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Higher-order statistical correlations in three-particle quantum systems with harmonic interactions

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Interaction information, a measure of higher-order statistical correlations, is examined in quantum systems consisting of three coupled and uncoupled oscillators, in position and in momentum space. The magnitudes of the interaction information are greater than zero, and equal in both spaces, in the uncoupled case. This is interpreted as a dominance of synergic effects due to the indistinguishability of particles, and is larger for symmetric wave functions compared to antisymmetric ones. In symmetric wave functions, the magnitude of interaction information increases with the coupling strength, and the inclusion of coupling reveals differences in behavior between the spaces. With attractive potentials, interaction information is positive in momentum space (synergic) and negative in position space (redundant). This is reversed with repulsive potentials. It is now position space which yields positive values, while momentum space gives negative ones. The inclusion of spin provides antisymmetric wave functions which yield that the overall tendencies are maintained. However, there are regions for both attractive and repulsive potentials where the sign of interaction information changes, with the interpretation that the balance changes from a dominance of synergic to that of redundant interactions, and vice versa. This suggests that the nature of the interactions in these systems can be tuned with the coupling strength.

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I. INTRODUCTION

Interaction is key to understanding the physical world. It is the electrons which interact among themselves and the nucleus to form atoms, the atoms which interact to form molecules, and the molecules which interact to form clusters and eventually different phases of matter. It is these interactions which are responsible for different phenomena at each level of organization. Thus, an appreciation of the interaction between elements within a larger set is important in understanding the behavior as a whole.

These ideas are not restricted to electrons, atoms, or molecules. It is the relations between neurons which lead to neural activity and between protein structures which yield a particular biological function. These are all aspects of what has been termed emergent behavior or the synergy among the elements belonging to the same set [1].

At the simplest level, it is the pairwise interactions that are responsible for observed behavior. However, truly emergent phenomena go beyond pairwise associations to consider higher-order ones between triples, quadruples, etc. It is these higher-order correlations that will be the focus of our study. The next relevant question is how to measure or quantify these so-called higher-order interactions or correlations. The term correlation is used here as a synonym to depict the presence of interactions between or among elements.

Correlation is a term taken from statistics, which should offer ideas about the measurement of pairwise and higher-order correlations. Indeed, it is a closely related field, information theory, which provides one answer of how to quantify these correlations. Information theory was conceived in the context of the analysis of communication signals but has since made an impact in many fields of study. Central to this is a framework for the analysis of probability distributions where inherent uncertainties and the correlation between variables can be quantified.

It should not be surprising that information theory has made an impact on quantum mechanics given that the dominant interpretation of quantum mechanics is that of a statistical theory based on probability densities or, more generally, density matrices or the density operator. In fact, it was realized earlier on that the Heisenberg uncertainty principle could be cast in terms of the information entropies, the uncertainty measures taken from information theory. This has led to an active discussion of the optimal manner of quantifying quantum uncertainties. This also begs the question of the best way to quantify correlations when the underlying distributions are quantum in nature.

The Heisenberg uncertainty principle is a statement about the optimal precision that can be attained when treating noncommuting observables, or incompatible representations, such as the position and momentum ones. The two are related, and correlated, via the uncertainty principle. This has led to considerations of joint probability distributions of both position and momentum which are called phase-space distributions. Among these is the Wigner function, which is a quasiprobability distribution since it can attain negative values. It is the marginals of the Wigner function which give the probability densities, in the position and in the momentum representation. The quantum correlations here would be the correlations between the conjugate x and p variables, and are not the topic of this investigation.

The sum of the information entropies in position and in momentum space, which form the basis of the uncertainty

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principle, can be thought of as emanating from the entropy of a separable phase-space distribution. Thus, the uncertainty principle demonstrates that the position and momentum space representations are equivalent and complementary formulations; however, the information that each representation carries is very different. One of the goals of this work is to examine the correlation effects in each representation, and to compare and contrast the similarities and differences.

The purpose of this work is to use three uncoupled and coupled quantum oscillators to probe the nature of higher-order or interaction information, in position and in momentum space. These systems are attractive since analytical solutions of the wave functions are available. We will examine how physical constraints imposed upon the system affect the behavior of the information measures and their interpretations. We use particle indistinguishability and the symmetry-antisymmetry of the wave function to probe the differences in the uncoupled case. In the coupled scenario, we will study the differences between attractive and repulsive potentials in symmetric wave functions and how these manifest with the coupling strength. Lastly, we will examine the measures when spin is included, yielding antisymmetric wave functions. In doing so, we will pay particular attention to the disparities or resemblances in behavior between the pairwise correlation measures and the interaction information (higher order) to examine how the particular degree of organization influences the interpretations obtained from these measures. Also of interest will be a comparison of the correlations among the position of the particles (position space) with the correlations among the momenta (momentum space) to examine their differences with regard to the nature and strength of the coupling potential.

There is current interest in examining effective three-body interactions [2–5] in these systems of interacting oscillators. Examination of the behaviors with regard to the strength of the two-body interaction potential is one way to gauge the influence of an effective potential that is generated by a three-body one. This work aims to use information measures to assess how the nature and strength of the interaction potentials influence the statistical correlation between (among) the three particles. In doing so, we examine the concept of higher-order statistical correlation among the three particles and compare its behavior to the well-studied and established pair correlations.

Sections II and III provide the definitions of the information and correlation measures, while Sec. IV gives the details about the coupled and uncoupled oscillators. This is followed by the presentation of the results in Sec. V, and lastly, the conclusions are outlined in Sec. VI.

II. INFORMATION MEASURES

Shannon entropies

We now proceed to give the definitions that are used in this work. Shannon entropies are measures of the uncertainties in the underlying distributions and have been used to examine quantum systems [6–28]. Shannon entropies of hydrogenic systems and the harmonic oscillator have been discussed in [6,7], while Bose-Einstein condensates have been studied via these entropies [29–32]. They have also been employed to study the nature of confined quantum systems [33–43]. Shannon information entropies of the Wigner function have also been explored [44,45].

In three-particle systems, such as the ones under consideration, there is the three-variable density corresponding to the wave function. The Shannon entropies for three-variables (particles), in position (x_1, x_2, x_3) and in momentum (p_1, p_2, p_3) space, are defined in terms of the wave functions as

$$S_\Psi = -\int |\Psi(x_1, x_2, x_3)|^2 \ln[|\Psi(x_1, x_2, x_3)|^2] dx_1 dx_2 dx_3, \tag{1}$$

$$S_\Phi = -\int |\Phi(p_1, p_2, p_3)|^2 \ln[|\Phi(p_1, p_2, p_3)|^2] dp_1 dp_2 dp_3. \tag{2}$$

These three-variable distributions may be reduced by integrating over one of the variables to yield a two-variable distribution. The two-variable or marginal distributions are

$$\Gamma(x_1, x_2) = \int |\Psi(x_1, x_2, x_3)|^2 dx_3, \tag{3}$$

$$\Pi(p_1, p_2) = \int |\Phi(p_1, p_2, p_3)|^2 dp_3. \tag{4}$$

The Shannon entropies of the two-variable reduced densities are

$$S_\Gamma = -\int \Gamma(x_1, x_2) \ln[\Gamma(x_1, x_2)] dx_1 dx_2, \tag{5}$$

$$S_\Pi = -\int \Pi(p_1, p_2) \ln[\Pi(p_1, p_2)] dp_1 dp_2. \tag{6}$$

Shannon pair entropies have been studied in different quantum systems [46–48].

