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Entropy and Wigner Distribution Functions Revisited

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Several expressions for quantum entropy proposed in the literature are evaluated within the Weyl–Wigner–Moyal phase-space representation of quantum mechanics, with emphasis on some important subtle points in this approach. It has been found that the Rényi–Süßmann entropy and its linearization are distinguished because of their properties.

KEY WORDS: phase-space quantum mechanics; Wigner distribution function; entropy; Rényi–Süßmann entropy; linear entropy.

1. INTRODUCTION

Entropy is, without any doubt, one of the most important physical concepts, not only in thermodynamics and statistical mechanics, but also in various areas of quantum theory. It also remains to be still one of the most mysterious quantities, especially outside the traditional phenomenological thermodynamics, where it can be directly connected with the amount of energy that becomes unavailable.

Information-theoretical entropy, calculated from the respective probability distributions, plays an important role in the study of fundamental aspects of quantum systems and their classical counterparts. As emphasized by Wehrl (1978) in his well-known review article, its correct definition is only possible within the framework of quantum mechanics, because classically *all* probability distributions are allowed, including those which are not physically realizable.

The situation could be improved by employing one of the various possible phase-space representations of quantum mechanics (QM), where quantum and classical concepts are put on equal footing. But as usual, there is a price tag attached to this convenient solution. Namely, the respective phase-space distribution functions are in general *not* probability distributions, in contrast to the classical sta-

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tistical mechanics. Moreover, the formalism involved may become arcane even for simple systems, depending on the particular choice of phase-space representation and the expression for entropy.

The purpose of the present paper is to evaluate some promising entropic expressions within the phase-space picture of QM, emphasizing at the same time important subtle points in this approach. Some of these points are often neglected, which can lead to confusion and incorrect results. As indicated in the title, our discussion will be focused on the Wigner phase-space distribution function (WDF) and the Weyl–Wigner–Moyal (WWM) representation, both occupying a unique position within the world of known phase-space representations of quantum mechanics. To make the paper self-contained, we begin with a short review of these topics. A more elaborate overview, containing also a brief guide to some landmark papers and an extensive reference list, could be found in Zachos, 2002.

2. THE WEYL–WIGNER–MOYAL REPRESENTATION

As in the classical statistical mechanics, the states of a quantum system and the respective dynamical variables are represented in the WWM formalism through the appropriate phase-space functions. The connection to the conventional operator approach is maintained via the Weyl transform (Leaf, 1968).

$$a^w(p,q) = h^{-N} \int d\tau \; \exp\left\{\frac{i}{\hbar} p\tau\right\} \left\langle q + \frac{\tau}{2} \left|\hat{A}\right| q - \frac{\tau}{2}\right\rangle \tag{1}$$

In consequence, phase-space functions corresponding to operator products cannot be obtained as ordinary (pointwise) products of the respective components. Instead, if the operator $\hat{A}$ corresponds to the phase-space function $a(p,q)$ and $\hat{B}$ corresponds to $b(p,q)$ then $\hat{A}\hat{B}$ is represented through $(a \star b)(p,q)$, which is defined as follows (Narcowich and Fulling, 1986):

$$\begin{aligned}(a \star b)(p,q) \equiv \left(\frac{2}{h}\right)^{2N} \int dP_1 dP_2 dQ_1 dQ_2 \; \exp\left\{\frac{2i}{\hbar}(Q_1P_2 - Q_2P_1)\right\} \\ \times\, a(P_1 + p, Q_1 + q) b(P_2 + p, Q_2 + q)\end{aligned} \tag{2}$$

For sufficiently regular phase-space functions (cf. Estrada *et al.*, 1989; Voros, 1977, 1978), the star product may be also expressed in a differential form (de Groot and Suttorp, 1972, Groenewold, 1946).

