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Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **65 (1992)**

Heft 4

PDF erstellt am: **23.09.2024**

Persistenter Link: https://doi.org/10.5169/seals-116505

Helv Phys Acta
Vol. 65 (1992)

0018-0238/92/040596-15$1.50+0.20/0

Critical points of the "entropy"-like functional for the quantum distribution functions

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(7. IX. 1990, revised 6. I. 1992)

Abstract. On the analogy of Kandrup's [43] functional of entropy for the Wigner's quantum distribution function a generalised "entropy"-like functional for, a larger class than Cohen's one of quantum distribution functions, is introduced. A variation of this functional, using the Gateaux derivatives and taking into account the properties of the distribution functions by means of Lagrange multipliers, leads to the existence of a class of specific distribution functions, the critical points of the functional. One of them is the distribution function introduced by Terletsky [4] and Margenau and Hill [6].

1. Introduction

Quantum distribution functions in phase space have been studied in parallel to the other approaches to the quantum mechanics. Many details of this development are traced out in the review of Hillery, O'Connell, Scully and Wigner [1]. In 1932 Wigner [2] introduced the first quantum distribution function for the purpose of studying quantum corrections to classical equilibrium distributions. In 1933 Kirkwood [3] proposed another quantum distribution function, having the disadvantage that is specifies a direction in phase space. Yet another distribution function was introduced by Terletsky [4] in 1937. It was investigated later by Blokhinzev [5]. This function was rediscovered as a particular case by Margenau and Hill [6].

To overcome the difficulties with the interpretation of negative values of the above distribution functions Husimi [7] invented a non-negative distribution function obtained by smoothing the Wigner distribution function with a Gaussian (see Englert [8]). The problem of existence of different kinds of non-negative quantum distribution functions was investigated by Bopp [9], Kano [10], Cohen [11], Mehta and Sudarshan [12], Kuryshkin [13], Zaparovanny [14] and many others (see [1]). They proved that the conventional quantum mechanics is not compatible with non-negative distribution functions. So, we are not going to deal with such functions.

In 1963 Glauber [15] and Sudarshan [16] introduced the so-called P-representation of the distribution functions for the aims of the quantum optics. Later Drummond, Gardiner and Walls [17] found some generalised P-representations. However, the disadvantage of the P-representation is that it fixes a scale (see [8]).

A rather general scheme for generating distribution functions was proposed by Cohen [18] and further studied by Summerfield and Zwaifel [19], Prugovecki [20], O'Connell and Wigner [21] and Springborg [22].

Here we will not concern the problem for the correspondence rules, discussed for example by Weyl [23], Groenewold [24], Moyal [25], Mehta and Sudarshan [26], Cahill and Glauber [27], Agarwal and Wolf [28], Springborg [22], Dunne [29] and many others.

Also, we will not deal with the more complicated relativistic distribution functions for particles with spin (see de Boer and van Weert [30], de Groot, van Leeuwen and van Weert [31], Gracia-Bondia and Várilly [32], Cariñena, Gracia-Bondia and Várilly [33] and others).

Thus, we restrict our investigation to the case of non-relativistic spinless representations of the distribution functions.

Here we need the following facts: 1) All the distribution functions can be written in terms of the Wigner distribution function taking derivatives and integrals (see Agarwal and Wolf [28], McKenna and Frisch [34], Haken [35], Leboeuf and Saraceno [36]); 2) There were established different relations between some of the above mentioned distribution functions (see Mehta [37], de Groot and Suttorp [38], Berezin and Shubin [39]).

Thus, the distribution functions do not seem to be independent one from the other. This idea was developed to its logical end by the proof of the statement that all the distribution functions from the Cohen's class can be expressed one by another using the convolution pseudodifferential operators (see Evtimova [40]).

The above facts raise the question about the existence of a criterion for a choice of the type of the distribution function among the whole variety of quantum distribution functions.

In the literature there exist some criteria connected mainly with the invariance properties of the distribution functions under arbitrary linear canonical transformations of the phase space, (see Englert [8], O'Connell and Wigner [21], Springborg [22], Fairlie [41], Krüger and Poffin [42]). This requirement, according to Springborg [22] "leads to the Wigner function as the only allowed phase space function".

The purpose of our work is to propose another criterion for the choice of the distribution function. It is based on a variational principle in the space of the quantum distribution functions. More precisely, we introduce a suitable functional $S(F)$ of the distribution function F and study its critical points. The representation of these critical points enables one to choose the type of the function F in the functional $S(F)$ and therefore to find a unique distribution function from Cohen's class.