A further reduction by integration can be carried out to yield the one-variable densities, which are

$$\rho(x) = \int |\Psi(x_1, x_2, x_3)|^2 dx_2 dx_3 = \int \Gamma(x_1, x_2) dx_2, \tag{7}$$

$$\pi(p) = \int |\Phi(p_1, p_2, p_3)|^2 dp_2 dp_3 = \int \Pi(p_1, p_2) dp_2. \tag{8}$$

The Shannon entropies of the one-variable distributions are

$$S_\rho = -\int \rho(x) \ln[\rho(x)] dx, \tag{9}$$

$$S_\pi = -\int \pi(p) \ln[\pi(p)] dp. \tag{10}$$

Particles are indistinguishable in quantum mechanics, and thus the reductions (integrations) can be made over any variable or pair of variables. Note also that the subscript has been suppressed on the one-particle densities to reflect the indistinguishability. The limits of integration are not specified, but are in the $[-\infty, \infty]$ range for each x or p variable since these are oscillator systems.

Furthermore, all densities are normalized to unity,

$$\int |\Psi(x_1, x_2, x_3)|^2 dx_1 dx_2 dx_3 = \int \Gamma(x_1, x_2) dx_1 dx_2 = \int \rho(x) dx = 1, \tag{11}$$

$$\int |\Phi(p_1,p_2,p_3)|^2 dp_1dp_2dp_3 = \int \Pi(p_1,p_2)dp_1dp_2 = \int \pi(p)dp = 1. \quad (12)$$

The interpretation of the Shannon entropies is that they are measures of the (de)localization in the underlying distributions, where larger values correspond to more delocalized distributions while smaller values are indicative of more localized ones.

The Shannon entropies have been used to quantify the uncertainties in the Heisenberg uncertainty relationship. These have led to the entropic uncertainty relations for D dimensions, where [7,49–51]

$$S_T^D = S(x) + S(p) \geqslant D(1 + \ln \pi). \quad (13)$$

The Shannon entropies at the $D = 1$ (one-), $D = 2$ (two-), and $D = 3$ (three)-variable levels form the basis from which one can construct the correlation measures, as will be outlined in the next section. The entropy sum has been proposed as a measure of basis set quality [6], as a correlation measure in atomic systems [52], and examined in different quantum systems [35,39,53].

III. CORRELATION MEASURES

A. Pairwise correlation

The pairwise correlation between two variables can be quantified in terms of the mutual information (MI) [54–58]. MI in the context of indistinguishable quantum systems is

$$I_x = I(x_1;x_2) = \int \Gamma(x_1,x_2)\ln\left[\frac{\Gamma(x_1,x_2)}{\rho(x_1)\rho(x_2)}\right]dx_1dx_2 \geqslant 0$$
$$= S_\rho - S(x_1|x_2) = 2S_\rho - S_\Gamma, \quad (14)$$

where the conditional entropy is defined as [54,59]

$$S(x_1|x_2) = -\int \Gamma(x_1,x_2)\ln\left[\frac{\Gamma(x_1,x_2)}{\rho(x_2)}\right]dx_1dx_2. \quad (15)$$

The interpretation is that it is a relative entropy between the two- variable distribution and a reference which is the product of the two marginals. Another interpretation is that it is the difference between the one-variable reduced entropy and the conditional entropy, that is, the entropy with knowledge of the other variable.

Pairwise-mutual information is bounded from below by zero, which corresponds to a separable distribution. It has been examined in a variety of different quantum systems and shown to increase with increasing correlation (coupling) in the system. One of the goals of this work is to compare and contrast the behavior of the correlation occurring between pairs of variables (MI) to that of the correlation among all three variables (interaction information), as given in the next section.

Note that for brevity, we will only provide the expressions in position space. The corresponding ones in momentum space are obtained by substituting $|\Psi(x_1,x_2,x_3)|^2$ with $|\Phi(p_1,p_2,p_3)|^2$, $\Gamma(x_1,x_2)$ with $\Pi(p_1,p_2)$, and $\rho(x)$ with $\pi(p)$.

B. Interaction information

One can also consider higher-order information that measures the correlation among three variables. There are a number of different ways in which this can be defined. The total correlation [60,61] is defined as

$$I_3(x_1;x_2;x_3) = \int |\Psi(x_1,x_2,x_3)|^2 \ln\left[\frac{|\Psi(x_1,x_2,x_3)|^2}{\rho(x_1)\rho(x_2)\rho(x_3)}\right] \times dx_1dx_2dx_3$$
$$= 3S_\rho - S_\Psi, \quad (16)$$

and measures all the distinct types of correlations in the system.

Perhaps the most compelling of the higher-order information is the interaction information (II) [54,62–66], which takes into account the correlation or interaction among the three variables. It is given as

$$I_x^3 = I^3(x_1;x_2;x_3) = I(x_1;x_2|x_3) - I(x_1;x_2), \quad (17)$$

where the first term is a conditional mutual information. Thus, II is defined as

$$I^3(x_1;x_2;x_3) = \int |\Psi(x_1,x_2,x_3)|^2 \ln\left[\frac{|\Psi(x_1,x_2,x_3)|^2\rho(x_3)}{\Gamma(x_1,x_3)\Gamma(x_2,x_3)}\right] \times dx_1dx_2dx_3 - (2S_\rho - S_\Gamma)$$
$$= 3S_\Gamma - 3S_\rho - S_\Psi, \quad (18)$$

and results from the fact that the marginal densities in the denominator of the logarithmic argument are conditioned by $\rho(x_3)$.

The interpretation is that it represents the difference in correlation between x_1 and x_2, when x_3 is known [first terms of Eqs. (17) and (18)] and when it is not known [second terms of Eqs. (17) and (18)]. It is important to note that unlike pairwise-mutual information, this quantity can either be positive or negative. Discrete versions have been utilized in the neurosciences to measure how neurons fire as a group [67–69] and also in the study of protein structure [70].

Interaction information may be rewritten as

$$I^3(x_1;x_2;x_3) = I(x_1;x_2,x_3) - I(x_1;x_2) - I(x_1;x_3) \quad (19)$$

or

$$I^3(x_1;x_2;x_3) = \int |\Psi(x_1,x_2,x_3)|^2 \ln\left[\frac{|\Psi(x_1,x_2,x_3)|^2}{\rho(x_1)\Gamma(x_2,x_3)}\right] \times dx_1dx_2dx_3 - I(x_1;x_2) - I(x_1;x_3)$$
$$= (S_\Gamma + S_\rho - S_\Psi) - 2I(x_1;x_2), \quad (20)$$

since the particles are indistinguishable [$I(x_1;x_2) = I(x_1;x_3)$].