$$(a \star b)(p,q) = a(p,q) \; \exp\left\{\frac{\hbar}{2i}\left(\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}\right)\right\} b(p,q) \tag{3}$$

where the arrows indicate the side to be processed. This form is especially useful in the case of simple polynomial or exponential phase-space functions, where even complicated expressions involving the star product cold be quite efficiently evaluated in a geometrical way (Zachos, 2000). The following simple relation involving the WWM $\star$-product will be useful later in this paper:

$$\int_\Gamma dpdq\,(a \star b)(p, q) = \int_\Gamma dpdq\, a(p, q) b(p, q) \tag{4}$$

It is evident from the above formulas that the $\star$-product is associative, but in general nonlocal and noncommutative. Together with the Weyl transform, the WWM $\star$-product establishes an isomorphism between the algebra of operators of the standard quantum mechanics and the algebra of phase-space function. Nonetheless, the WWM phase-space representation is a fully autonomous formulation of QM, which may operate independently of the standard approach.

3. THE WIGNER DISTRIBUTION FUNCTION

The states of a system are represented in the WWM formulation through the real-valued WDF (Wigner, 1932), which could be obtained from the respective wavefunction as

$$\rho^w(p, q) = h^{-N} \int d\tau\ \exp\left\{\frac{i}{\hbar} p\tau\right\} \left\langle q + \frac{\tau}{2} \middle| \Psi \right\rangle \left\langle \Psi \middle| q - \frac{\tau}{2} \right\rangle \tag{5}$$

Although named after Wigner, it was used in this form earlier by Dirac as a phase-space electron density in his study of the Thomas–Fermi model (Dirac, 1930).

WDFs corresponding to stationary states could be determined independently as solutions to the respective “star-genvalue” equations (see, e.g., Curtright *et al.*, 1998; Dahl, 1983 and references therein).

$$h^w(p, q) \star f(p, q) = f(p, q) \star h^w(p, q) = E f(p, q) \tag{6}$$

where $h^w(p, q)$ denotes the Weyl transform of the Hamiltonian. This two equations are equivalent to the stationary Schrödinger equation of standard QM.

The time dependence of WDF is given by the quantum Liouville equation.

$$i\hbar \frac{\partial \rho_t^w}{\partial t} = h^w \star \rho_t^w - \rho_t^w \star h^w \tag{7}$$

According to Eq. (3), the r.h.s. of Eq. (7) above could be formally split into a contribution resulting from the classical Liouville flow $\{h^w, \rho_t^w\}$ and “quantum corrections,” collecting the terms with *explicit* $\hbar$ dependence. Unfortunately, because of the *implicit* $\hbar$ dependence of WDF, these corrective terms do not always vanish in the $\hbar \to 0$ classical limit, as it could be expected.

Nevertheless, the WDFs share many features with classical phase-space distribution functions, the most important one is the possibility of calculation of expectation values in the same way as in classical statistical mechanics.

$$\langle \mathcal{A} \rangle = \int_\Gamma dpdq\, a^w(p,q)\rho^w(p,q) \tag{8}$$

But unlike to classical phase-space distribution functions, WDFs are not necessarily nonnegative, and they cannot be therefore regarded as phase-space probability densities.

Notice that the quantity $\int_\Gamma dpdq|\rho^w(p,q)|$ may become infinite for some normalizable WDFs, which precludes also the direct interpretation of a WDF as a "signed" or "extended" (Mückenheim, 1986) probability density.

It is well known (Pool, 1966) that normalizable (i.e., square-integrable) wave functions correspond to normalizable WDFs and vice versa. In this case:

$$\int_\Gamma dpdq\, \rho^w(p,q) = 1 \tag{9}$$

and

$$|\rho^w(p,q)| \leq \left(\frac{2}{h}\right)^N \tag{10}$$

which in combination gives immediately that the volume of the phase-space region, where a WDF takes nonzero values, cannot be smaller than $(\frac{h}{2})^N$. This relation is sometimes regarded as another, more illustrative formulation of the uncertainty principle, but it could be also misleading. Namely, one can get a wrong impression that it should be possibe to have a WDF supported on a sufficiently large but finite "phase-space cell." But one can prove that eactly the opposite is true: *if the support of a WDF is of finite measure, then this WDF have to be zero everywhere* (cf. Davidovič and Lalovič, 1992; Jaming, 1998; Janssen, 1998; Włodarz, 1988).

