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Flows of Information and Informational Trajectories in Chemical Processes

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1. Introduction

What is the importance of the concept of information measure in quantum mechanics? To answer, it is necessary to try to establish the importance of the concept of information, which is a general concept and perfectly applicable to any case. For example: What do they have in common codes used to send messages from a communications satellite and the bases of a DNA molecule? How does the second law of Thermodynamics and Communication, to the extent that is possible to speak of the entropy of a musical score? Why the intricate problems of probability is related to the way we express ourselves orally or in writing? The answer to all is *information* and the fact that one concept can link different ideas so reveals its great generality and power.

Until the forties, had not been defined information as a scientific term, and this definition was quite new, different from all the common meanings, and precisely because they were described with sufficient accuracy for mathematicians and engineers in telecommunications, the concept became more and more fascinating to the scientific community. The word began to regain some of its meanings that had fallen into disuse. The idea of information as an active agent, i.e. something that informs the material world in a manner similar to the messages of the genes that instruct the cellular machinery to build an organism.

This information emerged as a universal principle operating in the world that shapes, which specifies the special character of living forms, and even help determine, by means of special codes, forms of human thought. Thus, the information covers the disparate fields of computers, Communications Technologies, Physics, Biology, Chemistry, Mathematics, among others.

The information became a scientific concept when it began the era of electronic communication. Scientists were largely what their nineteenth-century predecessors did with the concept of energy. They turned it in theory, gave laws, festooned as usual equations and stripped it of vagueness and mystery. In its pure form, the information theory was discovered by engineer Claude E. Shannon. His most notable achievements were in the transmission of color television, the design of radar systems for warning and recovery of intact messages coming from a communications satellite. Shannon, of *Bell Telephone Laboratories*, presented the world in two papers published in *Bell System Technical Journal* in July and October 1948.

In essence, the Shannon articles contain a set of theorems dealing with the problem of fast delivery, economical and efficient messages from one place to another. But the vast and fascinating implications of Shannon's work focused on the fact that he managed to explain the concept of information with such logic and precision that can be placed within a formal framework of ideas.

By treating information in terms of clearly defined but totally abstract, Shannon was able to generalize and apply laws established not just for a few types of information, but for everyone, anywhere. Although his essays may seem rather abstract and technical in the first reading, provide new ways to analyze any system or process in which exchange messages.

Shannon trials dealing with issues involving shared intellectual concerns: order, disorder, error and control error, and realization of potential possibilities, uncertainty and limitations. Scientists still wonder why the processes of nature manifest such order, where the state would most likely be uncertainty and chaos, a surrender to the forces of disorder that seem so overwhelming universal and so natural. This is considered one of the great paradoxes of science related to the philosophical question of *why exists something instead of nothing?* In his essays, Shannon proved that contrary to what might be expected, *a part* of a message can persist in the middle of the *all* of a random disorder or noise.

The most amazing thing was that Shannon's expression for the amount of information, the first accurate measurement, scientific, satisfying the first definition of the twentieth century was shaped like an equation created many years ago, in the nineteenth century, to a law of physics peculiar and very elusive: *the entropy*, thereby Shannon established an equivalence between entropy and information, fully applicable to any system or process.

This is one of the few theories that have a well defined birth in time, having a birthday and has a parent. The father's name was Claude E. Shannon and the article gives rise to the Information Theory was published in 1948. Entitled *"A Mathematical Theory of Communication"* Shannon (1948) and appeared in Bell System Technical Journal Bell System company. It is curious that this theory has a birth so timely, because usually all important creations are collective creations. In 1998 celebrated fifty years of Information Theory and practice around the world appeared special issues in journals, commemorative symbols that demonstrate all that changed in a very short period of time. Of all the articles published were collected on the occasion of fifty years a series of studies which linked to Telecommunications and, of course, also in Mathematics, Statistics, Economics, Linguistics, Quantum Theory, Astrophysics, Atomic Physics, Genetics, Molecular Biology, Neural Networks and a number of areas that were originally outside the Shannon model.

In the mid 80's, part of the scientific community thought of combining information theory with Quantum Mechanics which led to the emergence of a new branch has been extended to include the until then unexplored territory of the transmission and processing quantum states, as well as the study of quantum information and its relationship with traditional forms of information. We could ask us why this did not happen before?, because some time ago has been accepted quantum principles as the foundation of Modern Physics. Until recently it we was thought the information in terms purely classical and Quantum Mechanics played only a minor role in the design of processing equipment and in setting limits on the rate at which we could send information by certain types of channels.

At a more fundamental level, it has become clear that an Information Theory based on the principles of Quantum Mechanics, expands and complements the Classical Information Theory Vedral (2002). In addition to the quantum generalizations of classical notions such

as sources, channels and codes, this new theory includes two complementary types of quantifiable data: classical information and quantum entanglement.
Finally, the purpose of this chapter is to present the idea that can improve our understanding of Nature by not only analyzing the behavior exclusively in terms of matter and energy, even at the level of elementary particles, but the study by the techniques and methods of modern physics and chemistry, integrate concepts and tools that allow us to comprehensively investigate the behavior of natural systems in order to deepen our understanding of them to incorporate information measures that take into account concepts such as entanglement, known since the early days of Quantum Mechanics, for which, however, there are no measures in classical theories.

2. Informational flows

During the study of quantum systems, is common to use phrases like "suppose the system is in state n", on the understanding that the state $|n\rangle$ is an eigenestate of a set of operators that commute with each other and that this specification is sufficient for our purposes. However a physical system, does not necessarily to be fulfilled this condition, i.e. not necessarily characterized by a wave function as $\psi_n(x) = \langle x \mid n\rangle$, it may be that we are interested in quantum ensemble, consists in turn by various subensembles, each one characterized by a wave function $\psi_1, \psi_2, \psi_3, \ldots$. For that, it is necessary to use a simple and elegant theory called *density matrix*, see for example Fano (1957); McWeeny (1960); Davidson (1976).
Then the description of a physical system in terms of a density matrix is the most general quantum description available; this formalism includes as particular case the description of pure states. To establish what it is a pure state in terms of the density matrix, we notice that if the system is in a state $|p\rangle$, then only in this state is done mixing, so the contribution to it from any other state $|q\rangle$ is null ($q \neq p$). Therefore the pure state is defined by the conditions

$$w_i = \delta_{pi} \tag{1}$$

and the density matrix is reduced to

$$\hat{\rho} = \sum_i w_i \, |i\rangle \langle i| = \sum_i \delta_{pi} \, |i\rangle \langle i| = |p\rangle \langle p| \, , \tag{2}$$

this is consistent with the projector state $|p\rangle$:

$$\hat{\rho} \, |p\rangle \langle p| = \hat{P}_p \tag{3}$$

And now, if we consider the density matrix in coordinate representation about pure state $\psi(x)$ is

$$\rho(x', x) = \langle x'| \, |p\rangle \langle p| \, |x\rangle = \psi_p(x')\psi_p^*(x), \tag{4}$$

from this is straightforward to show that

$$\hat{\rho} = |p\rangle \langle p| \, |p\rangle \langle p| = |p\rangle \langle p| \, , \tag{5}$$

so the density matrix of a pure state is idempotent:

$$\hat{\rho}^2 = \hat{\rho}. \tag{6}$$

This is property that is used to define a pure state.

As an algebraic relation between matrices is also valid for its eigenvalues, the eigenvalues of $\hat{\rho}$ of a density matrix of a pure state satisfy the equation $\hat{\rho}^2 = \hat{\rho}'$ so this values can be only 0 and 1. As $tr\hat{\rho} = 1$, only one of the eigenvalues can be 1, so that its diagonal representation the density matrix of the pure state $|p\rangle$ has a 1 in the diagonal element (pp) and other elements are zero.
In the case of a mixture that is true $tr\hat{\rho}^2 \leq 1$ an the equation (6) implies that equality will be only when the system is a pure state. This permit us define the degree of impurity a mixture as $I = 1 - tr\hat{\rho}^2 = tr(\hat{\rho} - \hat{\rho}^2) = tr\hat{\rho}(1 - \hat{\rho})$, this result represents the expected value of $1 - \hat{\rho}$ and 0 for a pure state and tends to a value of 1 with increasing impurity (when $tr\hat{\rho}^2 \ll 1$).[1]
For a pure state $|p\rangle$, we have

$$\left\langle \hat{A} \right\rangle = tr\hat{\rho}\hat{A} = tr\,|p\rangle\,\langle p|\,\hat{A} = \langle p|\,\hat{A}\,|p\rangle\,,$$

thus recover the expected value definition used in the quantum mechanics of pure states:

$$\left\langle \hat{A} \right\rangle = \langle p|\,\hat{A}\,|p\rangle\,.$$

We use these results to show that the superposition that characterizes a pure state is consistent. To show this, consider the state $|\psi\rangle$, we express the pure state as the superposition

$$|\psi\rangle = \sum_n q_n\,|n\rangle\,; \tag{7}$$

the density matrix is given by

$$\hat{\rho} = |\psi\rangle\,\langle\psi| = \sum_{n,m} q_n q_m^*\,|n\rangle\,\langle m| = \sum_{n=m} |q_n|^2\,|n\rangle\,\langle n| + \sum_{n\neq m} q_n q_m^*\,|n\rangle\,\langle m|\,. \tag{8}$$

The group of diagonal elements can be represented as

$$\sum_n |q_n|^2\,|n\rangle\,\langle n| = \sum_n |q_n|^2\,\hat{\rho}_n,$$

the sum is incoherent (without interference) contributions from each of the pure states $|n\rangle$, with the density matrix $\hat{\rho}_n = |n\rangle\,\langle n|$, the other terms in the expression for $\hat{\rho}$ constitutes the contribution of interference between the states $|n\rangle$ and $|m\rangle$, If the superposition was inconsistent these terms may not appear. In summary, understanding it with due care, we could say that the superposition is a property relative to a pure state (with respect to a base),

