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Information and quantum theories: an analysis in one-dimensional systems

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Abstract

We pedagogically present the information theory as originally established, explaining its essential ideas and paying attention to the expression employed to measure the amount of information. We also discuss relationships between information and quantum theories. In this context we determine the information entropies on the position, S_x, and momentum, S_p, spaces, in addition to the entropy sum, S_t. Here, we use the modified entropic expressions that are dimensionally consistent. We provide original explanations for the behaviors of the S_x, S_p and S_t values analyzing the probability densities and by means of the normalization constants and properties of Fourier transform. We validate the entropic uncertainty relation and inspect the standard deviation and information entropies as measures of quantum uncertainty. The systems of interest are unidimensional one-particle quantum systems in the ground and excited states.

Keywords: information theory, measures of quantum uncertainty, one-dimensional quantum systems, modified information entropies

(Some figures may appear in colour only in the online journal)

1. Introduction

The understanding and interpretation of the quantity known as entropy include at least three areas of knowledge; namely, thermodynamics, statistical mechanics and information theory. The entropy arises in the thermodynamic scope [1, 2], but with the atomistic assumption and statistical methods such concept gains a new meaning [3, 4]. It also emerges in the communications through use of the information entropy or Shannon entropy [5, 6]. Information entropies on the position, S_r, and momentum, S_p, spaces, in addition to the entropy sum, S_t, connect information theory and quantum mechanics [7, 8]. In this way, concepts and ideas find applicability in different areas aside from those originally defined.

Initially identified as an autonomous area, the mathematical theory of communication or information theory now has its fundamental concepts utilized in distinct fields of expertise, mainly through the informational entropy [9–11]. Information theory in the atomic, molecular and chemical physics context has generated a reasonable number of analyses [12–19]. Works about ions in plasma environments [20] and correlation measurements [21, 22] show great results in favor of the informational treatment. The examination of the strong confinement regime [23] and systems constrained by a dielectric continuum [24] apply the informational language. Also, the entropic expressions analyze the phenomena of localization or delocalization of the probability densities [25, 26].

One-dimensional quantum systems are a standard topic of the quantum theory studied in undergraduate courses of physics and related areas. They present important features as benchmark systems: they have exact solutions, reveal the existence of non-classical effects and do not present many difficulties in their solution as do higher dimensional systems. Research for one-dimensional systems using the informational entropy presents contributions to the infinite potential well (particle in a box) [27, 28] and to the harmonic potential (harmonic oscillator) [29, 30].

The goal of this work is to pedagogically show for teachers and students the relationships between information and quantum theories. We consider the connection provided by probability densities, emphasizing the modified entropic expressions that are dimensionally consistent. Applications to one-dimensional quantum systems are investigated.

The paper is organized as follows. In section 2 we present the information theory as originally established, explaining its essential ideas and paying attention to the expression employed to measure the amount of information. In section 3 we identify connections between information and quantum theories, highlighting certain subtleties. In section 4 we discuss the unidimensional one-particle quantum systems of interest, while in section 5 we present and analyze our results and compare them, when available, with those previously published. Finally, in section 6 we summarize the main aspects of the current study. In the appendix, we perform a dimensional analysis of the entropic expressions. In appendix A and B, we discuss how to reach the expression for S_t and we perform a dimensional analysis of the entropic expressions, respectively. All formalisms presented in this paper will be developed for one-dimensional systems.

2. Information theory

A mathematical theory of communication or information theory arose with the report of Shannon in 1948 [31]. Other works are significant for understanding the problem, including that of Nyquist [32], which suggest a quantity of telegraphic data, and Hartley [33], which delimits the meaning of information and shows its measurement by a logarithmic function. Weaver's explanation expands the applications of Shannon's research to include a spectrum of processes such as oral transmissions, music and photography [5].

The communication is considered as a process in which one mechanism affects another through a message. In this background, information is a measure of the choice of a message within an available repertoire. The essential question of information theory is how to replicate (or make as similar as possible) at a destination point a message transmitted from a point of origin [5].

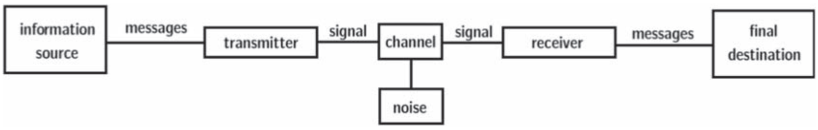

Figure 1. Diagram of a general communication system.

The model that defines a general communication system is illustrated in figure 1. In this diagram, the information source chooses a message from a possible group of them, so the transmitter codes the message into a signal that is sent by the communication channel. The message in the communication channel may be influenced by the noise, characterized as external changes imposed on the signal. The receiver decodes the original message to be delivered to the final destination.

In the sending and receiving process of a message, the semantic aspects are secondary ones. The expression employed to measure the amount of information generated in a message by a discrete information source is [31]

$$S(\{p_i\}) = -\sum_{i=1}^{j} p_i \log_2(p_i), \tag{1}$$

where $\{p_i\}$ represents the group of complete messages, j is the number of messages and p_i is the probability of occurrence of the ith message. These probabilities are constrained by the normalization condition, $\sum_{i=1}^{j} p_i = 1$, and non-negative condition, $_{pi} \geqslant 0, \forall\ i$. For $i = a$ and $p_a = 0$, this implies $p_a \log p_a \equiv 0$. In case of a continuous information source [31], equation (1) is written as

$$S(p(\alpha)) = -\int_{-\infty}^{\infty} \mathrm{d}\alpha\ p(\alpha)\log_2 p(\alpha), \tag{2}$$

where $p(\alpha)$ is a probability density in function of a continuous α variable, also constrained by the normalization condition, $\int_{-\infty}^{\infty} d\alpha\ p(\alpha) = 1$, and non-negative condition, $p(\alpha) \geqslant 0, \forall\ \alpha$. The values provided by equation (2) may be negative (see pg. 631 in [31]), where $p(\alpha)$ is bigger than 1 in some region of the α-domain. The expressions (1) and (2) are known as the information entropy or Shannon entropy[1].

