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LETTER TO THE EDITOR

On the zeros of the Husimi distribution

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Abstract. The basic features of the zeros of the Husimi phase-space density of a quantum eigenstate are discussed. It is demonstrated that some special properties of the harmonic oscillator related to the number of zeros and their location within the classical energy shell are not valid for anharmonic potentials, as illustrated by numerical examples for the Morse oscillator. Also discussed is the distribution of zeros in quantum Poincaré sections for systems with two degrees of freedom.

Quantum phase-space distributions are of increasing interest in studies of quantum chaos because they allow a direct comparison between classical and quantum dynamics (see, e.g., [1–3] and references therein). Of particular recent interest are the zeros of the Husimi distribution, which are organized, for example, on smooth curves or space filling for classically regular or chaotic dynamics, respectively [4–12].

In the present letter we discuss some properties of the Husimi phase-space distribution of a quantum state in order to clarify some frequent misconceptions. The Husimi density

$$\varrho^{(s)}(p,q) = \left| \int \phi^{(s)*}_{p,q}(q')\psi(q')\,\mathrm{d}q' \right|^2 \tag{1}$$

(normalization $\int \varrho^{(s)}(p,q)\,\mathrm{d}p\,\mathrm{d}q/2\pi\hbar = 1$) is given by the projection of the wavefunction ψ onto coherent states

$$\phi^{(s)}_{p,q}(q') = \langle q'|p,q;(s)\rangle = \sqrt[4]{\frac{s}{\pi\hbar}}\exp\left[\frac{-s(q'-q)^2}{2\hbar} + \mathrm{i}\frac{p}{\hbar}\left(q' - \frac{q}{2}\right)\right] \tag{2}$$

localized in phase space (p,q) with a minimum product of the uncertainties $\Delta p = \sqrt{\hbar s/2}$, $\Delta q = \sqrt{\hbar/2s}$. The squeezing-parameter $s = \Delta p/\Delta q$ can be adapted to the problem under investigation.

Expressed in terms of wavelet theory, the wavefunction ψ is analysed by means of the wavepackets (2), i.e. by a windowed Fourier transformation, where the size of the Gaussian window, s, can be chosen to maximize the resolution. The Husimi transform measures the probability to find a momentum p at position q in coarse-grained phase space. As shown by the inequality $\varrho^{(s)}(p,q) \leqslant 1$, the density cannot be concentrated in areas $< h = 2\pi\hbar$. In addition, the Husimi density (1) is clearly non-negative, in contrast to the Wigner distribution, which typically has negative values. The zeros of the Husimi function are simply the least probable points in phase space and appear at those points, where the positive and negative contributions of the Wigner function are equal, because the Husimi distribution (1) can be written as a Gaussian smoothed Wigner density.

The essential importance of the zeros, however, is based on the analytic properties in the complex $z = (sq + \mathrm{i}p)/\sqrt{2s\hbar}$ plane. The Bargmann transform [13] is

$$\langle z|\psi\rangle = \exp(-\tfrac{1}{2}|z|^2)F(z^*) \tag{3}$$

with $|z\rangle = |p, q; (s)\rangle$, where $F(z)$ is an entire function of order $\leqslant 2$, and the Weierstrass–Hadamard factorization

$$F(z) = z^m\, \mathrm{e}^{C_0+C_1z+C_2z^2} \prod_n \left(1 - \frac{z}{z_n}\right) \exp\left[\frac{z}{z_n} + \frac{1}{2}\left(\frac{z}{z_n}\right)^2\right] \tag{4}$$

expresses $F(z)$ in terms of the zeros $z_1, z_2, \ldots$ and a m-fold zero at the origin, i.e. the Husimi density $|\langle z|\psi\rangle|^2$ is completely determined by its zeros and the coefficients C_0, C_1,C_2. The 'geometry' of the quantum state can be essentially described by the distribution of the zeros, the so-called 'stellar representation' [8, 12].

Let us point out a few basic features of the Husimi zeros:

(i) The zeros are real or appear as complex conjugate pairs.

(ii) The position of the zeros is clearly affected by the squeezing parameter s. From the integral (2), we see that in the limit of large values of s the Husimi zeros approach the zeros of the wavefunction in coordinate space and for small s the zeros of the momentum distribution.

(iii) There is an upper limit of the density of zeros. In agreement with the uncertainty relation, there can be only one zero in an area $h = 2\pi\hbar$ [9] on the average.

(iv) It has been observed that the distribution of zeros differs for classically regular or chaotic systems and can be considered as a quantum indicator of classical chaos [4]. In the regular case, the zeros appear to be distributed along curves with distance $\mathrm{O}(\hbar)$. In the chaotic case, they fill the space between the large value regions like a gas with mean distance $\mathrm{O}(\sqrt{\hbar})$.

