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Higher-Order Information Measures from Cumulative Densities in Continuous Variable Quantum Systems

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Received: 29 September 2020; Accepted: 3 November 2020; Published: 6 November 2020



Abstract: A definition of three-variable cumulative residual entropy is introduced, and then used to obtain expressions for higher order or triple-wise correlation measures, that are based on cumulative residual densities. These information measures are calculated in continuous variable quantum systems comprised of three oscillators, and their behaviour compared to the analogous measures from Shannon information theory. There is an overall consistency in the behaviour of the newly introduced measures as compared to the Shannon ones. There are, however, differences in interpretation, in the case of three uncoupled oscillators, where the correlation is due to wave function symmetry. In interacting systems, the cumulative based measures are shown in order to detect salient features, which are also present in the Shannon based ones.

Keywords: higher order correlation; mutual information; cumulative densities; shannon entropy; quantum systems

1. Introduction

One interpretation of quantum mechanics is that of a statistical theory, thus analysis of the information obtained from the underlying densities of quantum systems is essential in understanding quantum phenomena. Important tools for interpreting this behaviour have evolved from consideration of position and momentum densities. A key theme in this regard is the measure of the uncertainty that is inherent in any probability distribution. A related concept for distributions with two or more variables is the quantification of the statistical correlation that exists between variables. One way to achieve these goals is with Shannon information theory [1,2], where the central quantity is an information entropy.

The original definition of Shannon entropy is in terms of N discrete random variables

$$S = - \sum_{i=1}^N p_i \ln p_i, \quad (1)$$

where $\sum_{i=1}^N p_i = 1$ and p_i is the probability of the i th event. This entropy has properties, such as being bounded and positive-definite ($S \geq 0$), since $0 \leq p_i \leq 1$. The interpretation of the entropy is that of a measure of uncertainty in a random variable. When these variables represent particles, as in quantum mechanics, the entropy can be interpreted as a measure that is related to the localization or (de)localization of particles. Smaller entropic values are indicative of a more localized distribution, while larger values imply a more delocalized one.

The differential Shannon entropy

$$S_x = - \int_{-\infty}^{\infty} \rho(x) \ln \rho(x) dx, \tag{2}$$

should be used when examining the probability densities with continuous variables. The density, $\rho(x)$, is normalized, $\int_{-\infty}^{\infty} \rho(x) dx = 1$, over the region $[-\infty, \infty]$. However, $\rho(x)$ is not necessarily bounded as in the discrete case, which can lead to negative values of the entropy. Furthermore, there has been discussion as to the dimensional consistency, in particular when the density inside the logarithmic argument contains units [3–6]. Nevertheless, the use of Shannon and related entropies has seen widespread application in the study of a variety of different quantum systems [5,7–43]. This popularity is perhaps due to the formulation of the Heisenberg uncertainty principle in terms of D -dimensional entropic uncertainty relationships [44,45]

$$S_T^D = S_x^D + S_p^D \geq D(1 + \ln \pi). \tag{3}$$

S_x^1 is given in Equation (2) by taking $\rho(x)$ as the position space density of quantum systems, while S_p^1 is obtained by substituting $\rho(x)$ with the corresponding momentum space density. This uncertainty relation has provided the motivation for the examination and discussion of Shannon entropies in both position and momentum representations.

One approach to overcome the difficulties that are presented by differential entropy is to examine cumulative probability densities, instead of the parent density, $\rho(x)$. These densities are bounded by unity, are positive-definite, and are dimensionless. The survival (cumulative residual), $su_x(a)$ and cumulative $cu_x(a)$ densities, are defined in terms of the parent density as

$$su_x(a) = P(x > a) = \int_a^{\infty} \rho(x) dx = 1 - cu_x(a) \quad \text{with} \quad cu_x(a) = P(x \leq a) = \int_{-\infty}^a \rho(x) dx. \tag{4}$$

In particular, one can define an entropy for the $su_x(a)$ density by

$$\epsilon_a = - \int_{-\infty}^{\infty} su_x(a) \ln su_x(a) da. \tag{5}$$

This definition is referred to as the cumulative residual entropy (CRE) [46]. Entropic definitions for the $cu_x(a)$ density have also been considered [46]. The question to be asked is, if the interpretations obtained from ϵ_a and S_x are consistent in nature, when applied to continuous variable quantum systems. The behaviours of S_x and ϵ_a have been compared and contrasted in some representative continuous variable quantum systems, where differences have been observed [47].

2. Two-Variable Information Measures

2.1. Entropies from Two-Variable Distributions

The definitions that were encountered in the previous section can also be applied to two-variable distributions. Such distributions are encountered when one considers two-particle (variable) quantum systems. The pair differential Shannon entropy is defined in terms of the joint or two-variable probability distribution $\Gamma(x_1, x_2)$, as

$$S_{\Gamma} = - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Gamma(x_1, x_2) \ln \Gamma(x_1, x_2) dx_1 dx_2. \tag{6}$$

The pair and one-variable Shannon entropies are related through

$$S_{\Gamma} = S_x + S(x_2|x_1), \tag{7}$$

where the second term is a conditional entropy or conditional expected value

$$E[S(x_2|x_1)] = S(x_2|x_1) = - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Gamma(x_1, x_2) \ln \left[\frac{\Gamma(x_1, x_2)}{\rho(x_1)} \right] dx_1 dx_2, \tag{8}$$

and $\rho(x_1) = \int_{-\infty}^{\infty} \Gamma(x_1, x_2) dx_2$. Note that, for indistinguishable quantum systems, $\rho(x_1) = \rho(x_2) = \rho(x)$, in the notation used.

A joint cumulative probability distribution can be defined in terms of the parent two-variable distribution as

$$cu_x(a, b) = P(x_1 \leq a, x_2 \leq b) = \int_{-\infty}^a \int_{-\infty}^b \Gamma(x_1, x_2) dx_1 dx_2, \tag{9}$$

while the joint survival (cumulative residual) density is

$$su_x(a, b) = P(x_1 > a, x_2 > b) = \int_a^{\infty} \int_b^{\infty} \Gamma(x_1, x_2) dx_1 dx_2. \tag{10}$$

It is possible to use the cumulative residual density to establish a pair cumulative residual entropy, analogous to the pair entropy, as

$$\epsilon_{ab} = - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} su_x(a, b) \ln su_x(a, b) da db. \tag{11}$$

However, there is difficulty in applying this definition, since the preceding integral diverges in the case of infinite support. On the other hand, it is convergent in the case of finite support.

To obtain a suitable definition of the pair cumulative residual entropy, one can consider the joint cumulative residual entropy (JCRE) [46], which is expressed in an analogous manner to Equation (7), as

$$JCRE = \epsilon_a + E[\epsilon(b|x_1)]. \tag{12}$$

The last term,

$$E[\epsilon(b|x_1)] = - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(x_1, x_2 > b) \ln \left[\frac{P(x_1, x_2 > b)}{\rho(x_1)} \right] db dx_1, \tag{13}$$

is the expected value of

$$\epsilon(b|x_1) = - \int_{-\infty}^{\infty} \frac{P(x_1, x_2 > b)}{\rho(x_1)} \ln \left[\frac{P(x_1, x_2 > b)}{\rho(x_1)} \right] db, \tag{14}$$

where

$$P(x_1, x_2 > b) = \int_b^{\infty} \Gamma(x_1, x_2) dx_2. \tag{15}$$

In the above, note that $E[\epsilon(b|x_1)] = E[\epsilon(a|x_2)]$, in quantum systems with indistinguishable particles. The behaviours of S_{Γ} and JCRE have been compared and contrasted in two-particle quantum systems [47].