The logarithmic base in equations (1) and (2) specifies the informational unit, e.g. hartleys and nats for 10 and neperian number logarithmic bases, respectively. When communication processes adopt base 2, the informational unit is the bit (binary digit). Note that a base change involves only a variation of scale.

3. Connection between information and quantum theories

Max Born, in the probabilistic interpretation of quantum mechanics [36], proposed the quantity $\rho(x)$ to be related to the probability density on position space and assigned it, in terms of the Schrödinger equation solution $\psi(x)$, as $\rho(x) = |\psi(x)|^2$. The Fourier transform of the function $\psi(x)$ is defined by $\widetilde{\psi}(p)$. In the same way, we establish a probability density on momentum space as $\gamma(p) = |\widetilde{\psi}(p)|^2$. In quantum theory, $\rho(x)$ has the dimension of the inverse of length and $\gamma(p)$ has the dimension of the inverse of momentum.

[1] The relationship between Boltzmann and Shannon entropies is a controversial point and the similarities are not so clear. Although definitions of both quantities are based on probability distributions, one should take care when comparing them. In this way, there are peculiar forms of comparing these distinct quantities [34, 35].

The dimensional adequate information entropies on position, S_x, and on momentum, S_p, spaces are given by [23]

$$S_x = -\int dx\ \rho(x) \ln(a_0\ \rho(x)) \tag{3}$$

and

$$S_p = -\int dp\ \gamma(p) \ln\left(\left(\frac{\hbar}{a_0}\right) \gamma(p)\right). \tag{4}$$

Here, the probability densities $\rho(x)$ and $\gamma(p)$ are normalized to unity. The equations (3) and (4) are characterized with the fundamental physical constants a_0, Bohr radius, and $\hbar$, the reduced Planck constant.

In the framework of union between information theory and quantum mechanics we obtain the entropic uncertainty relation. This relation is derived from the entropy sum of $S_x + S_p$ of the non-commuting position $\mathcal{X}$ and momentum $\mathcal{P}$ observables [37]. So, we have [23]

$$S_t = S_x + S_p = -\int\int dx\ dp\ \rho(x)\ \gamma(p)\ \ln(\hbar\rho(x)\ \gamma(p))\ \geqslant (1 + \ln \pi). \tag{5}$$

Note that the S_t value is bounded because it displays a minimum value for the entropy sum. In appendix A we discuss how to find the expression of S_t.

An adequate dimensional analysis in expressions (3)–(5) is guaranteed by the fundamental physical constants a_0 and $\hbar$. We examine in appendix B the dimensional balance of the entropic expressions in this work. We show that modified information entropies S_x and S_p, in addition to the modified entropic uncertainty relation are dimensionally adequate. The dimensional analysis does not consider any possible unit, thus the expressions proposed in reference [23] have a more general aspect than the relation regularly employed for the information entropies, e.g. reference [7].

In quantum theory, it is known that the measure of any two non-commuting observables $\mathcal{A}$ and $\mathcal{B}$ can only be done within a limit of accuracy. These quantitative descriptions are recognized as uncertainty relations. In this sense, Heisenberg's uncertainty principle presents this unpredictability in a conceptual way [38, 39]. In particular, for position $\mathcal{X}$ and momentum $\mathcal{P}$ observables, with their respective quantum operators $\hat{X}$ and $\hat{P}$, Kennard rigorously establishes the relation [40, 41]

$$\Delta\hat{X}\Delta\hat{P} \geqslant \frac{\hbar}{2}. \tag{6}$$

The standard deviations are

$$\Delta\hat{X} = \sqrt{\langle x^2\rangle - \langle x\rangle^2} \quad \text{and} \quad \Delta\hat{P} = \sqrt{\langle p^2\rangle - \langle p\rangle^2}, \tag{7}$$

where

$$\langle x\rangle = \int dx\ x\rho(x), \ \ \langle x^2\rangle = \int dx\ x^2\rho(x) \tag{8}$$

and

$$\langle p\rangle = \int dp\ p\gamma(p), \ \ \langle p^2\rangle = \int dp\ p^2\gamma(p). \tag{9}$$

Kennard's relation (6) establishes that it is not possible to simultaneously measure the position and momentum of a particle with arbitrary precision.

$\Delta\hat{X}$ or $\Delta\hat{P}$ quantities are dispersion (or spread) measures of the probability distributions in relation to the mean value $\langle x \rangle$ or $\langle p \rangle$. The S_x and S_p entropies are also types of dispersion or spread measures. However, in this specific case, they are calculated without taking into account reference points in the probability distributions, being therefore a genuine spread measure of the probability distributions. In this sense, the standard deviation and information entropies are a measure of uncertainty (localization or delocalization of the particle in the space) with different characteristics. The uncertainties can also be quantified by means of the Fisher information [42] and Tsallis and Rényi entropies [43], among others. The topic of which quantities are most consistent to measure quantum uncertainty is the object of discussion in the literature [44–47].

Uncertainty relations (5) and (6) reach their minimum values with the adoption of Gaussian-type wave functions such as in the ground state of the harmonic oscillator [29, 48]. The entropic uncertainty relation is considered as a stronger version of Kennard's relation, in the sense that from relation (5) we can deduce the relation (6) [37]. Still, uncertainty relations in terms of S_x and S_p are proposed to deal with situations where Heisenberg's uncertainty principle or Kennard's relation presents sensitivities [27, 28], as for instance, in the study of separable phase-space distribution [30, 49].

4. Systems of interest

The time-independent Schrödinger equation is written as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{10}$$

where m is the mass of the particle, E is the energy of the stationary state and $V(x)$ is the potential function.

A complete statement of the question is set when establishing the potential function $V(x)$ in equation (10) and boundary conditions for the wave function. The potential functions of interest in this paper are specified in sections 4.1 and 4.2.

