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Construction and analysis of statistical correlation measures through Diophantine equations

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In this work, we explore the connection between Diophantine equations and the construction of informational measures, particularly mutual information, total correlation, and higher-order interaction information. These information measures are calculated in continuous variable quantum systems comprised of three to fifty harmonic oscillators, and their bahavior was compared among them. By analyzing the ground state of quantum harmonic oscillators, we establish a mathematical framework where Diophantine constraints emerge naturally in the computation of these quantities. There is an overall consistency in the bahavior of the introduced measures as a function of the parameters of pairwise potential and the number of oscillators. Our results provide new insights into the interplay between number theory and quantum information, suggesting novel approaches to quantifying higher-order correlations in many-body quantum systems.

Keywords: Diophantine equations; Shannon entropies; higher-order correlation measures; quantum harmonic oscillators.

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1. Introduction

The study of informational measures in quantum systems provides a fundamental perspective on the nature of correlations and complexity in different quantum applications. Entropic quantities, such as Shannon entropy and mutual information [1,2], serve as essential tools for quantifying uncertainty and information content in quantum models [3-16]. Beyond these standard measures, higher-order correlation measures, such as total correlation and third-order information, offer deeper insights into the intricate structure of statistical correlations [17], particularly in many-body and continuous-variable systems.

Furthermore, there are not many proposals for higher-order correlation measures, and those that have been proposed are for discrete variables [18-21], thus there is a need to present new measures that capture the correlations that come from the physical interactions of the systems with continuous variables. Due to the above, one can think of some way to construct informational higher-order correlation measures and it seems possible through the use of Diophantine equations.

As part of this work, we analyze informational measures in the context of coupled quantum harmonic oscillators in their ground state. As one of the most fundamental models in quantum mechanics, harmonic oscillators provide a worthy yet analytically tractable framework for studying the emergence of correlations in quantum systems. Taking advantage of statistical definitions of information theory, we explore how mutual information, and higher-order correlation measures provide the structure of quantum interactions in the ground state harmonic oscillator model, by tuning control parameters such as the interaction intensity and number of oscillators.

The study of statistical correlations is fundamental to understand the behavior of complex quantum systems.

2. Quantum harmonic oscillators

We define the Hamiltonian of N-coupled one-dimensional oscillators in canonical coordinates in position space. In the pairwise interaction term with coupling constant λ, the positive sign is for the attractive potential, while the negative sign corresponds to a repulsive potential. Both λ and ω are real-valued and positive. The value of λ is bounded for the repulsive case by $\lambda < \omega/N$ to obtain a bound state, considering atomic units $(m = \hbar = 1)$ [22,23]

$$H_N = -\frac{1}{2}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}\omega^2\sum_{i=1}^{N}x_i^2 \pm \lambda^2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}(x_i - x_j)^2. \quad (1)$$

The Schrödinger equation can be solved exactly in the Jacobi coordinates, thus the Hamiltonian is rewritten in the new coordinates as

$$H = \frac{1}{2}\Bigg[\bigg(-\frac{\partial^2}{\partial R^2} + \alpha_1 R^2\bigg) + \bigg(-\frac{\partial^2}{\partial r_1^2} + \alpha_2 r_1^2\bigg) + \cdots + \bigg(-\frac{\partial^2}{\partial r_{N-1}^2} + \alpha_N r_{N-1}^2\bigg)\Bigg], \tag{2}$$

where the constants α_i depend on the potential parameters for one-body (ω) and two-bodies (λ), $\alpha_1 = \omega^2$ and $\alpha_2 = \cdots = \alpha_N = \omega^2 \pm N\lambda^2$. Thus, the Schrödinger equation is separable in the new coordinates

$$H\Psi_{n_R,n_{r_1},n_{r_2},\cdots,n_{r_{N-1}}}(R, r_1, r_2, \cdots, r_{N-1}) = E\Psi_{n_R,n_{r_1},n_{r_2},\cdots,n_{r_{N-1}}}(R, r_1, r_2, \cdots, r_{N-1}). \tag{3}$$

The eigenfunction is written as a product of eigenfunctions

$$\Psi_{n_R,n_{r_1},n_{r_2},\cdots,n_{r_{N-1}}}(R, r_1, r_2, \cdots, r_{N-1}) = \psi_{n_R}(R)\psi_{n_{r_1}}(r_1)\psi_{n_{r_2}}(r_2)\cdots\psi_{n_{r_{N-1}}}(r_{N-1}), \tag{4}$$

these subscripts $n_R, n_{r_1}, n_{r_2}, \cdots, n_{r_{N-1}} = 0$ are the ground state N-particle system quantum numbers, while R is for the center of mass and r_i is for each relative coordinate

$$\psi_0(R) = \left(\frac{\alpha_1^{\frac{1}{4}}}{\pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\sqrt{\alpha_1}R^2}, \tag{5}$$

$$\psi_0(r_i) = \left(\frac{\alpha_{1+i}^{\frac{1}{4}}}{\pi^{\frac{1}{2}}}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\sqrt{\alpha}r_i^2}. \tag{6}$$

The corresponding density for N-oscillators is

$$C_N = |\Psi_{000\cdots 0}(R, r_1, r_2, \cdots, r_{N-1})|^2, \tag{7}$$

where C_N is a normalization constant. An analogous procedure is performed to obtain the eigenfunction and density function in momentum space.