The functional, which we propose, resembles in form the functional of entropy in the classical statistical physics. In fact, given any distribution function $F(q, p)$, we consider the quantity

$$S(F) = -\iint F(q, p) \operatorname{Ln} F(q, p) \, dq \, dp. \tag{1.1}$$

Here q and p denote the position and momentum coordinates in the phase space and all the integrations are taken from $-\infty$ to $+\infty$.

In the above definition the functions $F(q, p)$ can be in general complex-valued ones. Hence the functional (1.1) will be also complex-valued. Kandrup [43] has already considered a similar quantity but only for the case when the function $F(q, p)$ is the real-valued Wigner function $F_W(q, p)$. He called the functional $S(F_W)$ "Wigner function entropy". Following his terminology we name $S(F)$ from (1.1) the distribution function "entropy"-like functional.

Next we shall make some comments concerning the notion of the entropy in quantum physics. As it was pointed out by Wehrl [44] the entropy is not an observable, i.e. there is no any operator in quantum physics such that its expectation value in some state could be its entropy. In his review [44] on general properties of entropy Wehrl considered two different interpretations that can be given to it: either as 1) "a measure of the amount of chaos within a quantum mechanical mixed state" or as 2) "a measure of the lack of information about a system". We are disposed to accept the idea that the entropy is a measure for the chaos in a quantum system. However, the definition (1.1) does not suppose that $S(F)$ is different from zero only in mixed states.

In a series of works Beretta [45], Wehrl [46], Thirring [47] and Uhlmann [48] studied the relation between classical entropy and the entropy of quantum thermodynamics in detail.

The most widely accepted definition of the notion of quantum entropy was suggested by von Neumann [49]:

$$S(\varrho) = -k \operatorname{Tr} (\varrho \ln \varrho), \tag{1.2}$$

where ϱ is the density matrix and k is a constant. This entropy is always equal to zero for pure states.

Some of the other definitions of the entropy existing in quantum physics are also considered by Wehrl [44]: "Shannon's expression for the information content of a discrete probability distribution", the expression of the von Neumann's entropy for the coherent states and its classical approximation, the relative entropy between two density matrices and so forth.

Beretta [45] managed to prove that the von Neumann's expression (1.2) in the classical limit $h \to 0$ tends to the classical entropy functional, provided some rather restrictive conditions hold and this proof is valid only for the Blokhintzev [5], Wigner [2] and Wehrl [46] phase space maps.

Many investigations of the properties of entropy, such as additivity, concavity, subadditivity, continuity, mixing, etc. have been done by Wehrl [44], Beretta [50], Narnhofer, Pflug and Thirring [51] and others.

Another important direction in the study of the entropy is the problem about its non-decrease with the time, connected with the second law of thermodynamics, see e.g. Wehrl [44], and Kandrup [52].

The main question that we raise in the work concerns the extremal properties of the "entropy"-like functional (1.1) in a set of quantum distribution functions larger than Cohen's class. For this purpose we need a strict definition of the above given formal expression of $S(F)$. Namely, a correct definition of a suitable logarithmic branch of $\operatorname{Ln} F(q, p)$ given by the assumption

(H.1) There exists an open one-connected domain $\mathcal{U} \in \mathbb{C}^*$, such that $0, \infty \notin \mathcal{U}$ and $\mu(\{(q, p); F(q, p) \notin \mathcal{U}\}) = 0$.

Here $\mu(\cdots)$ is the Lebesgue measure on $\mathbb{R}^{2n}$, while $\mathbb{C}^* = \mathbb{C} \cup \{\infty\}$.

The above assumption is fulfilled for a large class of distribution functions. As application we verify (H.1) for three important examples in Section 3.

To make the definition (1.1) of $S(F)$ rigorous we need also the validity of the following property

(H.2) $F(q, p) \in L^1(\mathbb{R}^{2n})$; $\quad F(q, p) \operatorname{Ln} F(q, p) \in L^1(\mathbb{R}^{2n})$.