Equations (19) and (20) represent the difference in the correlation between x_1 and (x_2x_3) as compared to the correlations between x_1x_2 and x_2x_3. All three terms are mutual information (relative entropy), and thus must be greater than or equal to zero by construction. The last two terms are also equal in quantum systems. Since these terms correspond to pairwise interactions, they can be considered as redundant (redundancies) when addressing higher-order correlations. What is most interesting is the first term, which contains the correlations among the three variables and is referred to as the synergy.

Thus, interaction information is a balance between the synergistic first term and the redundancies. It is positive valued when the synergic term is larger than the redundancies. On the other hand, a negative-valued II implies that the redundancies are larger than the synergic term, and the pairwise correlations prevail in this instance.

IV. INTERACTING HARMONIC OSCILLATORS

The Hamiltonian of a system of three one-dimensional interacting oscillators using position space canonical coordinates is

$$H = -\frac{1}{2}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right) + \frac{1}{2}\omega^2\left(x_1^2 + x_2^2 + x_3^2\right) \pm \frac{1}{2}\lambda^2[(x_1 - x_2)^2 + (x_1 - x_3)^2 + (x_2 - x_3)^2]. \tag{21}$$

We use units of $\hbar = m = 1$. This Hamiltonian is known as the Moshinsky atom in the literature [71,72] and has been employed in atomic physics and in quantum chemistry to study correlation effects. Moreover, ω is the natural frequency of the oscillator and λ is the coupling strength of the interaction potential between pairs of particles. The positive sign corresponds to attractive potentials, while the negative sign is for repulsive ones.

The canonical coordinates in position space (x_1, x_2, x_3) can be transformed into Jacobi coordinates (R, r_1, r_2) by applying the following changes of variable:

$$R = \frac{1}{\sqrt{3}}(x_1 + x_2 + x_3), \tag{22}$$

which corresponds to the center-of-mass coordinates, and

$$r_1 = \frac{1}{\sqrt{6}}(-2x_1 + x_2 + x_3), \quad r_2 = \frac{1}{\sqrt{2}}(x_2 - x_3), \tag{23}$$

which are the relative coordinates. The Hamiltonian is rewritten in the new coordinates as

$$H = \frac{1}{2}\left[\left(-\frac{\partial^2}{\partial R^2} + \alpha_1 R^2\right) + \left(-\frac{\partial^2}{\partial r_1^2} + \alpha_2 r_1^2\right) + \left(-\frac{\partial^2}{\partial r_2^2} + \alpha_3 r_2^2\right)\right], \tag{24}$$

where $\alpha_1 = \omega^2$ and $\alpha_2 = \alpha_3 = \omega^2 \pm 3\lambda^2$. The positive sign is for the attractive interactions, while the negative sign corresponds to repulsive interactions. Moreover, $\lambda < \frac{\omega}{\sqrt{3}}$, in the repulsive case, for the potential to be real valued [2]. Pair correlations in systems with harmonic interactions have been studied in two-particle systems [57,58] to N-particle ones [58].

The Schrödinger equation can be solved in the new coordinates using the Hamiltonian (24),

$$H\Psi_{n_R n_{r_1} n_{r_2}}(R, r_1, r_2) = E\Psi_{n_R n_{r_1} n_{r_2}}(R, r_1, r_2), \tag{25}$$

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial R^2} + \frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2}\right) + \frac{1}{2}\left(\alpha_1 R^2 + \alpha_2 r_1^2 + \alpha_3 r_2^2\right)\right] \times \Psi_{n_R n_{r_1} n_{r_2}}(R, r_1, r_2) = E\Psi_{n_R n_{r_1} n_{r_2}}(R, r_1, r_2). \tag{26}$$

The equation is separable in the new coordinates, and thus the eigenfunction $\Psi(R, r_1, r_2) \equiv |n_R n_{r_1} n_{r_2}\rangle$ is written as a product of three eigenfunctions,

$$\Psi_{n_R n_{r_1} n_{r_2}}(R, r_1, r_2) = \psi_{n_R}(R)\psi_{n_{r_1}}(r_1)\psi_{n_{r_2}}(r_2) = \left|n_R n_{r_1} n_{r_2}\right\rangle, \tag{27}$$

where we have

$$\psi_{n_R}(R) = \left(\frac{\alpha_1{}^{\frac{1}{4}}}{2^{n_R} n_R! \pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\sqrt{\alpha_1}R^2} H_{n_R}\left(\alpha_1^{\frac{1}{4}} R\right), \tag{28}$$

$$\psi_{n_{r_1}}(r_1) = \left(\frac{\alpha_2{}^{\frac{1}{4}}}{2^{n_{r_1}} n_{r_1}! \pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\sqrt{\alpha_2}r_1^2} H_{n_{r_1}}\left(\alpha_2^{\frac{1}{4}} r_1\right), \tag{29}$$

$$\psi_{n_{r_2}}(r_2) = \left(\frac{\alpha_3{}^{\frac{1}{4}}}{2^{n_{r_2}} n_{r_2}! \pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\sqrt{\alpha_3}r_2^2} H_{n_{r_2}}\left(\alpha_3^{\frac{1}{4}} r_2\right), \tag{30}$$

and $H_n(x)$ is an n-order Hermite polynomial.

In addition, the corresponding eigenvalue is

$$\begin{aligned} E &= E_R + E_{r_1} + E_{r_2}, \\ E &= \omega\left(n_R + \frac{1}{2}\right) + \sqrt{\omega^2 \pm 3\lambda^2}\,\left(n_{r_1} + n_{r_2} + 1\right). \end{aligned} \tag{31}$$

It is important to note that the permutation of x_1, x_2, or x_3 does not necessarily result in a state that is indistinguishable from the original $|n_R n_{r_1} n_{r_2}\rangle$ one. This can be seen from the definition of the relative coordinates in Eq. (23). Thus, we will focus our attention in this work on the ground state $|000\rangle$, which is symmetric to particle exchange. We will see in the following section that the inclusion of spin offers a route to obtain antisymmetric wave functions.

The wave function in momentum space, $\Phi(p_1, p_2, p_3)$, can be obtained by applying the Fourier transform to the wave function in position space, $\Psi(x_1, x_2, x_3)$,

$$\Phi(p_1, p_2, p_3) = \left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}} \int \Psi(x_1, x_2, x_3) \times e^{-i(p_1x_1 + p_2x_2 + p_3x_3)/\hbar} dx_1 dx_2 dx_3. \tag{32}$$