3. Correlation measures and Diophantine equations

Shannon entropies [1,2] are measures of the uncertainties in the underlying distributions. The interpretation of the Shannon entropies is that they are measures of the (de)localization in the corresponding distributions, where larger values correspond to more delocalized distributions while smaller values are indicative of more localized ones. We define the corresponding reduced densities as $\rho(x), \Gamma(x_1, x_2)$ and $\Theta(x_1, x_2, x_3)$, which are obtained by integrating the density for N-oscillators.

With these densities we can define the entropies for one variable

$$S_x = -\int \rho(x)\ln[\rho(x)]dx, \tag{8}$$

two variables

$$S_{x_1x_2} = -\int \Gamma(x_1, x_2)\ln[\Gamma(x_1, x_2)]dx_1dx_2, \tag{9}$$

and three variables

$$S_{x_1x_2x_3} = -\int \Theta(x_1, x_2, x_3)\ln[\Theta(x_1, x_2, x_3)]dx_1dx_2dx_3, \tag{10}$$

where the interval of integration is $[-\infty, \infty]$.

The pairwise correlation between two variables can be quantified in terms of the mutual information [2]

$$I_x = \int \Gamma(x_1, x_2)\ln\left[\frac{\Gamma(x_1, x_2)}{\rho(x_1)\rho(x_2)}\right]\mathrm{d}x_1\mathrm{d}x_2 = 2S_x - S_{x_1x_2}. \tag{11}$$

This measure can be interpreted as a relative entropy between the two-variable distribution and a reference, which is the product of the two marginals.

On the other hand, one can also consider higher-order information that measures the correlation among three variables, this measure is the total correlation [24,25]

$$I_{3x} = \int \Theta(x_1, x_2, x_3)\ln\left[\frac{\Theta(x_1, x_2, x_3)}{\rho(x_1)\rho(x_2)\rho(x_3)}\right]dx_1dx_2dx_3 = 3S_x - S_{x_1x_2x_3}, \tag{12}$$

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

The pair-particle correlation is another and is defined as

$$I^p_{3x} = \int \Theta(x_1,x_2,x_3) \ln \left[\frac{\Theta(x_1,x_2,x_3)\rho(x_1)}{\Gamma(x_1,x_2)\Gamma(x_1,x_3)}\right] dx_1dx_2dx_3 = 2S_{x_1x_2} - S_x - S_{x_1x_2x_3}. \quad (13)$$

The interaction information, which takes into account the correlation or interaction among the three variables [26-29], is given as

$$I^{3x} = \int \Theta(x_1,x_2,x_3) \ln \left[\frac{\Theta(x_1,x_2,x_3)\rho(x_1)\rho(x_2)\rho(x_3)}{\Gamma(x_1,x_2)\Gamma(x_1,x_3)\Gamma(x_2,x_3)}\right] dx_1dx_2dx_3 \quad (14)$$

$$= 3S_{x_1x_2} - 3S_x - S_{x_1x_2x_3}. \quad (15)$$

Equation (15) may be written as

$$I^{3x} = (S_x + S_{x_1x_2} - S_{x_1x_2x_3}) - 2I_x, \quad (16)$$

where the first term in parentheses is known as the synergy and expressed as

$$I^s_{3x} = \int \Theta(x_1,x_2,x_3) \ln \left[\frac{\Theta(x_1,x_2,x_3)}{\rho(x_1)\Gamma(x_2,x_3)}\right] dx_1dx_2dx_3 = S_x + S_{x_1x_2} - S_{x_1x_2x_3}. \quad (17)$$

The above is a summary of some pairwise and higher-order correlation information theory measures that have been used to study quantum systems in continuous variables.