4.1. Harmonic potential

As an initial approximation, this model expresses the relative motion of atoms in molecules and solids. The harmonic potential is given by

$$V(x) = \frac{1}{2}m\omega^2x^2, \tag{11}$$

where ω is the angular frequency of the classical oscillator and x is the displacement of the mass m regarding the equilibrium position in the origin of the coordinate framework. From now on we will call this system a harmonic oscillator. The angular oscillation frequency ω relates to the force constant k by the expression $\omega = \sqrt{k/m}$.

The resolution of equation (10) for the potential function (11) can be done by different procedures such as the algebraic [48] and the analytical [50] ones. The eigenvalues and eigenfunctions are respectively

$$E_n = \hbar\omega(n + 1/2) \tag{12}$$

$$\psi_n(x) = A_n e^{-\frac{\beta x^2}{2}} H_n(\sqrt{\beta}x), \tag{13}$$

where $A_n = 2^{-n/2}\pi^{-1/4}(n!)^{-1/2}\beta^{1/4}$ is the normalization constant, the β parameter is $m\omega/\hbar$ and $H_n(\sqrt{\beta}x)$ represents the Hermite polynomials [51]. The quantum number n takes non-negative values and specifies the quantum state of the system.

4.2. Infinite potential well

The infinite potential well is defined by

$$V(x) = \begin{cases} \infty & \text{to} \quad |x| \geqslant x_c/2 \\ 0 & \text{to} \quad |x| < x_c/2 \end{cases}, \tag{14}$$

where x_c is the confinement distance (width of the box). From now on we will call this system a particle in a box. For the x range of values between $-x_c/2$ and $x_c/2$, the particle is free. The boundary conditions, $\psi(x = \pm x_c/2) = 0$, force the confinement.

The general solution of equation (10) for the potential function (14) is given by [52]

$$\psi(x) = Ae^{ikx} + Be^{-ikx}. \tag{15}$$

By imposing the boundary conditions in equation (15) and choosing a nontrivial solution, we find

$$\psi_n(x) = A_n \cos(k_n x) \tag{16}$$

and

$$\psi_n(x) = B_n \sin(k_n x), \tag{17}$$

with the eigenvalues given as

$$E_n = \frac{\pi^2\hbar^2 n^2}{2mx_c^2}. \tag{18}$$

Normalization constants A_n and B_n are equal and independent of the state; they only depend on $x_c^{-1/2}$. The parameter $k_n = n\pi/(2x_c)$ is identified as the wave number. Furthermore, n specifies the quantum number and determines the fundamental and excited states of the system. The cosine-type solution adopts $n = 1, 3, 5, \ldots$, while for the sine type, n takes the values $2, 4, 6, \ldots$.

5. Results and discussion

In sections 5.1 and 5.2, we examine the data for the harmonic potential and for the infinite potential well. We use the atomic units (a.u.) system, which is common in atomic and molecular physics works. This system uses the mass, m_e, and the elementary charge, e, of the electron, the constant of electrostatic force, $1/4\pi\varepsilon_0$, and the reduced Planck constant, $\hbar$, as standard units of their quantities. The atomic unit system, beyond simplifying the main equations in quantum theory for atoms and molecules, has computational advantages in numerical computations. We used the software Maple13 to perform the calculations. In all calculations we consider $m = m_e$.

5.1. Harmonic potential

We investigated the three lowest energy states $n = 0$, 1 and 2 of the harmonic oscillator. The values of modified information entropies S_x and S_p as a function of ω are presented in table 1, jointly with the entropy sum S_t. With a decrease of the ω value, the S_x value increases, while the S_p value decreases. Moreover, S_t is constant with ω and increases with n. The reference

Table 1. Modified information entropies S_x and S_p, in addition to the entropy sum, S_t, as a function of ω for the harmonic oscillator to the three lowest energy states. All values in atomic units system.

	S_x			S_p			S_t		
ω	$n=0$	$n=1$	$n=2$	$n=0$	$n=1$	$n=2$	$n=0$	$n=1$	$n=2$
0.0600	2.4791	2.7494	2.9053	−0.3343	−0.0640	0.0919	2.1447	2.6855	2.9972
0.0800	2.3352	2.6056	2.7615	−0.1905	0.0799	0.2357	2.1447	2.6855	2.9972
0.2000	1.8771	2.1474	2.3033	0.2676	0.5380	0.6939	2.1447	2.6855	2.9972
0.4000	1.5305	1.8009	1.9568	0.6142	0.8846	1.0405	2.1447	2.6855	2.9972
0.5000	1.4189	1.6893	1.8452	0.7258	0.9962	1.1520	2.1447	2.6855	2.9972
1.0000	1.0724	1.3427	1.4986	1.0724	1.3427	1.4986	2.1447	2.6855	2.9972
2.0000	0.7258	0.9962	1.1520	1.4189	1.6893	1.8452	2.1447	2.6855	2.9972
3.0000	0.5231	0.7934	0.9493	1.6217	1.8920	2.0479	2.1447	2.6855	2.9972
4.0000	0.3792	0.6496	0.8055	1.7655	2.0359	2.1918	2.1447	2.6855	2.9972
5.0000	0.2676	0.5380	0.6939	1.8771	2.1474	2.3033	2.1447	2.6855	2.9972
6.0000	0.1765	0.4468	0.6027	1.9682	2.2386	2.3945	2.1447	2.6855	2.9972
7.0000	0.0994	0.3698	0.5257	2.0453	2.3157	2.4716	2.1447	2.6855	2.9972
8.0050	0.0323	0.3027	0.4586	2.1124	2.3828	2.5386	2.1447	2.6855	2.9972

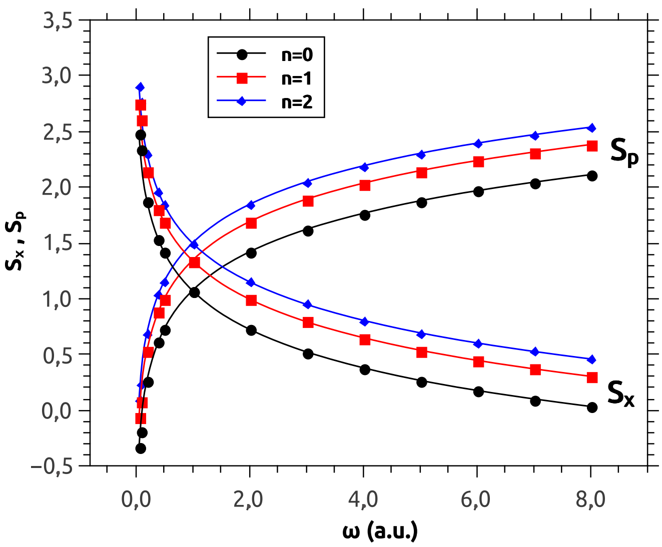

Figure 2. Modified information entropies S_x and S_p as a function of ω for the harmonic oscillator to the three lowest energy states.