(v) There are states without zeros, for example, the Husimi distribution of the coherent states (2) is a Gaussian density in phase space

$$\varrho^{(s)}(p, q) = \left|\int \phi^{(s)*}_{p,q}(q')\phi^{(s)}_{p_0,q_0}(q')\,\mathrm{d}q'\right|^2 = \hbar^{-1} \exp\left(\frac{-(q-q_0)^2}{2(\Delta q)^2} - \frac{(p-p_0)^2}{2(\Delta p)^2}\right). \tag{5}$$

In addition to these well known features, there are various more or less explicit statements in discussions or even in the literature, which are simply based on folklore. It is the aim of the following to correct this misleading view. Let us point out the most frequent conjectures (to exclude complications, which are important, but not essential for the present discussion, we confine ourselves to the simple case of bound states of a particle with unit mass in a one-dimensional potential $H(p, q) = -\frac{1}{2}\{p^2 + V(q)\}$).

(a) The number of nodes of the wavefunction is equal to the number of zeros, i.e. the quantum state number n has exactly n Husimi zeros.

(b) The zeros are restricted to the classically allowed region inside the energy contour $H(p, q) = E$.

(c) In the case of a harmonic oscillator, all zeros accumulate at the origin $(p, q) = (0, 0)$.

All these frequent statements are wrong and can be traced back to a straightforward generalization of results for a simplified harmonic oscillator. In the following we will—after revisiting the harmonic case—try to clarify the properties of the Husimi zeros by means of a few instructive numerical illustrations for an anharmonic potential, the Morse oscillator.

Let us start with the case of a harmonic oscillator with frequency $\omega = 1$,

$$V(q) = \tfrac{1}{2}q^2 \tag{6}$$

where the coherent states agree with the minimum uncertainty wavepackets (2) in the coordinate representation for a squeezing parameter $s = 1$. For the standard choice, where the analysing wavepacket (2) is taken as a harmonic oscillator coherent state for $\omega = 1$, i.e. $s = 1$, the Husimi density of an oscillator eigenstate n is given by

$$\varrho^{(1)}(p,q) = \mathrm{e}^{-(1/2\hbar)(p^2+q^2)} \frac{1}{n!} \left(\frac{1}{2\hbar}(p^2+q^2) \right)^n . \tag{7}$$

The distribution is a radially symmetric function of the action variable $I = \frac{1}{2}(p^2+q^2)$, a gamma distribution $\mathrm{e}^{-I/\hbar}(I/\hbar)^n/n!$ with mean value $\langle I \rangle = \hbar n$ and variance $\Delta I = \hbar\sqrt{n}$. In the limit $\hbar \to 0$, the distribution concentrates on the classical energy shell, as expected in general. We note that this distribution possesses an n-fold zero at the origin. Figure 1(c) shows the distribution for the state $n = 3$ ($\hbar = 1$).

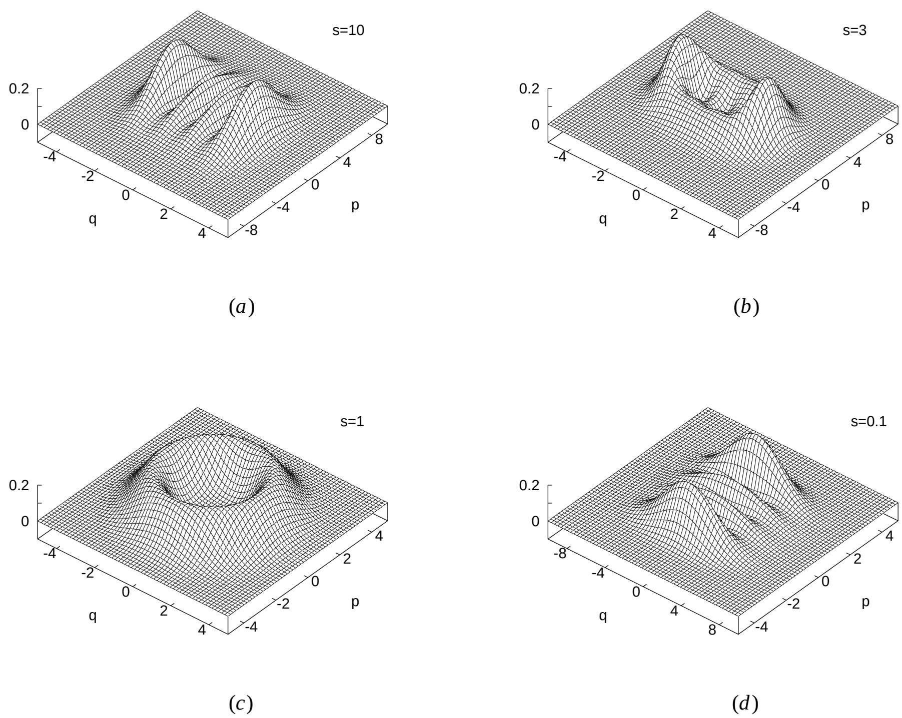

Figure 1. Husimi distributions for a harmonic oscillator eigenstate $n = 3$ for selected values of the squeezing parameter ($s = 10$, 3, 1 and 0.1) illustrating the transition from 'coordinate-like' to 'momentum-like' distributions.