However, we will use the following Hamiltonian to get the wave function in the momentum space:

$$H = \frac{1}{2}\left[\left(Q^2 - \alpha_1\frac{\partial^2}{\partial Q^2}\right) + \left(q_1^2 - \alpha_2\frac{\partial^2}{\partial q_1^2}\right) + \left(q_2^2 - \alpha_3\frac{\partial^2}{\partial q_2^2}\right)\right], \tag{33}$$

where the coordinates (Q, q_1, q_2) correspond to the Jacobi coordinates in the momentum space which are obtained using the same Eqs. (22) and (23) with respect to the canonical coordinates (p_1, p_2, p_3). The wave function in momentum space is expressed as

$$\Phi_{n_Q n_{q_1} n_{q_2}}(Q, q_1, q_2) = \phi_{n_Q}(Q)\phi_{n_{q_1}}(q_1)\phi_{n_{q_2}}(q_2) = \left|n_Q n_{q_1} n_{q_2}\right\rangle, \tag{34}$$

where

$$\phi_{n_Q}(Q) = \left(\frac{1}{\alpha_1{}^{\frac{1}{4}} 2^{n_Q} n_Q! \pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} e^{-\frac{1}{2\sqrt{\alpha_1}}Q^2} H_{n_Q}\left(\frac{Q}{\alpha_1^{\frac{1}{4}}}\right), \tag{35}$$

$$\phi_{n_{q_1}}(q_1) = \left(\frac{1}{\alpha_2{}^{\frac{1}{4}} 2^{n_{q_1}} n_{q_1}! \pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} e^{-\frac{1}{2\sqrt{\alpha_2}}q_1^2} H_{n_{q_1}}\left(\frac{q_1}{\alpha_2^{\frac{1}{4}}}\right), \tag{36}$$

$$\phi_{n_{q_2}}(q_2) = \left(\frac{1}{\alpha_3{}^{\frac{1}{4}} 2^{n_{q_2}} n_{q_2}! \pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} e^{-\frac{1}{2\sqrt{\alpha_3}} q_2^2} H_{n_{q_2}}\left(\frac{q_2}{\alpha_3^{\frac{1}{4}}}\right). \tag{37}$$

Noninteracting oscillator wave functions are obtained by setting $\lambda = 0$ in the Hamiltonian in Eq. (21). In this case, the equation is now separable in the canonical coordinates with solutions which are products of the harmonic oscillator wave function,

$$\phi_n(x) = \sqrt{\frac{\omega^{1/2}}{2^n n! \pi^{1/2}}} e^{-\omega x^2/2} H_n(\sqrt{\omega} x). \tag{38}$$

Symmetric (S) and antisymmetric (A) wave functions are built from these orbitals by considering (anti)symmetrized determinantal products,

$$\Psi^{A,S}(x_1, x_2, x_3) = \frac{1}{\sqrt{6}} \left| \phi_{n_1}(x_1) \phi_{n_2}(x_2) \phi_{n_3}(x_3) \right|, \tag{39}$$

and n_1, n_2, and n_3 are the three quantum numbers.

The momentum-space representation of the orbitals in Eq. (38) is

$$\tilde{\phi}_n(p) = \sqrt{\frac{1}{2^n n! (\omega\pi)^{1/2}}} e^{-p^2/2\omega} H_n\left(\frac{p}{\sqrt{\omega}}\right). \tag{40}$$

Thus, symmetric and antisymmetric wave functions in momentum space are obtained by forming the orbital products in an analogous manner to Eq. (39).

Interacting harmonic oscillators with spin

Antisymmetric wave functions considering spin functions $|\sigma_1, \sigma_2, \sigma_3\rangle = |\pm, \pm, \pm\rangle$ can be constructed [2] using the cyclic permutation of Jacobi coordinates (R, r_1, r_2),

$$R = R' = R'' = \frac{1}{\sqrt{3}}(x_1 + x_2 + x_3), \tag{41}$$

$$r_1' = \frac{1}{\sqrt{6}}(x_1 - 2x_2 + x_3), \quad r_1'' = \frac{1}{\sqrt{6}}(x_1 + x_2 - 2x_3), \tag{42}$$

$$r_2' = \frac{1}{\sqrt{2}}(x_3 - x_1), \quad r_2'' = \frac{1}{\sqrt{2}}(x_1 - x_2). \tag{43}$$

Quantum numbers can 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 antisymmetric wave functions are constructed $\Psi_{n_R n_{r_1} n_{r_2}}(R, r_1, r_2)$ for indistinguishable particles (electrons) considering spin as

$$\begin{aligned} N\Big[\Big(&\big|n_{R''} n_{r_1''} n_{r_2''}\big\rangle |{+}{+}{-}\rangle + \big|n_{R'} n_{r_1'} n_{r_2'}\big\rangle |{+}{-}{+}\rangle \\ &+ \big|n_R n_{r_1} n_{r_2}\big\rangle |{-}{+}{+}\rangle\Big)\Big], \end{aligned} \tag{44}$$

for odd values of n_{r_2}.

The three-variable density function is built from the antisymmetric wave function in Eq. (44). We then integrate with respect to the spin variables, $|\sigma_1, \sigma_2, \sigma_3\rangle$, where there are terms that are canceled due to orthogonality of the spin functions. Thus, we obtain the spin-traced density function in position space as

$$\begin{aligned} N^2\Big[&\big|n_R n_{r_1} n_{r_2}\big\rangle\big\langle n_R n_{r_1} n_{r_2}\big| + \big|n_{R'} n_{r_1'} n_{r_2'}\big\rangle\big\langle n_{R'} n_{r_1'} n_{r_2'}\big| \\ &+ \big|n_{R''} n_{r_1''} n_{r_2''}\big\rangle\big\langle n_{R''} n_{r_1''} n_{r_2''}\big|\Big]. \end{aligned} \tag{45}$$

One- and two-particle densities are obtained by integrating the three-particle density function in Eq. (45) with respect to one or two of the canonical coordinates (x_1, x_2, x_3). The functions and densities in momentum space are built in an analogous manner to Eqs. (44) and (45) for position space.

There is also one further point that should be mentioned here. With $\lambda = 0$, one does not return to the antisymmetrized noninteracting systems, since a combination of functions have been used to build the antisymmetric function in Eq. (44). In this work, we will center our attention on the $|001\rangle$ state.

V. RESULTS

The results are divided into two sections. The results from the first section on noninteracting oscillators offer an analysis of the influence of the wave-function symmetry on the entropies and on the pair and higher-order information measures. The section on interacting oscillators examines the effects of the strength and nature (attractive or repulsive) of the interaction potential on the entropies and information measures. We begin each section with a discussion of the behavior of the information entropies since these are the basis from which the correlation measures are constructed. Subsequently, the correlation measures are then presented and discussed.

A. Noninteracting oscillators

We now discuss the influence of the wave-function symmetry on the information measures.

Figure 1 shows the behavior of the three-variable entropies, in position and in momentum space, as a function of the inverse of the one-body potential $(1/\omega)$. The one- and two-variable entropies are not shown, but are very similar in behavior to the three-variable ones. The $|012\rangle$ state with antisymmetric wave function was chosen. The corresponding symmetric wave function yields plots which are very similar to the antisymmetric ones, and are also not presented. The values, however, of the entropies from symmetric and antisymmetric wave functions are different.

One can see that the position-space entropies increase with $1/\omega$, while the momentum-space entropies decrease. The interpretation is that the position-space densities localize with increasing ω, while the momentum-space densities delocalize. Important to note is that all three entropy sums are constant with $1/\omega$. That is, the increase in value in position space is equal in magnitude to the decrease in momentum space. Note that there is no interaction potential here $(\lambda = 0)$. This observed behavior of the entropy sums will be important in the subsequent discussion of the interacting oscillators.

Figure 2 compares the behavior of the pair mutual information with that of the interaction information for symmetric and antisymmetric wave functions with the same quantum numbers. There is no interaction potential in these noninteracting systems so all of the correlation is due to the particular symmetry of the wave function.

