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Uncertainties and statistical correlations in quantum systems

Robin P. Sagar

Departamento de Química, Universidad Autónoma Metropolitana Iztapalapa,
Av. Ferrocarril San Rafael Atlixco 186, Col. Leyes de Reforma 1a Sección, Iztapalapa, 09340 Ciudad de México.

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A survey of recent ideas and goals, along with a brief history behind the quantification of uncertainties and statistical correlation in quantum systems is presented. The focus is on ideas and connections taken from information theory, in particular, the quantification of uncertainties via Shannon entropies, the entropic uncertainty relation, and statistical correlation by mutual information. A discussion of phase-space distributions and their use in information theory is also given. An incomplete list of applications, with emphasis on confined quantum systems, is provided. The article concludes by addressing future challenges in these directions.

Keywords: Uncertainty quantification; statistical correlation; entropic uncertainty relation; phase-space distributions; quantum systems.

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1. Perspectives from quantum chemistry

One of the first papers concerning Shannon entropies that appeared in the quantum chemistry/atomic and molecular physics literature was devoted to a study of the entropies of the neutral atoms, in position and in momentum space [1]. Shannon entropies in atomic excited states were also considered as well as the harmonic oscillator. This work provided the basis for our interest in these quantities. Among the results was the conclusion or conjecture that the Shannon entropy sum (sum of position and momentum space Shannon entropies) is a measure of wave function quality. Quantum chemistry addresses how one obtains accurate wave function approximations, so the idea of a quantity that quantifies this was certainly intriguing.

These ideas were later tested in atomic and molecular systems [2, 3]. The interest in the entropies was due to the fact that it is a functional of the electron density, and a lot of attention was being placed on the development of density functional theory. Moreover, the electron density is accessible from x-ray crystallography. At this time, further interest in the electron density was also provided by the Quantum Theory of Atoms in Molecules (QTAIM), which was also under development [4]. The interest in the entropy sum also put emphasis on what information is acquired through consideration of momentum space, a theme related to the development of momentum space quantum chemistry [5]. The impetus here is provided by $(e, 2e)$ spectroscopy from which the momentum density is experimentally accessible.

Besides the idea of the entropy sum as a measure of wave function quality, there were other conceptual interpretations as to what exactly these measures provided. The entropy sum was proposed as a measure of correlation in atomic systems [6]. Such a concept resembles the link that was provided between the position space Shannon entropy and the correlation energy of the weakly inhomogeneous electron gas [7]. Furthermore, the position space Shannon entropy has been shown to be related to the mean excitation energy within the local plasma approximation, a quantity that is experimentally accessible via stopping power measurements [8]. We should also mention that a discrete form of the Shannon entropy, using the eigenvalues of the one-particle reduced density matrix (natural orbital occupation numbers) [9], has been related to the correlation energy in atomic systems.

2. Uncertainties and information entropies: Entropic uncertainty relation

The Heisenberg uncertainty principle (HUP) lies at the heart of phenomena in quantum mechanics. Simply put, it exists because the objects in quantum mechanics exhibit wave-like properties [10]. The Kennard-Robertson formulation [11] in terms of the product of the standard deviations (Δ) of position and momentum is

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{1}$$

In recent years, entropic formulations of the uncertainty principle have gained attention [12–16] and offer certain advantages to the traditional textbook one in terms of standard deviations. For example, the underlying basis for the use of variance-based measures is the assumption of a Gaussian or normal distribution. Many quantum distributions, including those of atomic and molecular systems, deviate from such a form.

The Shannon entropy formulation of the uncertainty relation is (for D dimensions)

$$S_t = S_x + S_p \geq D(1 + \ln \pi), \tag{2}$$

where the Shannon entropies in position (x) and in momentum (p) space are defined in terms of the respective wave functions ($D = 1$) or densities as

$$S_x = -\int |\Psi(x)|^2 \ln |\Psi(x)|^2 dx, \tag{3}$$

$$S_p = -\int |\Phi(p)|^2 \ln |\Phi(p)|^2 dp. \tag{4}$$

We employ one-dimensional variables throughout for simplicity, with the understanding that these are replaced with vectors in atoms and molecules.