[53] establishes the values of S_x and S_p for the first six quantum states of the harmonic oscillator for $\omega = 1.0000$ a.u. This study indicates that the information entropy values increase with n. The present paper endorses the reference [53] and generalizes this characteristic for some values of ω.

In figure 2, the curves of S_x and S_p versus ω are presented. The crossing points of the curves for the three lowest energy states occur in $\omega = 1.000$ a.u. to $S_x = S_p = 1.0724$ for $n = 0$, to $S_x = S_p = 1.3427$ for $n = 1$ and to $S_x = S_p = 1.4986$ for $n = 2$. For this ω value, the Hamiltonian is given by $H = \frac{1}{2}p^2 + \frac{1}{2}x^2$ in a.u. So the probability densities on the position and momentum spaces have the same prevalence on the system; that is, they are equally balanced. Furthermore, the values of S_x and S_p at the crossing points increase with the increment of n.

The analysis of probability densities is related to the wave function in ground state, in this case a Gaussian wave function. The variation of ω in the function modifies its amplitude, transforming the spreading of this probability distribution. Thus, we can consider the localization or delocalization of a particle.

In figure 3 we present the curves of $|\psi_0(x)|^2$ and $|\widetilde{\psi}_0(p)|^2$ for distinct values of ω. Decreasing the values of ω, the spreading of $|\psi_0(x)|^2$ increases, implying a growth of delocalization, i.e. the S_x value increases. The decrease of the ω value comes together with a decrease of $|\widetilde{\psi}_0(p)|^2$ spreading, unveiling the uncertainty decreases on particle momentum, corresponding to a plunge in the S_p curves.

For ω values equal to 0.5000 a.u., 2.5000 a.u. and 5.0000 a.u. to the ground state, the $\Delta\hat{X}$ values are 1.0000 a.u., 0.4472 a.u. and 0.3162 a.u., and the $\Delta\hat{P}$ values are 0.5000 a.u., 1.1180 a.u. and 1.5811 a.u., respectively. Still, the S_x values for such frequencies are 1.4189, 0.6142 and 0.2676, while the S_p values are 0.7258, 1.5305 and 1.8771, respectively. In all cases, $\Delta\hat{X}\Delta\hat{P} = 1/2$ a.u. and $S_t = 2.1447$. The standard deviation and information entropies are equivalent measures for Gaussian-type probability distribution, having the same qualitative behavior, and satisfactorily describing the spread.

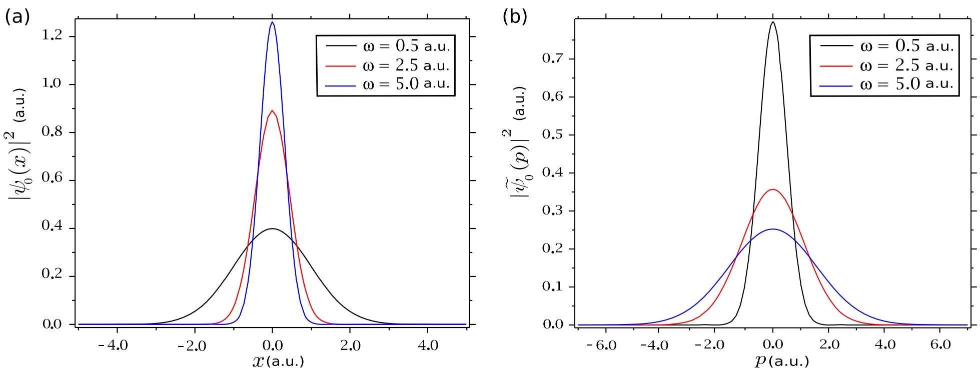

Figure 3. For the harmonic oscillator the probability densities (a) on position space $|\psi_0(x)|^2$ and (b) on momentum space $|\widetilde{\psi}_0(p)|^2$. The angular frequencies of ω are 0.5000 a.u., 2.5000 a.u. and 5.0000 a.u.

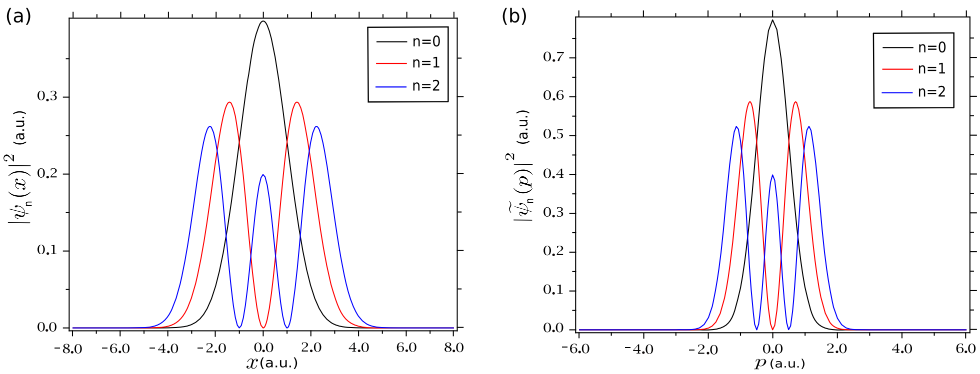

Figure 4. For the harmonic oscillator the probability densities (a) in position space $|\psi_0(x)|^2$, $|\psi_1(x)|^2$ and $|\psi_2(x)|^2$ and (b) in momentum space $|\widetilde{\psi}_0(p)|^2$, $|\widetilde{\psi}_1(p)|^2$ and $|\widetilde{\psi}_2(p)|^2$. The angular frequency is $\omega = 0.5000$ a.u.