By examining the expressions of the mutual information, the total correlation, the interaction information and the others, it is inferred that it is possible to construct them from the definition of certain coefficients associated with a linear combination of Shannon entropies as

$$I(x) = nS_x + mS_{x_1x_2} + lS_{x_1x_2x_3}, \quad (18)$$

for the indistinguishable case. We can see that in each of the correlation measures reviewed above, the entropy coefficient multiplied by the corresponding number of variables (associated with the entropies) is equal to zero. This is because there is a cancellation of dimensions in the logarithmic argument. Thus, we define a homogeneous Diophantine equation associated with the information measures

$$n + 2m + 3l = 0, \quad (19)$$

where the solution coefficients of the Diophantine equation are

$$n = c_1, \quad (20)$$

$$m = c_1 + 3c_2, \quad (21)$$

$$l = -c_1 - 2c_2, \quad (22)$$

and $c_1, c_2 \in \mathbb{Z}$. Also by construction, $m = -1$ is set for $N = 2$ (two variables) and $l = -1$ for $N = 3$ (three variables).

We can assign the corresponding values to the coefficients and obtain all the informational measures from the definition of the Diophantine equation

$$(c_1,c_2) = (3,-1) \rightarrow I_{3x},$$
$$(c_1,c_2) = (1,0) \rightarrow I^s_{3x},$$
$$(c_1,c_2) = (-1,1) \rightarrow I^p_{3x},$$
$$(c_1,c_2) = (-3,2) \rightarrow I^{3x}.$$
$$\vdots$$

¿ ?

At this point, we wonder whether it is possible to obtain other informational measures at the level of three variables by exploring other values of c_1 and c_2. In the same sense, can new information measures be generated with four, five, six and more variables? Furthermore, if different informational measures can be constructed, which ones have physical relevance in many-body models?

In future work, we hope to answer these open questions.

4. Ground state of coupled harmonic oscillators

In this section, we present and analyze the N-dependent behavior of the correlation measures and their dependencies on the pairwise interaction strength. Additionally, we examine correlation measures with respect to particle number dependencies N when attractive or repulsive interparticle potentials are present. Momentum space measures are defined in an analogous manner to their position space counterparts, using the respective momentum space densities.

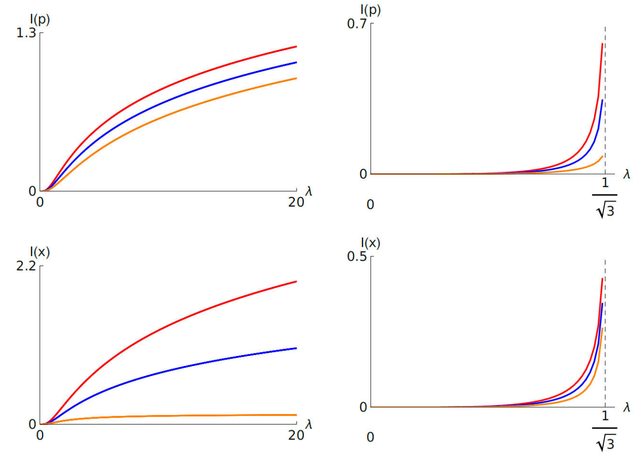

FIGURE 1. First row: Plots of the momentum space total correlation I_{3p} (red), synergy I_{3p}^{s} (blue) and pair-particle correlation I_{3p}^{p} (yellow) *vs* λ. Second row: Plots of the position space I_{3x} (red), I_{3x}^{s} (blue) and I_{3x}^{p} (yellow) *vs* λ. The left column corresponds to results for an attractive potential, while results for a repulsive one are presented in the right column. The vertical dashed line in the case of the repulsive potential is the respective bound, $\lambda = 1/\sqrt{3}$. The value of ω is set at unity and $N = 3$, for the ground state systems.

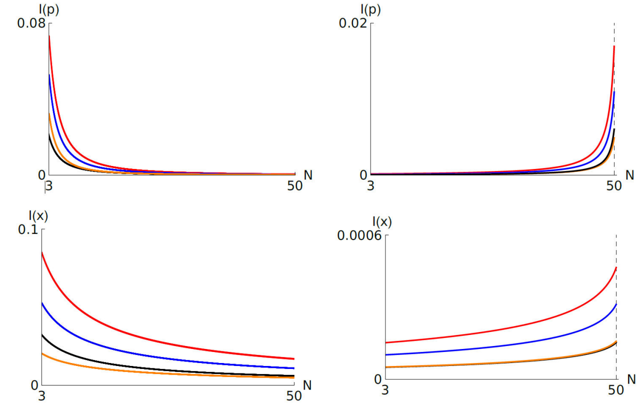

FIGURE 3. First row: Plots of the momentum space mutual information I_p (black), total correlation I_{3p} (red), synergy I_{3p}^{s} (blue) and pair-particle correlation I_{3p}^{p} (yellow) *vs* N. Second row: Plots of the position space I_x (black), I_{3x} (red), I_{3x}^{s} (blue) and I_{3p}^{p} (yellow) *vs* N. The left column corresponds to results for an attractive potential while results for a repulsive one are presented in the right column. The vertical dashed line in the case of the repulsive potential is the respective bound, $\lambda = 1/\sqrt{3}$. The values of ω and λ are set at unity for the ground state systems.