The Born interpretation of the wave function in terms of probability densities provides the connection for their use in the definition of the entropies. Notably, the product of standard deviations in Eq. (1) is changed into a sum of entropies (S_t) in Eq. (2). The Shannon entropies [17,18] are measures of the uncertainties in the underlying distributions. Larger values are associated with a more delocalized distribution, while smaller values have localized ones.

Thus, it should not be surprising that the Shannon entropy has attracted attention in chemistry where delocalization is a key concept. Note also that the Shannon entropy is a global measure of the delocalization in the underlying distribution, in contrast to the local measures of localization that are frequently employed in quantum chemistry. We also stress that our interest here is directed toward continuous variable quantum systems in position and in momentum, thus the measures are defined in terms of integrals and not sums.

Quantum information theory, as understood from the computational viewpoint of information shared between two or more states in a superposition, goes beyond the densities of a classical system, to consider the density matrix and the non-local behaviour of quantum systems. A relevant question here is the limitation of Shannon entropies defined in terms of densities, and not density matrices or density operators. Densities, and their probabilistic interpretations, invoke the conception of the quantum object as a particle, not as a wave. The diagonal of the density matrix contains information about populations, not coherences.

We will argue and illustrate later on, that considering the sum of the entropies, rather than a particular component, is indeed an approximation to the consideration of the density operator, and thus contains non-local behaviour. This non-local aspect can be appreciated since the momentum space wave function is the Dirac-Fourier transform of the position space one,

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int \Psi(x) e^{-ipx/\hbar} dx. \tag{5}$$

Furthermore, it should be noted that the Shannon entropies in Eqs. (3) and (4) are defined in terms of a one-particle wave function. For N-particle systems, reduced densities, which have been integrated over the remaining $N-1$ particles, are employed in the definitions. We will see later on that it is possible to consider Shannon entropies of pair or higher-order densities.

The Shannon entropies are not the only measures that have been used to quantify uncertainties in quantum systems. The Rényi measure (R_α) [19], defined in terms of a density, $\rho(x)$, is characterized and generalized by the introduction of a parameter α,

$$\left(\frac{1}{1-\alpha}\right) \log \int \rho(x)^\alpha dx, \alpha > 0, \alpha \neq 1, \tag{6}$$

and reverts to the Shannon entropy as $\alpha \to 1$. This measure has been studied in atoms [20].

Likewise, the Tsallis entropy (T_q) from statistical physics [21] is

$$T_q = \left(\frac{1}{q-1}\right)\left(1 - \int \rho(x)^q dx\right), \tag{7}$$

and also returns to the Shannon entropy as $q \to 1$. This entropy has been examined in the context of electron correlation [22]. A relevant feature of both R_α and T_q is their dependence on the parameters and their possible physical interpretations. We note that there are corresponding uncertainty relations for the Rényi entropies [23]. We should also mention the interest in the Fisher information [24], a measure of localization, and studies with complexity measures [25,26].

The prevalent idea is that information is encoded in the wave function and the task at hand is how to extract this information from uncertainty measures. Among the most important unresolved questions here are: (i) What is the most appropriate measure to capture (quantum) uncertainties? (ii) What do quantum uncertainties tell us about the system? (iii) The uncertainty relation is a statement about position-momentum correlation. How does one measure or examine this? This will be the topic of the next section.

3. Phase-space distributions

The question of defining joint position-momentum distributions has a long history in quantum mechanics. One can formulate the problem by transiting from densities to density matrices or density operators. The phase-space Wigner function [27] is defined as (Weyl-Wigner transform)

$$W(x,p) = \frac{1}{\hbar\pi} \int dy \Psi(x+y) \Psi^*(x-y) e^{-2ipy/\hbar}, \tag{8}$$

and can be seen as a particular representation of the density matrix or operator. It is not surprising that due to the Heisenberg uncertainty principle, and the problem associated with defining the probability of finding a particle with a certain position and momentum, the Wigner function has regions where it is negative-valued. Thus, it is usually referred to as a quasi-probability function. On one hand, one can view this as the principal reason to discard it from consideration, while on the other, one can view the negative regions as a signature of quantum behaviour.