[1] The equation (6) can be written as

$$\sum w_n^2\,|n\rangle\,\langle n| = \sum w_n\,|n\rangle\,\langle n|\,,$$

allows us to establish that $w_n^2 = w_n$, i.e. a density matrix weights can only contain 0 or 1. But as the condition on the trace implies that only one of these weights may be different from zero, the condition (6) of idempotency is necessary and sufficient to define a pure state.
At the end opposite the pure case corresponds to a situation where the total lack of information on the possible status of any of the subsystems leads to assign equal weight to all of them, which gives, if the mixture has a total of N components, $w_n \frac{1}{N}$. In this case we obtain

$$tr\hat{\rho}^2 = \sum_{n=1}^{N} w_n^2 = \sum_{n=1}^{N} \frac{1}{N^2} = \frac{1}{N}.$$

For $N \longrightarrow \infty$ this amount can be taken arbitrarily small values.

it is irreducible to a mixture (as well as in the first case is consistent, while the second is incoherent).
Moreover, the uncertainty of a quantum system can be determined from the collection of probabilities $p_i(A)$ of an observable A by von Neumann entropy, von Neumann (1955)

$$S(A) = -\sum_{i=1}^{n} p_i(A) \ln p_i(A), \tag{9}$$

where $\sum_{i=1}^{n} p_i(A) = 1$ y $p_i(A)$ correspond to the elements of a diagonalized density matrix, and will be a maximum when $p_1(A) = p_2(A) = \cdots = p_i(A) = 1/n$, with this condition $S_{\max}(A) = \ln n$, and for a pure estate $S(A) = 0$. Then, within the context of Quantum Chemistry, we consider a pure state as one whose values of the reduced density matrix, fulfilled with the condition $1/p_{11}(A) = 1/p_{22}(A) = \cdots = 1/p_{nm}(A)$. This condition only be satisfied by a monodeterminantal methodologies, such as Hartree-Fock or Density Functional Theory. In this perspective, has been used the Shannon entropy as a measure of correlation in atomic systems Ziesche (1995). Moreover it is important to notice that the Shannon entropy, $S(\vec{r}) = -\int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r}$ is not equal or equivalent to the von Neumann entropy, $S(\rho) = -Tr\{\rho \ln \rho\}$. To show this, consider an observable A found in the state ρ, whose expected value is

$$\langle A \rangle = -tr\{\rho, A\}, \tag{10}$$

then if the state is described by a density matrix ρ, the corresponding entropy of that state is

$$S(\rho) = -tr\{\rho \ln \rho\}, \tag{11}$$

while the entropy of the observable is given by

$$S(\rho, A) = -tr\{(\rho, A) \ln(\rho, A)\}, \tag{12}$$

therefore the entropies $S(\rho)$ and $S(\rho, A)$ are not equal or equivalent. The Shannon entropy determines the classical information of the system and is defined in terms of an observable, while von Neumann entropy determines the quantum information of the system and is defined in terms of a density matrix.
Both entropies are subject to

$$S(\rho) \leq S(\rho, A) \tag{13}$$

and will be equal if and only if $[\rho, A] = 0$. That is, only when the values of the observables commute with their density matrix.
From the definition of the uncertainty of a quantum system characterized by its density matrix and using different definitions we can define the following entropies

$$H(A) = -\sum_{i=1}^{n} \sum_{j=1}^{m} P_{i,j}(A, B) \ln \sum_{j=1}^{m} P_{i,j}(A, B), \tag{14}$$

$$H(A \mid B) = -\sum_{i=1}^{n} \sum_{j=1}^{m} P_{i,j}(A, B) \ln P_{i,j}(A \mid B), \tag{15}$$

$$H(A, B) = -\sum_{i=1}^{n} \sum_{j=1}^{m} P_{i,j}(A, B) \ln P_{i,j}(A, B), \tag{16}$$

$$H(A : B) = \sum_{i=1}^{n} \sum_{j=1}^{m} P_{i,j}(A, B) \ln \frac{P_{i,j}(A, B)}{\sum_{i=1}^{n} P_{i,j}(A, B) \sum_{j=1}^{m} P_{i,j}(A, B)}, \tag{17}$$

which, in previous studies have shown the use of von Neumann marginal entropies applied to simple chemical processes, Flores & Esquivel (2008); Flores (2010), where $P_{i,j}(A,B)$ is the joint probability, i.e. the probability from a collection of events $(A_i,B_j) \in \xi$, where ξ is the a set of probabilities obtain form first order density matrix, we can establish which is the probability that a random event occurs with a set of probabilities $\{A\}_i$ when a event $\{B\}_j$ occurs this is given by

$$P\left\{(A_i,B_j) \in \xi\right\} = \sum_{i,j\in\xi}^{n,m} P_{i,j}(A,B) = \sum_{i=1}^{n}\sum_{j=1}^{m} P_{i,j}(A,B) = 1. \tag{18}$$

Also, we can define the marginal probability of the set $\{A\}$ as

$$P(A) = \sum_{j=1}^{m} P_{i,j}(A,B) \tag{19}$$

and the conditional probability $P(A \mid B)$ as

$$P(A \mid B) = \frac{\sum_{i=1}^{n}\sum_{j=1}^{m} P_{i,j}(A,B)}{\sum_{i=1}^{n} P_{i,j}(A,B)}. \tag{20}$$

In all cases, the marginal probabilities are subject to

$$\sum_{i=1}^{n}\sum_{j=1}^{m} P_{i,j}(A,B) = \sum_{i=1}^{n} P(A) = \sum_{i=1}^{n}\sum_{j=1}^{m} P(A \mid B) = 1. \tag{21}$$

The equations (14-17) are interrelated. For example,

$$H(A,B) = H(A) + H(B \mid A) = H(B) + H(A \mid B) \tag{22}$$

and

$$H(A:B) = H(A) - H(A \mid B) = H(B) - H(B \mid A). \tag{23}$$

this equations have been classified as a *informational balance* Guiaşu (1977). The equations (14-17) are generally represented by the following mnemonic diagram shown in Figure (1).

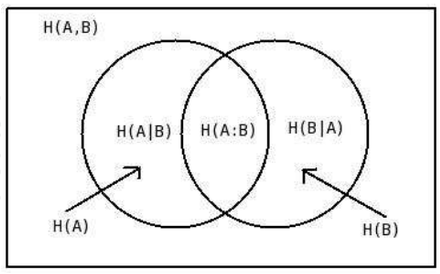


Fig. 1. Relationship between the informational entropies.

The informational entropies have the following properties:

1. The joint entropy and mutual entropy are invariants operationally:

$$H(A,B) \equiv H(B,A)$$

and

$$H(A:B) \equiv H(B:A).$$

2. The conditional entropy always is positive, $H(A \mid B) \geq 0$, consequently

$$H(A:B) \leq H(B)$$

and will be equal if and only if B is a function of $A, B = f(A)$.

3. Subadditivity,

$$H(A,B) \leq H(A) + H(B),$$

will be equal if and only if A and B are independent variables.

4. As $H(A \mid B) \leq H(A)$. Consequently $H(A:B) \geq 0$ and will be equal if and only if A and B are independent variables.

5. Strong subadditivity,

$$H(A,B,C) + H(B) \leq H(A,B) + H(B,C).$$

6. The conditioning reduces the entropy

$$H(A \mid B,C) \leq H(A \mid B).$$

In this case, we can determine the maximum amount of information allows us to quantify each Eqns. (14-17), for which we use the probability distribution that maximizes entropy, which in this case is $\sum_{i=1}^{n} P_{i,j}(A,B) = 1/n + m$, $\sum_{j=1}^{n} P_{i,j}(A,B) = 1/m + n$ and $\sum_{i=1}^{n}\sum_{j=1}^{m} P_{i,j}(A,B) = 1/n + 1/m$, with which we obtain

$$H_{\max}(A) = -\left(\frac{n+m}{nm}\right)\ln\left(\frac{1+nm}{n}\right), \tag{24}$$

$$H_{\max}(A \mid B) = -\left(\frac{n+m}{nm}\right)\ln\left(\frac{n+m}{n(1+nm)}\right), \tag{25}$$

$$H_{\max}(A,B) = -\left(\frac{n+m}{nm}\right)\ln\left(\frac{n+m}{nm}\right), \tag{26}$$

$$H_{\max}(A:B) = \left(\frac{n+m}{nm}\right)\ln\left(\frac{n+m}{(1+nm)^2}\right). \tag{27}$$

To calculate the informational entropies is necessary to construct the density matrix of the system of interest with the purpose of having a collection of probabilities, in this case are obtained from the density matrix of first order, in this context there is ample number of population analysis techniques allow us to obtain these values, for example Reed et al (1985); Löwdin (1955); Bruhn et al. (2006). In previous work Flores & Esquivel (2008); Carrera et al (2010); Flores (2010) have shown that the population analysis of Weinhold Reed et al (1985) and the Lowdin-Davidson Bruhn et al. (2006) this population analysis follows this criteria:

1. Are orthonormal orbitals of maximum occupancy, obtained from sub-blocks of atomic symmetry of the density matrix of first order, located on each atom.
2. Being orthogonal occupations are never negative and sum correctly to the number of electrons.
3. The obtained atomic blocks reflect the most compact description of the density around the isolated atom to which they correspond.

4. The density of natural atomic orbitals is v-representable by obtaining atomic block the first order density matrix and correspond to the potential generated by the Hamiltonian of the isolated atom.
5. The blocks obtained from first-order density matrix reflect intrinsic properties of the wave function and therefore do not have a strong dependence on the choice of the base.
6. Are rotationally invariant, which is appropriate to define the subsystems A and B used to calculate each one of the entropies.
7. Unlike the occupation numbers of Löwdin are not delocalized throughout the molecular orbital and the transform as irreducible representations of the molecular point group and this allow us the study of atomic subsystems and their interaction.

