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LETTER TO THE EDITOR

On the probability density interpretation of smoothed Wigner functions

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Abstract. It has been conjectured that averages of the Wigner function over phase space volumes, larger than those of minimum uncertainty, are always positive. This is true for Gaussian averaging, so that the Husimi distribution is positive. However, we provide a specific counterexample for the averaging with a discontinuous hat function. The analysis of the specific system of a one-dimensional particle in a box also elucidates the respective advantages of the Wigner and the Husimi functions for the study of the semiclassical limit.

The falsification of the averaging conjecture is shown not to depend on the discontinuities of the hat function, by considering the latter as the limit of a sequence of analytic functions.

There are many problems concerning the semiclassical limit of quantum mechanics that still remain open. One of the difficulties in comparing classical and quantal properties is that a classical solution is best portrayed as a phase-space trajectory, whereas the usual quantal solution takes the form of a wavefunction in coordinates $\langle \boldsymbol{q}|\psi\rangle$ *or* momenta $\langle \boldsymbol{p}|\psi\rangle$. The uncertainty principle forbids the knowledge of both $\boldsymbol{q}$ snd $\boldsymbol{p}$ simultaneously.

Nonetheless the Wigner function [1]

$$W(\boldsymbol{q},\boldsymbol{p}) = (2\pi\hbar)^{-L}\int \langle \boldsymbol{q}+\boldsymbol{y}/2|\psi\rangle\langle\psi|\boldsymbol{q}-\boldsymbol{y}/2\rangle \exp(\mathrm{i}\boldsymbol{p}\boldsymbol{y})/\hbar)\,\mathrm{d}\boldsymbol{y} \qquad (1)$$

(where L is the number of freedoms) does provide a phase-space 'view' of the quantum state, which projects into the correct marginal probability densities:

$$\int W(\boldsymbol{q},\boldsymbol{p})\,\mathrm{d}\boldsymbol{p} = |\langle \boldsymbol{q}|\psi\rangle|^2 \qquad \text{and} \qquad \int W(\boldsymbol{q},\boldsymbol{p})\,\mathrm{d}\boldsymbol{q} = |\langle \boldsymbol{p}|\psi\rangle|^2. \qquad (2)$$

The problem with trying to interpret the Wigner function as a phase-space probability density is that although $W(\boldsymbol{q},\boldsymbol{p})$ is real, it is necessarily negative in some regions of phase space [2]. Even so, the uncertainty principle may be invoked to wash out the phase-space structure in volumes smaller than $(2\pi\hbar)^L$. The conjecture that the averaged value of the Wigner function in any such volume would yield a positive value, recovers then the desired interpretation [3].

Husimi [4] showed that a Gaussian smoothing of $W(\boldsymbol{q},\boldsymbol{p})$ is indeed positive and hence suitable for a probability density. In fact we may interpret the resulting *Husimi function* as the wave intensity in the coherent state representation [5]. However this result does not settle the 'averaging conjecture', since it depends on the specific properties of the smoothing function.

It should be noticed that the requirement on smoothed Wigner functions to be both real and positive implies that they cannot have the correct marginals as in (2) [1, 6].

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This is a price one has to pay to have the probability interpretation. Generalizations of the Wigner function with the correct marginals have been extensively studied [7] but those do not allow for a probability interpretation.

In this letter we calculate and compare the Wigner and the Husimi functions for a very simple example: a particle in a one-dimensional box. As a result we obtain a transparent counterexample to the 'averaging conjecture': the Wigner function averaged over suitably chosen areas larger than $2\pi\hbar$ can be negative. This shows that Gaussian smoothing is essential for guaranteeing positiveness; that is, the contribution of the Gaussian tail is what ensures a positive result.

The problem we are going to study is defined by the potential function

$$V(x)=\begin{cases}0 & \text{if } -d/2<x<d/2\\ \infty & \text{otherwise.}\end{cases} \tag{3}$$

The even parity stationary solutions of the Schrödinger equation are

$$\psi(x)=\sqrt{\frac{2}{d}}\cos\left(\frac{p_0 x}{t}\right) \tag{4}$$

where

$$p_0=\frac{(2N+1)\pi\hbar}{d}. \tag{5}$$

The Wigner function defined by (1) can be computed immediately to give [8]

$$W(q,p)=C_+ + C_- + C_0 \tag{6}$$

where

$$C_\pm \equiv \frac{1}{2\pi d}\,\frac{\sin[d(p\mp p_0)/\hbar]}{p\mp p_0} \tag{7}$$

and

$$C_0 \equiv \frac{1}{2\pi d}\,\frac{\sin(dp/\hbar)}{p}\,2\cos(2p_0 q/\hbar). \tag{8}$$