The Husimi function [28] represents a Wigner function that has been passed through a Gaussian filter (Gauss-Weierstrass transform)

$$H(x,p) = \frac{1}{\pi\hbar} \int\int W(x,p) e^{\frac{-(x-x')^2}{2s^2}} \times e^{\frac{-(p-p')^2 2s^2}{\hbar^2}} \mathrm{d}x' \mathrm{d}p'. \tag{9}$$

It is now positive-definite and does not have the negative regions of the Wigner function. On the other hand, much of the interesting nodal structure that is present in Wigner function is lost [29]. Both Wigner and Husimi functions obey the probabilistic property that they normalize to unity.

The Wigner function is also attractive because its marginals are the position [$\rho(x)$] and momentum space [$\pi(p)$] densities. That is,

$$\int dpW(x,p) = \rho(x), \qquad \int dxW(x,p) = \pi(p). \tag{10}$$

The entropies of these marginals, S_x and S_p, are given in Eqs. (3) and (4) for one-particle systems. For $N > 1$ systems, the squared modulus of the wave functions is replaced by reduced densities.

On the other hand, the Husimi function marginals [$\rho_H(x)$ and $\pi_H(p)$] are not the position and momentum space densities

$$\int dpH(x,p) = \rho_H(x), \qquad \int dxH(x,p) = \pi_H(p), \tag{11}$$

that is, in general, $\rho(x) \neq \rho_H(x)$ and $\pi(p) \neq \pi_H(p)$.

The Shannon entropies of the Husimi function marginals are

$$S_H^x = -\int \rho_H(x) \ln \rho_H(x) dx, \tag{12}$$

$$S_H^p = -\int \pi_H(p) \ln \pi_H(p) dp. \tag{13}$$

Most importantly, the Shannon entropies of the Wigner function [30] and the Husimi function (Wehrl entropy) [31] are

$$S_W = -\int W(x,p) \ln W(x,p) dxdp, \tag{14}$$

$$S_H = -\int H(x,p) \ln H(x,p) dxdp. \tag{15}$$

The price to be paid in the definition of the Shannon entropy of the Wigner function is that it is a complex-valued valued quantity, due to the negative regions in the Wigner function. However, the imaginary component is proportional to the volume of the negative regions, which have been associated with quantum correlations [30].

A comparison of the behaviour of the Wehrl and Wigner function entropies in the harmonic oscillator showed that the absolute values of S_W and S_H increase with quantum number and display qualitatively similar behaviours [29]. The Wehrl entropy has been used in the study of a vibron-model quantum phase transition [32] and in entanglement [33]. Rényi entropies of phase-space distributions in density functional theory have also been discussed [34].

After discussing phase-space distributions, we now return to the discussion of the entropy sum to illustrate and to stress its significance. The entropy sum can be interpreted as the entropy of a *separable* phase-space distribution

$$-\int \rho(x)\pi(p) \ln \left[\rho(x)\pi(p)\right] dxdp = S_x + S_p, \tag{16}$$

where this distribution, [$\rho(x)\pi(p)$], is defined as the product of the Wigner function marginals, that is, the position and momentum space densities. This phase-space entropy (entropy sum) is known as the Leipnik entropy [35, 44]. The question of units and dimensions in the logarithmic argument in the Shannon entropy is also addressed here [35]. It should be mentioned that the Wigner function has this particular product form for a harmonic oscillator in the ground state, and where it also saturates the bound in Eq. (2).

4. Statistical correlations

Correlations, or interactions between or among objects in physical systems, provide the framework for the understanding of a wide variety of natural phenomena. Indeed, a noninteracting world would be a nondescript place, devoid of the richness in behaviour induced by such interactions. Thus, there is keen interest in measures that can quantify the extent of such interactions.

This has been the case in quantum chemistry. The correlation energy introduced by Löwdin [38] uses the Hartree-Fock wave function as the reference. Thus, a Hartree-Fock wave function is not correlated from this perspective, even though there are correlations between same-spin electrons due to the antisymmetry of the wave function. The idea of examining and quantifying in turn the statistical correlations in a system has a long history [45], probably due to the statistical interpretation of the wave function.