2.2. Pairwise Statistical Correlation Measures

Another fundamental quantity in information theory is the Mutual Information (MI). It quantifies the pairwise correlation between two variables [2], and it is defined as

$$\begin{aligned}
 I_x &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Gamma(x_1, x_2) \ln \left[\frac{\Gamma(x_1, x_2)}{\rho(x_1)\rho(x_2)} \right] dx_1 dx_2 \geq 0, \\
 &= S_x - S(x_1|x_2),
 \end{aligned}
 \tag{16}$$

where the last term is the expectation, $E[S(x_1|x_2)] = S(x_1|x_2)$. Measures of pairwise statistical correlation have been used in order to interpret the types and strength of interparticle correlations present in quantum systems [48]. The idea here is that the statistical correlation measures can be used to examine how particle interaction is encoded into the densities and wave functions of quantum systems.

Measures, such as the correlation energy [49], are employed in quantum chemistry to gauge the correlation effects in approximate wave functions. The correlation coefficient has also been used to quantify and examine correlation in quantum systems [50,51]. It is defined in terms of the covariance as

$$\tau_x = \frac{Cov(x_1, x_2)}{\sigma_{x_1}\sigma_{x_2}} = \frac{\langle x_1 x_2 \rangle - \langle x_1 \rangle \langle x_2 \rangle}{\sqrt{\langle x_1^2 \rangle - \langle x_1 \rangle^2} \sqrt{\langle x_2^2 \rangle - \langle x_2 \rangle^2}}.
 \tag{17}$$

The expectation values are

$$\langle x_1 x_2 \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_1 x_2 \Gamma(x_1, x_2) dx_1 dx_2,
 \tag{18}$$

$$\langle x_1 \rangle = \langle x_2 \rangle = \langle x \rangle = \int_{-\infty}^{\infty} x \rho(x) dx,
 \tag{19}$$

$$\langle x_1^2 \rangle = \langle x_2^2 \rangle = \langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 \rho(x) dx,
 \tag{20}$$

for indistinguishable quantum systems. τ_x is known to be sensitive to linear correlations. MI, on the other hand, is a more general measure of correlation, which is capable of detecting non-linear dependencies. However, the correlation coefficient is bounded by $-1 < \tau_x < 1$; thus, it is able to detect differences between positive and negative correlations. That is, when the variables move in the same or opposite directions. The behaviours and properties of MI and the correlation coefficient have been examined in two-particle quantum systems [48].

The second expression that is given in Equation (16) can be used to establish an analogous definition of MI in terms of cumulative entropies, which is called the cross cumulative residual entropy (CCRE) [46,52,53],

$$CCRE = \epsilon_a - E[\epsilon(b|x_1)].
 \tag{21}$$

CCRE and MI have been compared in two-particle quantum systems [47]. The questions to be addressed are the following: are the behaviours and interpretations obtained from the cumulative-based measures, consistent with the Shannon-based ones, when addressing continuous variable systems? Are there systems that present inconsistencies in the interpretations that arise from the two sets of measures? These two-variable cumulative measures, along with three-variable ones that will be presented in subsequent sections, have not been examined in three-particle (variable) quantum systems. Two-variable measures in this case depend on the properties of the reduced two-variable (particle) densities.

3. Three-Variable Information Measures

3.1. Entropies from Three-Variable Distributions

The focus of this work is the study of the information quantities in three-variable (particle) quantum systems. The Shannon differential entropy for the three-variable case is defined in terms of the wave function, as

$$S_\Psi = - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\Psi(x_1, x_2, x_3)|^2 \ln \left[|\Psi(x_1, x_2, x_3)|^2 \right] dx_1 dx_2 dx_3. \tag{22}$$

In such systems, the two-variable density is a reduced one and it is defined as

$$\Gamma(x_1, x_2) = \int_{-\infty}^{\infty} |\Psi(x_1, x_2, x_3)|^2 dx_3, \tag{23}$$

where the integration can be carried out over any of the three variables due to indistinguishability.

A chain relation similar to Equation (7) exists for the three-variable entropy [2] as

$$S_\Psi = S_x + S(x_2|x_1) + S(x_3|x_1x_2) = S_\Gamma + S(x_3|x_1x_2), \tag{24}$$

where the last term is a conditional expected value

$$E[S(x_3|x_1x_2)] = S(x_3|x_1x_2) = - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\Psi(x_1, x_2, x_3)|^2 \ln \left[\frac{|\Psi(x_1, x_2, x_3)|^2}{\Gamma(x_1, x_2)} \right] dx_1 dx_2 dx_3. \tag{25}$$

Equation (24) above can be used in order to obtain an analogous expression for the three-variable cumulative residual entropy *TCRE*

$$TCRE = \epsilon_a + E[\epsilon(b|x_1)] + E[\epsilon(c|x_1x_2)] = JCRE + E[\epsilon(c|x_1x_2)], \tag{26}$$

where

$$\epsilon(c|x_1x_2) = - \int_{-\infty}^{\infty} \frac{P(x_1, x_2, x_3 > c)}{\Gamma(x_1, x_2)} \ln \left[\frac{P(x_1, x_2, x_3 > c)}{\Gamma(x_1, x_2)} \right] dc, \tag{27}$$

and

$$E[\epsilon(c|x_1x_2)] = - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(x_1, x_2, x_3 > c) \ln \left[\frac{P(x_1, x_2, x_3 > c)}{\Gamma(x_1, x_2)} \right] dx_1 dx_2 dc, \tag{28}$$

with

$$P(x_1, x_2, x_3 > c) = \int_c^{\infty} |\Psi(x_1, x_2, x_3)|^2 dx_3. \tag{29}$$

We emphasise that this definition of *TCRE* has not, to our knowledge, been presented before, nor has it been studied in continuous variable quantum systems.

3.2. Triple-Wise Statistical Correlation Measures

The concept of pairwise statistical correlation is a standard one, which has been applied in many fields of science. On the other hand, the quantification and examination of triple-wise correlations are not nearly so well-established. These higher-order correlations represent the interactions among the three particles (variables) as a group, and go beyond the pairwise interactions. There is current interest in quantifying higher-order or triple-wise correlations in various disciplines, which range from the neurosciences [54–56], to applications in big data analysis [57]. One of the goals of this work is to examine these higher-order correlations in continuous variable systems, and to extend the definitions of higher-order correlations to the consideration of cumulative densities. Higher-order measures have been examined in systems with discrete distributions [58,59], but little has been done to extend these studies to continuous variable systems [60,61].

The interaction information [2,58–63] takes into account the correlation or interaction among the three variables and it is expressed as

$$\begin{aligned} I_x^3 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\Psi(x_1, x_2, x_3)|^2 \ln \left[\frac{|\Psi(x_1, x_2, x_3)|^2 \rho(x_1) \rho(x_2) \rho(x_3)}{\Gamma(x_1, x_2) \Gamma(x_1, x_3) \Gamma(x_2, x_3)} \right] dx_1 dx_2 dx_3, \\ &= 3S_\Gamma - 3S_x - S_\Psi = (S_\Gamma + S_x - S_\Psi) - 2I_x. \end{aligned} \tag{30}$$

The last equality or grouping is meant to express I_x^3 as a difference between two positive terms. The second one is referred to as the redundancy because it contains information about the pairwise correlation ($2I_x$). The first term has the information regarding how the three variables are correlated as a group. This term is called the synergy. I_x^3 is positive when the synergic first term dominates, while it is negative when the redundancy, or twice the pair correlation, is larger than the synergic term.