Figure 1 shows the behaviour of these three functions at $q=0$. It is clear that in the

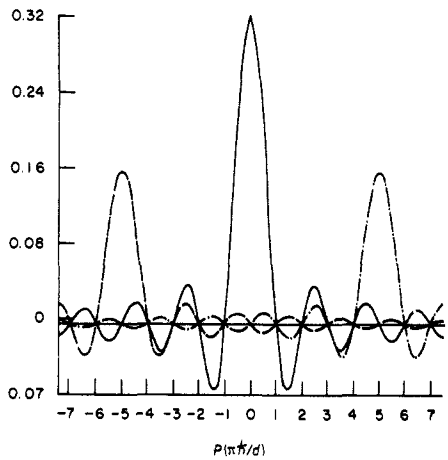

Figure 1. The three functions $C_\pm$ and C_0 at $q=0$.

limit $\hbar \to 0$, we get two delta-functions at $p = \pm p_0$, plus an extra non-classical delta at $p = 0$ modulated by $2\cos(2p_0 q/\hbar)$. The amplitude of this third delta oscillates increasingly as $\hbar \to 0$, as will the value of $W(q, p)$ at any point where $p \neq \pm p_0$.

The oscillations also increase as p_0 (or N) becomes large. Figure 2 shows contour plots of the positive (a) and negative (b) parts of $W(q, p)$ for three different values of N and $\hbar = 1$. Note the intricate weaving of the positive with the negative parts, and the fact that the non-classical maxima at $p = 0$ are twice as large as the maxima at $p = \pm p_0$.

Next we compute the Husimi distribution, defined by [5]

$$H(q,p) = \frac{1}{\pi\hbar}\int \mathrm{d}q'\,\mathrm{d}p'\; W(q',p')\exp[-(q-q')^2/2b^2 - (p-p')^2 b^2/2\hbar^2]$$

$$= \left|\frac{1}{(2\pi b^2)^{1/4}}\int_{-d/2}^{d/2} \psi(x)\exp[-(q-x)^2/4b^2 - \mathrm{i}p(x-q/2)]\,\mathrm{d}x\right|^2. \tag{9}$$

Instead of presenting the full analytical result in terms of error functions, we replace the limits in (9) by $\pm\infty$, thus obtaining

$$H(q,p) \simeq \frac{\sqrt{2\pi}\,b}{d}(\exp[-2(p-p_0)^2 b^2/\hbar^2] + \exp[-2(p+p_0)b^2/\hbar^2]$$

$$+ 2\exp[-(p^2+p_0^2)b^2/\hbar^2]\cos 2qp_0/\hbar). \tag{10}$$

For $b \ll d$, this will only be a poor approximation near the edges $\pm d/2$, but in this region the wavefunction goes to zero anyway. Notice that we still have three terms here (compare with equation (6)) but now $H(q, p) \geqslant 0$ with only isolated zeros at $p = 0$ and $q = \pi\hbar(2k+1)/2p_0$. Contour plots of $H(q, p)$ are shown in figure 3 for $N = 1$, $\hbar = 1$ and different values of b.

Much interest has recently been devoted to the semiclassical limit of both Wigner and Husimi functions of chaotic and non-integrable systems [9] and the question of which would be most appropriate for specific purposes has been raised. It is readily seen that the underlying classical motion is displayed much more clearly by the Husimi function *if* the parameter b is conveniently chosen. If b is too small compared with typical oscillations, the Gaussian average will include non-local features leading to very non-classical structures, as can be seen in figure 3(c).