4.1. Pairwise correlations

This idea was introduced and explored in quantum chemistry/atomic physics by examining the correlation coefficient [46,47]

$$\sigma_x = \frac{\langle x_1 x_2\rangle - \langle x\rangle^2}{\langle x^2\rangle - \langle x\rangle^2}. \tag{17}$$

The correlation coefficient can also be defined and examined in momentum space by calculating the corresponding expectation values. Its values are bounded between zero and ± 1. A perfect correlation of $+1$ corresponds to when the variables are perfectly correlated and move in the same direction, while -1 corresponds to perfect correlation but in opposite directions. A zero-valued σ corresponds to no correlation or a separable pair of distribution. Note that a pair density is required for the calculation of the $\langle x_1 x_2\rangle$ expectation value, while the other expectation values are calculated with the marginals of the pair density. The numerator is the covariance, where the $\langle x\rangle^2$ term is a consequence of particle indistinguishability, particular to quantum systems.

The pair density can be obtained from the wave function in two-particle systems as, $|\Psi(x_1,x_2)|^2 = \rho(x_1,x_2)$, or obtained from an $N > 2$ particle wave function by reducing over $N-2$ remaining particles. It is convenient to consider that these types of correlation measures do not use an external reference. That is, correlation is quantified by comparing expectation values pertaining to the same system or same level of calculation. This is different from the correlation energy where the energy of the correlated system is compared to the Hartree-Fock one. Furthermore, all types of correlation, due to interaction and wave function symmetry, are included in such statistical measures.

There is another pairwise measure of statistical correlation that has attracted attention in many diverse fields. Mutual information is defined as

$$\begin{aligned} I_x &= \int \rho(x_1,x_2)\ln\left[\frac{\rho(x_1,x_2)}{\rho_1(x_1)\rho_2(x_2)}\right]dx_1dx_2 \\ &= S_{x_1}+S_{x_2}-S_{x_1x_2}\geq 0, \end{aligned} \tag{18}$$

where I_p in momentum space is defined in an analogous manner. I_x can be interpreted as a relative entropy, or distance between a pair density and a reference one consisting of the product of its marginals, since $\rho_1(x)$ and $\rho_2(x)$ are obtained by integration of the pair density over x_2 and x_1 respectively. It is also instructive to examine the physical nature of this reference density. For distinguishable systems, it is a Hartree-like product density, while for indistinguishable ones, it is a Bose condensate-like one where all particles occupy the same state.

Mutual information is generally accepted as a more general measure of correlation since it can capture non-linear correlations, while the correlation coefficient can only capture linear ones. On the other hand, mutual information does not distinguish between positive and negative correlation, as in the case of the correlation coefficient. Mutual information is lower-bounded by zero (separable pair density) and increases in value with larger correlation. In principle, there is no upper bound to its value. Note that when applied to quantum systems, $S_{x_1}=S_{x_2}$, as $\rho_1(x)=\rho_2(x)$, due to particle indistinguishability, and the statistical correlation as measured by mutual information is twice the one-variable Shannon entropy minus the two-variable one. This illustrates the relation between uncertainties and statistical correlation.

Mutual information has been employed in various contexts in quantum systems [36, 37, 39–41]. We also remark that statistical correlation measures could conceivably form part of the discussion in any re-examination of the electron correlation problem [42, 43].

At this juncture, it is worthwhile to take a step back, and appreciate that questions raised about measures of uncertainties and statistical correlations that pertain to quantum systems, are the same types of questions that have been raised in data science. Subtle differences involve the use of continuous or discrete distributions. One can expect that there will be interactions between these communities in the future.

One can also address position-momentum correlation by using mutual information measures defined in terms of Wigner [29, 30, 48] or Husimi functions [33],

$$\begin{aligned} I_W &= \int W(x,p)\ln\left[\frac{W(x,p)}{\rho(x)\pi(p)}\right]dxdp \\ &= S_x+S_p-S_W, \end{aligned} \tag{19}$$

$$\begin{aligned} I_H &= \int H(x,p)\ln\left[\frac{H(x,p)}{\rho_H(x)\pi_H(p)}\right]dxdp \\ &= S_H^x+S_H^p-S_H. \end{aligned} \tag{20}$$

where I_W is complex-valued due to S_W. Both the absolute values of I_W and I_H, exhibit a similar increasing behaviour as the quantum number increases in the harmonic oscillator [29].