Not all WDF are normalizable. A prominent example may be furnished by the WDF describing the EPR (Einstein *et al.*, 1935) state

$$\rho^w_{\mathrm{EPR}}(p_1, p_2, q_1, q_2) = C\delta(q_1 - q_2 + q_0)\delta(p_1 + p_2) \tag{11}$$

discussed by Bell (1987) and others (Banaszek and Wódkiewicz, 1999a,b; Cohen, 1997; Johansen, 1997) more recently. An even simpler example is given by the WDF for a one-dimensional plane wave state.

$$\langle x|k\rangle = \frac{1}{\sqrt{(2\pi)}} \exp\{ikx\} \tag{12}$$

where the corresponding WDF can be easily obtained via Eq. (5) as (cf. Balazs and Jennings, 1984).

$$\rho^w_k(p,q) = \hbar\delta(p - \hbar k) \tag{13}$$

One can easily verify that $\rho^w_k(p,q)$ above, although singular, fulfills the condition that a given phase-space function $f(p,q)$ should satisfy to be a WDF (cf.

Eq. 2.19b) in Hillery *et al.*, 1984)

$$\int_{\Gamma} dpdq\ f(p,q)\rho^{w}_{\psi}(p,q) \geq 0 \tag{14}$$

for any WDF $\rho^{w}_{\psi}(p,q)$ corresponding to a pure state $|\psi\rangle$. Indeed, inserting Eq. (13) into Eq. (14) we immediately get

$$\int dq\ \rho^{w}_{\psi}(\hbar k, q) = |\langle \hbar k|\psi\rangle|^2 \tag{15}$$

which is obviously nonnegative in all cases.

This result could be extended to general straight-line-supported δ-distributions $\delta(\xi_1 p + \xi_2 q + \xi_3)$ (Włodarz, 1999). Moreover, it could be shown that $\delta(\xi_1 p + \xi_2 q + \xi_3)$ are the only δ-shaped WDFs possible, since the other would violate the position-momentum uncertainty principle (cf. App. C in (Balazs, 1980).

4. QUANTUM ENTROPY

Going through the literature, one can find various expressions for quantum entropy, obtained mainly through relaxing one or more constraints, which are usually imposed on the information-theoretical entropy. For a quantum state per se, i.e., without any measurements being involved, and represented through a density operator $\hat{\rho}$, the "canonical" quantum entropy may be defined after von Neumann (1927) as

$$S = -\mathrm{Tr}(\hat{\rho} \ln \hat{\rho}) \tag{16}$$

This expression is the only one fulfilling all the constraints contained in the Shannon theorem (Shannon, 1948) and also some other important criteria (Gyftopoulos and Çubukçu, 1997). Moreover, in the case of a thermal ensemble it becomes the well-known thermodynamical entropy. Therefore, it seems to be a perfect entropic expression. But in some situations, e.g., for nonextensive physical systems, these constraints may be too restrictive, affecting the possibility of getting the correct description of such systems. The increasingly popular formalism, introduced by Tsallis (1988) and based on the following expression for entropy:

$$S_q = \frac{1 - \mathrm{Tr}(\rho^q)}{q - 1}, q \in \mathcal{R} \tag{17}$$

appears to cure this problem in many cases.

The Tsallis entropy S_q is nonnegative, extremal at equiprobability, concave for $q > 0$, but pseudoadditive.

$$S_q(\rho_A \otimes \rho_B) = S_q(\rho_A) + S_q(\rho_B) + (1-q)S_q(\rho_A)S_q(\rho_B) \tag{18}$$

It reduces to the canonical von Neumann entropy for $q \to 1 : S_1 \equiv S$.

Another popular family of entropic expressions are Rényi entropies (Rényi, 1970).

$$R_\alpha = \frac{1}{1-\alpha} \ln \mathrm{Tr}(\hat{\rho}^\alpha) \tag{19}$$

known also as so-called α-entropies (Thirring, 1980). Rényi entropies are additive and therfore they are filling in a sense the gap between the von Neumann and Tsallis entropies. Namely, the Tsallis expression Eq. (17) may be seen as a linearization of the Rényi expression Eq. (19) with respect to $\mathrm{Tr}(\hat{\rho}^\alpha)$.