In order to study the critical points of $S(F)$ we introduce a new and a larger class of distribution functions, which includes the Cohen's class of distribution functions. This new class of distribution functions is suggested by the following

Lemma 1. *If $F(q, p)$ is a distribution function from the Cohen's class then the following conditions hold*

$$\int F(q, p)\, dp = \langle \Psi(q) \mid \Psi(q) \rangle^2 \tag{1.3a}$$

$$\int F(q, p)\, dq = \langle \Psi(p) \mid \Psi(p) \rangle^2 \tag{1.3b}$$

$$\int qpF(q, p)\, dq\, dp = (\Psi \mid \hat{q}\hat{p} \mid \Psi) + c(\Psi \mid \Psi) \tag{1.4}$$

where c is a complex constant and $\Psi(p)$ is the Fourier transform of the state function $\Psi(q)$; $\langle \cdot \mid$ and $\mid \cdot \rangle$ are the Dirac bra and ket representations of the state vectors; $(\cdot \mid \cdot)$ is the scalar product in the Hilbert space; $\hat{q}$ and $\hat{p}$ are the operators corresponding to the position q and momentum p; $(\Psi \mid \hat{q}\hat{p} \mid \Psi)$ is the quantum average of the operator $\hat{q}\hat{p}$. The equations (1.3) express the well-known marginal conditions and the equation (1.4) is proved in the Appendix.

Hence the new class of distribution functions can be introduced by the following

Definition 1. Given any state $\Psi(q) \in \mathbb{C}(\mathbb{R}^n)$ and any complex number c, denote by $\Lambda(\Psi, c)$ the set of continuous functions $F(q, p) \in \mathbb{C}(\mathbb{R}^{2n})$ satisfying the properties (H.1) and (H.2) and the conditions (1.3) and (1.4).

Definition 2. $\Lambda(\Psi) = \bigcup_c \Lambda(\Psi, c)$.

Now the main problem of the work can be stated more precisely a representation formula for the critical points of the quantum distribution function "entropy"-like functional $S(F)$ over $\Lambda(\Psi)$ is to be found.

The main result of the paper is the following.

Theorem 2. *The distribution function $F(q, p)$ is a critical point of the functional $S(F)$ over $\Lambda(\Psi)$ if and only if it has the form*

$$F(q, p) = v(q)\eta(p) \exp(cqp). \tag{1.5}$$

The proof of the theorem is based on the notion of Gateaux derivative of the functional $S(F)$.

$$\delta S(F, h) = \lim_{t \to 0} \{S(F + th) - S(F)\}/t, \qquad 0 < t < 1, \tag{1.6}$$

where h is a continuous function.

The necessity to use the Gateaux derivatives when one investigates variational problems in quantum physics has been pointed out by Sharma and Rebelo [53] and Fonte [54]. Fonte especially underlines that a rigorous variational calculus on complex spaces has to be based on differentials which contain linear and antilinear terms.

There is an essential difference in (1.6) and the definition used by Fonte: the functional $S(F)$ in (1.6) is complex-valued while the functionals regarded by Fonte are real-valued.

Hence the main difficulty which arises here has the following origin: since $F \in \Lambda(\Psi)$ then $(F + th)$ must be from $\Lambda(\Psi)$ too. To satisfy this assumption it is necessary to guarantee that supp h is a compact.

It is easy to see that Terletsky's function satisfies (1.5) in the case when $c = i$. Hence, we conclude that some of the critical points of $S(F)$ lie in the Cohen's class of distribution functions.

An important question arising from the result of Theorem 2 is whether $\Lambda(\Psi)$ is essentially larger than the Cohen's class. This is naturally true, since the distribution functions from the Cohen's class F_C satisfy (1.3) and the requirement (see Springborg [22])

$$(\Psi \mid \hat{G}(\hat{q}, \hat{p}) \mid \Psi) = \int F_C(q, p; f) G(q, p) \, dq \, dp. \tag{1.7}$$

Here $(\Psi \mid \hat{G} \mid \Psi)$ is the expectation value of the quantum mechanical operator $\hat{G}(\hat{q}, \hat{p})$ and $G(q, p)$ is its classical counterpart; f is a continuous function introduced by Cohen to describe the correspondence rule $\hat{G} \to G$.

It is well-known that $\hat{G}(\hat{q}, \hat{p})$ and $G(q, p)$ are regarded as polynomials or functions in general. Hence, the comparison of the conditions (1.7) and (1.4), since $\hat{q}\hat{p}$ and qp are included as monomials in the latter, shows that one can derive the following.

Corollary 3. $\Lambda(\Psi)$ *does not coincide with the Cohen's class.*

The plan of the work is as follows: In Section 2 we prove the Theorem 2; in Section 3 we consider three examples—we verify the hypotheses (H.1) and (H.2) for the cases of a harmonic oscillator, a potential well and a basic state of the hydrogen atom.

