I included an exploration of some entanglement features of an exactly solvable SU2 many-body model.

In Chapter 3 I investigated extended Landauer-like principles that were based amongst others on the conservation of information of divergenceless dynamical systems. Conservation of information within the framework of general probabilistic theories, which included the classical and quantum mechanical probabilities as particular instances, was explored. Furthermore, in the context of general

probabilistic theories, Zurek's information transfer theorem and the no-deleting theorem were generalized.

In Section 3.1 I developed extended Landauer-like principles valid within scenarios involving general dynamical systems exhibiting divergenceless phase space flows. Two fundamental features of Shannon's information measure $S[F]$ lead to these Landauer-like results:

- The conservation of S under the Liouville's ensemble dynamics associated with divergenceless systems.
- The subadditive character of S.

The profound links between Landauer's principle and the second law of thermodynamics [22] suggest that the present results may help to explore analogues of the second law in non-standard contexts, like the biological ones discussed in [150, 151].

The lack of subadditivity exhibited by some important non-logarithmic information or entropic functionals seems to be a serious difficulty for deriving generalizations of Landauer's principle in terms of the non-standard maxent formalisms that are nowadays popular for the study of non-equilibrium, meta-stable states. On the other hand, the Beck-Cohen approach allows for the extension of Landauer's principle to some of those scenarios. This important issue, however, needs further exploration and the idea would be to obtain a valid formulation of Landauer-like principles directly based upon generalized, non-standard entropic measures.

Conservation of information within the framework of general probabilistic theories, which include the classical and quantum mechanical probabilities as particular instances, was explored in Section 3.2. That is, information-related aspects of the BBLW framework for probabilistic physical theories were analyzed and within this general setting I investigated the main features of a fidelity measure between pairs of states that reduced, in the case of quantum theory, to the standard fidelity measure between statistical operators. We showed that our generalized fidelity measure complies with all the basic properties (excepting

Uhlmann's theorem) satisfied by the quantum fidelity measure for density matrices. All the alluded properties admitted direct derivations not involving specific features of standard quantum theory, such as the Hilbert space formalism or the properties of density matrices.

I used the aforementioned fidelity measure to obtain a generalization to the BBLW family of probabilistic theories of Zurek's recent extension of the quantum no-cloning theorem. We considered two systems $\mathcal{S}$ and $\mathcal{A}$ interacting in such a way that a finite amount of information was transferred from $\mathcal{S}$ to $\mathcal{A}$. No matter how little information about the state of $\mathcal{S}$ was finally stored in $\mathcal{A}$ (as long as it was not strictly zero) the only initial states of $\mathcal{S}$ that were left unchanged by this process were restricted to a set of states with vanishing mutual fidelity.

In Chapter 4 I investigated several separability criteria for fermions. Criteria for the detection of entanglement were developed, based either on the violation of appropriate uncertainty relations or on inequalities that involved entropic measures.

In Section 4.1 I derived a separability criterion for states (pure or mixed) of two fermions with a single-particle Hilbert space of dimension four ($s = \frac{3}{2}$) based on the violation of local uncertainty relations. The violation of these relations provided a means of entanglement detection and also a quantitative indicator of entanglement. Then we developed separability criteria for fermion systems using sums of variances of appropriate projector operators. We implemented this type of criterion for two-fermion systems with four-dimensional ($s = \frac{3}{2}$) and six-dimensional ($s = \frac{5}{2}$) single-particle Hilbert spaces, and for systems of three identical fermions with a six-dimensional single-particle Hilbert space. In the latter two instances no analytical, closed expression for the concurrence, nor a necessary and sufficient separability criterion exists. Therefore, the present criteria for entanglement detection provided in these cases a valuable tool for the identification of families of entangled mixed states. The violation of entropic uncertainty relations was then investigated as a means of entanglement detection. Criteria were established using the Shannon, Tsallis and Rényi entropies. I also provided illustrations of families of entangled states that were detected by our

separability criteria.

In Section 4.2 new entropic entanglement criteria for systems of two identical fermions were advanced. These criteria had the form of appropriate inequalities involving the entropy of the density matrix associated with the total system, on the one hand, and the entropy of the single-particle reduced density matrix, on the other hand. I obtained entanglement criteria based upon the von Neumann, the linear, and the Rényi entropies. The criterion associated with the von Neumann entropy constituted a special instance, corresponding to the particular value $q \to 1$ of the Rényi entropic parameter, of the more general criteria associated with the Rényi family of entropies. Extensions of these criteria to systems constituted by N identical fermions were also considered.

I applied our entanglement criteria to various illustrative examples of parameterized families of mixed states, and studied the dependence of the entanglement detection efficiency on the entropic parameter q. For the two-fermion states we considered, the entanglement criterion improved as q increased and was the most efficient in the limit $q \to \infty$. For the two-fermion states with single-particle Hilbert space of dimension four, we illustrated the fact that the quantities $D_{\rm vN}$, D_L and R_q involved in the entanglement criteria that were advanced here could also be regarded as entanglement indicators, in the sense that states which exhibited large values of these quantities had higher entanglement.

In the three-fermion case we had seen that the entropic criterion based on the Rényi entropy $S_\infty^{(R)}$ was also a sufficient criterion for full three-particle entanglement. Incidentally, this was another manifestation of the fact that the most powerful entropic entanglement criterion based upon the Rényi entropy corresponds to the limit $q \to \infty$.

In Chapter 5 I introduced an approach for the analysis of quantum correlations in fermion systems which was based upon the state disturbances generated by the measurement of "local" observables (that is, quantum observables represented by one-body operators). The concomitant concept of quantum correlations in systems of identical fermions differs from entanglement. According to this approach

the quantum states of two identical fermions exhibiting the minimum amount of quantum correlations ("classical" states) are those that are diagonal in a Slater basis (induced by a single-particle basis). We proposed a quantitative measure for the quantum correlations of two-fermion systems, and computed it analytically for some relevant states. In the case of pure states of two identical fermions the present concept of quantum correlations coincided with entanglement, and the measure of quantum correlations reduced to the amount of entanglement exhibited by the fermionic state.

6.1 The End

What we call the beginning is often the end,

And to make an end is to make a beginning.

The end is where we start from...

And the end of all our exploring

Will be to arrive where we started

And know the place for the first time.
T.S. Eliot

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