In this chapter, we present a new application of these entropies, that consist in determinate the informational flows and their trajectories of a system that is involved in a chemical process. To do this, start by defining the information amount that a pair of subsystems can be exchanged, i.e.

$$\begin{aligned} H(A) - H(B) &= -\sum_{i=1}^{n}\sum_{j=1}^{m} P_{i,j}(A,B) \ln \sum_{j=1}^{m} P_{i,j}(A,B) + \sum_{i=1}^{n}\sum_{j=1}^{m} P_{i,j}(A,B) \ln \sum_{i=1}^{n} P_{i,j}(A,B), \\ &= -\sum_{i=1}^{n}\sum_{j=1}^{m} P_{i,j}(A,B) \ln \left(\frac{\sum_{j=1}^{m} P_{i,j}(A,B)}{\sum_{i=1}^{n} P_{i,j}(A,B)} \right). \end{aligned} \tag{28}$$

From this result we notice that the difference $H(A) - H(B)$ represent the amount of information that a pair of subsystems can be exchanged in a process.
Similarly, we can define what level of conditioning that will have the amount of information exchanged, i.e.:

$$H(A \mid B) - H(B \mid A) = -\sum_{i=1}^{n}\sum_{j=1}^{m} P_{i,j} \ln \frac{\sum_{j=1}^{m} P_{i,j}(A,B)}{\sum_{i=1}^{n} P_{i,j}(A,B)}. \tag{29}$$

Notice that $H(A) - H(B) \equiv H(A \mid B) - H(B \mid A)$, henceforth denote this result as $H(\dot{AB})$.
In applying the above result to a chemical process, we can interpret $H(\dot{AB})$ as the amount of information transferred in the system. This quantity has the following properties

$$H(\dot{AB}) = -\sum_{i=1}^{n}\sum_{j=1}^{m} P_{i,j}(A,B) \ln \frac{\sum_{j=1}^{m} P_{i,j}(A,B)}{\sum_{i=1}^{n} P_{i,j}(A,B)} = \begin{cases} \{A\} > \{B\} \Rightarrow H(\dot{AB}) < 0 \\ \{A\} \equiv \{B\} \Rightarrow H(\dot{AB}) = 0 \\ \{A\} < \{B\} \Rightarrow H(\dot{AB}) > 0 \end{cases}. \tag{30}$$

We can interpret this result as follows, if $H(\dot{AB}) > 0$, informational flow is given in the form $\{A\} \rightarrow \{B\}$, if $H(\dot{AB}) < 0$, the informational flow $\{B\} \rightarrow \{A\}$, while if $H(\dot{AB}) \equiv 0$ imply that the informational flow is completely equivalent in both directions, i.e. $\{A\} \leftrightarrow \{B\}$, so it is then convenient to define the net flow of information as $H(\dot{AB}) = \|H(A) - H(B)\|$.
As in the case of informational entropy, in this case we can also determine the maximum flow of information, taking into account the probability distributions that maximize this flow to obtain

$$H_{\max}(\dot{AB}) = \left| \frac{n+m}{nm} \ln \frac{n}{m} \right|. \tag{31}$$

3. Informational trajectories

In previous section we defined the amount of information that a system can be exchanged, either between the subsystems that constitute or their environment and other interesting point to study is the possible informational trajectory that follow the amount of information that the subsystems interchanged. To do this, we return the definition informational flow that we defined in the previous section, $H(\dot{AB})$, which allows us to establish or determine the amount of information that a pair of subsystems can exchange with each other, however, it is also important to determine what would be the trajectory that these informational flows.
To do this, is necessary define the informational trajectory that follow the informational flow,

$$H(\vec{AB}) = \int_C H(\dot{AB}) dP(A,B), \tag{32}$$

which has explicit form,

$$H(\vec{AB}) = \int_C H(\dot{AB}) H'(\dot{AB}) d(AB), \tag{33}$$

i.e.

$$H(\vec{AB}) = -\int_C \left[\sum_{i=1}^{n} \sum_{j=1}^{m} P_{i,j}(A,B) \ln \left(\frac{\sum_{j=1}^{m} P_{i,j}(A,B)}{\sum_{i=1}^{n} P_{i,j}(A,B)} \right) \left(\frac{1}{\sum_{i=1}^{n} P_{i,j}(A,B)} - \frac{1}{\sum_{j=1}^{m} P_{i,j}(A,B)} \right) \right] dP(A,B), \tag{34}$$

the last equation can be written explicitly as follow

$$H(\vec{AB}) = -\int_C \left[\frac{\sum_{i=1}^{n} \sum_{j=1}^{m} P_{i,j}(A,B) \left[\sum_{i=1}^{n} P_{i,j}(A,B) - \sum_{j=1}^{m} P_{i,j}(A,B) \right]}{\sum_{i=1}^{n} P_{i,j}(A,B) \sum_{j=1}^{m} P_{i,j}(A,B)} \ln \left(\frac{\sum_{j=1}^{m} P_{i,j}(A,B)}{\sum_{i=1}^{n} P_{i,j}(A,B)} \right) \right] dP(A,B), \tag{35}$$

notice that $\frac{\sum_{i=1}^{n} \sum_{j=1}^{m} P_{i,j}(A,B)}{\sum_{i=1}^{n}} = P(A \mid B)$ and $\frac{\sum_{i=1}^{n} \sum_{j=1}^{m} P_{i,j}(A,B)}{\sum_{j=1}^{m}} = P(B \mid A)$, so

$$H(\vec{AB}) = -\int_C (P(B \mid A) - P(A \mid B)) \ln \frac{\sum_{j=1}^{m} P_{i,j}(A,B)}{\sum_{i=1}^{n} P_{i,j}(A,B)} dP(A,B), \tag{36}$$

this integral, is subject to

$$H(\vec{AB}) = \begin{cases} \sum_{i=1}^{n} P_{i,j}(A,B) \equiv \sum_{j=1}^{m} P_{i,j}(A,B);\ H(\vec{AB}) = 0 \\ \sum_{i=1}^{n} P_{i,j}(A,B) > \sum_{j=1}^{m} P_{i,j}(A,B);\ H(\vec{AB}) > 0 \\ \sum_{i=1}^{n} P_{i,j}(A,B) < \sum_{j=1}^{m} P_{i,j}(A,B);\ H(\vec{AB}) > 0 \end{cases}. \tag{37}$$

This would imply that any process, physical, chemical, physicochemical, has a positive informational trajectory which is related to a corresponding flow and informational exchange, so we could postulate the following axiom, *Any system that is subject to a natural process exchanges information*.

As in the flow of information, we can obtain the maximum informational trajectory, using the probability distributions that maximize the flow,

$$H_{\max}(\vec{AB}) = \int_C \left(\frac{n^2 - m^2}{nm}\right) \ln\left(\frac{n}{m}\right) d(n,m), \tag{38}$$

$$= \left(\frac{n^2}{2} + \frac{m^2}{2}\right) \left[\frac{1}{2} \ln\left(\frac{m}{n}\right) + 1\right], \tag{39}$$

and

$$H_{\max}(\vec{BA}) = \left(\frac{n^2}{2} + \frac{m^2}{2}\right) \left[\frac{1}{2} \ln\left(\frac{n}{m}\right) + 1\right], \tag{40}$$

the maximum trajectory $H_{\max}(\vec{AB})$ is subject to the follow conditions

$$H_{\max}(\vec{AB}) = \begin{cases} n > m \Rightarrow H_{\max}(\vec{AB}) > 0 \\ n \equiv m \Rightarrow H_{\max}(\vec{AB}) \equiv 1 \\ n < m \Rightarrow H_{\max}(\vec{AB}) > 0 \end{cases}. \tag{41}$$

4. Informational flows and informational trajectories in chemical processes

Within the context of quantum chemistry, one of the principal interests is sorting systems or chemical processes, in general, this is accomplished by using certain models and approaches in order to obtain and quantify certain parameters of the system or process and to give a physical interpretation of what is possibly happening. Generally, these parameters are: energy, electron density, molecular electrostatic potential, Laplacian of the Density, Molecular or Atomic charges, Chemical Reactivity Parameters (like Hardness, Softness, Chemical Potential, Electrophilicity Parr & Yang (1989), Frequencies, among others.
Reactivity parameters we use in this work are defined as Parr & Yang (1989):

$$\eta = \frac{1}{2}\left(\frac{\partial \mu}{\partial N}\right)_v = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_v,$$

and

$$S = \frac{1}{2\eta} = \left(\frac{\partial N}{\partial \mu}\right)_v$$

$$\mu = \left(\frac{\partial E}{\partial N}\right)_v,$$

where μ is the chemical potential, N is the number of particles in the system, E is the total energy of the system and v is the external potential. These parameters of reactivity, can be approximated by the Koopmans theorem and finite differences as

$$\eta = \frac{I - A}{2} = \frac{E^{LUMO} - E^{HOMO}}{2},$$

where I is the firts ionization potential and A is the electronic affinity, E^{LUMO} is the energy of Lowest Unoccupied Molecular Orbital and E^{HOMO} is he energy of the Highest Occupied

Molecular Orbital, with this approximation we can calculate the softness and the chemical potential,

$$S = \frac{1}{2\eta}$$

and

$$\mu = \frac{E^{LUMO} + E^{HOMO}}{2}.$$

Under this scheme, in this section show that by applying this parameters and the informational entropies to describe a chemical process its possible obtain trends, which, through its interpretation enable us to establish a link between the parameters commonly obtained with respect to information of the system, we intend to show that changes in the amount of information system are also related to changes in the two principal parameters in the context of the Quantum Chemistry: the electron density and the energy.
In the next section we present some applications concerning the applications of the entropies informational, informational flows and informational trajectories. In each of the examples presented here we used Gaussian 03 program Gaussian (2003), for the electronic occupation probability we used the program NBO 5.0 Glendening et al (2004) and finally the isosurfaces of the molecular electrostatic potential and the Laplacian of the density were obtained with MOLDEN program Schaftenaar & Noordik (2000).