The magnitudes of the correlation at the pair and higher-order levels are equal in both position and momentum space. Thus, the correlation due to indistinguishability of particles offers no distinction between the spaces. This will be further

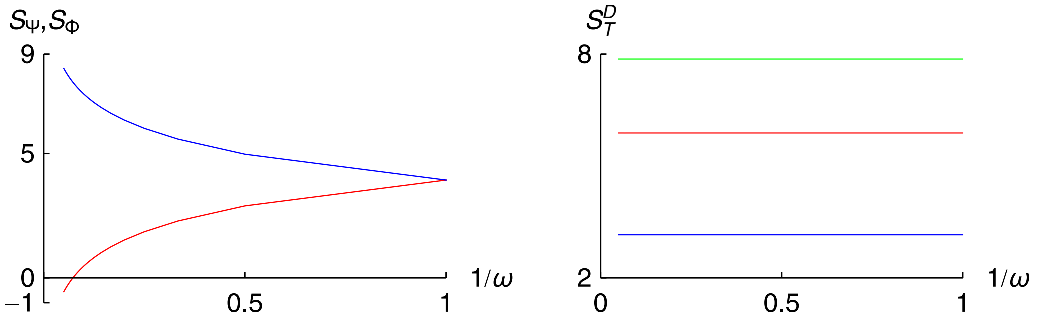

FIG. 1. Left: Plots of the position-space S_Ψ (red, lower curve) and momentum-space S_Φ (blue, upper curve) entropies vs $\frac{1}{\omega}$. Right: Plots of the entropic sum S_T^D vs $\frac{1}{\omega}$ for $D = 3$ (green, upper curve), $D = 2$ (red, middle curve), and $D = 1$ (blue, lower curve).

commented on when interacting oscillators are discussed. These magnitudes are also constant with $1/\omega$ since there is no interaction potential present.

The magnitude of the pair correlation is larger for the antisymmetric wave function compared to the symmetric one. This is expected due to the presence of the Fermi hole in the antisymmetric functions.

On the other hand, it is the symmetric wave functions which have the largest interaction information. This is distinct from the pair mutual information. Both symmetric and antisymmetric functions have positive-valued interaction information. Thus, the synergic first term from Eq. (20) outweighs the redundancies in the second term. The interpretation here is that indistinguishability in these three-particle systems leads to a synergic type of dominant statistical interaction.

B. Interacting oscillators

We now turn our attention to examine the impact of attractive and repulsive interaction potentials on the information measures. We will also analyze the contributions from the redundancies and synergy terms to the interaction information.

Three-variable Shannon entropies for oscillators interacting with attractive potentials as a function of coupling strength, λ, are presented in Fig. 3 for the antisymmetric $|001\rangle$ state. Note that we set the value of ω at one for all calculations involving interacting oscillators. Results with different values of ω are qualitatively the same. The position-space entropies diminish with increasing λ as the densities localize, while the momentum-space entropies increase as the corresponding densities delocalize. The one- and two-variable entropies are not shown but display similar tendencies.

The entropy sum is constant with coupling strength, similar to the behavior in the noninteracting oscillators with $1/\omega$. However, the entropy sums for the reduced one- and two-variable densities are not constant and increase with λ. This is different from the behavior in the uncoupled oscillators. Thus, the effect of the interaction potential is inherent in the entropy sums of the reduced quantities.

Figure 4 presents the entropies for the repulsive interaction potential. The behaviors of S_Ψ and S_Φ are now opposite to that observed for the attractive potential. The position-space entropies increase as the underlying densities delocalize with increasing λ and the momentum-space entropies decrease as the corresponding densities localize.

The plots of the entropy sums show the same type of behavior as in the attractive potential. The three-variable sum is not dependent on the coupling strength, while the reduced one- and two-variable entropy sums increase with λ, particularly for larger values of the coupling strength.

Plots of the reduced one-particle position- and momentum-space densities, for two values of the coupling strength, are presented in Fig. 5. These figures illustrate how the densities change in the respective spaces, with an increase in λ. One observes that the position-space density delocalizes with an increased repulsive potential. This is translated into an increase in the corresponding entropic value. On the other hand, the momentum density localizes with a decrease in the entropic value. The entropic sum (S_T^1) as shown in Fig. 4 seems constant in the interval of $\lambda = 0.1$–0.4; however, it increases

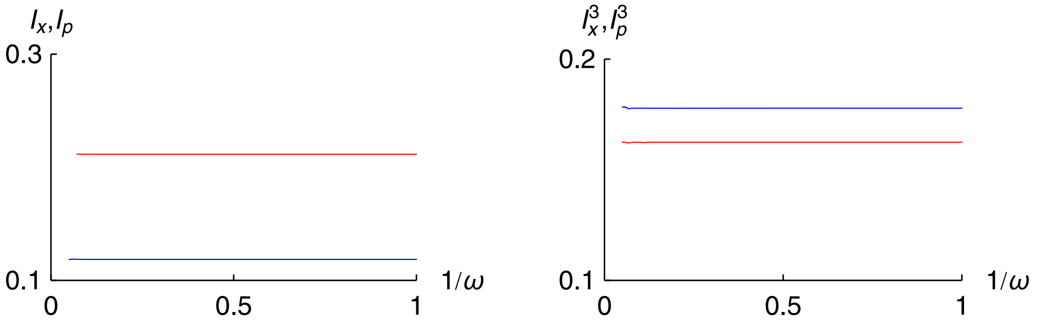

FIG. 2. Left: Plots of the mutual information ($I_x = I_p$) vs $\frac{1}{\omega}$ for symmetric (blue, lower curve) and antisymmetric (red, upper curve) wave functions of the $|012\rangle$ state. Right: Plots of the interaction information ($I_x^3 = I_p^3$) vs $\frac{1}{\omega}$ for symmetric (blue, upper curve) and antisymmetric (red, lower curve) wave functions.