4.2. Higher-order correlations

To date, most of the attention and emphasis has been directed towards the study of pairwise interactions and correlations in physical systems. This is not to say that higher-order correlations, or those arising from the coupling among three or more objects, do not play a role in physical phenomena. For example, such interactions are related to the concept of emergent behaviour in physical systems [49] and are also studied to understand how neurons interact as a group. It is thought that information is stored in the higher-order interactions among them as a group. In machine learning, higher-order correlations are necessary in order to introduce context into decision-making algorithms.

It is thus important to have available measures to quantify such higher-order correlations. Interaction information, is one such measure that quantifies the correlations among three objects that go beyond the pairwise ones. It is defined as

$$\begin{aligned} I^{3x} &= \int \rho(x_1,x_2,x_3)\ln\left[\frac{\rho(x_1,x_2,x_3)\rho(x_1)\rho(x_2)\rho(x_3)}{\rho(x_1,x_2)\rho(x_1,x_3)\rho(x_2,x_3)}\right]dx_1dx_2dx_3 \\ &= (S^2_{x_1x_2}+S^2_{x_1x_3}+S^2_{x_2x_3})-(S^1_{x_1}+S^1_{x_2}+S^1_{x_3})-S^3_{x_1x_2x_3}=3S^2_{x_1x_2}-3S^1_x-S^3_{x_1x_2x_3}. \end{aligned} \tag{21}$$

$\rho(x_1,x_2,x_3)$ is a three-variable or triple density and the last equality is particular to indistinguishable quantum systems. It is not the only higher-order measure, however, a defining feature is that it can be negative-valued, in contrast to others including the pairwise mutual information. It has been applied to the studies of physical systems [37, 50–52]. One can hope that future work will serve to establish the nature and importance of higher-order correlations in physical systems, and in particular, the physical interpretations behind negative-valued interaction information. A pertinent question here will also be the development of measures for four and more objects or variables.

One could also consider the application of higher-order measures to the analysis of two-particle or two-variable Wigner and Husimi functions. These are defined as

$$W(x_1,p_1,x_2,p_2) = \frac{1}{(\pi\hbar)^2}\int dy_1 dy_2 \Psi(x_1+y_1,x_2+y_2)\Psi^*(x_1-y_1,x_2-y_2)e^{-2i(p_1y_1+p_2y_2)/\hbar}, \tag{22}$$

$$H(x_1,p_1,x_2,p_2) = \frac{1}{(\pi\hbar)^2}\int\int W(x_1,p_1,x_2,p_2)e^{\frac{-\left[(x_1-x_1')^2+(x_2-x_2')^2\right]}{2s^2}} e^{\frac{-\left[(p_1-p_1')^2+(p_2-p_2')^2\right]2s^2}{\hbar^2}} \mathrm{d}x_1'\mathrm{d}p_1'\mathrm{d}x_2'\mathrm{d}p_2'. \tag{23}$$

For example, one can define a mutual information measure in terms of the two-particle phase-space distributions that would take into account total correlations using the Wigner function

$$I_{xp}^W = \int W(x_1,p_1,x_2,p_2)\ln\left[\frac{W(x_1,p_1,x_2,p_2)}{\rho(x_1)\pi(p_1)\rho(x_2)\pi(p_2)}\right] \times dx_1dp_1dx_2dp_2, \tag{24}$$

or in the case of the Husimi function

$$I_{xp}^H = \int H(x_1,p_1,x_2,p_2) \times \ln\left[\frac{H(x_1,p_1,x_2,p_2)}{\rho_H(x_1)\pi_H(p_1)\rho_H(x_2)\pi_H(p_2)}\right] dx_1dp_1dx_2dp_2. \tag{25}$$