Figure 4 presents the probability densities on position space $|\psi_1(x)|^2$, $|\psi_2(x)|^2$ and $|\psi_3(x)|^2$ and on momentum space $|\widetilde{\psi}_1(p)|^2$, $|\widetilde{\psi}_2(p)|^2$ and $|\widetilde{\psi}_3(p)|^2$, for $\omega = 0.5000$ a.u. Note that the probability densities in the position and momentum spaces increase their spreading in the respective x and p domains of the wave function with the increase of the quantum number. This represents an increasing uncertainty in the position and momentum of a particle, a result that corroborates with the increase of S_x and S_p with n that is presented in table 1.

The results obtained for the entropy sum as a function of ω are also given in table 1 and the behavior presented in figure 5. The S_t value increases with the increment of n. Moreover, despite the S_x and S_p changes, the entropy sum remains constant for each state of the system. The properties of Fourier transform, a topic studied in undergraduate physics courses, can explain these results. Since Parseval's theorem states that Fourier transform is unitary, i.e. the integral of $\rho(x)$ has the same value as the integral of $\gamma(p)$, and the normalization constant of $\widetilde{\psi}(p)$ is equal to the normalization constant of $\psi(x)$. The normalization constant of wave functions on the position and momentum spaces depends on $\beta^{1/4}$. As $\psi(x) \equiv \psi(\sqrt{\beta}x) \propto \beta^{1/4}\phi(\sqrt{\beta}x)$, the scale property of Fourier transform states that

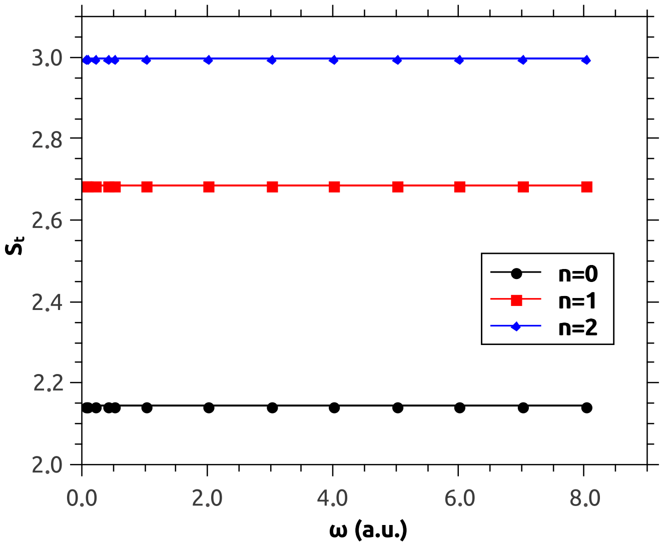

Figure 5. Entropy sum S_t as a function of ω for the harmonic oscillator to the three lowest energy states.

$\widetilde{\psi}(p) \equiv \widetilde{\psi}(p/\sqrt{\beta})/\sqrt{\beta} \propto \widetilde{\phi}(p/\sqrt{\beta})/\beta^{1/4}$, where $\phi(x)$ and $\widetilde{\phi}(p)$ are the non-normalized wave functions on the position and momentum spaces, respectively. So

$$S_t = -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\ dp\ \bar{\rho}(\sqrt{\beta}x)\ \bar{\gamma}(p/\sqrt{\beta})\ \ln(\bar{\rho}(\sqrt{\beta}x)\ \bar{\gamma}(p/\sqrt{\beta})). \tag{19}$$

Here, $\bar{\rho}(\sqrt{\beta}x) \propto \sqrt{\beta}|\phi(\sqrt{\beta}x)|^2$ and $\bar{\gamma}(p/\sqrt{\beta}) \propto |\widetilde{\phi}(p/\sqrt{\beta})|^2/\sqrt{\beta}$. Replacing $\sqrt{\beta}x$ by x and $p/\sqrt{\beta}$ by p, the entropy sum is written as

$$S_t = -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\ dp\ \bar{\rho}(x)\ \bar{\gamma}(p)\ \ln(\bar{\rho}(x)\ \bar{\gamma}(p)). \tag{20}$$

In this way, the entropy sum is independent of β, and consequently of ω too.

5.2. Infinite potential well

We investigated the particle confined in a box in the ground ($n = 1$) and also in the two first excited ($n = 2$ and 3) states by equations (16) and (17). The values of modified information entropies S_x and S_p for some values of x_c are given in table 2 and displayed in figure 6. Note that the values of S_x are identical for different quantum states.

A mathematical explanation is given by normalization constants. Normalization constants for the probability density $\rho(x)$ are the same for different states, and depend only on ${x_c}^{-1}$ for the different wave functions in equations (16) and (17). In this way, the integrand of equation (3) for different states is related by a scaling factor equal to n to the same confinement distance. For the cosine solution (16)

$$\begin{aligned} S_x &= -\int_{-x_c}^{x_c} dx\ |A|^2\cos^2(nx)\ln(a_0\ |A|^2\cos^2(nx)) \\ &= -\frac{1}{n}\int_{-nx_c}^{nx_c} dx\ |A|^2\cos^2(x)\ln(a_0\ |A|^2\cos^2(x)). \end{aligned} \tag{21}$$

Table 2. Modified information entropies S_x and S_p, in addition to the entropy sum S_t as a function of x_c for the confined particle in a box to the three lowest energy states. All values in atomic units system.