One can obtain an expression for higher-order or triple-wise correlation, based on cumulative densities ($TCCRE$), by substituting the expressions for S_Ψ and S_Γ from Equations (7) and (24), into Equation (30), to yield

$$\begin{aligned} TCCRE &= 2E[\epsilon(b|x_1)] - \epsilon_a - E[\epsilon(c|x_1x_2)], \\ &= (JCRE + CRE - TCRE) - 2CCRE. \end{aligned} \tag{31}$$

Another triple-wise information measure that can be formulated is the total correlation [64,65]

$$\begin{aligned} I_3^x &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\Psi(x_1, x_2, x_3)|^2 \ln \left[\frac{|\Psi(x_1, x_2, x_3)|^2}{\rho(x_1)\rho(x_2)\rho(x_3)} \right] dx_1 dx_2 dx_3, \\ &= 3S_x - S_\Psi. \end{aligned} \tag{32}$$

Taking the difference, $(I_3^x - I_x^3)$, yields $3I_x$, which shows that the correlations that are included in I_3^x , which are not present in I_x^3 , are pairwise ones.

Thus, the corresponding total cumulative correlation $TcCCRE$ in terms of cumulative densities is defined as

$$TcCCRE = 3CRE - TCRE. \tag{33}$$

$TCCRE$ and $TcCCRE$ have not been previously discussed in the literature.

It is also possible to extend the concept of the correlation coefficient in order to consider triple-wise correlations, by using moments of the distribution to define the correlation in terms of joint cumulants. The second joint cumulant is the covariance or numerator of the correlation coefficient. The third joint cumulant of interest here is

$$\begin{aligned} \kappa(x_1x_2x_3) &= \langle x_1x_2x_3 \rangle - \langle x_1x_2 \rangle \langle x_3 \rangle - \langle x_1x_3 \rangle \langle x_2 \rangle - \langle x_2x_3 \rangle \langle x_1 \rangle + 2\langle x_1 \rangle \langle x_2 \rangle \langle x_3 \rangle, \\ &= [\langle x_1x_2x_3 \rangle - \langle x_2x_3 \rangle \langle x_1 \rangle] - Cov(x_1, x_2) \langle x_3 \rangle - Cov(x_1, x_3) \langle x_2 \rangle, \end{aligned} \tag{34}$$

where

$$\langle x_1x_2x_3 \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_1x_2x_3 |\Psi(x_1, x_2, x_3)|^2 dx_1 dx_2 dx_3. \tag{35}$$

One can highlight the similarities between the cumulant and higher-order Shannon measures by considering the indistinguishable case,

$$\begin{aligned} \kappa(x_1x_2x_3) &= \langle x_1x_2x_3 \rangle - 3\langle x_1x_2 \rangle \langle x \rangle + 2\langle x \rangle^3, \\ &= [\langle x_1x_2x_3 \rangle - \langle x_1x_2 \rangle \langle x \rangle] - 2Cov(x_1, x_2) \langle x \rangle. \end{aligned} \tag{36}$$

This last expression is similar in nature to the last equality for I_x^3 in Equation (30), where there is a subtraction of the pair correlation, through the $2I_x$ term. Taking the difference between $\langle x_1x_2x_3 \rangle - \langle x \rangle^3$, and $\kappa(x_1, x_2, x_3)$ from the previous equation yields $3Cov(x_1, x_2) \langle x \rangle$. This expression, which quantifies the pair correlation, resembles the $3I_x$ term, is obtained from the $(I_3^x - I_x^3)$ difference.

The goal of this work is to compare and contrast the behaviour of the measures that are based on the cumulative densities, with their counterpart measures from Shannon theory. Special emphasis is placed on the higher-order measures, since the definitions for $TCRE$, $TcCCRE$, and $TCCRE$ introduced here are new ones. Furthermore, the one- and two-variable cumulative measures have not been examined in three-particle systems. That is, when the parent densities are ones that have been

reduced by integration. Pertinent results from both position and momentum space are presented. The cumulative based measures have not been previously studied in momentum space. All of the measures in momentum space are easily obtained by replacing $\Psi(x_1, x_2, x_3)$ with $\Phi(p_1, p_2, p_3)$, $\Gamma(x_1, x_2)$ with $\Pi(p_1, p_2)$, and $\rho(x)$ with $\pi(p)$, in the corresponding position space expressions. These measures are not explicitly given for the sake of brevity.

Three-particle uncoupled and coupled oscillator systems, whose wave functions are analytically representable, are used in this study. In the coupled scenario, we examine the effects of the presence of an attractive or repulsive pair potential on the information measures. In the uncoupled case, the effects of indistinguishability on the information measures are explored. The next section presents the uncoupled and coupled wave functions.

4. Three Uncoupled and Coupled Oscillators

Non-interacting oscillator wave functions are orbital products of the harmonic oscillator wave function

$$\phi_n(x) = \sqrt{\frac{\omega^{1/2}}{2^n n! \pi^{1/2}}} e^{-\omega x^2/2} H_n(\sqrt{\omega}x), \tag{37}$$

where we consider (anti)symmetrized determinantal products to build symmetric and antisymmetric wave functions

$$\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{6}} |\phi_{n_1}(x_1)\phi_{n_2}(x_2)\phi_{n_3}(x_3)|. \tag{38}$$

The momentum space representation of the orbitals is

$$\tilde{\phi}_n(p) = \sqrt{\frac{1}{2^n n! (\omega\pi)^{1/2}}} e^{-p^2/2\omega} H_n\left(\frac{p}{\sqrt{\omega}}\right), \tag{39}$$

with wave functions

$$\Phi(p_1, p_2, p_3) = \frac{1}{\sqrt{6}} |\tilde{\phi}_{n_1}(p_1)\tilde{\phi}_{n_2}(p_2)\tilde{\phi}_{n_3}(p_3)|. \tag{40}$$

The Hamiltonian for the three interacting oscillators is

$$H = -\frac{1}{2} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) + \frac{1}{2} \omega^2 (x_1^2 + x_2^2 + x_3^2) + \frac{1}{2} \lambda^2 [(x_1 - x_2)^2 + (x_1 - x_3)^2 + (x_2 - x_3)^2]. \tag{41}$$

We use units of $\hbar = m = 1$. ω can be identified with the natural frequency of the oscillators, while λ controls the strength of the two-particle interactions. The positive sign corresponds to attractive potentials while the negative sign to repulsive ones.