The simplest expression for quantum entropy is definitely furnished by

$$S_2 = 1 - \mathrm{Tr}(\hat{\rho}^2) \tag{20}$$

known in the literature as linear or linearized entropy (Zurek *et al.*, 1993). This quantity is obviously a measure of "impurity" of the quantum state, but it has been recently used also as a succesful measure of decoherence (de Oliveira *et al.*, 2001; Dodonov *et al.*, 2000; Facchi *et al.*, 1999, 2000, 2001; Mokarzel *et al.*, 2002; Watanabe, 1939), entanglement (Angelo *et al.*, 2001; Dodonov *et al.*, 2002; Furuya *et al.*, 1998; Munro *et al.*, 2001; Zanardi *et al.*, 2000), complexity (López-Ruiz *et al.*, 1995; Sugita and Aiba, 2002), and mixedness (Ghosh *et al.*, 2001) of quantum systems. Moreover, it is also the simplest, but fairly good approximation of von Neumann quantum entropy in many cases.

In a recent paper, Brukner and Zeilinger (1999) defined the lack of information or uncertainty, regarding the n possible discrete outcomes from an experiment, as a discrete version of linear entropy

$$U = 1 - \sum_{i=1}^{n} p_i^2 \tag{21}$$

emphasizing that this quantity refers directly to the experimental results of mutually complementary measurements, unlike the von Neumann quantum entropy, which is applicable when the measurements reveal a preexisting property. Therefore, the linear entropy seems to be much more than only a mere approximation to the von Neumann expression.

In mathematical statistics, Eq. (21) is known as the Simpson diversity index and it has been extensively used in various studies (cf., e.g., Patil and Taillie, 1982).

5. PHASE-SPACE QUANTUM ENTROPY

The presence of the $\ln \hat{\rho}$ term precludes an easy translation of von Neumann quantum entropy Eq. (16) to the WWM or similar phase-space representation of quantum mechanics, mainly because of the nonlocal star products of phase-space distributions involved. Other expressions for quantum entropy have enormous advantages here, especially the simplest to handle, like the S_2 and R_2 entropies in the WWM picture, where the star product could be explicitly eliminated in the integrand, i.e.,

$$\int_\Gamma dpdq\, \rho^w(p,q) \star \rho^w(p,q) \equiv \int_\Gamma dpdq(\rho^w(p,q))^2 \tag{22}$$

by virtue of Eq. (4). Notice that this is *not* a common property of all phase-space representations, but rather an exception, equivalent to demanding that the underlying phase-space representation is *self-dual* (Włodarz, 1994, 2001), like the WWM one.

Hence, the expression for linear quantum entropy Eq. (20) has a direct transcription to the WWM picture of the form

$$S_2 = 1 - (2\pi\hbar)^D \int_\Gamma dpdq(\rho^w(p,q))^2 \tag{23}$$

Because of its importance, the WWM linear entropy is discussed separately in the next Section.

Another way to generate expressions for quantum entropy within a phase-space representation of QM is to substitute *classical* phase-space probability distributions in *classical* entropic expressions through the respective *quantum* phase-space distributions, or their "smoothed" versions, in order to avoid the problems resulting from negative or even complex values taken by the original distributions in some representations. This in general abusive practice may lead to different end results, which may be well-founded as well as nonsensical, depending on the applied "smoothing" or "positivization" procedure and its physical meaning.

For example, the "coarse graining" of a WDF, performed over small phase space cells of finite size, known from classical statistical mechanics, does not lead in general to a nonnegative, "coarse" phase-space distribution function, in contrast to the widespread belief (cf. Włodarz, 2002 and references therein). Consequently, a "coarse-grained" phase-space quantum entropy would be in general an ill-defined quantity, too.