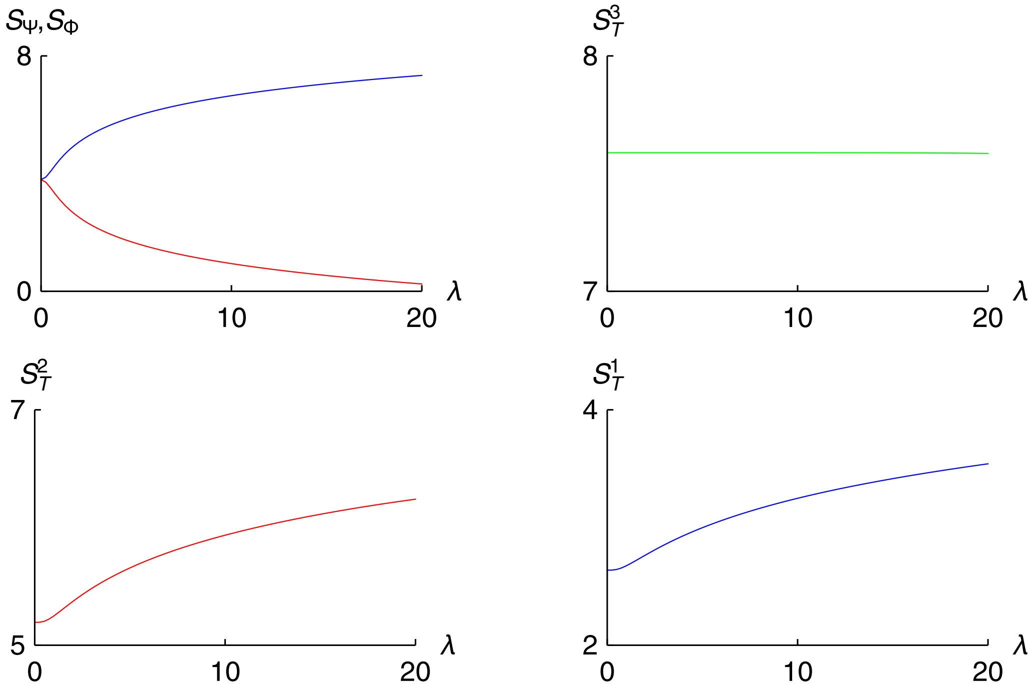

FIG. 3. Upper left: Plots of the position-space S_Ψ (red, lower curve) and momentum-space S_Φ (blue, upper curve) entropies vs the coupling strength λ for the $|001\rangle$ state with attractive potential. Upper right: Plot of the entropic sum S_T^3 (green) vs the coupling strength λ. Lower row: Plots of the entropy sums, S_T^2 (red) and S_T^1 (blue), vs the coupling strength λ.

slightly in this given range. Thus the effects of delocalization in position space are not matched by an equivalent localization in momentum space, with increasing λ.

The entropies obtained from the symmetric $|000\rangle$ state are not presented but have very similar behaviors to those presented in Figs. 3 and 4.

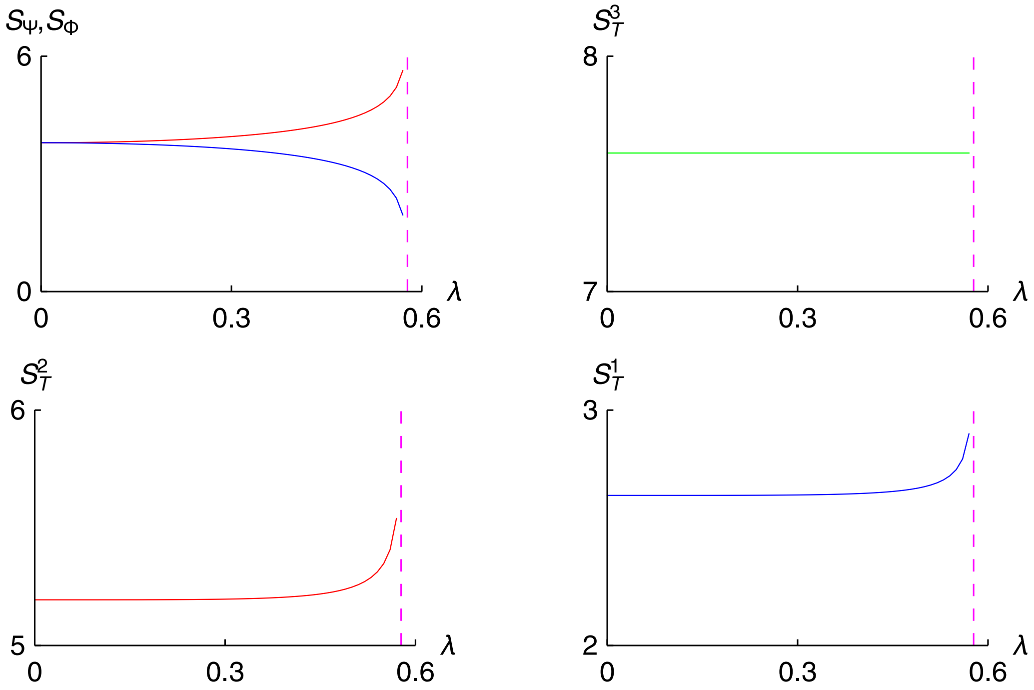

FIG. 4. Upper left: Plots of the position-space S_Ψ (red, upper curve) and momentum-space S_Φ (blue, lower curve) entropies vs the coupling strength λ for the $|001\rangle$ state with repulsive potential. Upper right: Plot of the entropic sum S_T^3 (green) vs the coupling strength λ. Lower row: Plots of the entropy sums, S_T^2 (red) and S_T^1 (blue), vs the coupling strength λ. The dashed vertical line bounds the range in which the potential is real valued.

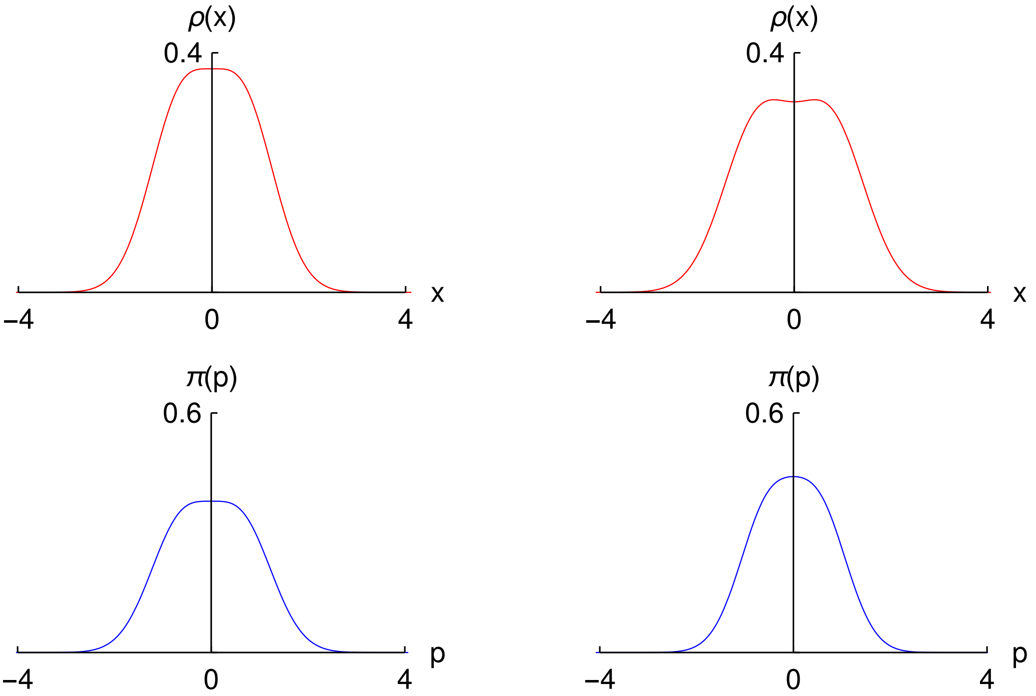

FIG. 5. Upper row: Plots of the one-variable densities $\rho(x)$ (red) vs x, for a repulsive potential with $\lambda = 0.1$ (left) and $\lambda = 0.4$ (right). Bottom row: Plots of the one-variable densities $\pi(p)$ (blue) vs p, for a repulsive potential with $\lambda = 0.1$ (left) and $\lambda = 0.4$ (right).