Now we come to the main aim of this letter, which is construct a hat function defined by a rectangle of area greater than $2\pi\hbar$, where the averaged value of $W(q, p)$ is negative. We start by choosing p_0 large enough so as to separate the contribution to $W(q, p)$ of the three peaks in (6) (actually it will be enough to take $N \geqslant 1$ in (5)). Next, we calculate the average of the Wigner functio, $\bar{W}$, in the rectangle $(-\delta < q \leqslant \delta$, $-\varepsilon < p \leqslant \varepsilon)$ with

$$\varepsilon = 2\pi\hbar/d. \tag{11}$$

This choice of ε ensures that the average values of $C_\pm$, given by (7), will be negative and therefore

$$\bar{W} < \bar{C}_0 = (\pi\,\mathrm{d}p)^{-1}\,\overline{\sin(pd/\hbar)}\;\overline{\cos(2p_0 q/\hbar)}. \tag{12}$$

The average of the first term is clearly positive, since

$$\int_{-2\pi\hbar/d}^{2\pi\hbar/d} \frac{\sin(pd/\hbar)}{p}\,\mathrm{d}p = 2\int_0^{2\pi}\frac{\sin x}{x} \simeq 2.8. \tag{13}$$

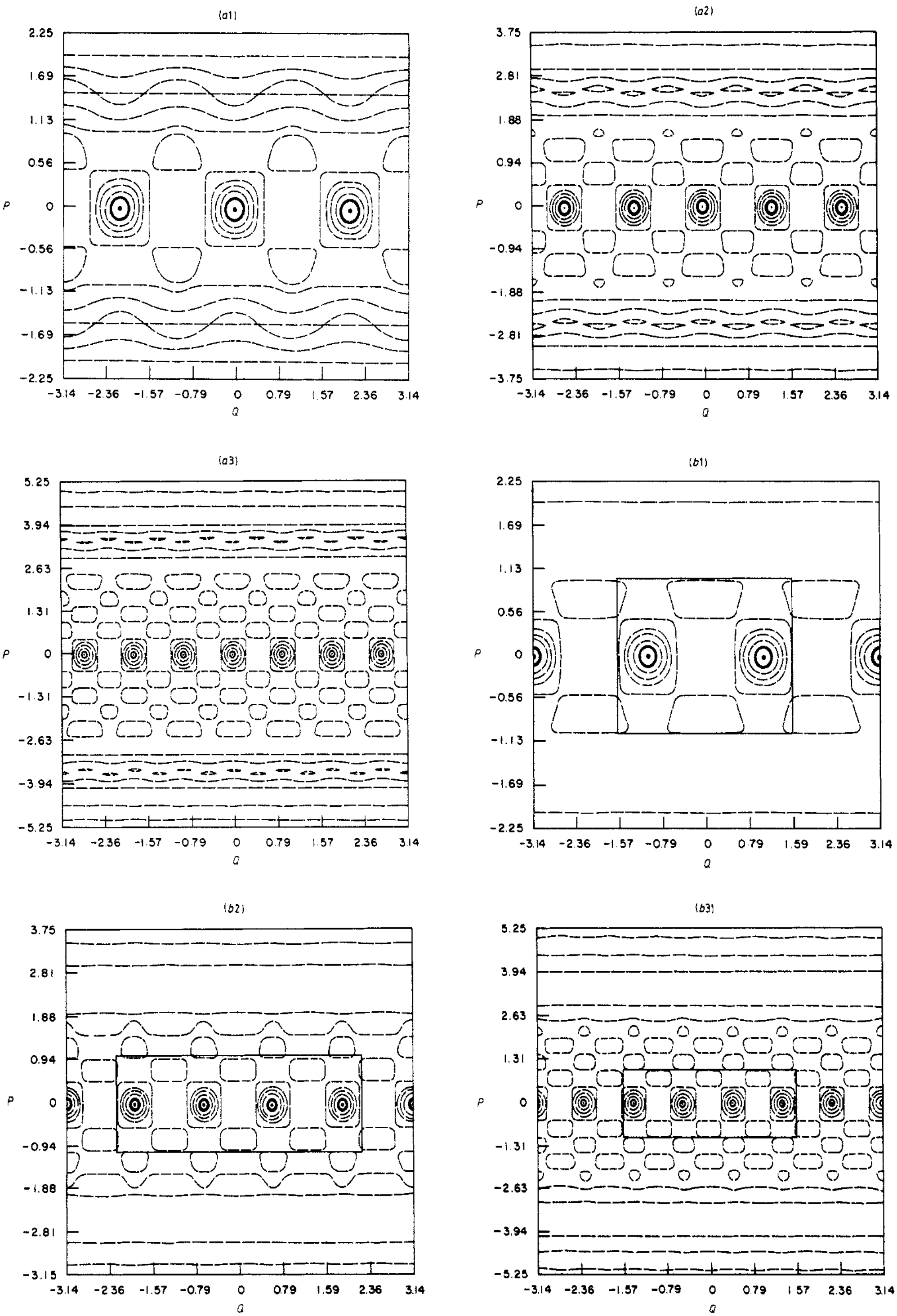

Figure 2. (a) Positive part of $W(q,p)$ for $N=1$, 2 and 3. (b) Negative part of $W(q,p)$ for $N=1$, 2 and 3. The rectangle shows the hat function where the average of $W(q,p)$ is negative.