The eigenfunctions for three interacting harmonic oscillators are written as a product of three harmonic oscillator eigenfunctions in Jacobi coordinates [66,67]

$$\Psi_{n_R n_{r_1} n_{r_2}}(R, r_1, r_2) = \psi_{n_R}(R)\psi_{n_{r_1}}(r_1)\psi_{n_{r_2}}(r_2) = |n_R n_{r_1} n_{r_2}\rangle, \tag{42}$$

where

$$\psi_{n_R}(R) = \left(\frac{\alpha_1^{1/4}}{2^{n_R} n_R! \pi^{1/2}} \right)^{1/2} e^{-\frac{1}{2} \sqrt{\alpha_1} R^2} H_{n_R} \left(\alpha_1^{1/4} R \right), \tag{43}$$

$$\psi_{n_{r_1}}(r_1) = \left(\frac{\alpha_2^{1/4}}{2^{n_{r_1}} n_{r_1}! \pi^{1/2}} \right)^{1/2} e^{-\frac{1}{2} \sqrt{\alpha_2} r_1^2} H_{n_{r_1}} \left(\alpha_2^{1/4} r_1 \right), \tag{44}$$

$$\psi_{n_{r_2}}(r_2) = \left(\frac{\alpha_3^{1/4}}{2^{n_{r_2}} n_{r_2}! \pi^{1/2}} \right)^{1/2} e^{-\frac{1}{2} \sqrt{\alpha_3} r_2^2} H_{n_{r_2}} \left(\alpha_3^{1/4} r_2 \right). \tag{45}$$

The cyclic permutation of Jacobi coordinates (R, r_1, r_2)

$$R = R' = R'' = \frac{1}{\sqrt{3}}(x_1 + x_2 + x_3), \tag{46}$$

$$r_1 = \frac{1}{\sqrt{6}}(-2x_1 + x_2 + x_3), \quad r'_1 = \frac{1}{\sqrt{6}}(x_1 - 2x_2 + x_3), \quad r''_1 = \frac{1}{\sqrt{6}}(x_1 + x_2 - 2x_3), \tag{47}$$

$$r_2 = \frac{1}{\sqrt{2}}(x_2 - x_3), \quad r'_2 = \frac{1}{\sqrt{2}}(x_3 - x_1), \quad r''_2 = \frac{1}{\sqrt{2}}(x_1 - x_2), \tag{48}$$

allows for quantum numbers to be defined as $n_R = n_{R'} = n_{R''}$ for the center-of-mass coordinates R , and $n_{r_1} = n_{r'_1} = n_{r''_1}$ and $n_{r_2} = n_{r'_2} = n_{r''_2}$, for the relative coordinates r_1 and r_2 .

The wave function in momentum space can be obtained by either applying the Fourier transform or solving the Hamiltonian in the momentum representation. These procedures lead to wave functions that are analogous to Equations (42)–(45), by making the substitutions $R \rightarrow Q$, $r_1 \rightarrow q_1$ and $r_2 \rightarrow q_2$. Q , q_1 and q_2 are defined similarly to Equations (46)–(48), by substituting $x_i \rightarrow p_i$ and $\alpha_j \rightarrow 1/\alpha_j$.

On the other hand, antisymmetric wave functions for interacting harmonic oscillators with spin included are obtained [67]

$$N[(|n_{R''}n_{r'_1}n_{r''_2}\rangle |++-) + |n_{R'}n_{r'_1}n_{r'_2}\rangle |+-+) + |n_Rn_{r_1}n_{r_2}\rangle |-+ +)], \tag{49}$$

for odd values of n_{r_2} . Through this procedure we obtain the spin-traced density function in position space as

$$N^2 \left[|n_Rn_{r_1}n_{r_2}\rangle \langle n_Rn_{r_1}n_{r_2}| + |n_{R'}n_{r'_1}n_{r'_2}\rangle \langle n_{R'}n_{r'_1}n_{r'_2}| + |n_{R''}n_{r''_1}n_{r''_2}\rangle \langle n_{R''}n_{r''_1}n_{r''_2}| \right]. \tag{50}$$

5. Results

The presentation of the results is divided into subsections for the uncoupled and coupled oscillators. The behaviours of the information measures in the uncoupled oscillators are examined as a function of the ω frequency. We then turn our attention to the coupled oscillators, and how the measures vary with the coupling strength λ , in the presence of an attractive or repulsive pair potential. The principal goal of this discussion is the comparison of the Shannon and cumulative density measures in different environments. Appendix A presents a discussion of the entropic sums for these systems.

5.1. Uncoupled Oscillators

Figure 1 presents the behaviour of the Shannon and cumulative entropies as a function of ω . All of the entropies decrease with ω , thus the cumulative and Shannon entropies are consistent in their interpretation. That is, the underlying densities localize with increasing ω . Note that S_Ψ and S_Γ become negative-valued at larger values of ω . However, $TCRE$ and $JCRE$ remain positive, illustrating the property of the cumulative survival densities to be bounded between zero and one, which provides positive-valued entropies.

The second row of Figure 1 shows the Shannon and cumulative correlation measures. The two sets of measures exhibit a major difference in their behaviours. The Shannon measures are constant with ω . The interpretations from these measures are that both the pair and higher-order statistical correlations, due to the symmetry of the wave function, are constant with ω . On the other hand, the cumulative based measures all decay with ω . Thus, the magnitude of the correlations decrease with ω . The interpretations that were obtained from the two distinct viewpoints are not consistent. The correlation coefficient is constant with ω and negative-valued. Hence, the behaviours of I_x and τ_x are consistent.

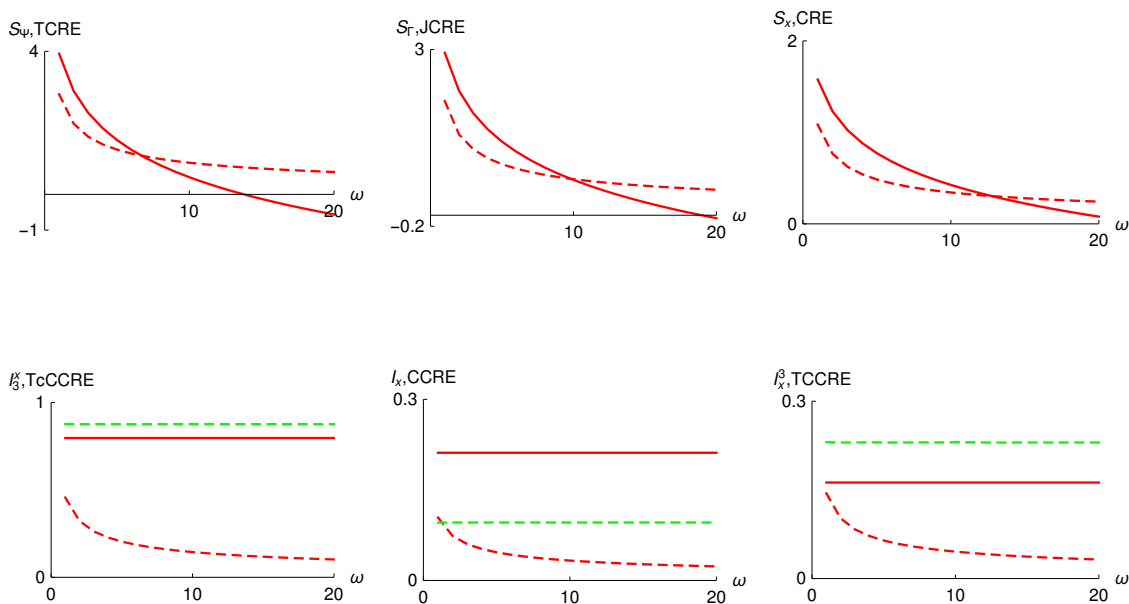


Figure 1. First row: Plots of three-, two-, and one-variable Shannon entropies (solid lines) and *TCRE*, *JCRE* y *CRE* (dashed lines) in position space vs ω . Second row: Plots of I_3^2 , I_x and I_x^2 (solid lines) and *TcCCRE*, *CCRE* y *TCCRE* (dashed lines) in position space vs ω . The green dashed lines are $0.2 * TcCCRE/CCRE$, $CCRE/CRE$ and $0.3 * TCCRE/CCRE$, respectively. All of the plots correspond to the antisymmetric wave function of the $|012\rangle$ state.