2. Proof of Theorem 2

The first step in this section is the verification of the existence and correctness of the "entropy"-like functional for the quantum distribution functions $F(q, p)$

$$S(F) = -\int F(q, p) \operatorname{Ln} F(q, p)\, dq\, dp \tag{2.1}$$

provided the assumptions (H.1) and (H.2) are fulfilled.

Indeed, let $\mathscr{U}$ be the open domain chosen according to the assumption (H.1). Set $L \equiv L(F) = \{(q, p); F(q, p) \in \mathscr{U}\}$. Let $\operatorname{Arg} z = \operatorname{Arg}_{\mathscr{U}} z$ be any branch of the function $\operatorname{Arg} z$ defined in $\mathscr{U}$. Then we have

$$\operatorname{Ln} F(q, p) = \ln |F(q, p)| + i \operatorname{Arg}_{\mathscr{U}} F(q, p)$$

for $(q, p) \in L$. The assumption (H.1) guarantees that $\mu(\mathbb{R}^{2n} - L) = 0$. Since any branch of $\operatorname{Arg} z$ satisfies the estimate

$$|\operatorname{Arg} z| \leqslant C,$$

we obtain the estimate

$$|F \operatorname{Ln} F| \leqslant C(|F| + |F| \ln |F|)$$

on L. Now the Lebesgue convergence theorem and the assumption (H.1) imply that $F \operatorname{Ln} F \in L^1(\mathbb{R}^{2n})$. Thus, we conclude the definition (2.1) is correct.

In order to study the critical points of the "entropy"-like functional $S(F)$ (2.1) we recall the definition of the Gateaux variation of $S(F)$ determined by

$$\delta S(F, h) = \lim_{t \to 0} \frac{S(F + th) - S(F)}{t}, \tag{2.2}$$

provided the limit in the right-hand side of this equality exists.

The next step in this section is the determination of a star-shaped neighbourhood of F in $\Lambda(\Psi, c)$ in order to be sure that the quotient in the right-hand side of (2.2) is correctly defined.

Lemma 2.1. *Let* $F \in \Lambda(\Psi, c)$, *let* $\mathscr{U}$ *be determined according to the assumption* (*H*.1) *and let* K *be a compact subset in*

$$L = \{q, p; F(q, p) \in \mathscr{U}\}.$$

Then one can find $\varepsilon > 0$, *such that for any continuous function* $h(q,p)$, *which satisfies the requirements*

$$\operatorname{supp} h \subset K, \max_K |h| \leqslant \varepsilon, \tag{2.3}$$

$$\int h(q,p)\,dp = \int h(q,p)\,dq = \int q \cdot ph(q,p)\,dq\,dp = 0, \tag{2.4}$$

we have $(F + th) \in \Lambda(\Psi, c)$ *for* $0 \leqslant t \leqslant 1$.

Proof. The properties

$$(F + th) \in L^1, |F + th| \ln |F + th| \in L^1, \quad 0 \leqslant t \leqslant 1$$

are fulfilled, since $F \in \Lambda(\Psi, c)$, h is a continuous function and $\operatorname{supp} h$ is included in K. It is easy to see that (2.4) imply the conditions (1.3) and (1.4) for the function $(F + th)$. The main difficulty is the verification of the assumption (H.1) for the function $F + th$. Let $0 \leqslant t \leqslant 1$ be fixed. Since $F \in \Lambda(\Psi, c)$ we can choose the open domain $\mathscr{U}$ according to the property (H.1). Our goal is to define a branch of $\operatorname{Ln}[F(q,p) + th(q,p)]$ for $(q,p) \in \mathscr{U}$. To do this take

$$\varepsilon = \min_K |F(q,p)|/2.$$

The facts that $K \subset L$ and F is a continuous function guarantee that $\varepsilon > 0$. Then we define

$$\operatorname{Ln}(F + th) = \operatorname{Ln} F - \sum_{k=1}^{\infty} k^{-1}(-th)^k F^{-k} \tag{2.5}$$

on L. Note that our choice of ε shows that the inequality

$$\max_K |h| \leqslant \varepsilon$$

leads to the estimate $|h/F| \leqslant 1/2$ on $\operatorname{supp} h$. Hence $\operatorname{Ln}(F + th)$ is defined correctly by the series expansion in (2.5) for $0 \leqslant t \leqslant 1$. This completes the proof of the lemma.

Now we can turn to the following.