	S_x			S_p			S_t		
r_c	$n=1$	$n=2$	$n=3$	$n=1$	$n=2$	$n=3$	$n=1$	$n=2$	$n=3$
0.1000	−2.6094	−2.6094	−2.6094	4.8215	5.2164	5.3625	2.2120	2.6070	2.7531
0.2000	−1.9163	−1.9163	−1.9163	4.1283	4.5232	4.6694	2.2120	2.6070	2.7531
0.3000	−1.5108	−1.5108	−1.5108	3.7229	4.1178	4.2639	2.2120	2.6070	2.7531
0.4000	−1.2231	−1.2231	−1.2231	3.4352	3.8301	3.9762	2.2120	2.6070	2.7531
0.5000	−1.0000	−1.0000	−1.0000	3.2120	3.6070	3.7531	2.2120	2.6070	2.7531
1.0000	−0.3069	−0.3069	−0.3069	2.5189	2.9138	3.0599	2.2120	2.6070	2.7531
1.5009	0.0992	0.0992	0.0992	2.1128	2.5077	2.6538	2.2120	2.6070	2.7531
2.0000	0.3863	0.3863	0.3863	1.8257	2.2207	2.3668	2.2120	2.6070	2.7531
2.5000	0.6094	0.6094	0.6094	1.6026	1.9975	2.1437	2.2120	2.6070	2.7531
3.0000	0.7918	0.7918	0.7918	1.4203	1.8152	1.9613	2.2120	2.6070	2.7531
3.5000	0.9459	0.9459	0.9459	1.2661	1.6611	1.8072	2.2120	2.6070	2.7531
4.0000	1.0794	1.0794	1.0794	1.1326	1.5275	1.6737	2.2120	2.6070	2.7531
4.5000	1.1972	1.1972	1.1972	1.0148	1.4098	1.5559	2.2120	2.6070	2.7531
5.0000	1.3026	1.3026	1.3026	0.9094	1.3044	1.4505	2.2120	2.6070	2.7531
6.0000	1.4849	1.4849	1.4849	0.7271	1.1221	1.2682	2.2120	2.6070	2.7531
7.0000	1.6391	1.6391	1.6391	0.5730	0.9679	1.1140	2.2120	2.6070	2.7531
8.0000	1.7726	1.7726	1.7726	0.4394	0.8344	0.9805	2.2120	2.6070	2.7531
9.0050	1.8909	1.8909	1.8909	0.3211	0.7160	0.8621	2.2120	2.6070	2.7531

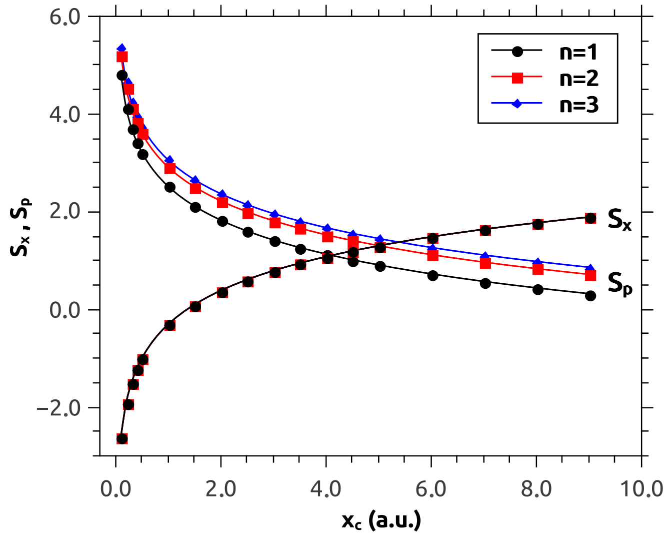

Figure 6. Modified information entropies S_x and S_p for the confined particle in a box as a function of x_c to the three lowest energy states.

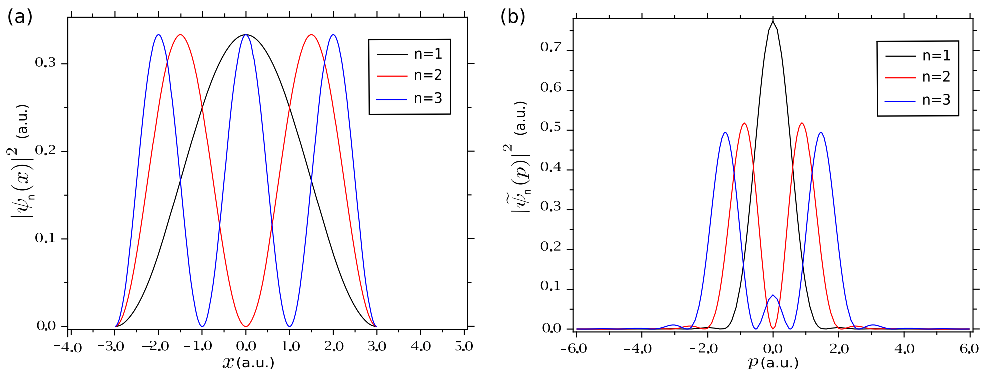

Figure 7. For the confined particle in a box the probability densities (a) in position space $|\psi_1(x)|^2$, $|\psi_2(x)|^2$ and $|\psi_3(x)|^2$ and (b) in momentum space $|\widetilde{\psi}_1(p)|^2$, $|\widetilde{\psi}_2(p)|^2$ and $|\widetilde{\psi}_3(p)|^2$. The confinement distance is $x_c = 6.0000$ a.u.

Here, nx was replaced by x. The integrand is a periodic function and it has full periods in the interval $[-x_c, x_c]$. To integrate in the new interval is the same as multiplying the S_x for the fundamental state by n. However, the factor $1/n$ keeps the integral values for excited states the same as for the fundamental one. For sine solutions (17), an identical answer is obtained since sine and cosine functions are equal by a $\pi/2$ phase shift.