A constant behaviour as a function of ω can be recovered from the cumulative measures, if one rescales the quantities. These curves are presented in Figure 1. *CCRE/CRE*, *TcCCRE/CCRE* and *TCCRE/CCRE*, are constant for all values of ω . This result illustrates that the one-, two-, and three-variable cumulative entropies possess the same ω -dependence. Rescaling thus allows one to recapture an interpretation which is consistent with the Shannon measures. That is, the pairwise and higher-order correlations are constant in these uncoupled systems.

Figure 2 presents the measures in momentum space. The Shannon and cumulative entropies now all increase with ω , and are consistent in their behaviour. That is, the momentum space densities delocalize with increasing ω . The Shannon based correlation measures are all constant, as in position space, while the cumulative based measures now increase with ω . Thus, the inconsistencies in the interpretations that were obtained from the Shannon and cumulative based measures are also present in momentum space. Furthermore, the interpretation from the cumulative measures is that the magnitude of the correlation increases with ω , in momentum space, while it decreases in position space. The correlation coefficient here is constant with ω and positive-valued. Hence, I_x and τ_p are consistent in their behaviour. As in position space, rescaling the cumulative measures yields a constant behaviour, which is consistent with the Shannon measures. The same types of results were also observed for the corresponding symmetric state wave function and are not presented.

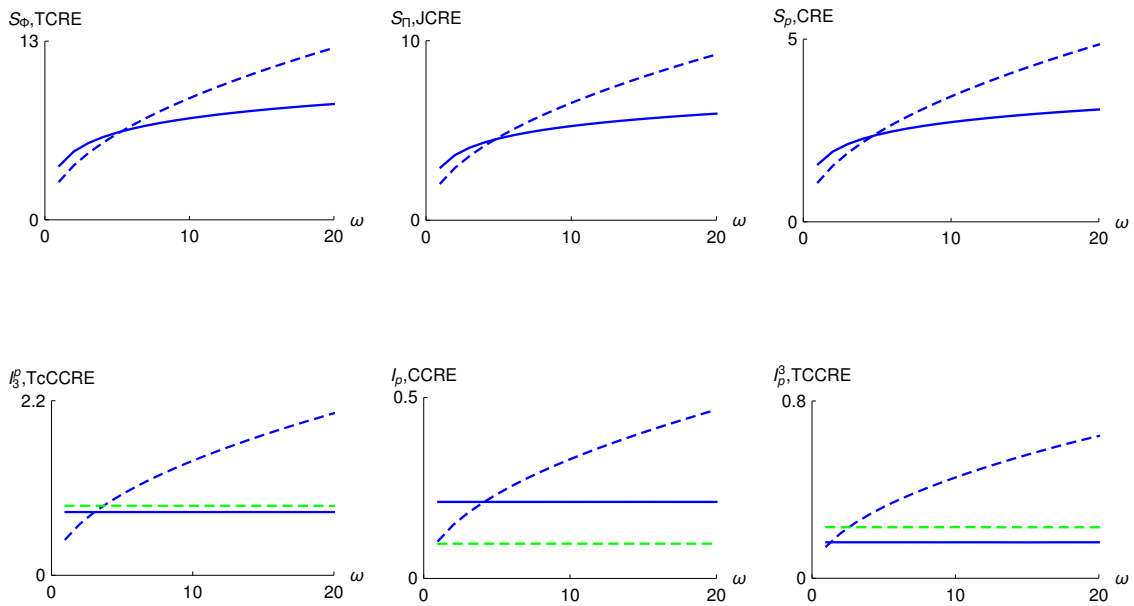


Figure 2. First row: plots of three-, two-, and one-variable Shannon entropies (solid lines) and $TCRE$, $JCRE$ y CRE (dashed lines) in momentum space vs ω . Second row: plots of I_3^p , I_p and I_p^3 (solid lines) and $TcCCRE$, $CCRE$ y $TCCRE$ (dashed lines) in momentum space vs ω . The green dashed lines are $0.2 * TcCCRE/CCRE$, $CCRE/CRE$ and $0.3 * TCCRE/CCRE$, respectively. All of the plots correspond to the antisymmetric wave function of the $|012\rangle$ state.

5.2. Interacting Oscillators: Symmetric Wave Function

We now turn our attention to the interacting system $|000\rangle$ with attractive pair potential, in position space and $\omega = 1.0$. Figure 3 shows the behaviours of the entropic measures as a function of coupling strength λ .

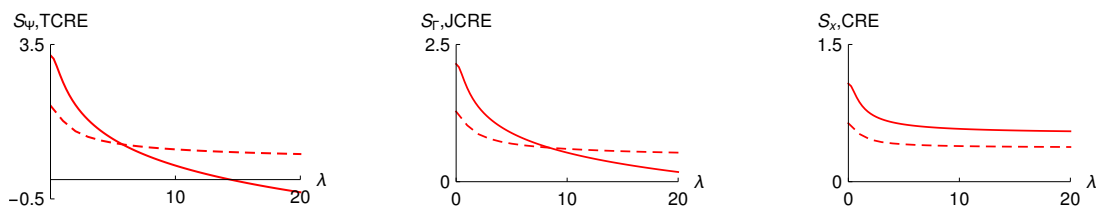


Figure 3. Plots of three-, two-, and one-variable Shannon entropies (solid lines) and $TCRE$, $JCRE$, and CRE (dashed lines) vs the coupling strength λ , in position space, for the $|000\rangle$ state with attractive potential and $\omega = 1.0$.

The Shannon and cumulative entropies decrease with increasing λ and are consistent in their behaviour, although the exhibited functional forms are different. $TCRE$ retains its positivity at larger λ , while S_Ψ is negative-valued.

The left column of Figure 4 presents plots of the one-variable reduced parent and survival densities in position space. One can appreciate the differences between the two forms of densities. One can also observe how the increase in intensity of the attractive pair potential leads to a localization of both densities around the origin. This localization is captured by decreasing entropies in Figure 3. There is another difference between the parent and survival densities. While the parent densities are analytically representable, there are no closed form expressions for the survival densities in these systems. These survival densities are calculated by the numerical integration of the parent densities.