4.1 Dissociation of HCl

In previous work Flores & Esquivel (2008); Esquivel et al (2009) have shown that changes in the informational entropies are associated with physical and chemical changes of a system, such as electron density, atomic charges, molecular electrostatic potential, normal modes of vibration, among others.
In this section we show some applications of informational flows and informational paths Eqns. (28) and (37), presented in such processes. In this case, we present the results for the dissociation HCl, which were calculated with B3LYP/6-311G.
In the Figure 2(a), shows the energy profile of the process of dissociation of the HCl in which we see that the equilibrium internuclear distance is 1.3 Å, and energy is -460.77606 Hartrees. In the Figures 2(b), 3(c) and 3(d) shows the contour surfaces of molecular electrostatic potential at a distance of 1.3 Å, and 4.0 Å, respectively.
From these figures we can notice several important aspects regarding the set of parameters used to characterize this process: i) trends obtained only allow us to get an idea of what is happening in this process based on it, apply or guess that's what happens in the process, and ii) The parameters used, the cases do not necessary represent some of the critical points that may be important to better classify the system and thus seek to identify some important aspect of it.
In the Figures 3(e) - 3(g) present the trends of informational entropy, which were obtained with the Eqn. (14), previously reported Flores & Esquivel (2008), in these trends we define the set $\{A\}$ as the natural atomic probabilities of hydrogen atom and the set $\{B\}$ as the set natural atomic probabilities of chlorine atom. In the Figure 3(e) we present the trends of $H(A)$ and $H(B)$ in which we can see that $H(A)$ has a minimum in $R = 0.45$ Å, and a local maximum in the trend $H(B)$ in the same internuclear distance, to compare trends of the charge density (Figure 2(b)) in this Figure we notice that the change in the curvature trend occurs in the same internuclear distance in both trens of the subsystems, this change of curvature can be attributed to the instability of the system, however, could also say that from this equilibrium

internuclear distance the system starts stabilized due to a redistribution of electron density, which can be viewed through the contour map of the Laplacian Density, see Figures 3(a)-3(b). At a distance of 0.65 Å, the entropy $H(A)$ have a maximum which can be attributed at the beginning in the redistribution of electron density of hydrogen atom which would schedule at the beginning of stabilization of the molecular system to reach equilibrium internuclear distance this is reflected in an abrupt change in the slope of the trend of the entropy. While in the case of the tendency of the entropy $H(B)$, notice how it behaves the chlorine atom in the molecular environment shows a maximum at 1.3 Å, this corresponds to minimum energy, this is agree with a thermodynamic interpretation of the systems. We can also say that in this case, the behavior of the entropy $H(A)$ show a inflexion points in the trend are associated with the physical and chemical changes that occur in this process.

Moreover, in the Figure 3(f), shows the trends of the conditional entropy, which we can interpret them as follows *how the hydrogen atom are conditionated by the presence of chlorine atom* or in a more general form, *how the subsystem* $\{A\}$ *is conditionated by the presence of the subsystem* $\{B\}$, notice the generality of this interpretation, because is it a guideline for board a discussion theme fundamental in the modern chemistry, *What is an atom in a molecule?* Parr et al (2005), Is possible that through the application of the conditional von Neumann informational entropies we can give a opinion to respect.

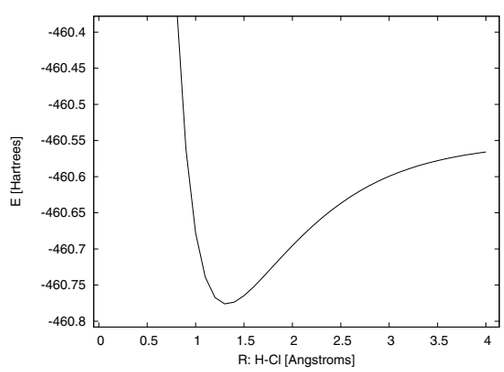
In the trends of the informational entropies, we can notice that $H(A)$ trend, have basically, the same structure of the $H(A \mid B)$ and $H(A, B)$, see Figures 3(g). This leads us to hypothesize that the hydrogen atom, which plays an important role in the process of this nature, for example, in a natural process, this subsystem has primary responsibility for carrying out a transfer of density. With this context, basically recovered several interpretations of the concepts and descriptions commonly used in Chemistry.

Finally, in the Figure 3(h) shows the trends of the flow of information and informational trajectory integral, notice that in this case, both trends have the same structure, this implied that in this process, the trajectory and informational flow depend of the electron density that the subsystems can be transferred to each other, in both cases, the critical points of these trends are the same critical points observed in the trends of informational entropy, Eqns. (14) - (17), which can be attributed to charge transfer process.

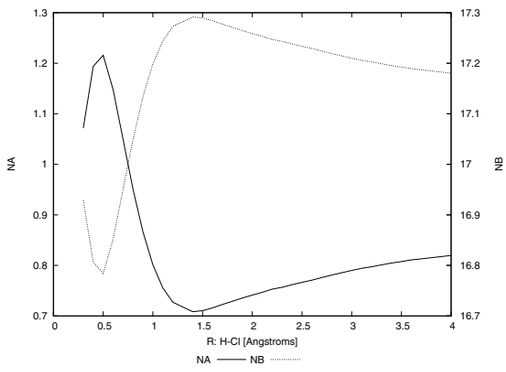
Furthermore, in the trends of $H(A, B)$ and $H(A : B)$, Figure 3(g), find that the mutual entropy, $H(A : B)$, the measure information that subsystems share increase this allows us to establish the nonclassical behavior of this system, because from a classical interpretation, we hope that in the limit when $R \longrightarrow \infty$, classically, the subsystems should not be any interaction between them, however, the entropy $H(A : B)$ shows that the subsystems A y B present a nonclassical types of interaction that is evident when the classical interactions decrease, this is, notice that $H(A : B) \neq 0$, while the total information system $H(A, B) \neq H(A) + H(B)$ and observe that it tends to a constant value. This behavior could be considered as possible evidence of quantum nonlocality Aspect (2007), i.e. evidence shows a strong correlation between pairs of subsystems, which can be separated by an arbitrarily large distance without communication (known) between them. This allows us to incorporate concepts of quantum mechanics such as entanglement, teleportation, among others.

In experimental field, the entanglement of the systems has been determined by ion trap Molmer & Sorensen (1999); Cirac & Zoller (1995); Sorensen & Molmer (1999); Kreuter et al (2004); Schlosser (2001); Monroe et al (1995), by photons Molmer & Sorensen (1999); Tittel et al (1998), phonons Jian-Wei et al (2000), by NMR Ladd et al (2002); Braunstein et al (1999). This property has also been applied to quantum cryptography Beveratos et al (2002); Jenneweinm

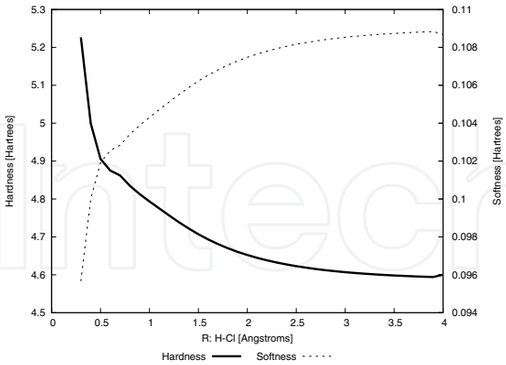
et al (2000); Gisin et al (2002). In such experiments have been used primarily: *Ca*, *Be* and *Mg*. For this circumstance, it is interesting to analyze the processes of dissociation of these systems in order to determine if they have quantum behavior as described above. Notice that these systems are clustered on the block "*s*" of the periodic table, this permit us establish the hypothesis that it is possible to find a quantum behavior in the other elements of the block and try to determine if this property have a periodical pattern that allows us to predict if a chemical system will manifest some type of quantum behavior.
In the following example, we show the characterization of a simple chemical reaction, which is characterized with concepts of modern chemistry, such as; internuclear equilibrium distances, variation of the subsystems charges, normal modes of vibration, as well as concepts of chemical reactivity, such as hardness, softness, chemical potential. In this example, we show, quantitatively, the dependence of the flow of information and the informational trajectory with the charge density of the subsystems, the internuclear distances, and so on.



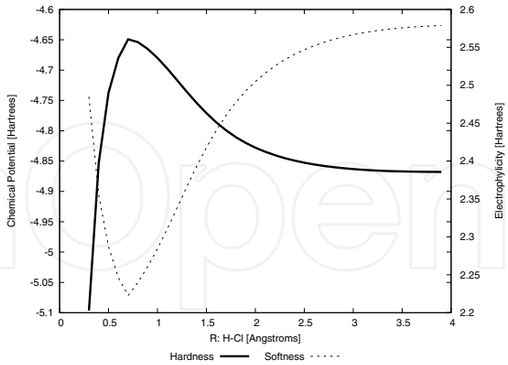
(a) Energy profile of the process of dissociation of *HCl*



(b) Trend charge density of the process dissociation*HCl*

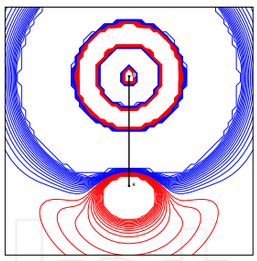


(c) Trends of the hardness and softness of the process of dissociation of *HCl*

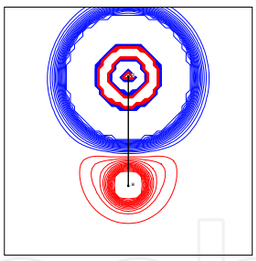


(d) Trend of chemical potential and electrophilicity in the process of dissociation of *HCl*

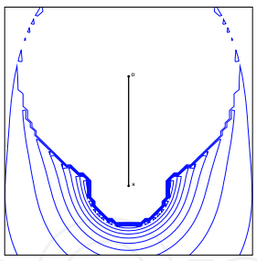
Fig. 2. Parameters that depend of energy and the electron density in the process of dissociation of *HCl*.