Proof of Theorem 2. Suppose $F \in \Lambda(\Psi, c)$ is a critical point of the "entropy"-like functional $S(F)$, i.e.

$$\delta S(F) = 0$$

for any continuous function h satisfying the properties (2.3) and (2.4) of Lemma 2.1. Then the continuous function h satisfies the relations

$$\int h(q,p)\,dp = 0, \tag{2.6a}$$

$$\int h(q,p)\,dq = 0, \tag{2.6b}$$

$$\int q \cdot ph(q,p)\,dq\,dp = 0. \tag{2.6c}$$

To find a suitable parametrization of the marginal conditions (2.6a) and (2.6b) we put

$$h(q,p) = g(q,p)\left(\int g(q',p')\,dq'\,dp'\right) - \left(\int g(q,p')\,dp'\right)\left(\int g(q',p)\,dq'\right), \quad (2.7)$$

where g is a continuous function. Let $h(g) : g \to h$ be the map given by (2.7). Then the conditions (2.6a) and (2.6b) are always fulfilled for $h(g)$. The relation (2.6c) takes the form

$$\left(\int g(q,p)\,dp\,dp\right)\left(\int qpg(q,p)\,dq\,dp\right)$$
$$= \left(\int pg(q,p)\,dq\,dp\right)\left(\int qg(q,p)\,dq\,dp\right). \quad (2.8)$$

Take a compact $K \subset L = \{q, p; F(q,p) \in \mathscr{U}\}$ and choose $\varepsilon > 0$ according to Lemma 2.1. Then one can find $\delta_1 = \delta_1(F, K) > 0$, so that for any continuous function $g(q,p)$ satisfying (2.8) and

$$\operatorname{supp} g \subseteq K, \max_K |g| \leqslant \delta_1 \quad (2.9)$$

We have $\max |h| \leqslant \varepsilon$ with $h(q,p)$ determined by (2.7). Further, a simple calculation shows that we have the relation

$$\delta S(F, h(g)) = \iint (1 + \operatorname{Ln} F) h(g)(q,p)\,dq\,dp.$$

The assumption that F is a critical point of the "entropy"-like functional $S(F)$ and the conditions (2.6) imply

$$\iint (1 + \operatorname{Ln} F) h(g)(q,p)\,dq\,dp = 0 \quad (2.10)$$

for any continuous function $g(q,p)$ satisfying (2.8), (2.9). Denote by $M(F, K, \delta)$ the set of all continuous functions $g(q,p)$ satisfying (2.8) and (2.9). Further, we denote by $N(F, K, \delta)$ the set of all continuous functions satisfying (2.9) only. Since the functional

$$g \to \iint (1 + \operatorname{Ln} F) h(g)(q,p)\,dq\,dp$$

is identically zero over $M(F, K, \delta)$, we can apply the technique of the Lagrange multipliers and conclude that any $g \in M(F, K, \delta)$ is a critical point of the functional

$$\mathscr{I}(g) = \iint (1 + \operatorname{Ln} F) h(g)(q,p)\,dq\,dp$$
$$+ c\left\{\left(\int g(q,p)\,dq\,dp\right)\left(\int qpg(q,p)\,dq\,dp\right)\right.$$
$$\left. - \left(\int pg(q,p)\,dq\,dp\right)\left(\int qg(q,p)\,dq\,dp\right)\right\}$$

over $N(F, K, \delta)$. Here c is a Lagrange multiplier. Take $g^* \in M(F, K, \delta)$ so that $\int g^*(q, p)\, dq\, dp \neq 0$ and fix g^*. Then the above observation yields

$$\delta \mathscr{J}(g^*, g) = 0$$

for any $g \in N(F, K, \delta)$.

Putting

$$H(q, p) = (1 + cqp + \operatorname{Ln} F(q, p)) \iint g^*(q, p)\, dq\, dp,$$

we obtain

$$0 = \delta \mathscr{J}(g^*, g) = \iint [H(q, p) - \lambda(q) - \mu(p) - D] g(q, p)\, dq\, dp, \tag{2.11}$$

where

$$\lambda(q) = \int H(q, p) \int g^*(q, p)\, dq\, dp \left(\iint g^*(q, p)\, dq\, dp \right)^{-1},$$

$$\mu(p) = \int H(q, p) \int g^*(q, p)\, dp\, dq \left(\iint g^*(q, p)\, dq\, dp \right)^{-1},$$

$$D = \iint H(q, p) g^*(q, p)\, dp\, dq \left(\iint g^*(q, p)\, dq\, dp \right)^{-1}.$$

Our assumptions guarantee that $\lambda(q)$, $\mu(p)$ are continuous functions. Hence, the relations (2.11) lead to the identity

$$H(q, p) = \lambda(q) + \mu(p) + D$$

and the representation formula of $H(q, p)$ leads to the equality

$$\operatorname{Ln} F = \left(\iint g^*(q, p)\, dq\, dp \right)^{-1} (\lambda(q) + \mu(p) + D - 1 - cqp).$$

Thus, we conclude that F has the form

$$F(q, p) = v(q) \eta(p) e^{cpq},$$

where $v(q)$, $\eta(p)$ are continuous functions on $\mathbb{R}^n$, while c is a complex constant.