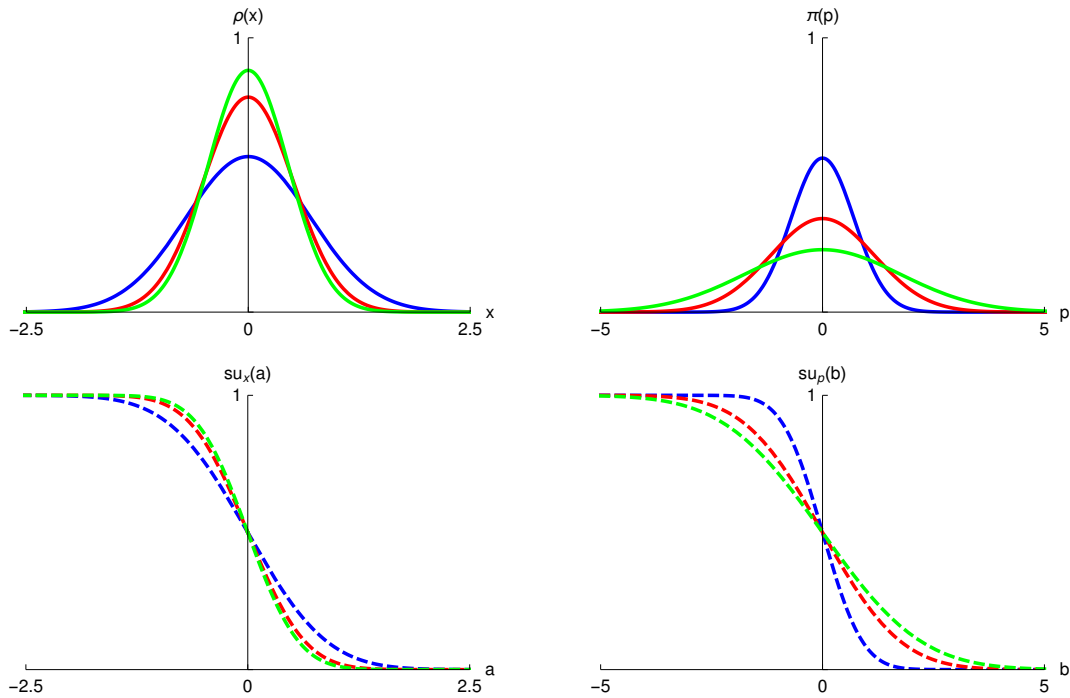


Figure 4. Plots of one-variable reduced parent and cumulative survival densities in position space (left column) and in momentum space (right column) for attractive potentials $\lambda = 0.1$ (blue), $\lambda = 2$ (red) and $\lambda = 5$ (green) in the $|000\rangle$ state with $\omega = 1.0$.

The magnitudes of the Shannon and cumulative correlation measures in Figure 5, increase with λ , and are consistent in their behaviour. Thus, pairwise and higher-order statistical correlations increase with the strength of the pair potential. This consistency among the behaviours of the Shannon and cumulative measures is distinct from the non-interacting case presented in Figure 1. Hence, the interpretation that was obtained from the two sets of measures is now consistent, when interaction is included. Rescaling the cumulant measures results in curves that have a similar behaviour to the unscaled curves. Thus we do not pursue this further in these cases. Note also that both I_x^3 and $TCCRE$ are increasingly negative-valued with λ . The interpretation here from both measures is that the dominant higher-order interactions are redundant in nature. All of the correlation measures go to zero as the coupling is turned off ($\lambda \rightarrow 0$).

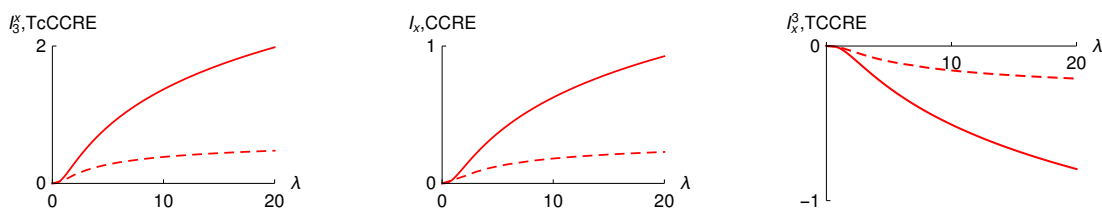


Figure 5. Plots of I_3^3 , I_x and I_x^3 (solid lines) and $TcCCRE$, $CCRE$ and $TCCRE$ (dashed lines) vs. the coupling strength λ , in position space, for the $|000\rangle$ state with attractive potential and $\omega = 1.0$.

The top row of Figure 6 shows the behaviour of the Shannon and cumulative measures for the $|000\rangle$ state in momentum space. One can observe that the Shannon and cumulative entropies increase with λ . Both sets of measures are consistent in their interpretations. That is, the underlying densities delocalize with an increasing intensity of the attractive potential. The delocalization of the one-variable densities in momentum space, as λ increases, can be seen from the group of plots in the right hand column of Figure 4.

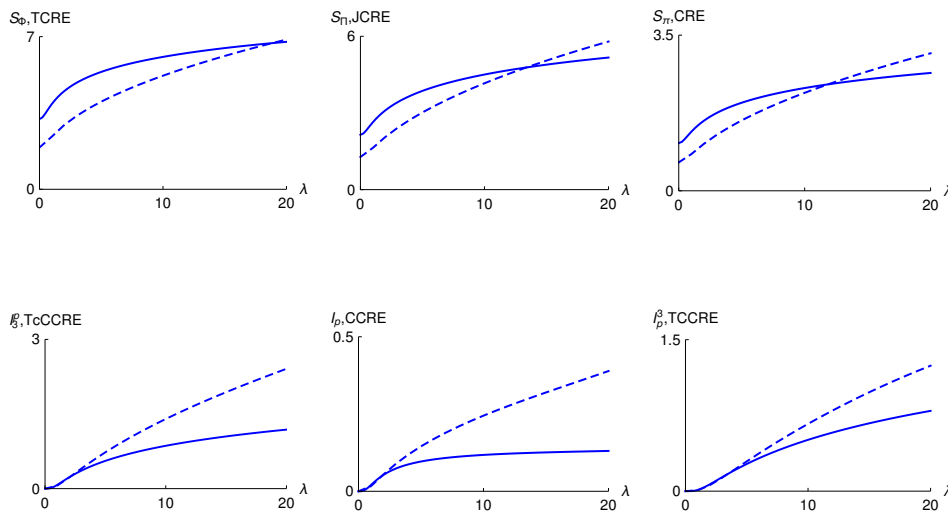


Figure 6. First row: plots of three-, two- and one-variable Shannon entropies (solid lines) and $TCRE$, $JCRE$ and CRE (dashed lines) vs the coupling strength λ , in momentum space. Second row: Plots of I_3^p , I_p and I_p^3 (solid lines) and $TcCCRE$, $CCRE$, and $TCCRE$ (dashed lines) vs. the coupling strength λ , in momentum space. All of the plots correspond to the $|000\rangle$ state with attractive potential and $\omega = 1.0$.

The bottom row of Figure 6 illustrates that the respective Shannon and cumulative correlation measures have a consistent behaviour in momentum space, since all measures increase with λ . All of the measures are zero with no coupling. This consistency in behaviour is different from the previously examined case of non-interacting oscillators, as presented in Figure 2. The results for the state with a repulsive potential are not presented. All Shannon and cumulative measures in these systems were observed to display consistent behaviour.

5.3. Interacting Oscillators: Antisymmetric Wave Function

The results for the interacting $|001\rangle$ state with attractive potential in position space, and repulsive one in momentum space, are presented in this section. These examples were chosen since the Shannon measures present interesting behaviour [60]. We will focus our attention here on the statistical correlation measures. All Shannon and cumulative entropies for this state, with attractive and repulsive potentials and, in position and momentum space, exhibit a consistent behaviour as in the previous figures. These plots are not presented.

Figure 7 gives the behaviour of the correlation measures for the attractive potential in position space. There are minima present that are features of this state [60]. The minima indicate that correlation actually decreases with increasing λ , before it begins to increase at larger coupling strength. It is significant that the minimum in I_3^x at smaller λ , is also captured by $TcCCRE$. The corresponding minimum in I_x also appears in $CCRE$. However, note that the locations of the minima in the Shannon measures are slightly different from the cumulative-based ones. This is especially true for the I_x , $CCRE$ pair.