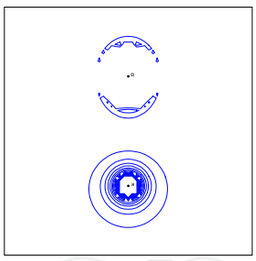
(a) LAP in R = 0.4 Å



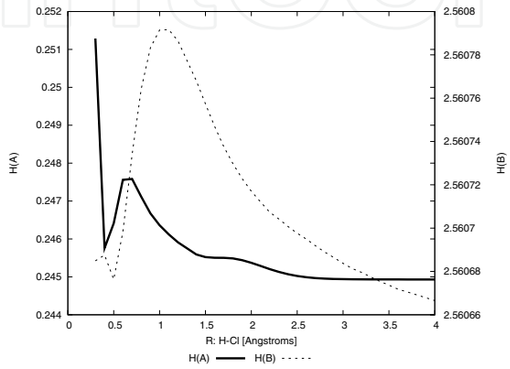
(b) LAP in R = 0.65 Å



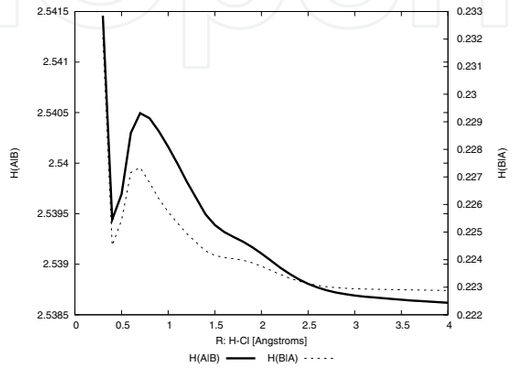
(c) MEP in R = 1.3 Å



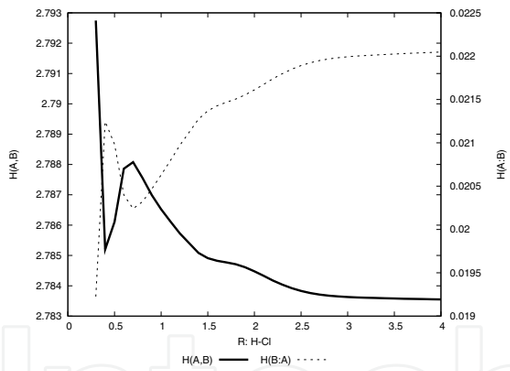
(d) MEP in R = 4 Å



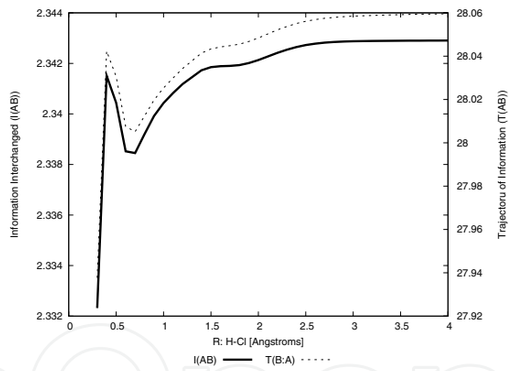
(e) $H(A)$ and $H(B)$



(f) $H(A \mid B)$ and $H(B \mid A)$



(g) $H(A,B)$ y $H(A:B)$



(h) Informational flow and informational trajectory.

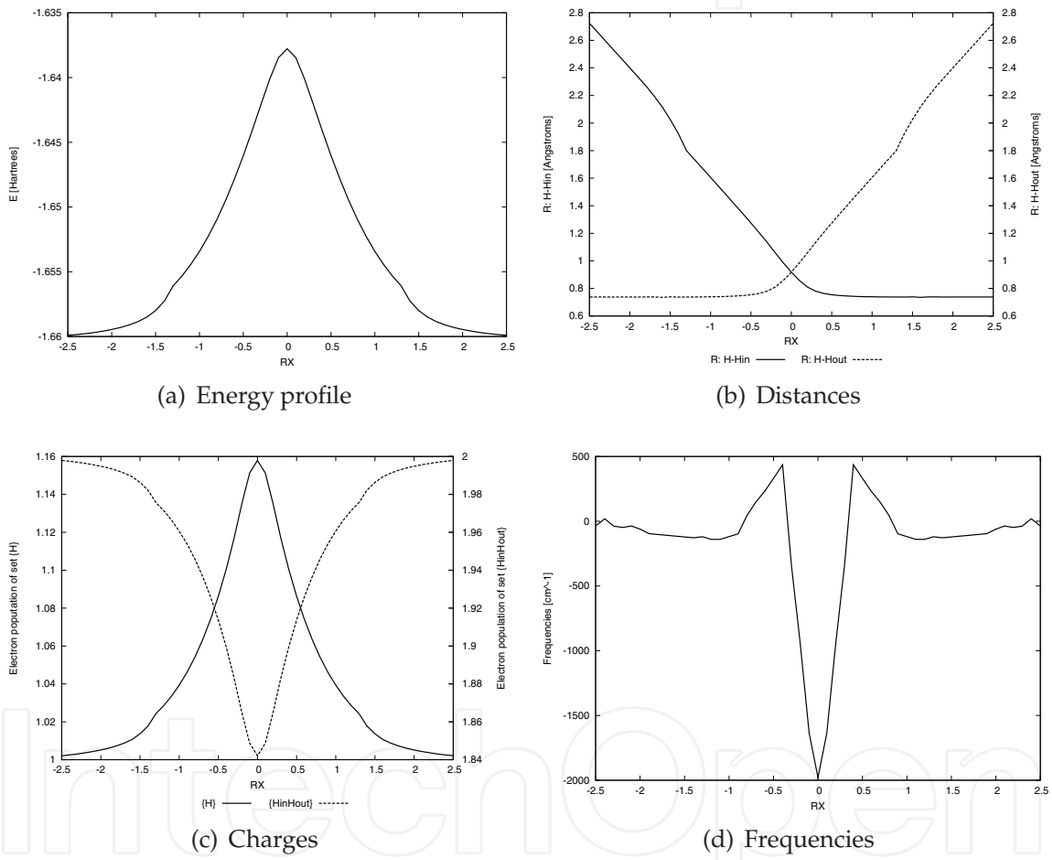
Fig. 3. Trends in informational entropies in the process of dissociation of HCl, LAP (Laplacian of Electron Density), MEP (Molecular Electrostatic Potential).

4.2 Process $H_2 + H^- \longrightarrow H_2 + H^-$

For this case study, we use the method UMP2 with the function basis set 6-311++G** to find the transition state structure. The IRC and each point of the reaction path were also obtained with the same method and function basis set, in each point of the path we verified the wave function stability Seeger & Pople (1977); Bauernschmitt & Ahlrichs (1996). The nomenclature used for this reaction is: $HH_{out} + H_{in} \longrightarrow HH_{in} + H_{out}$. From which, it is possible to generate two analysis. In the first case, selecting the set $\{A\} = H$ and the set $\{B\} = H_{in}H_{out}$, and in

the second analysis is possible take; $\{A\} = HH_{out}$ y $\{B\} = H_{in}$. In this case we just present the firts of them.
In the Figure 4(a) presents the energy profile for this reaction. In which we observe a transition structure that has a maximum, equilibrium internuclear distances at this point are 0.91808 Å, and the energy is -1.63778 Hartrees.
In the Figures 4(b), 4(c) and 4(d) correspond to the trends of the equilibrium internuclear distances, changes in the electronic population of each subsystem, the normal mode of vibration for this process, changes in hardness and softness of the system, which are chemical parameters are related to chemical reactivity.
In the Figures 5(c) - 6(b) we present the trends of the informational entropies, Eqns. (14-17), for this process. In this case two possible combinations were analyzed to generate the sets that allow us to define the joint probability, in the first case was selected set of probabilities of occupation $\{A\}$ how H_2 subsystem and the set $\{B\}$ with the occupation probabilities of H_{in}.
In the Figure 5(c) we shows the $H(A)$ trend, Eqn. (14), which basically shows how is the informational behavior of the H atom, which is directly involved in the process of rupture and formation of the chemical bond. In this figure we notice that from a distance $RX > -1.4$, $H(A)$ exhibits a change of curvature, which is attributed to the beginning of the process of breaking of the chemical bond, and can be visualized by isosurfaces of the molecular electrostatic potential, Figures 6(c) - 6(f), in which there is a decrease of the charge density in the central part of the H_2 molecule. In the coordinate $RX = -0.4$, the $H(A)$ trend shows a change in curvature, this change is associated with the process of breaking and formation of chemical bond, see Figures 6(g) - 6(j), where are the maps of molecular electrostatic potential, from such maps, we can observe a redistribution of electron density in the bond zone of the H_2 molecule, where a decrease in electron density, which is due to a decrease in the internuclear distance of the hydrogen atom which increases the interactions between these systems.
A similar behavior can be observed by comparing the trend of the normal modes of vibration of the system in Figure 4(d), which when compared with the trend of $H(A)$ we notice an excellent agreement with the normal mode of vibration, both trends have a two maximum in $RX = -0.4$ and $RX = 0.4$, these maxima we have attributed to a transition state zone Esquivel et al (2009).
As in the case of the dissociation process of HCl, we notice that $H(A, B) \neq H(A) + H(B)$, Figure 6(a), and $H(A : B) \neq 0$, Figure 6(b), the first result allows us to interpret a new way this kind of results and processes, on the one hand, urges us to leave the classic way of interpreting this type of process, i.e., an even though the subsystems are physically separated and in principle there any known interaction between them, either chemistry or physics, these systems preserve some classical types of interaction. Such results allow us to issues and philosophical implications of Quantum Mechanics, for example, if we accepts the result could be concluded that the interpretation of the results of this process using Quantum Mechanics is inconsistent with local realistic interpretation. This has important consequences. For example must be concluded that quantum systems do not have objective properties, pre measure whose values are simply revealed by the experiment. In the Copenhagen interpretation is accepted contextuality that is inferred here as a fact of Nature, so the value assigned to A, depends if you are determined jointly with B.
There has been a large number of experiments to verify the Bell inequalities Bell (1966), are fulfilled or violated Tittel et al (1998); Aspect (2007); Timothy et al (2007). Generally considered that experiments have shown that the Bell inequalities are violated, and therefore local realism has been refuted in experiments. Notice carefully the nature of this results because imply

a metaphysical dilemma *Is it valid or not local realism in nature?*, which is resolved through empirical issue that has been classified in experimental metaphysics. In some way, the only precedent in physics of this situation was the EPR theorem Einstein et al (1935).
The reason for the popularity of the Bell inequalities lies in the fact that they can lead the experimental field, which opens the way for long discussions on the fundamental problems of Quantum Mechanics (determinism *vs.* indeterminism, location *vs.* holism, objectivity *vs.* subjectivity, etc.) leave the realm of speculation to go to the empirically verifiable (or refutable as desired). However, the fact is that here the discussions and disagreements persist, and there is good reason for it. Accepting the validity of the quantum description, the proposed scheme is to reject outright the existence of hidden variables, and return with it to indeterminism, or consider the final theory is deterministic, but not necessarily local.