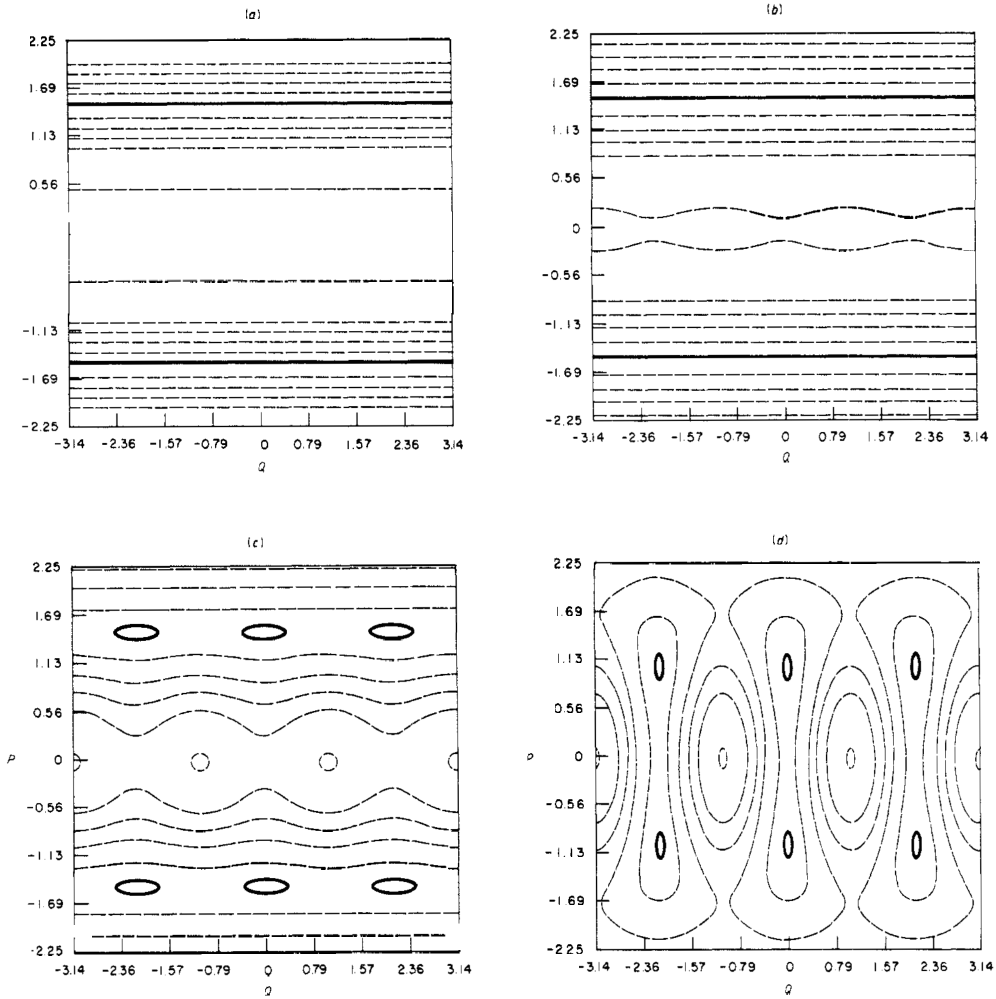

Figure 3. Husimi function for $N=1$ and (*a*) $b=1.571$; (*b*) $b=1.178$; (*c*) $b=0.785$; (*d*) $b=0.524$.

Therefore, we just have to choose δ such that

$$\int_{-\delta}^{\delta} \cos(2p_0q/\hbar)\,\mathrm{d}q=\frac{\hbar}{p_0}\sin\left(\frac{2p_0\delta}{\hbar}\right)<0 \tag{14}$$

and

$$d/4\leqslant\delta\leqslant d/2. \tag{15}$$

These inequalities can easily be achieved for $N\geqslant 1$! Therefore $\bar{W}<0$ and $(2\varepsilon)(2\delta)\geqslant 2\pi\hbar$. The appropriate choice of δ includes a single extra valley more than the number of humps in the cosine oscillation. These rectangles are shown in figure 1(*b*) by full lines.