Such measures in the case of the Wigner function have been discussed in the case of coupled oscillators [48]. Here, the pair densities, $\rho(x_1,x_2)$ and $\pi(p_1,p_2)$, in each space, are the marginals of the two-particle Wigner function, so it is also possible to conceive of higher-order measures that involve these densities. For example,

$$I_{xp}^2 = \int W(x_1,p_1,x_2,p_2)\ln\left[\frac{W(x_1,p_1,x_2,p_2)}{\rho(x_1,x_2)\pi(p_1,p_2)}\right] \times dx_1dp_1dx_2dp_2, \tag{26}$$

is another candidate [48]. Similar to the interpretation of the entropy sum in terms of a separable phase-space distribution in Eq. (16), the mutual information sum, $I_x + I_p$, represents the correlation present in a two-particle separable phase-space distribution

$$I_x + I_p = \int \rho(x_1,x_2)\pi(p_1,p_2)\ln\left[\frac{\rho(x_1,x_2)\pi(p_1,p_2)}{\rho(x_1)\pi(p_1)\rho(x_2)\pi(p_2)}\right] \times dx_1dp_1dx_2dp_2. \tag{27}$$

5. Applications in confined quantum systems

The interest in the study and application of uncertainties, correlations, and in general information theory, has witnessed a growth in the scope of applications to physical systems in past years. Specific examples, among others, include studies of particles with Bose-Einstein and Fermi-Dirac statistics [53], Bose-Einstein condensates [54–56], quantum time revivals [57], chemical reactivity theory [58], density functional reactivity theory [59, 60], and gravity as an emergent entropic force [61].

There has also been significant interest placed in the application of information theoretical ideas to the study of confined quantum systems [62–75]. These mentioned works provide a basis for a representation, which is by no means complete. One always incurs risk, or uncertainty, by projecting onto a particular basis. The interest in confined systems is due in part to their use as models in the understanding of technologically important devices such as quantum dots.

Here, the emphasis is on understanding behaviour when the particle(s) is (are) confined by hard or soft boundaries, by confining potentials, and by applied external fields. Various entropies, including the Shannon entropy sum, have been used to determine how the system reacts in terms of localization or delocalization, upon application of these physical constraints. Behind these studies lies the more general question of the use of information entropies in the tailoring of quantum control.

A related question, which has not been as yet fully explored, is how particle interaction in confined systems influences the behaviour, and if such interactions can be used as a resource in quantum control. Hopefully, future works will yield more insights into the nature of inter-particle interactions, and how they manifest in confined quantum systems. More generally, one can ask if the Heisenberg uncertainty principle, or its entropic formulation, can be used as a resource for quantum devices. To answer this, efforts need to be devoted to understanding the physical reasons and principles associated with the entropy sum moving away or towards the bound, and its dependence on the physical parameters of the system.

6. Future challenges

We now present some ideas that might present further insights into the role of uncertainties and statistical correlations in quantum systems. There is a relatively large amount of work that has employed Shannon entropies of the one-body densities, but the works employing the two-body or pair densities have been relatively scarce. Shannon pair entropies, and pairwise mutual information, in position and in momentum space, have been studied in neutral atoms and in ions [76–78], in ground and excited states. Fisher information measures for pair distributions have also been examined [24]. Such work needs to be extended to molecular systems where particular interest could be placed on the examination and interpretation of the chemical bond from information theoretical concepts. A major challenge here will be the development of fast algorithms for the numerical evaluation of higher-dimensional integrals.

As previously mentioned, further work needs to be done to understand the nature of entropy sums and mutual information sums, and their relation with the Heisenberg uncertainty principle. More attention is needed in the development, understanding and interpretation of higher-order correlation measures. If interconnectedness is a prevalent feature rather than an exception in physical systems, such measures would serve to quantify these effects.

The Shannon entropies of phase-space distributions and their associated mutual information in chemical systems are also of interest; however, the first step would entail the ability of to calculate Husimi and Wigner functions in atomic and molecular systems. The development of higher-order mutual information measures here is also necessary.

Lastly, although there have been applications of information theoretical concepts to study time-dependent phenomena [39–41, 44, 57, 79, 80], this avenue has not been sufficiently exploited, and one can expect that there will be future endeavours in this regard.

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