Conversely, if $F(q, p)$ has the above given form, then the equalities (2.6) show that $\delta S(F, h) = 0$ for any continuous function h satisfying the property (2.7). This completes the proof of the Theorem 2.

3. Examples

In this section we shall verify the assumptions (H.1) and (H.2) for the important cases of a harmonic oscillator, a potential well and the basic state of a hydrogen atom. Everywhere in the expressions of the distribution functions we use the units in which $(h/2\pi) = 1$ with h being the Planck's constant.

Throughout this section the phase space will be two-dimensional.

To check (H.1) we shall use the following.

Lemma 3.1. *Let $\mathscr{D}$ be an open connected domain in $\mathbb{R}^n$, $n \geqslant 1$, and let $f(x)$ be a smooth function on $\mathscr{D}$ in $\mathbb{C}^n$. Then*

$$\mu_{\mathbb{R}^n}\{x; f(x) = 0\} = 0.$$

Proof. Set $x' = \{x_2, \ldots, x_n\}$ and $A(x') = \{x_1; f(x_1, x') = 0\}$, $A(x) = \{x; f(x) = 0\}$, Denoting by χ_B the characteristic function of any set B and applying the Fubini theorem we get

$$\mu(A) = \int_{\mathbb{R}^n} \chi_A(x)\, dx = \int_{\mathbb{R}^{n-1}} \left(\int \chi_{A(x')}(x_1)\, dx_1 \right) dx' = \int_{\mathbb{R}^{n-1}} \mu_{\mathbb{R}}(A(x'))\, dx.$$

Since $f(x_1, x')$ can be extended as an analytic function of x_1, we conclude that the roots of the equation $f(x_1, x') = 0$ with respect to x_1 form a set of Lebesgue measure zero. Hence $\mu_{\mathbb{R}}[A(x')] = 0$. This proves the Lemma.

Example 1. A harmonic oscillator.

Introduce new variables $x = (m\omega/2)^{1/2}q$, $y = (2m\omega)^{-1/2}p$, where m is the mass and ω is the frequency of the oscillator. The Wigner function in the case has the form (cf. [1])

$$F_W^n(x, y) = (-1)^n \exp(-x^2 - y^2) L_n(2x^2 + 2y^2)/\pi, \qquad n = 0, 1, \ldots \tag{3.1}$$

where L_n is the Lagerre polynomial of order n. From (3.1) one can see directly that (H.2) is fulfilled.

Further we turn to the assumption (H.1). Take $\mathscr{U} = \mathbb{C}^* - i\mathbb{R}_+$. The fact that F_W^n is a real-valued function guarantees it is sufficient to show that the Lebesgue measure of the set

$$\{(x, y); F_W^n(x, y) \notin \mathscr{U}\} = \{(x, y); F_W^n(x, y) = 0\} = \{(x, y); L_n(2x^2 + 2y^2) = 0\}$$

on $\mathbb{R}^2$ is zero. This follows directly from Lemma 3.1, since $L_n(2x^2 + 2y^2)$ is an analytic function on $\mathbb{C}^2$.

The Terletsky's distribution function has the form

$$F_n^T(x, y) = (2^{3/2})^{-1} H_n(x) P_n(y) e^{-(x^2 + y^2)/2} e^{i(xy + n\pi/2)} \tag{3.2}$$

where $n = 0, 1, 2, \ldots$, H_n is the Hermite polynomial of degree n and $P_n(y)$ is a polynomial determined by

$$P_n(y) = e^{y^2/2} \sum_{m=0}^{[n/2]} \partial_n^{n-2m} (e^{-y^2/2})/(4^m m!(n-2m)!),$$

$[c]$ is the integer of the real number c.

Again it is clear that the assumption (H.2) holds if $F(x, y)$ is given by the expression (3.2).