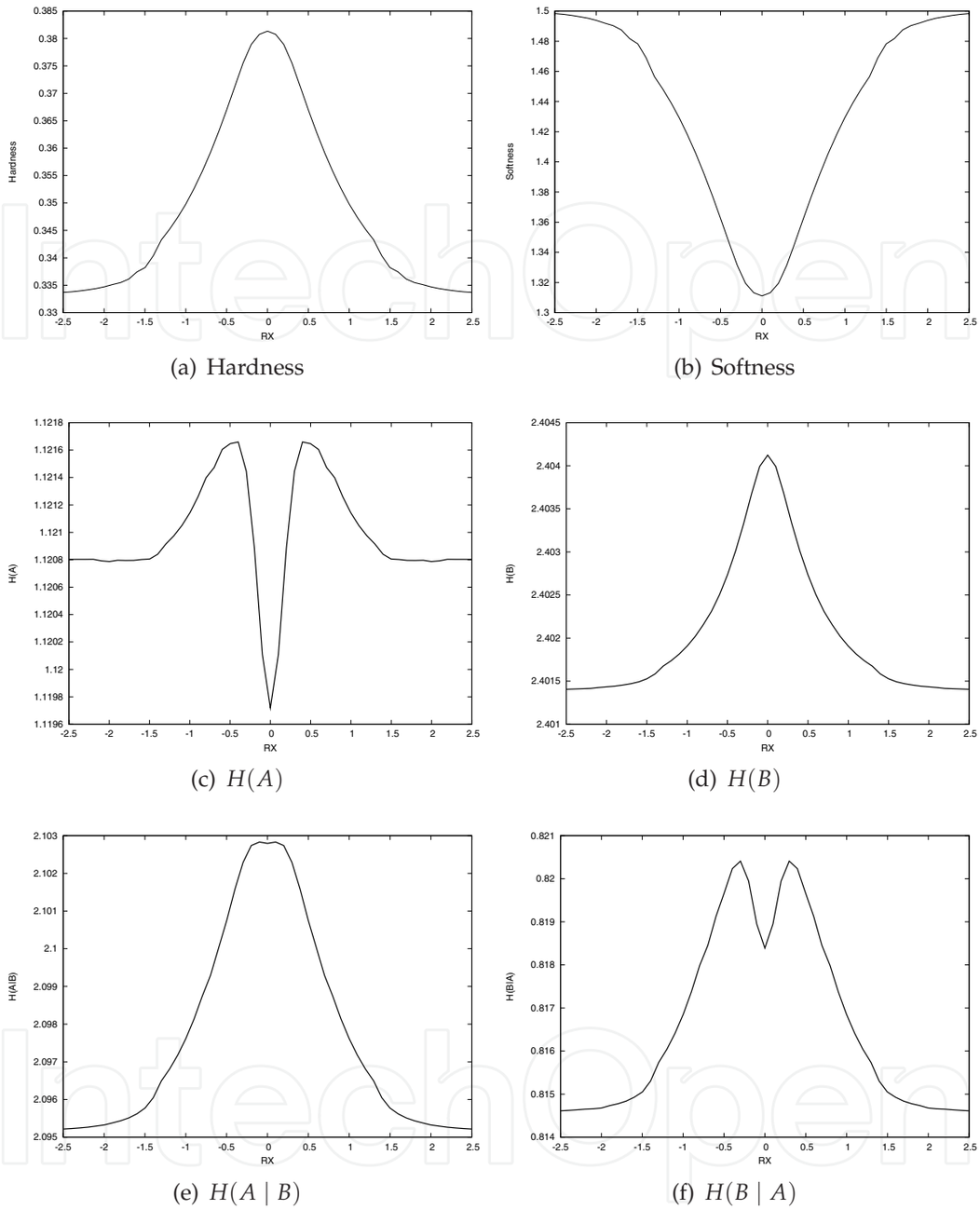


(a) Energy profile (b) Distances

(c) Charges (d) Frequencies

Fig. 4. Parameters characterizing the process $H_2 + H^- \longrightarrow H_2 + H^-$.

One of the most valuable aspects of each of the above figures is that the informational entropies permit us define clearly, there are areas where physical and chemical changes involved in this process. This leads us to establish the following hypothesis; *in any natural process, there is an exchange of matter, energy and information*.
The Figure 7(a) show a contour map which shows as the subsystems exchange information among themselves. In this figure we notice that approximately 1.2,1.2 coordinates correspond to the area where the flow of information is greatest, when comparing this region with the equilibrium internuclear distances Figure 4(b) we can establish a rank in the reaction



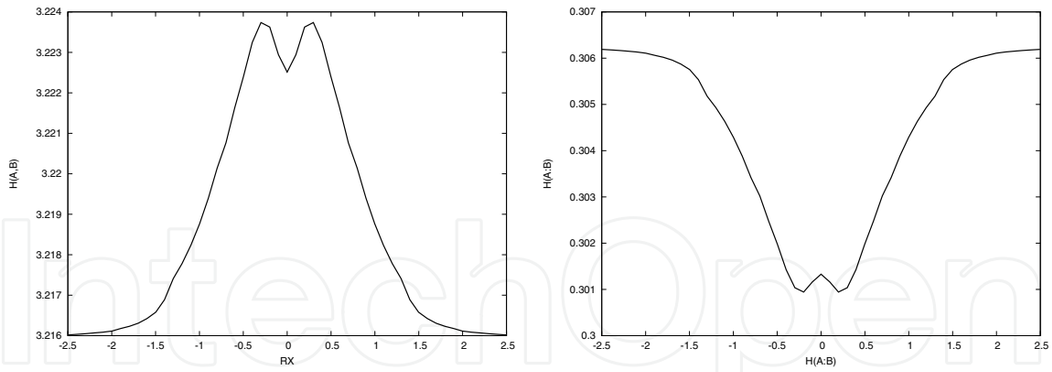
(a) Hardness (b) Softness

(c) $H(A)$ (d) $H(B)$

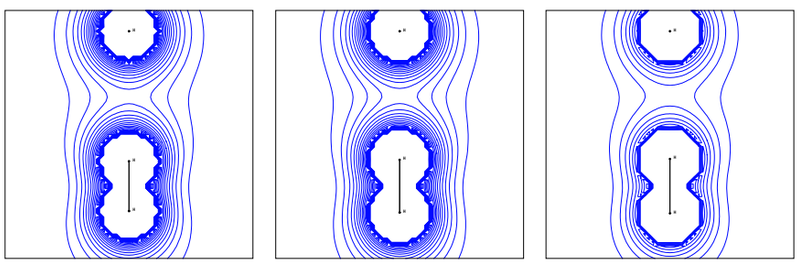
(e) $H(A \mid B)$ (f) $H(B \mid A)$

Fig. 5. Trends of informational entropies, using $\{A\} = \{H\}$ and $\{B\} = H_{in}H_{out}$ in the process $H_2 + H^- \longrightarrow H_2 + H^-$.

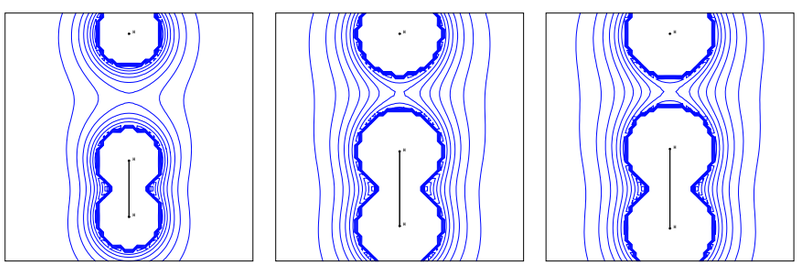
coordinate of $-0.5 < RX < 0.5$, which when compared with the trend of the normal modes of vibration, Figure 4(d), we notice that this is the same range in are the peaks we define the transition zone, also in this range we can say that the charge transfer occurs between the subsystems, see Figure 4(c), this leads us to infer that the area defined by the maximum flow of information is the area where important physical and chemical changes involved in this



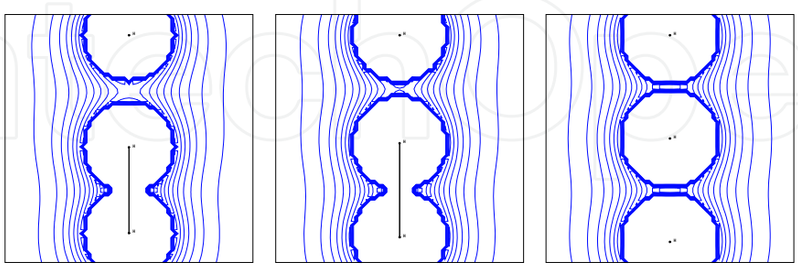
(a) $H(A,B)$ (b) $H(A:B)$



(c) RX = -2.49852 (d) RX = -2.39853 (e) RX = -2.29854



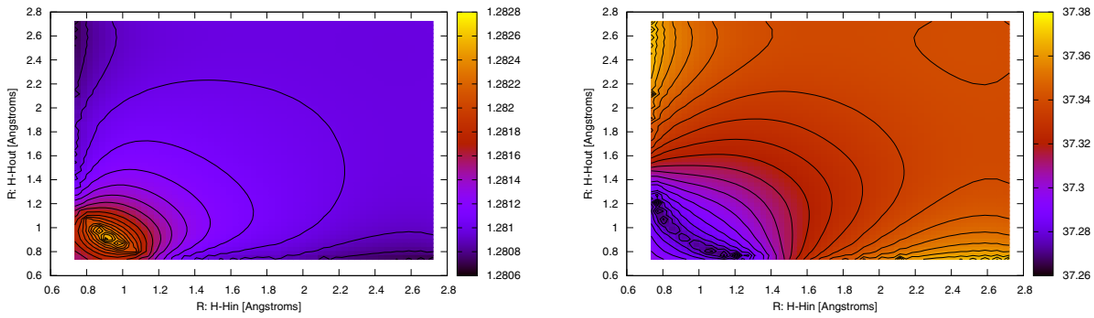
(f) RX = -2.19858 (g) RX = -1.49883 (h) RX = -1.39883



(i) RX = -1.29884 (j) RX = -1.19884 (k) RX = 0.00000 (Transition State)

Fig. 6. Trends of $H(A,B)$, $H(A:B)$ using $\{A\} = \{H\}$ and $\{B\} = H_{in}H_{out}$ and the Molecular Electric Potential in different points of the reaction coordinate in the process $H_2 + H^- \longrightarrow H_2 + H^-$.