We now turn our attention to the comparison of the behaviors of pair mutual information and interaction information, in position and momentum space, in the antisymmetric $|001\rangle$ and symmetric $|000\rangle$ cases. Note that the following comparisons do not strictly demonstrate the effects of spin or symmetry since the quantum numbers are different. The $|001\rangle$ spin-free function is not indistinguishable, while the $|000\rangle$ antisymmetric function with spin included is zero.

Figure 6 presents the behavior for the attractive potential. First, the magnitudes of both measures are different in each space. This result is different from that of the uncoupled oscillators presented in Fig. 2, where they are equal. Thus, the presence of the interparticle potential separates the magnitudes of the measures in the two representations.

The pairwise correlation in the spin-free case (top row) increases with coupling strength and is larger in position space compared to momentum space. On the other hand, the magnitudes of the interaction information are equal, $I_p^3 = |I_x^3|$, and both increase with coupling strength. The interpretation here is that the balance of interactions is synergic in momentum space (positive), while in position space it is the redundancies or the pairwise correlations that dominate the balance.

The inclusion of spin in the wave function modifies these results. This can be seen from comparing the top and bottom rows of Fig. 6. In the antisymmetric case, $I_p^3 \neq |I_x^3|$. Furthermore, there is now a region at smaller coupling strength where the pair correlation in position space is smaller than the corresponding momentum-space one, and passes through a shallow minimum. That is, in this region, the pair correlation is smaller for a larger value of the coupling strength. In the minimum, the condition $2\partial S_\rho/\partial\lambda = \partial S_\Gamma/\partial\lambda$ is obeyed. This provides a relationship between the changes at the two-variable and one-variable levels. For larger values of λ, the information measures behave as the ones without the spin included.

The behavior of the interaction information in momentum space does not seem to be modified by the inclusion of spin. However, in position space, there is a region, again at smaller λ, where the interaction information is positive. This is distinct from the spinless case, where it was observed to be negative in the range of λ.

At larger λ, both cases have a consistent behavior in that the interaction information is negative valued. The positive-valued region would be interpreted as a balance in favor of synergic interactions. The zero corresponds to the particular value of the coupling strength, where the magnitudes of the synergic and redundant interactions are equal. This also suggests that the balance between the synergic and redundant interactions can be tuned with the coupling strength.

The results from the repulsive interaction potential are presented in Fig. 7. In the spinless case, the pairwise correlation is now larger in momentum space for the entire range of coupling strength. This is the reverse of the behavior from the attractive potential in Fig. 6 where position space is larger.

The behaviors of the interaction information are also opposite to that of the attractive potential. It is the position-space measure which is now positive valued, while the momentum space one is negative valued. Thus, it is now position space which exhibits the synergic interactions and which increases in magnitude with the coupling strength. Momentum space, on the other hand, displays redundancies. What is shared with the attractive potential is that the magnitudes are equal, $I_x^3 = |I_p^3|$.

The comparison of spin free (top row) and spin (bottom row) also demonstrates differences. Pairwise correlation with

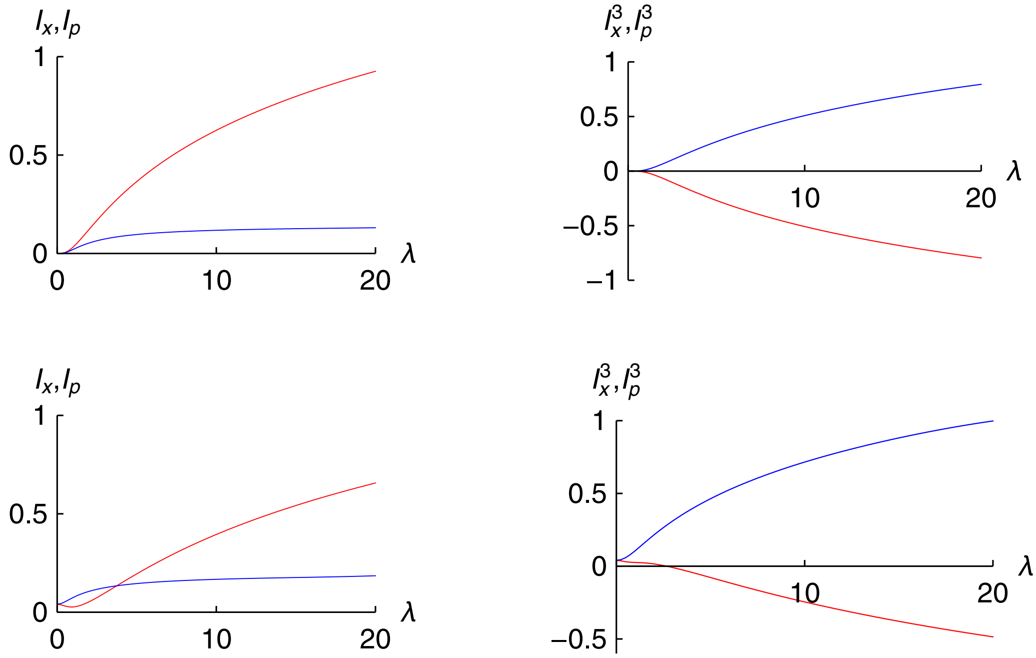

FIG. 6. Left column: Plots of the mutual information I_x (red, upper curve [larger λ]) and I_p (blue, lower curve [larger λ]) vs the coupling strength λ, with attractive potential, for the $|000\rangle$ symmetric state (upper) and the $|001\rangle$ antisymmetric state (lower). Right column: Plots of the interaction information I_x^3 (red, lower curve) and I_p^3 (blue, upper curve) vs the coupling strength λ, with attractive potential, for the $|000\rangle$ symmetric state (upper) and the $|001\rangle$ antisymmetric state (lower).

the inclusion of spin is larger in position space than in momentum space. Also notable is that the pair correlation in momentum space passes through a minimum at relatively larger values of the coupling strength before increasing to the limiting value of λ. The condition $2\partial S_\pi/\partial\lambda = \partial S_\Pi/\partial\lambda$ is obeyed at this minimum. Thus, in a large region of coupling