To check the assumption (H.1) for the case we consider $\mathcal{U} = \mathbb{C}^* - \mathbb{R}_-$. Here we have to find the Lebesgue measure of the set

$$\{(x, y); F_T^n(x, y) \notin \mathcal{U}\} = \{(x, y); F_T^n(x, y) \in \mathbb{R}_-\}.$$

Since the following inclusion

$$\{(x, y); F_T^n \in \mathbb{R}_-\} \subset \{(x, y); \operatorname{Im} F_T^n = 0\} \tag{3.3}$$

is valid, we can apply Lemma 3.1 for the second set in (3.3). Because

$$\operatorname{Im} F_T^n = (2^{3/2}\pi)^{-1} H_n(x) P_n(y) e^{-(x^2+y^2)/2} \sin(xy + n\pi/2)$$

is a smooth function that can be extended as analytic function in $\mathbb{C}^2$, Lemma 3.1 yields

$$\mu(\{(x, y); \operatorname{Im} F_T^n = 0\}) = 0.$$

Consequently, the inclusion (3.3) shows that

$$\mu(\{(x, y); F_T^n \in \mathbb{R}_-\}) = 0$$

and we see the assumption (H.1) is fulfilled.

Example 2. A potential well.

Here it is suitable to represent the Wigner distribution function in the form

$$F_W^n(x, y) = F_1 + F_2 + F_3, \tag{3.4}$$

where

$$F_1 = \cos[n\pi(1 + 2x)] \sin[y(1 - 2|x|)](\pi y)^{-1},$$

$$F_2 = \sin[(y + n\pi)(1 - 2|x|)][2\pi(y + n\pi)]^{-1},$$

$$F_3 = \sin[(y - n\pi)(1 - 2|x|)][2\pi(y - n\pi)]^{-1}.$$

Here $x \in [-1/2, 1/2]$, $y \in \mathbb{R}$ and $x = q/a$, $y = pa$, a being the size of the potential well.

To verify the assumption (H.2) we use the fact that (3.4) is a smooth function which can be estimated as follows

$$|F_W^n| \leqslant \text{const}\, |y|^{-2}$$

if y is sufficiently large. This estimate yields (H.2).

To check (H.1) we choose $\mathcal{U} = \mathbb{C}^* - (i\mathbb{R}_+)$. The real-valued smooth function (3.4) satisfies the relation

$$\{(x, y); F_W^n(x, y) \notin \mathcal{U}\} = \{(x, y); F_W^n(x, y) = 0\}.$$

From (3.4) we see that the function F^n_W can be extended as analytic function in a neighbourhood of $(-1/2, 1/2) \times \mathbb{R}$. The above observation shows that we can apply Lemma 3.1 and conclude that the condition (H.1) holds.

Similar argument can be applied for the Terletsky's distribution function which, for the considered case, can be represented in the form

$$F^n_T(x, y) = F_1 + F_2,$$

where

$$F_1 = 2(n\pi - y)^{-1} \sin(n\pi(x + 1/2))\, e^{i[xy + (n+1)\pi/2]} \sin((n\pi - y)/2),$$

$$F_2 = 2(-1)^n(n\pi + y)^{-1} \sin(n\pi(x + 1/2))\, e^{i[xy + (n+1)\pi/2]} \sin((n\pi + y)/2)$$

for $x \in (-1/2, 1/2)$, $y \in \mathbb{R}$. Now we choose $\mathscr{U} = \mathbb{C}^* - \mathbb{R}_-$ and use the inclusion

$$\{(x, y); F^n_T(x, y) \notin \mathscr{U}\} \subset \{(x, y); \operatorname{Im} F^n_T(x, y) = 0\}.$$

The application of Lemma 3.1 for the function $\operatorname{Im} F^n_T(x, y)$ leads to the property (H.1).

Example 3. Basic state of a Hydrogen atom.

Denoting by r and k the radial position and momentum variables we have the following expression for Terletsky's distribution function (see [55])

$$F^H_T(r, k) = \frac{C\, e^{-\beta r}}{(k^2 + \beta^2)^{3/2}} \left\{ \sum_0^\infty \frac{\Gamma(p - 1/2)}{p!} \left(\frac{k^2}{k^2 + \beta^2} \right)^p \right\} \frac{\sin(k \cdot r)}{(k \cdot r)}$$

where C and β are constants, and $\Gamma(\cdot)$ is the well-known gamma-function (see [56]).

Because of the fact that

$$|F^H_T(r, k)| \leqslant C\, e^{-\beta r} |k|^{-4}$$

if k and r are sufficiently large we conclude that the assumption (H.2) is fulfilled.