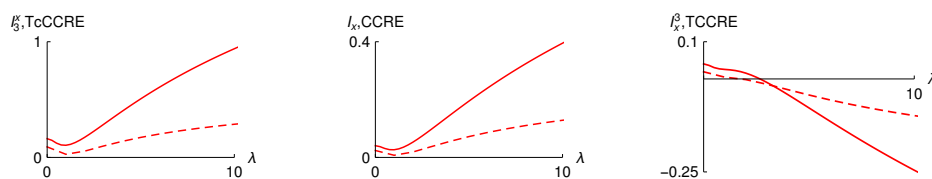


Figure 7. Plots of I_3^x , I_x and I_x^3 (solid line) and $TcCCRE$, $CCRE$ and $TCCRE$ (dashed line) vs. the coupling strength λ , in position space for the $|001\rangle$ state with attractive potential and $\omega = 1.0$.

The synergic behaviour, when the dominant interactions occur as a group, is picked up by both I_x^3 and $TCCRE$ (positive valued), at smaller values of λ . The transition from synergic to redundant dominance (positive to negative) in I_x^3 is also caught by $TCCRE$. Thus, the interpretations that were obtained from the Shannon and cumulative-based measures are consistent. The correlation measures here do not go to zero as the interaction is turned off. This is due to the wave function symmetry. That is, the wave function when λ is zero, is not a separable one.

The presence of the minima in I_x and $CCRE$ can be investigated by examining τ_x . This is presented in Figure 8. The location of the minima in I_x and $CCRE$, correspond to the regions of λ where τ_x changes sign. This value of λ is where the reduced pair density transitions from being negatively correlated to positively correlated. τ_x is zero-valued at this point since $\langle x_1 x_2 \rangle$ is also zero-valued. This point is also characterised by the transition of $\langle x_1 x_2 \rangle$ from negative to positive values. On the other hand, I_x and $CCRE$ cannot be negative, by construction. Thus, these measures detect this transition with the presence of a minimum.

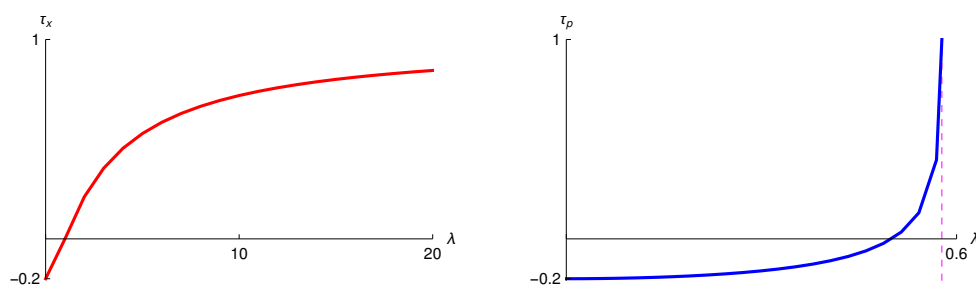


Figure 8. Plots of correlation coefficient τ vs the coupling strength λ for the $|001\rangle$ state, with attractive potential in position space (**left**), and repulsive potential in momentum space (**right**), with $\omega = 1.0$. The dashed vertical line bounds the range in which the repulsive potential is real-valued.

One could also consider comparing the behaviour of I_x^3 and $TCCRE$ with $\kappa(x_1 x_2 x_3)$. However, $\kappa(x_1, x_2, x_3)$ is zero for all values of λ in these systems and, thus, is unable to capture the effects of higher-order or triple-wise correlation. This value of zero does not result from a cancellation of the terms in Equation (36), but rather that both the one- and three-variable expectation values are zero-valued. This occurs in both position and momentum space.

The corresponding plot for the $|001\rangle$ state, with a repulsive potential, in momentum space, is presented in Figure 9. As in position space, all of the measures have non zero values with no coupling. There are also minima in I_3^p and $TcCCRE$, and in I_p and $CCRE$, but now at larger values of λ . Both I_3^p and $TCCRE$ exhibit a transition from positive to negative values, at larger λ . Thus, the behaviours of the Shannon and cumulative measures are similar, and consistent, in momentum space. The point here is that $TcCCRE$ and $CCRE$ are able to detect the minima that are present in I_3^p and I_p . The higher-order measure, $TCCRE$, detects the positive to negative transition, which is present in I_3^p at larger λ .

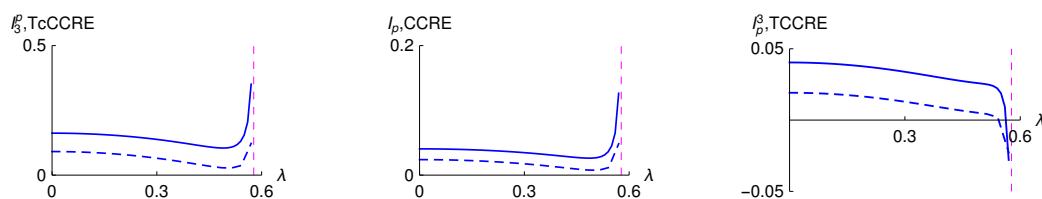


Figure 9. Plots of I_3^p , I_p and I_3^3 (solid lines) and $TcCCRE$, $CCRE$ and $TCCRE$ (dashed lines) vs. the coupling strength λ , in momentum space, for the $|001\rangle$ state with repulsive potential and $\omega = 1.0$. The dashed vertical line bounds the range in which the potential is real-valued.

Figure 8 shows the behaviour of τ_p , which can be compared to I_p and $CCRE$ in Figure 9. τ_p transits from negative to positive values, in the region of λ , where I_p and $CCRE$ exhibit minima. Both τ_x and τ_p approach unity (perfect correlation), in the limit of large λ .

6. Conclusions

An expression for three-variable entropy, which is based on cumulative residual densities, is introduced, and it is used to construct higher-order (triple-wise) correlation measures. The cumulative based measures are compared to the corresponding Shannon ones in continuous variable quantum systems. These systems consist of three coupled and uncoupled oscillators, with attractive and repulsive pair potentials, in position and in momentum space. The results show that the behaviours of the one-, two-, and the newly introduced three-variable cumulative entropies, are consistent with those obtained from the Shannon entropies, in all studied systems. However, the Shannon correlation (mutual information) measures are constant as a function of oscillator frequency in the uncoupled systems, while the cumulative based measures decrease in position space, and increase in momentum space, as a function of the frequency. Rescaling the cumulative based measures leads to a constant behaviour, which is consistent with the interpretation that was obtained from the Shannon ones. On the other hand, the presence of an attractive or repulsive pair potential in the coupled systems yields that both the Shannon and cumulative correlation measures are consistent in their interpretations, when examined as a function of coupling strength. This is particularly relevant in the discussion of the newly introduced higher-order cumulative measures. The results also give credence to the interpretations that were obtained from the Shannon ones. The cumulative-based measures detect the presence of minima, which are also present in the Shannon measures. These minima occur in the regions of coupling strength where the correlation coefficient changes its sign.

Author Contributions: Conceptualization, S.J.C.S., H.G.L. and R.P.S.; methodology, S.J.C.S., H.G.L. and R.P.S.; formal analysis, S.J.C.S., H.G.L. and R.P.S.; investigation, S.J.C.S., H.G.L. and R.P.S.; writing—original draft preparation, S.J.C.S. and R.P.S.; writing—review and editing, S.J.C.S., H.G.L. and R.P.S. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Acknowledgments: S.J.C.S. would like to thank CONACyT for a graduate fellowship.

Conflicts of Interest: The authors declare no conflict of interest.

Appendix A. Entropic Sums

The entropy sums at the one (S_T^1), two (S_T^2) and three (S_T^3) variable levels, as defined in Equation (3), have been the object of increasing attention and study, due to their connection with the uncertainty principle. Thus, we will compare and contrast their behaviour to the sums of the position and momentum space cumulative measures (CRE_T , $JCRE_T$ and $TCRE_T$).