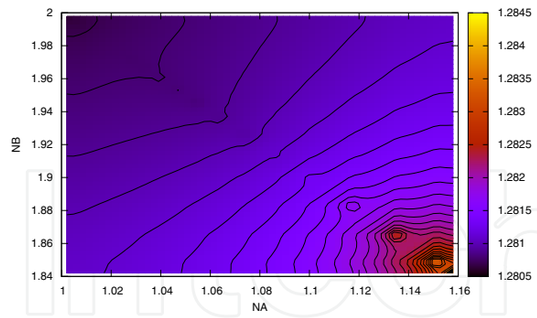
process is carried out and while the flow of information in the $-0.5 < RX < 0.5$ is maximum, the trajectory informational, Figure 7(b), decreases when the internuclear distance increases.
This same behavior leads to the conjecture that when carrying out a physical or chemical process exist gradients of information, this gradients must be associated with the electronic distribution system, therefore, in Figure 8(a) we present a contour map representing the variation of subsystems charges with respect to information flow. Using this figure we try to relate the informational content of the subsystems that are involved in this process with the charge density from which we notice that when the charge density of the subsystem A, is approximately the values $1.13 < NA < 1.16$ and B of the subsystem at $1.84 < NB < 1.87$, thereby when there are major differences in charges between the subsystems is when we observe the flow of information between the subsystems is maximal.



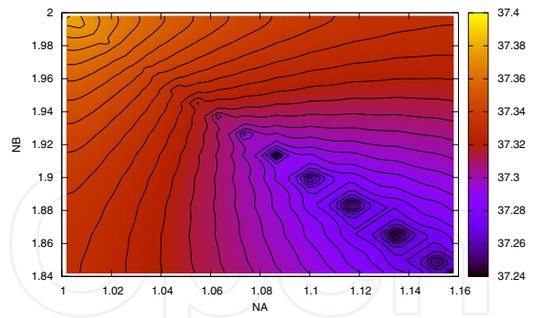
(a) Internuclear distances with informational flow (b) Inter nuclear distances with informational trajectory

Fig. 7. Contour maps of the informational flow and informational trajectories in the process $H_2 + H^- \longrightarrow H_2 + H^-$.

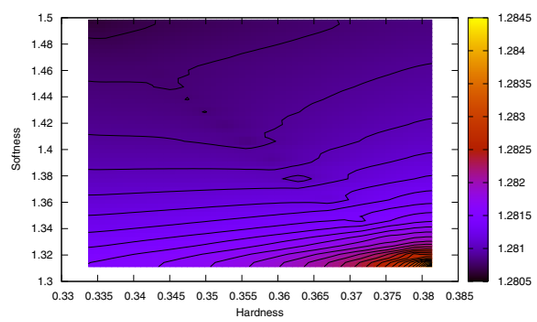
Also, notice that this flow is not constant during the process and is associated with the difference of the charge densities of the various subsystems which leads us to infer that there must be gradients of information which in turn must be related to the charge density of the subsystems, and in Figures 8(a) and 8(b) shows the contour maps showing the change of the charge density of the subsystems with the flow and informational trajectory. This also leads us to establish a conjecture about the existence of gradients of information. This permit us relate these gradients information changes with some parameters of chemical reactivity such hardness and softness.
In Figures 8(c) and 8(d) we present maps of the variation of hardness respect to the flow of information and informational trajectory. Figure 8(c) shows the surface that relates the change in hardness, softness in the information flow, in this case we notice that with the coordinates $0.36 < \eta < 0.385$ and $1.3 < S < 1.33$ we define the area where the information flow is maximum, this area also is an area of $-0.25 < RX < 0.25$, see Figures 5(a) and 5(b) thereby in this range of the intrinsic reaction coordinate important chemical and physical changes occurs, such as charge transfer which is closely related to the process of break and formation of a chemical bond.
Finally, with this example we have tried to link information from a system that is subjected to a process with the physical and chemical changes. Thus, we have linked the concept of *information*, which is an epistemological concept completely with ontological concepts and



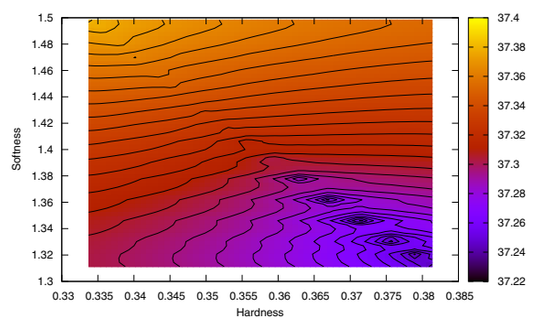
(a) Density charge of subsystems with informational flow



(b) Density charge of subsystems with informational trajectory



(c) Plane of the Hardness-Softness variation, and the informational flow.



(d) Plane of the Hardness-Softness variation and the informational trajectory.

Fig. 8. Contour maps of the informational flow and informational trajectories in the process $H_2 + H^- \longrightarrow H_2 + H^-$.

the solution concepts or interpretation of the results allows us feedback on these concepts in ontological terms, according to the author, abstract and more general.
By other part, is probable that today do not exist a ortodoxical definition of what actually is the *information*, beyond that presented by Shannon and its guidelines, criteria, characterization of it, among other things, the interpretation and the relationship with other concepts such as: energy, electron density, chemical reactivity parameters and many others need be discussed to try of establish a formal relation between concepts.
So, there is no doubt that both knowledge and the praxis and reality as knowledge scientific understanding and also, is it clear that information concept and the model itself is interdisciplinary or transdisciplinary. The concept and moreover, the model itself, promotes a systematic relation with causal analogies and parallelism with scientific knowledge, which transcends the framework of the source domain and extend in various directions, thus making the knowledge acquires an unusual resonance, as this, we believe it is feasible to complement the explanations of natural processes and natural systems.

This model is not intended that the manner of the old school, that using metaphysical substance, the particularities of the processes reveal themselves to us in the end as a progressive manifestation of homogeneous order or a unitary whole and absolute. It is simply to promote and implement a partnership scheme which promises analog route and cover knowledge in a way easier.
Thereby, one of the first goals of the Information Theory that can be invoked to find the link to Modern Chemistry is that through such a link is possible to restore a space for dialogue in this branch of science that in some cases lost or greatly reduced mended because the large number of specialized topics and concepts, thereby, with this scenario is possible consolidate a new vanguard line of research.

5. Conclusion

As the reader will appreciate the above discussion, Information Theory allows us to postulate that in any macroscopic system can identify an attribute inherent in its nature the electron density, energy and entropy. Each of them has a clear and precise physical meaning and its definition is accompanied by an operational rule to quantify it, that is, assigning numerical values. Thus we speak of universal axioms that govern natural processes.
However, we can make the question of what is now known about the informational entropy, which is related to the informational content of a classical or quantum observables and the same. So is there a universal axiom of incontrovertibly establish the relationship between information system with observables?
Thus, the study of physical processes and systems relatively simple physicochemical located within a general outline more or less well understood. But obtaining results that can compare with the experiment is a not a goal yet, in our point of view, it is therefore necessary to understand and apply a theory general enough to try to describe, explain and understand the behavior of natural systems.
For complex systems, like a biological, geophysical, or juts systems constitutes by a large particle number. We think that we are very far from being able to offer a convincing theory.
Finally we can say that now days the interest shifts to the study of systems far from equilibrium or complex processes that interact around through the exchange of matter, energy and information.

6. References

Nelson Flores-Gallegos and Rodolfo O. Esquivel. von Neumann Entropies Analysis in Hilbert Space for the Dissociation Processes of Homonuclear and Heteronuclear Diatomic Molecules. *J. Mex. Chem. Soc.*, Vol. 52, No. 1, (2008) 19-30, ISSN 1870-249X.

Rodolfo O. Esquivel, Nelson Flores-Gallegos, Cristina Iuga, Edmundo M. Carrera, Juan Carlos Angulo, Juan Antolín. Phenomenological description of the transition state, and the bond breaking and bond forming processes of selected elementary chemical reactions: an information-theoretic study. *Theor. Chem. Acc.*, Vol. 240, 445-460 (2009), ISSN 1432-881X.

Edmundo M. Carrera, Nelson Flores-Gallegos, Rodolfo O. Esquivel. Natural atomic probabilities in quantum information theory. *Journal of Computational and Applied Mathematics.*, Vol. 233, 1483-1490 (2010), ISSN 0377-0427.

V. Vedral, The Role of relative entropy in quantum information theory. *Rev. Mod. Phys.*, Vol. 74, 197-234 (2002), ISSN 0034-6861.

C. E. Shannon, A mathematical theory of communication. *The Bell System Technical Journal*. Vol. 27, 379-423, 623-656, July, October (1948), ISSN 0005-8580.

Reed A. E., Weinstock R. B., Weinhold F. Natural Population Analysis. *J. Chem. Phys*. Vol. 83, No. 2, (1985) 735-747 , ISSN 0021-9606.