A better approach, so called "smoothing," is based on convolution of the WDF with a properly chosen "weight function," defined on the whole phase space. In this case, any legitimate WDF is a perfect candidate for a weight function. Moreover, it can be then interpreted as a "quantum ruler" representing the measuring device. The resulting operational phase-space distributions and so-called sampling entropies are well-defined quantities with nice properties (Bužek *et al.*, 1995).

The well-known Wehrl entropy (Wehrl, 1979), defined as follows:

$$S_W = -\int_\Gamma dpdq\, \rho^H(p,q;\kappa))\, \ln \rho^H(p,q;\kappa) \tag{24}$$

where ρ^H denotes the respective Husimi phase-space distribution function parametrized with some arbitrary positive constant κ, is a prominent example of sampling entropy, using minimum-uncertainty states as quantum rulers. One can prove (Beretta, 1984) that in the classical limit ($\hbar \to 0$) von Neumann quantum entropy becomes Wehrl "classical" entropy. Therefore, the Wehrl entropy is often regarded as the closest quantity to the classical Boltzmann–Gibbs–Shannon entropy and is extensively applied in various studies.

6. WWM LINEAR ENTROPY

The WWM expression for linear entropy Eq. (23) has a very simple functional form and is not sensitive to negative values of the underlying WDF, which makes it extremely attractive for various applications. However, a precaution is needed when using this quantity in some cases.

A simple but important example of ill behavior is furnished by a MaxEnt procedure employing Eq. (23) with the constraint appropriate for the microcanonical ensemble: $\int dpdq\rho^w(p,q) = 1$ (cf. Manfredi and Feix, 2000). Namely, the resulting phase-space distribution which extremize the linear entropy: $\rho(p,q) = \text{const} = 1/\Omega$, where $\Omega = \text{vol}(\text{supp}\rho)$, cannot be regarded as a valid WDF.

The employment of smoothed WDFs may be also problematic, because it is in general equivalent to a *representation switch* to another phase-space picture of QM. For example, the usage of Gaussian-smoothed WDFs, which are Husimi distribution functions, means a representation switch to the Husimi picture, with all consequences for the derived results.

Therefore, the linear entropy calculated from a smoothed WDF, say a Husimi distribution function

$$S_2^H = 1 - (2\pi\hbar)^D \int_\Gamma dpdq(\rho^H(p,q))^2 \tag{25}$$

is a *different* quantity on its own right, defined in a *distinct* (Husimi) phase-space representation. Notice also that Eq. (25), in contrast to WWM linear entropy Eq. (23), does *not* correspond directly to the linear entropy expression of Eq. (20).

7. RÉNYI–SÜßMANN ENTROPY

The conventional formulation of the position-momentum uncertainty relation uses standard deviations of position and momentum observables as uncertainty measures. A more accurate uncertainty measure, especially in situations when position and momentum are highly correlated, has been proposed by Süßmann (1997) as

$$\delta[p,q] \equiv \frac{1}{\int_\Gamma dpdq[\rho^w(p,q)]^2} \tag{26}$$

This quantity represents the effective phase-space volume occupied by the particular quantum state.

In general, $\delta[p, q] \geq h^N$, but for any pure state we have always that $\delta[p, q] = h^N$, i.e., each pure quantum state is a minimum uncertainty state in the meaning of the Süßmann phase-space uncertainty measure, occupying effectively a phase-space volume of the order h^N, like a microstate in statistical termodynamics.

This enables one to define an entropic expression, reflecting the statistical weight of a quantum state in the phase space:

$$S_\delta = \ln \frac{\delta[p, q]}{h^N} \tag{27}$$

This quantity, let it call the Rényi–Süßmann entropy, is manifestly additive and equal to the WWM transcription of the Rényi R_2 entropy. Its linearization gives in turn the WWM linear entropy Eq. (23).

8. SUMMARY AND CONCLUSIONS

In this paper, several expressions proposed for quantum entropy were evaluated within the WWM phase-space representation of QM. We have shown that with sufficient precaution, at least some of these entropic expressions may be easily translated to the WWM picture and succesfully applied in various studies. It has been also found that the Rényi–Süßmann entropy and its linearization, the WWM linear entropy, are distinguished as quantities with a clear physical interpretation and useful properties.

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