A qualitative explanation of the behavior of modified entropies for different states can be obtained by analysis of the probability densities in the position and momentum spaces. In figure 7 the curves of these probability densities are presented for $x_c = 6.0000$ a.u. For example, the curves $|\psi_1(x)|^2$, $|\psi_2(x)|^2$ and $|\psi_3(x)|^2$ are spread by same range of x values (confinement limits $x = \pm x_c/2$), leading to equal values of S_x for all states. On the other

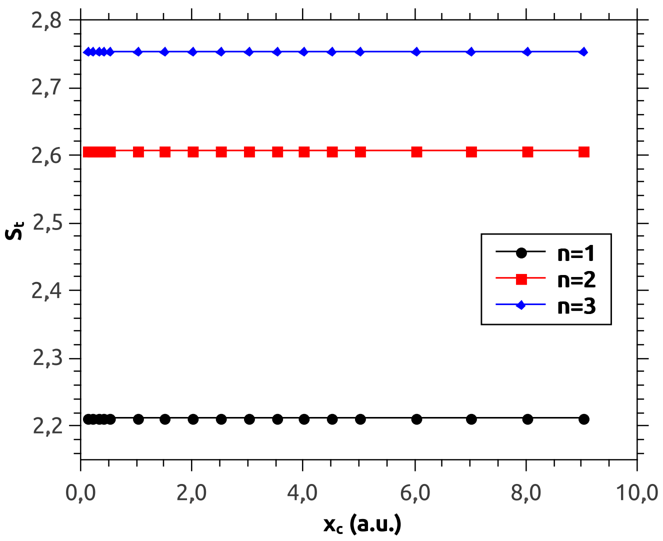

Figure 8. Entropy sum S_t as a function of x_c for the confined particle in a box to the three lowest energy states.

hand, the curves of $|\widetilde{\psi}_1(p)|^2$, $|\widetilde{\psi}_2(p)|^2$ and $|\widetilde{\psi}_3(p)|^2$ are spread for increasing ranges of p values increasing n, which explains the increase in S_p with the increment of n.

These results indicate that, in this sense, the information entropies S_x and S_p represent an uncertainty measure of the particle in the position and momentum spaces. The values of S_x decrease when confinement becomes stronger, then the uncertainty in the particle's location decreases too. The values of S_p increase with the confinement increment and affect the states more as the order of energy increases. The behaviors of S_x and S_p are the same as found in reference [30].

On the other hand, $\Delta\hat{X}$ values, calculated for $x_c = 6.0000$ a.u. for the $n = 1$, 2 and 3 states, are 1.0845 a.u., 1.5950 a.u. and 1.6725 a.u., respectively. In contrast with the behavior of S_x, the $\Delta\hat{X}$ values vary with the n increment. $\Delta\hat{X}$ is a measure of uncertainty that not only depends on x_c, but also considers a specific point of the probability distributions as a reference, so variation with n is expected. On the other hand, S_x is an entropic measure of uncertainty in the location of the particle in a box that only depends on x_c.

In figure 6 crossings can be observed between curves S_x and S_p for particular values of x_c. Approximately, for $n = 1$, the crossing point occurs at $x_c = 4.0000$ a.u., to $S_x = S_p = 1.0794$. For $n = 2$ and $n = 3$ crossing points respectively occur at $x_c = 5.0000$ a.u. to $S_x = S_p = 1.3026$ and $x_c = 5.3975$ a.u. to $S_x = S_p = 1.3653$. This indicates that the values of the crossing points of the curves S_x and S_p increase with the increase of the quantum number.

The values of the entropy sum S_t as a function of x_c are also found in table 2 and its curve is presented in figure 8. For each quantum state, the value of S_t remains constant despite changes in S_x and S_p. The reason is the same as that given in the harmonic oscillator case, but the parameter is now x_c^{-1}, in spite of explicitly $\beta^{1/2}$, or implicitly $\omega^{1/2}$. Additionally, S_t assumes its lowest value for the ground state and it increases with the increment of n; this is similar to the results of reference [53]. The entropic uncertainty relation is respected for the different values of x_c and n since it is above its minimum defined in equation (5).

Note in tables 1 and 2 that some of the S_p and S_x values are negative. These values correspond to regions where the probability densities are highly localized. This fact can also be observed in the spherically confined hydrogen atom [23, 54] and systems with static screened Coulomb potential [55].

5.3. Considerations about both systems

The probability densities of excited quantum states have a nodal structure (points in the space of positions that assume null values) that increase with increasing quantum number n. For the harmonic oscillator the nth excited state has n nodes; in figure 4 one can appreciate the nodal structure in the (a) position and (b) momentum space for the first three quantum states. For the confined particle in a box the nth excited state has $n - 1$ nodes (the boundary conditions are not nodes), and in figure 7 we observed the nodal structure in the (a) position and (b) momentum space for the $n = 1$, 2 and 3 states.

Generally the increase in the number of nodes causes spreading of the probability distribution in position space. For the harmonic oscillator this causes an increase in the S_x values with n increments in table 1. However, such spreading is avoided by the infinite potential barriers of the box in which the particle is confined, thus promoting values of S_x independent of the quantum number in table 2. This aspect again highlights the difference between the standard deviation and information entropy, because $\Delta\hat{X}$ increases for both considered systems. On the other hand, the S_p values of the studied quantum systems always increase when n also increases, and the entropic uncertainty relation remains valid.

Another interesting observation is the influence of the nodal structure of probability densities on the value of S_t. In either case, S_t is always constant for each n and their values increase when the quantum number n grows. Moreover, for the ground state the S_t value of the confined particle in a box is of 2.2120; that is, greater than the harmonic oscillator which is 2.1447 (minimum value of the entropic uncertainty relation). For excited states, the S_t values are smaller for the confined particle in a box than the respective harmonic oscillator due to the invariance of S_x values in relation to the n increments (see tables 1 and 2 for numerical values).

We can also note in both systems that the growth rate of S_t decreases when the quantum number n increases. Meanwhile, the $\Delta\hat{X}\Delta\hat{P}$ quantity varies linearly with n (or the node number) for the harmonic oscillator and near-linearly for the confined particle in a box[2]. This feature makes the value of $\Delta\hat{X}\Delta\hat{P}$ smaller for the harmonic oscillator than the confined particle in a box for the first three quantum states, when an inversion occurs.

6. Conclusions

We pedagogically explored some elements of information theory and provided a link to quantum theory through the information entropies. The physical significance of these entropies was discussed and a comparison with the standard deviations and Kennard's relation was performed.