P. O. Löwdin. Quantum Theory of Many-Particle Systems I. Physical Interpretation by Means of Density Matrices, Natural Spin-Orbitals, and Convergence Problems in the Method of Configuration Interaction. *Phys. Rev.*, Vol. 97 (1955) 1474-1489, ISSN 0031-9007.

G. Bruhn, E. R. Davidson, I. Mayer, and A. E. Clark. Löwdin Population Analysis With and Without Rotational Invariance. *Int. Jour. of Quantum Chem.*, Vol. 106 (2006) 2065-2072, ISSN 0020-7608.

Nelson Flores-Gallegos *Teoría de información cuántica como lenguaje conceptual en Química*. Tesis Doctoral. Universidad Autónoma Metropolitana-Iztapalapa. México D.F. (2010).

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr. T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewsk, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople 2004, Gaussian Inc. Wallingford CT, Gaussian 03 Revision D.01.

Glendening, E. D., Badenhoop, J. K., Reed, A. E., Carpenter, J. E., Bohmann, J. A., Morales, C. M., Weinhold, F., NBO 5.0, Theoretical Chemistry Institute 2001, University of Wisconsin, Madison.

Schaftenaar, G., Noordik, J. H. MOLDEN: a pre- and post-processing program for molecular and electronic structures., *J. Comput. Aided Mol. Design* Vol. 14 (2000) 123-134, ISSN 0920-654X.

Parr, R. G. & Yang, W. (1989). *Density-Functional Theory of Atoms and Molecules*, Oxford University Press. ISBN 0-19-504279-4, United States of America.

Guiaşu, S. (1977). *Information Theory with Applications*, MacGraw-Hill International Book Company. ISBN 0-07-025109-6, Great Britain.

von Neumann, J. (1955). *Mathematical foundations of quantum mechanics*, Princeton, N. J.: Princeton University Press. L.C.Card 53-10143, London: Geoffrey Cumberlege.

Johnson, B. G., Gonzales, C. A., Gill, P. M. W. Pople, J. A. A density functional study of the simplest hydrogen abstraction reaction. Effect of self-interaction correction. *Chem. Phys. Lett.*, Vol. 221 (1994) 100-108, ISSN 0009-2614.

Ziesche, P. Correlation Strengh and Information Theory., *Int. J. Quantum Chem.* Vol. 56 (1995) 363-369, ISSN 0020-7608.

Parr, R. G., Ayers, P. W. and Nalewajski, R. F., What is an atom in a molecule?. *J. Phys. Chem.*, Vol. 109 (2005) 3957-3959, ISSN 1089-5639.

Fano, U., Descriptions of States in Quantum Mechannics by Density Matrix and Operador Techniques., *Rev. Mod. phys.*, Vol. 29 (1957) 74-93, ISSN 0034-6861.

McWeeny, R., Some Recent Advances in Density Matrix Theory., *Rev. Mod. Phys.*, Vol. 32 (1960) 335-369, ISSN 0034-6861.

Davidson, E. R. (1976). *Reduced Density Matrices in Quantum Chemistry.*, Academic Press Inc. (London), ISBN 0-12-205850-X.

Molmer, K. Sorensen, A. Multiparticle Entanglement of Hot Trapped Ions. *Phys. Rev. Lett.*, Vol. 82 (1999) 1835-1838, ISSN 1079-7114.

Cirac, J. I. and Zoller, P., Quantum Computations with Cold Trapped Ions. *Phys. Rev. Lett.*, Vol. 74 (1995) 4091-4094, ISSN 1079-7114.

Sorensen, A. and Molmer, K., Qantum Computation with Ions in Thermal Motion. *Phys. Rev. Lett.*, Vol. 82 (1999) 1971-1974, ISSN 1079-7114.

Kreuter, A. Becher, C. Lancaster, G. P. T. Mundt, A. B. Russo, C. Haffner, H., Roos, C., Eschner, J., Schmidt-Kaler, F., Blatt, R., Spontaneous Emission Lifetime of a Single Trapped Ca^{+} Ion in a High Finesse Cavity., *Phys. Rev. Lett.*, Volume 92 (2004) 203002-203006, ISSN 1079-7114.

Schlosser, N., Reymond, G., Protsenko, I., Grangier, P., Sub-poissonian loading of single atoms in a microscopic dipole trap., *Nature*, Vol. 411 (2001) 1024-1027, ISSN 0028-0836.

Monroe, C., Meekhof, D. M., King, B. E., Itano, W. M., Wineland, D. J., Demostration of a Fundamental Quantum Logic Gate. *Phys. Rev. Lett.*, Vol. 75 (1995) 4714-4717, ISSN 1079-7114.

Tittel, W., Brendel, J. Gisin, B. Herzog, T., Zbinde, H., Gisin, N., Experimental demostration of quantum correlations over more than 10 km., *Phys. Rev. A.*, Vol. 57 (1998) 3229-3232, ISSN 1050-2947.

Jian-Wei, P., Bouwmeester, D., Daniel, M., Experimental test of quantum nonlocality in three-photon., *Nature*, Vol. 403 (2000) 515-519, ISSN 0028-0836.

Ladd, T. D., Goldman, J. R., Yamaguchi, F., Yamamoto, Y., All-Silicon Quantum Computer., *Phys. Rev. Lett.*, Vol. 89 (2002) 017901-017905, ISSN 1079-7114.

Braunstein, S. L., Caves, C. M., Jozsa, R., Linden, N., Popescu, S. Schack, R., Separability of Very Noisy Mixed States and Implications for NMR Quantum Computing., *Phys. Rev. Lett.*, Vol. 83 (1999) 104-107, ISSN 1079-7114.

Beveratos, A., Brouri, R., Gacoin, T., Villing, A., Poizat, J.-P., Grangier, P., Single Photon Quantum Cryptography., *Phys. Rev. Lett.*, Vol. 89 (2002) 187901-187905, ISSN 1079-7114.

Jennewein, T., Simon, C., Weihs, G., Weinfurter, H. Zeilinger, A., Quantum Cryptography with Entangled Photons., *Phys. Rev. Lett.*, Vol. 84 (2000) 4729-4732, ISSN 1079-7114.

Gisin, N., Ribordy, G., Tittel, W. Zbinden, H., Quantum cryptography., *Rev. Mod. Phys.*, Vol. 74 (2002) 145-195, ISSN 0034-6861.

Horodecki, M., Oppenheim, J., Winter, A., Partial quantum information., *Nature*, Vol. 436 (2005) 673-676, ISSN 0028-0836.

Divincenzo, D., Horodecki, M., Leung, D., Smolin J., Terha, B., Locking classical correlation in quantum states., *Phys. Rev. Lett.*, Vol. 92 (2004) 067902-067906, ISSN 1079-7114.

Horodecki, M., Oppenheim, J., Horodecki, R., Are the laws of entanglement theory thermodynamical?., *Phys. Rev. Lett.*, Vol. 89 (2002) 240403-240407, ISSN 1079-7114.

Horodecki, R., Horodecki, P., Horodecki, M., Violating Bell inequality by mixed spin $-\frac{1}{2}$ image states: necessary and sufficient condition., *Phys. Lett. A.*, Vol. 200 (1995) 340-344, ISSN 0375-9601.

Hoderecki, R., Hoderecki, M., Information-theoretic aspects of inseparability of mixed states., *Phys. Rev. A.*, Vol. 54 (1996) 1838-1846, ISSN 0375-9601.

Horodecki, M., Horodecki, P., Horodecki, R., Separability of mixed states: necessary and sufficient conditions., *Phys. Lett. A.*, Vol. 223 (1996) 1-8, ISSN 0375-9601.

Horodecki, P., Separability criterion and inseparable mixed states with positive partial transposition., *Phys. Lett. A.*, Vol. 232 (1997) 333-339, ISSN 0375-9601.

Horodecki, M., Horodecki, P., Horodecki, R., Mixed–State Entanglement and Distillation: Is there a "Bound" Entanglement in Nature?., *Phys. Rev. Lett.*, Vol. 80 (1998) 5239-5242, ISSN 1079-7114.

Horodecki, R., Horodecki, P., Horodecki, M., Horodecki, K., Quantum Entanglement., *Rev. Mod. Phys.*, Vol. 81 (2009) 865-942, ISSN 0034-6861.

Aspect, A., Quantum Mechanics: To be or not to be local., *Nature* Vol. 446 (2007) 866-867, ISSN 0028-0836.

Timothy, Y., Ayman, F., Abouraddy Bahaa E., A., Saleh Malvin C., Teich., Experimental Violation of Bell's Inequality in Spatial-Parity Space., *Phys. Rev. Lett.*, Vol. 99 (2007) 170408-1704012, ISSN 1079-7114.

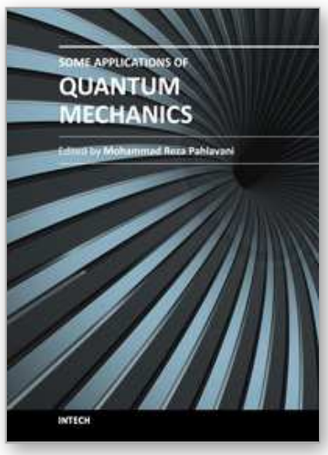
Einstein, A., Podolsky, B., Rosen, N., Can Quantum–Mechanical Description of Physical Reality Be Considered Complete?, *Phys. Rev.*, Vol. 47 (1935) 777-780, ISSN 1943-2879.

Bell, J. S., On the Problem of Hidden variables in Quantum Mechanics., *Rev. Mod. Phys.*, Vol. 38 (1966) 447-452, ISSN 0034-6861.

Seeger, R. and Pople, J. A., Self-Consistent Molecular Orbital Methods. 28. Constraints and Stability in Hartree-Fock Theory., *J. Chem. Phys.*, Vol. 66 (1977) 3045-3050, ISSN 0021-9606.

Bauernschmitt, R. and Ahlrichs, R., Stability analysis for solutions of the closed shell Kohn-Sham equation., *J. Chem. Phys.*, Vol. 104 (1996) 9047-9052, ISSN 0021-9606.

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