We see from (10) that the term corresponding to $\bar{C}_0$ in the Husimi function can also be negative, but in this case we cannot make $\bar{C}_\pm$ negative as well. In fact they are always positive and large enough to overcome $\bar{C}_0$, yielding a positive final result.

(Notice that the terms in $\bar{H}$ are *not* the separate smoothing of the terms of $W(q,p)$, but a complicated combination of them.)

Now we finally show that the above result is not a consequence of the sharp cutoff presented by the hat function. To see this, consider the sequence of smooth (actually analytic) functions

$$f_n(q-q',p-p') = A_n \exp\left[-\left(\frac{q-q'}{\delta}\right)^{2n} - \left(\frac{p-p'}{\varepsilon}\right)^{2n}\right]$$

where A_n is determined by the condition

$$\int f_n(q-q',p-p')\, dq'\, dp' = 4\varepsilon\delta$$

(notice that $\lim_{n\to\infty} A_n = 1$. Clearly, this sequence approaches the hat function $\bar{f}(q-q',p-p')$ as $n\to\infty$. Let

$$\overline{W_n(q,p)} = \int dq'\, dp'\; W(q',p') f_n(q-q',p-p')$$

and

$$\overline{W(q,p)} = \int dq'\, dp'\; W(q',p')\bar{f}(q-q',p-p').$$

Then, the difference between $\bar{W}$ and $\bar{W}_n$ is given by

$$\Delta_n \equiv \left|\int dq'\, dp'\; W(q',p')[\bar{f}(q-q',p-p') - f_n(q-q',p-p')]\right|$$

$$\leqslant \frac{2}{h}\left|\int dq'\, dp'(\bar{f}(q',p') - f(q',p'))\right|$$

since [10] $|W(q,p)| \leqslant 2/h$. The remaining integral can be divided into four regions where estimates can be made:

Region 1. $|q'| < \delta$ and $|p'| < \varepsilon$.

$$I_1 \equiv \int_{R1} dq'\, dp'(1-f_n) < 4\int_0^{\delta} dq' \int_0^{\varepsilon} dp'\left[\left(\frac{q'}{\varepsilon}\right)^{2n} + \left(\frac{p'}{\varepsilon}\right)^{2n}\right] = \frac{4(\varepsilon+\delta)}{2n+1}.$$

Region 2. $|q'| < \delta$ and $|p'| > \varepsilon$.

$$I_2 \equiv \int_{R2} dq'\, dp'\, f_n < 4\int_0^{\delta} dq' \int_{\varepsilon}^{\infty} dp'\left(\frac{p'}{\varepsilon}\right)^{-2n} = \frac{4\delta}{2n-1}.$$

Region 3. $|q'| > \delta$ and $|p'| < \varepsilon$.

$$I_3 \equiv \int_{R3} dq'\, dp'\, f_n < 4\int_{\delta}^{\infty} dq' \int_0^{\varepsilon} dp'\left(\frac{q'}{\delta}\right)^{-2n} = \frac{4\varepsilon}{2n-1}.$$

Region 4. $|q'| > \delta$ and $|p'| > \varepsilon$.

$$I_4 \equiv \int_{R4} dq'\, dp'\, f_n < 4\int_{\delta}^{\infty} dq' \int_{\varepsilon}^{\infty} dp'\left(\frac{q'}{\delta}\right)^{-2n}\left(\frac{p'}{\varepsilon}\right)^{-2n} = \frac{4}{(2n-1)^2}.$$

And, therefore

$$\Delta_n < \frac{2}{h}|I_1 - I_2 - I_3 - I_4| < \frac{2}{h}(I_1 + I_2 + I_3 + I_4)$$

since all $I_k > 0$. So as $n \to \infty, \Delta_n \to [8(\delta+\varepsilon)/h]/n$ and, if for a given point (q, p) $\overline{W(q, p)} = -A$, with $A > 0$ there exists N such that for $n > N$, $\overline{W_n(q, p)} < 0$. This extends our counterexample to analytic smoothing functions.

We conclude that it is necessary to make restrictions on the minimum uncertainty smoothing function, if we are to interpret the Wigner function as a phase-space probability density. Gaussian smoothing certainly belongs to this allowed class, but the positive property of Husimi function is not trivial.

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