Consider the assumption (H.1). Here we can choose $\mathscr{U} = \mathbb{C}^* - i\mathbb{R}_+$. Since $F^H_T(r, k)$ is a real-valued function it is sufficient to show that the Lebesgue measure of the set

$$\{(r, k); F^H_T(r, k) \notin \mathscr{U}\} = \{(r, k); F^H_T(r, k) = 0\} = \{(r, k); \sin(k, r) = 0\}$$

on $\mathbb{R}^2$ is zero. As $\sin(k, r)$ is an analytical function, the application of Lemma 3.1 to the last set leads to (H.1).

Appendix

Here we shall describe briefly the proof of Lemma 1. Let $F_C(q, p; f)$ be any function from the Cohen's [18] class, i.e.

$$F_C(q, p; f) = \int e^{i(-\vartheta q - \tau p + \vartheta u)} f(\vartheta, \tau) \Psi^*(u - \tau/2) \Psi(u + \tau/2)\, d\Omega, \qquad \text{(A.1)}$$

where $d\Omega = d\vartheta\, d\tau\, du/4\pi^2$. The function $f(\vartheta, \tau)$ satisfies the conditions

$$f(0, \tau) = f(\vartheta, 0) = 1. \tag{A.2}$$

We start with the relation

$$\int qpF_C(q, p; f)\, dq\, dp = \int (i\,\partial_\vartheta\, e^{-i\vartheta q})(i\,\partial_\tau\, e^{-i\tau p})J(\vartheta, \tau, u)\, d\Omega\, dq\, dp, \tag{A.3}$$

where $J(\vartheta, \tau, u) = e^{i\partial u}\Psi^*(u - \tau/2)\Psi(u + \tau/2)f(\vartheta, \tau)$.

A double integration by parts in the last integral yields the right-hand side in (A.3) is equal to

$$-4\pi^2 \int \delta(\vartheta)\, \delta(\tau)\, \partial_\vartheta\, \partial_\tau \{e^{i\vartheta u}f(\vartheta, \tau)\Psi^*(u - \tau/2)\Psi(u + \tau/2)\}\, d\Omega. \tag{A.4}$$

Taking advantage of (A.2) we see that the expression (A.4) becomes

$$4\pi^2 \int \{u\, \delta(\tau)(-i\,\partial_\tau) - \delta(\vartheta)\, \delta(\tau)\, e^{i\vartheta u}[\partial_\tau\, \partial_\vartheta f(\vartheta, \tau)]\}j(u, \tau)\, d\Omega, \tag{A.5}$$

where $j(u, \tau) = \Psi^*(u - \tau/2)\Psi(u + \tau/2)$.

Since we have the relation

$$\partial_\tau\, \Psi^*(u \pm \tau/2) = \pm(1/2)\, \partial_u\, \Psi^*(u \pm \tau/2) \tag{A.6}$$

and $\partial_\vartheta\, \partial_\tau f(0, 0)$ does not depend on u, we find that (A.5) goes into

$$(1/2) \int \{u[i(\partial_u\, \Psi^*(u))\Psi(u) - i\Psi^*(u)\, \partial_\tau\, \Psi(u)] - 2\partial_{\theta\tau} f(0, 0)\Psi^*(u)\Psi(u)\}\, du.$$

Hence we obtain the equality

$$\int qpF_C\, dq\, dp + [\partial_{\vartheta\tau} f(0, 0)](\Psi \mid \Psi)$$
$$= \int (u/2)[(-i\,\partial_u\, \Psi(u))^*\Psi(u) + \Psi^*(u)(-i\,\partial_u\Psi(u))]\, du.$$

Now we can exploit the identity

$$\int u(-i\,\partial_u\, \Psi(u))^*\Psi(u)\, du = \int u\Psi^*(u)(-i\,\partial_u\, \Psi(u))\, du - i(\Psi \mid \Psi)$$

and derive the relation

$$\int qpF\, dq\, dp = [\partial_{\theta\tau} f(0, 0) + i/2](\Psi \mid \Psi) + \int u\Psi^*(u)(-i\,\partial_u\, \Psi(u))\, du.$$

Consequently, taking $u = \hat{q}$, $(-i\,\partial_u) = \hat{p}$ and $c = c_f = i/2 + \partial_{\tau\vartheta} f(0, 0)$, we conclude that the equality (1.4) does hold.

Acknowledgements

We would like to thank Prof. A. Anastassov for the suggestion of the idea that Terletsky's function has some extremal properties in the set of functions from Cohen's class.

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