In particular, we applied the modified entropic expressions in one-dimensional quantum systems to the ground and two first excited states. For S_x, S_p and S_t, we provided an original explanation of their behaviors analyzing the probability densities and by means of the normalization constants and properties of Fourier transform.

In the harmonic oscillator problem, the value of S_x increases and S_p decreases when the ω value reduces. An increase of S_x and S_p implies an increase in the uncertainty of the position and momentum of a particle, i.e. an increase in the spreading of the respective probability

[2] In this case, $\Delta\hat{X}\Delta\hat{P}$ grows linearly with the quantum number when n tends to infinity.

densities in their domains. For the confined particle in a box, the values of S_x are equal for all considered quantum states and decrease when confinement becomes stronger. The values of S_p increase with the n increment and advance of confinement.

For the studied physical systems, despite the changes in S_x and S_p, the value of S_t remains constant for each quantum state and takes its smallest value for the ground state. The value of S_t for the harmonic oscillator ground state is the minimum value of the entropic uncertainty relation. But, for the excited states the values of S_t are smaller for the confined particle in a box. The entropic uncertainty relation is respected for the considered systems.

Moreover, for the ground state of the harmonic oscillator, the standard deviation and information entropies are equivalent measures of the spread of the probability distributions or the quantum uncertainty. On the other hand, for the confined particle in a box the $\Delta\hat{X}$ values, contrasting with the S_x values, vary with the increment of n. These results highlight the different characteristics of $\Delta\hat{X}$ ($\Delta\hat{P}$) and S_x (S_p) as measures of spread or uncertainty. This fact already justifies the interest in introducing to undergraduate physics students the ideas of information entropy and theory of information in the quantum mechanics context.

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Appendix A.

In the context of quantum theory the dimensional adequate information entropies on position, S_x, and on momentum, S_p, spaces for one-dimensional systems are [23]

$$S_x = -\int dx\ \rho(x)\ln((a_0)\ \rho(x)) \tag{A.1}$$

and

$$S_p = -\int dp\ \gamma(p)\ln\left(\left(\frac{\hbar}{a_0}\right)\gamma(p)\right). \tag{A.2}$$

Using the equations (A.1) and (A.2) to compose the entropy sum we have

$$S_t = S_x + S_p = -\int \rho(x)\ln((a_0)\ \rho(x))dx - \int \gamma(p)\ln\left(\left(\frac{\hbar}{a_0}\right)\gamma(p)\right)dp. \tag{A.3}$$

Rewriting the expression to S_t we get

$$S_t = -\int\int\ dx\ dp\ [\rho(x)\ \gamma(p)]\left[\ln((a_0)\rho(x)) + \ln\left(\left(\frac{\hbar}{a_0}\right)\gamma(p)\right)\right]. \tag{A.4}$$

Making a convenient choice and working with the properties of the logarithmic function we can write

$$S_t = -\int\int dx\ dp\ [\rho(x)\ \gamma(p)]\left[\ln\left((a_0)\left(\frac{\hbar}{a_0}\right)\rho(x)\gamma(p)\right)\right]. \tag{A.5}$$

Thus, we find the expression of the entropy sum in terms of the fundamental constant $\hbar$, that is,

$$S_t = -\int\int dx\ dp\ [\rho(x)\ \gamma(p)][\ln(\hbar\ \ \rho(x)\ \gamma(p))]. \tag{A.6}$$

From the entropy sum we derive the entropic uncertainty relation. The inequality of equation (5) is obtained by defining the (q, n)-norm of the Fourier transform. For a further study see the reference [37].

Appendix B.

The modified information entropies S_x and S_p in one dimension are defined by equations (3) and (4). In the dimensional analysis of S_x, where a_0 and dx have dimensions of length $[L]$, and $\rho(x)$ has the dimension of the inverse of length $1/[L]$, we have

$$S_x[=][L]\left[\frac{1}{L}\right]\ln\left[[L]\left[\frac{1}{L}\right]\right], \tag{B.1}$$

consequently S_x is a dimensionless quantity. Here $[\ =\ ]$ refers to dimensional equality.

Realizing the dimensional analysis of S_p, where $\hbar/a_0$[3] and dp have the dimension of momentum $[P]$, and $\gamma(p)$ has the dimension of the inverse of momentum $1/[P]$, we have

$$S_p[=][P]\left[\frac{1}{P}\right]\ln\left[[P]\left[\frac{1}{P}\right]\right], \tag{B.2}$$

so S_p is also a dimensionless quantity.

Insofar as the entropy sum corresponds to an addition between two dimensionless quantities, it is also a dimensionless one. In the dimensional analysis of S_t, where $[\hbar] = [E]$ $[T]$, being $[E]$ the dimension of energy and $[T]$ the dimension of time, we have

$$S_t[=][L][P]\left[\frac{1}{L}\right]\left[\frac{1}{P}\right]\ln\left[[E][T]\left[\frac{1}{L}\right]\left[\frac{1}{P}\right]\right][=][1]. \tag{B.3}$$

Remembering that $[E] = \frac{[M][L]^2}{[T]^2}$, where $[M]$ is the dimension of mass, we have

$$S_t[=][1]\ln\left[\frac{[M][L]^2}{[T]^2}[T]\left[\frac{1}{L}\right]\left[\frac{1}{P}\right]\right]. \tag{B.4}$$

And, $[P] = \frac{[M][L]}{[T]}$, i.e.

$$S_t[=][1]\ln\left[\frac{[M][L]^2}{[T]^2}[T]\left[\frac{1}{L}\right]\left[\frac{1}{\frac{[M][L]}{[T]}}\right]\right]. \tag{B.5}$$

Finally,

$$S_t[=][1]\ln[1]. \tag{B.6}$$

[3] In the dimensional analysis of $\left(\frac{\hbar}{a_0}\right)$ we have $\left[\frac{\hbar}{a_0}\right][=]\left[\left(\frac{[E][T]}{[L]}\right)\right][=]\frac{[M][L]^2[T]}{[L][T]^2}[=]\frac{[M][L]}{[T]}[=][P]$.

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