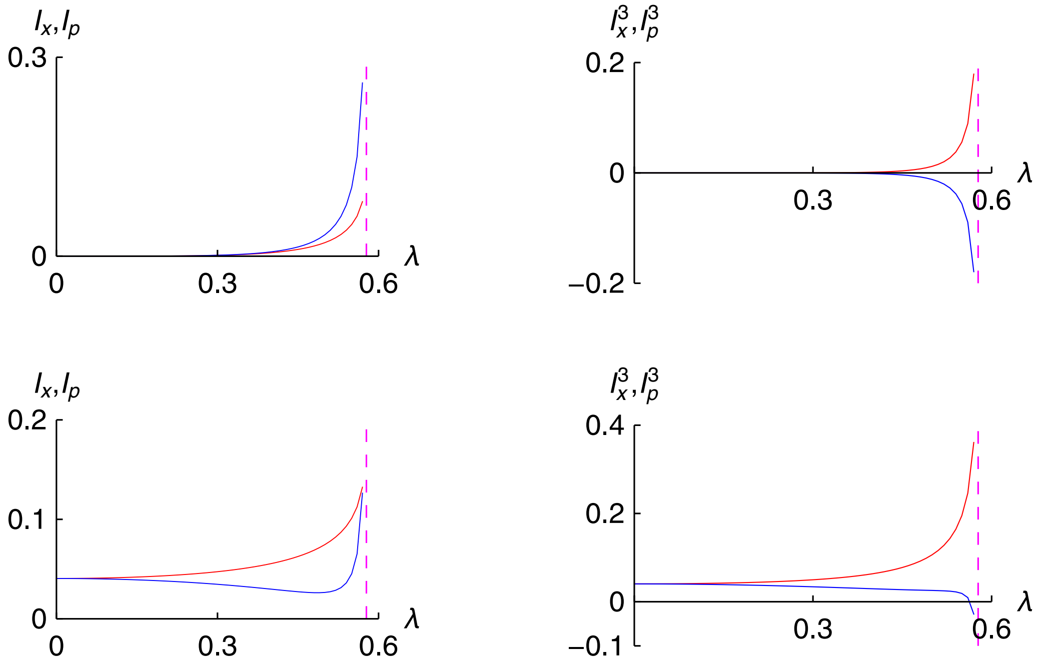

FIG. 7. Left column: Plots of the mutual information I_x (red, lower curve) and I_p (blue, upper curve) vs the coupling strength λ, with repulsive potential, for the $|000\rangle$ symmetric state (upper) and the $|001\rangle$ antisymmetric state (lower), I_x (red, upper curve) and I_p (blue, lower curve). Right column: Plots of the interaction information I_x^3 (red, upper curve) and I_p^3 (blue, lower curve) vs the coupling strength λ, with repulsive potential, for the $|000\rangle$ symmetric state (upper) and the $|001\rangle$ antisymmetric state (lower). The dashed vertical line bounds the range in which the potential is real valued.

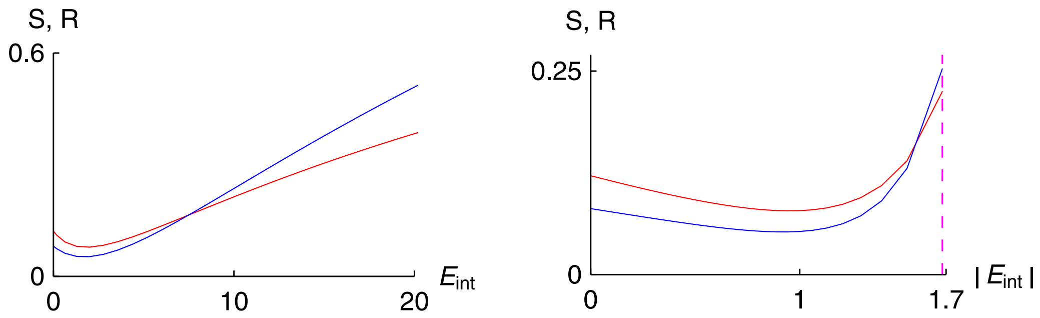

FIG. 8. Left: Plots of the synergic S (red, upper curve [smaller $E_{\rm int}$]) and redundancy R (blue, lower curve [smaller $E_{\rm int}$]) components of I_x^3 vs interaction energy $E_{\rm int}$, for the $|001\rangle$ state with attractive potential. Right: Plots of the synergic S (red, upper curve [smaller $|E_{\rm int}|$]) and redundancy R (blue, lower curve [smaller $|E_{\rm int}|$]) components of I_p^3 vs interaction energy $|E_{\rm int}|$, for the $|001\rangle$ state with repulsive potential. The dashed vertical line bounds the range in which the potential is real valued.

strength, from small to large, the pair correlation in momentum space is actually decreasing with larger values of coupling strength.

Interaction information in position space behaves similarly in the spin and spin-free scenarios. However, there are marked differences in momentum space. The measure is now positive for a wide range of λ, before eventually turning negative in the limit of large coupling strength. Thus, similar to position space with the attractive potential (Fig. 6), the measure passes through a value of λ where it is zero, and changes from a dominance of synergic interactions to one where there are redundancies. Thus the type of dominant interaction can be tuned with the coupling strength. The difference here is that this change occurs at larger coupling strength, while in the attractive potential this occurs at smaller coupling strength.

The behaviors of the synergic (S) and redundancy (R) components of II are presented for attractive (position-space) and repulsive (momentum-space) potentials, corresponding to the $|001\rangle$ state, in Fig. 8. We chose to plot the measures as a function of $E_{\rm int}$, which is defined as the difference in energy from the noninteracting system (NI) ($\lambda = 0$),

$$E_{\rm int} = E - E_{\rm NI} = \left(\sqrt{\omega^2 \pm 3\lambda^2} - \omega\right)\left(n_{r_1} + n_{r_2} + 1\right). \quad (46)$$

One observes that the two components have similar behaviors. Note that R is twice the pair-mutual information. The crossing points correspond to where the interaction information changes sign, and separates the regions of dominance by one of the components over the other. Important to note is that both components increase with $E_{\rm int}$. Also, the R component (twice the pair-mutual information) dominates in both cases at relatively larger values of $E_{\rm int}$ or pairwise interaction. The total correlation, defined in Eq. (16), exhibited the same behavior as R.

VI. CONCLUSIONS

Interaction information and pairwise-mutual information correlation measures are examined in quantum systems consisting of three coupled and uncoupled oscillators, in position and momentum space. The idea here is to gauge how the level of organization (pairwise or higher order) influences the interpretations obtained for these systems. The magnitudes of the correlation measures in position and momentum space are equal, in the case of uncoupled oscillators. For pairwise correlations, the antisymmetric wave functions are more correlated than the symmetric ones. In the interaction information, it is the symmetric functions which are more correlated. Both symmetric and antisymmetric functions yield positive values for the interaction information. The interpretation is that indistinguishability can be thought of as provoking a dominance of synergic interactions. With the inclusion of coupling, the magnitudes of the correlation measures in each space are now distinct. For symmetric wave functions and attractive interparticle potentials, the pairwise correlation is greater in position space, while for repulsive potentials, this correlation is larger in momentum space. In the attractive case, the interaction information is positive in momentum space and grows with the coupling strength, while it is negative in position space. However, the magnitudes are equal in both spaces. The interpretation here for the attractive potential is that interaction information is dominated by synergic interactions in momentum space and redundant ones in position space. With repulsive potentials, it is now the interaction information in position space which is positive valued, while the momentum space one is negative valued. Thus, the dominant interactions are synergic in position space and redundant in momentum space. Hence, the type of interaction potential (attractive or repulsive) controls the dominant contribution (synergic or redundant) to the interaction information, in each space. The inclusion of spin to obtain antisymmetric wave functions is also studied. This results in the appearance of regions in the interaction information where the sign switches from positive to negative values. This occurs in position space at smaller coupling strength with attractive potentials and in momentum space at larger coupling strengths with repulsive potentials. This suggests that the dominant influence to the interaction information (synergic or redundant) can be tuned with the coupling strength. The next step could be a comparison of these results with other potentials such as the Coulombic one [73,74] to examine similarities or differences. The inclusion of explicit three-body terms in the Hamiltonian in order to compare and to contrast with the present results, via the use of variational wave functions, is also contemplated.

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