Figure A1 compares the behaviours for the $|012\rangle$ antisymmetric non-interacting state. One can appreciate differences between the two sets of measures. All Shannon entropy sums are constant with ω while the cumulative measures all increase with ω . The constant behaviour observed in the Shannon entropy sums is a result of symmetry. That is, the localization of the position space density with increasing ω , which results in a smaller position space Shannon entropy, is exactly matched by an increase in the momentum space Shannon entropy, due to the delocalization of the momentum density with larger ω . The net effect in the Shannon sum is the observed constant behaviour. The cumulative measures do not preserve this symmetry. The increase in the momentum space measure, due to delocalization of the density with increasing ω , is not matched by an equivalent decrease in the position space measure, due to localization. These same types of behaviour were also observed for the $|012\rangle$ symmetric non-interacting state.

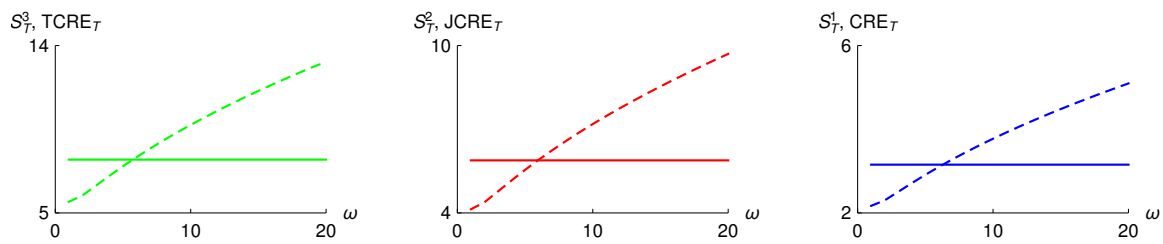


Figure A1. Position and momentum space Shannon entropy sums (solid lines) for one (S_T^1), two (S_T^2) and three (S_T^3) variables, along with the corresponding cumulative entropy sums (dashed lines), (CRE_T , $JCRE_T$, $TCRE_T$), as a function of the strength of the harmonic potential ω , for three non-interacting oscillators in the antisymmetric $|012\rangle$ state.

The entropy sums in interacting systems are presented in Figure A2 for the $|001\rangle$ antisymmetric state in the presence of attractive and repulsive potentials. S_T^3 is constant with the interaction strength (λ), for both attractive and repulsive potentials, similar to the non-interacting case, and the symmetry is preserved. However, S_T^2 and S_T^1 , obtained from reduced densities, are increasing functions of λ . Thus, the symmetry is broken in these cases. The increasing behaviour of S_T^2 and S_T^1 with λ is matched by the $JCRE_T$ and CRE_T measures. On the other hand, the constant behaviour displayed by S_T^3 is not matched by the $TCRE_T$ measure, which increases with λ . For the repulsive potential, all measures display a roughly constant behaviour for smaller values of λ . Similar behaviours were also observed for the $|000\rangle$ symmetric state. All bounds for the Shannon entropy sums in Equation (3) are obeyed in the plots of Figures A1 and A2.

Bounds for the cumulative measures, such as those presented in Equation (3) for the Shannon sums, have not been reported to date. The ground state harmonic oscillator represents the lower bound for S_T^1 in Equation (3). S_T^1 along with CRE_T , is presented in Figure A3 for a single oscillator, in order to contrast the behaviours. The Shannon entropy sum is invariant to the strength of the ω potential and forms the lower bound of Equation (3), while CRE_T is an increasing function of the ω potential. This behaviour is similar to the case of the three non-interacting and interacting oscillators presented in Figures A1 and A2.

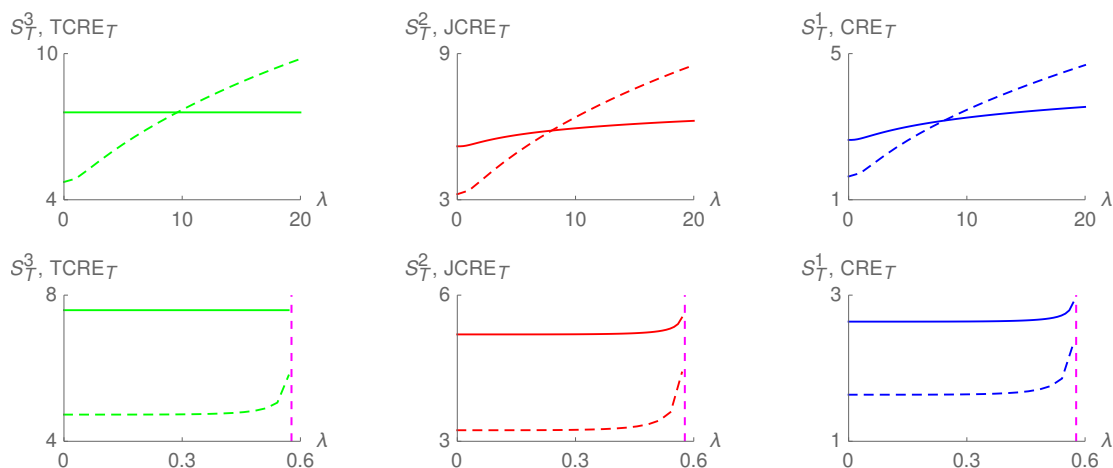


Figure A2. Position and momentum space Shannon entropy sums (solid lines) for one (S_T^1), two (S_T^2) and three (S_T^3) variables, along with the corresponding cumulative entropy sums (dashed lines), (CRE_T , $JCRE_T$, $TCRE_T$), as a function of the interaction strength λ , for three interacting oscillators in the antisymmetric $|001\rangle$ state. The top row presents the measures in the presence of attractive potentials while the bottom row corresponds to repulsive ones.

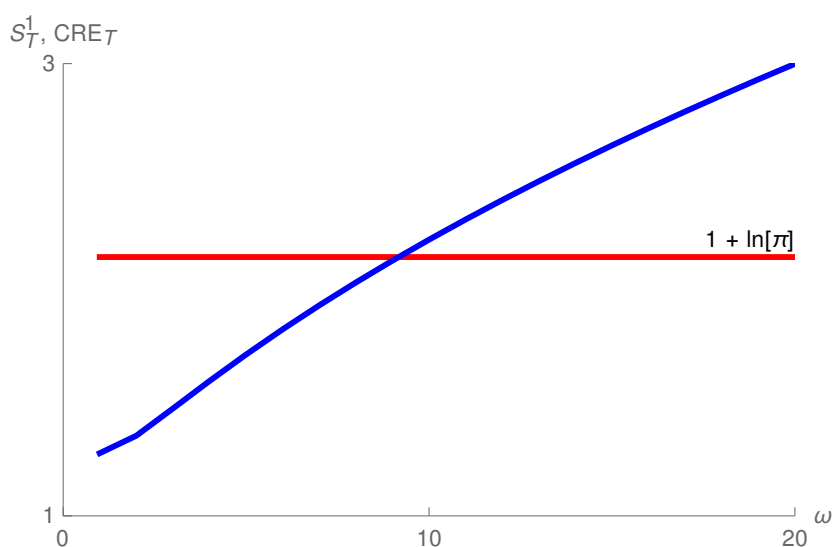


Figure A3. Shannon entropy sum, S_T^1 (red line), and cumulative entropy sum, CRE_T (blue curve) for a ground state harmonic oscillator, as a function of potential strength ω .

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