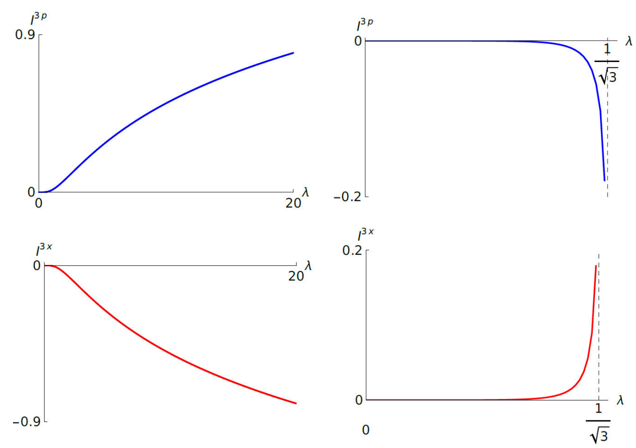

FIGURE 2. First row: Plots of the momentum space interaction information I^{3p} (blue) *vs.* λ. Second row: Plots of the position space I^{3x} (red) *vs.* λ. The left column corresponds to results for an attractive potential while results for a repulsive one are presented in the right column. The vertical dashed line in the case of the repulsive potential, is the respective bound, $\lambda = 1/\sqrt{3}$. The value of ω is set at unity and $N = 3$, for the ground state systems.

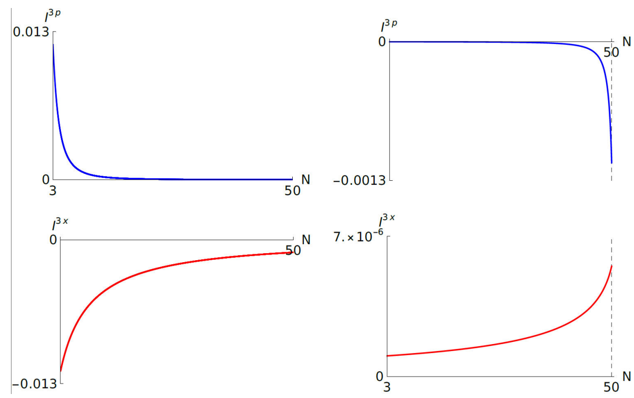

FIGURE 4. First row: Plots of the momentum space interaction information I^{3p} (blue) *vs.* N. Second row: Plots of the position space I^{3x} (red) *vs.* N. The left column corresponds to results for an attractive potential, while results for a repulsive one are presented in the right column. The vertical dashed line in the case of the repulsive potential is the respective bound, $\lambda = 1/\sqrt{3}$. The values of ω and λ are set at unity for the ground state systems.

The results of the correlation measures in both spaces with respect to pairwise interaction with attractive and repulsive interaction potentials are presented in Fig. 1. First, the magnitudes of the correlation measures are different in each space. At this point, all correlation measures increase as the magnitude of the pairwise potential rises. Furthermore, we see that pair-particle correlation is lower than the other higher-order correlation measures in both spaces. However, in all cases the total correlation is the highest magnitude.

The interaction information measures present changes of sign with the type of potential in Fig. 2 [17]. All informational measures in both spaces increase in absolute value as the value of the parameter λ increases, in both the attractive and repulsive cases.

Figure 3 [30] presents the correlation measures, which decrease in magnitude as the value of the parameter N increases in the attractive case. The correlation measures grow in magnitude as the number of oscillators N increases in the repulsive case up to the respective bound. Likewise, the same ordering between the correlation measures is presented as in Fig. 2.

The difference in Fig. 4 [30] is that in the attractive potential the correlation measures change occurs with a lower coupling force, while in the repulsive potential this occurs with a higher coupling force. The dashed vertical line delimits the range in which the potential is real-valued. Furthermore, we observe, as in Fig. 2, that the interaction information measures present opposite signs.

5. Conclusions

Higher-order interaction information measures are examined in quantum systems consisting of three to fifty coupled oscillators in the ground state, in position and momentum spaces. We observe a consistent behavior between the higher-order measures, upon tuning the λ and N parameters. Furthermore, interaction information is positive or negative-valued depending on whether the interparticle potential is repulsive or attractive. The sign also switches on going from position to momentum space. It would be interesting to explore these results in other kinds of systems, as in excited state coupled oscillator systems or in higher dimensionalities. Finally, we are also interested in defining new correlation measures by solving Diophantine equations.

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