Let us now look at the behaviour of the zeros when the squeezing parameter s of the analysing state is varied (note that for a general potential different from the harmonic oscillator, there is no 'true' or intrinsic value that could be chosen for the squeezing parameter s). Here, the Husimi distribution is a bit more complicated [14]:

$$\varrho_n^{(s)}(p,q) = \frac{\sqrt{s}}{(s+1)2^{n-1}n!} \left| \frac{s-1}{s+1} \right|^n \exp\left(-\frac{p^2+sq^2}{\hbar(s+1)} \right) \left| H_n\left(\frac{sq+\mathrm{i}p}{\sqrt{\hbar(s-1)(s+1)}} \right) \right|^2 \tag{8}$$

which agrees for $s \to 1$ with (7). For large values of s, we observe a 'coordinate-like' distribution, which transforms for small s into a 'momentum-like' behaviour [15]. The zeros of the Husimi distribution are confined to the real q-axis for $s > 1$ and to the imaginary p-axis for $s < 1$ (all zeros of the Hermite polynomials in (8) are real valued). For $n = 3$, there are three zeros, a zero at the origin and a symmetric pair. When s is decreased from infinity, the zeros move along the real q-axis towards the origin, where they coincide for $s = 1$ and separate again along the imaginary axis, until they finally reach their position on the imaginary (momentum) axis for $s \to 0$. In all cases, the zeros are inside the circle $(p^2 + q^2)/2 = E_n = \hbar(n + 1/2)$, i.e. inside the classical energy shell. A very similar behaviour is found if the frequency ω is different from unity, with the only difference of a scaling of the axes. The n zeros now appear inside an ellipse, the classical energy shell, and the most classical-like behaviour of the Husimi density is found for a squeezing parameter $s = \omega$.

These results for the harmonic oscillator should, however, not be generalized too easily to non-harmonic potentials. As an example, we will discuss the Morse oscillator

$$V(q) = D(1 - \mathrm{e}^{-aq})^2. \tag{9}$$

Choosing $a = (2D)^{-1/2}$, the potential approaches (6) for small q. The normalized Morse wavefunctions are given by [16, problem 70]

$$\psi_n(q) = A_n\, \mathrm{e}^{-\zeta/2} \zeta^{\sigma_n}\, {}_1\mathrm{F}_1(-n; 2\sigma_n + 1; \zeta) \tag{10}$$

with $\zeta = 4D\,\mathrm{e}^{-aq}$, $\sigma_n = 2D - n - 1/2$, $A_n = (2\sigma_n + 1)_n \{2a\sigma_n/n!\Gamma(4D - n)\}^{1/2}$ and ${}_1\mathrm{F}_1$ is the confluent hypergeometric function (for a recurrence relation see [17]). The Morse–Husimi distributions have been computed by evaluating the integral (1) numerically.

In order to demonstrate the effects of anharmonicity, we consider the case $D = 2$, where the potential has $[2D + 1/2] = 4$ bound states with energies $E_n = (n + 1/2) - (n + 1/2)^2/4D$, $n = 0, \ldots, 3$.

Figure 2 shows the Husimi distributions (for an analysis of the Wigner density see [17]) as a contour diagram of ϱ and of the phase function $\arg(\langle z|\psi\rangle)$. The squeezing parameter is chosen as $s = 1$. As expected from the harmonic oscillator, the density plots for the eigenstates n show n strong zeros, which are, however, no longer coincident at the origin because of the anharmonicity of the potential. The zeros are more pronounced in the phase diagrams also shown in figure 2, where they appear as topological defects, i.e. as phase jumps along a loop encircling a zero. One observes that there may be more than n zeros of a Husimi distribution for state n. In general—for the case of a non-compact phase space, which is considered here—there is an infinite number of zeros, most of which are, however, far away in the complex plane, i.e. in regions where the density is extremely small. In these regions, where the Husimi density is, for example, of the order of $\varrho \sim 10^{-10}$, the numerical results are very sensitive with respect to computational accuracy. As a clear demonstration of the existence of these weak zeros even for the ground state, figure 3 shows a contour diagram of the phases of the Husimi function (3) for the ground state of a strongly anharmonic Morse oscillator ($D = 1/2$, $s = 1$).

In the following, we will show that also the conjecture (b) is wrong. For large values of the squeezing parameter s, the zeros of the Husimi distribution for an eigenstate n are close to the nodes of the wavefunction in the coordinate representation, which are located inside the classically allowed region $V(q) \leqslant E_n$ (for a simple proof see, e.g. [19, Ch 5.5]). The zeros are real and simple and, therefore, they cannot leave the real axis when the squeezing parameter s is decreased (the complex zeros appear as complex conjugate pairs). So the only possibility is that the zeros move toward each other, collide and separate as a complex conjugate pair.

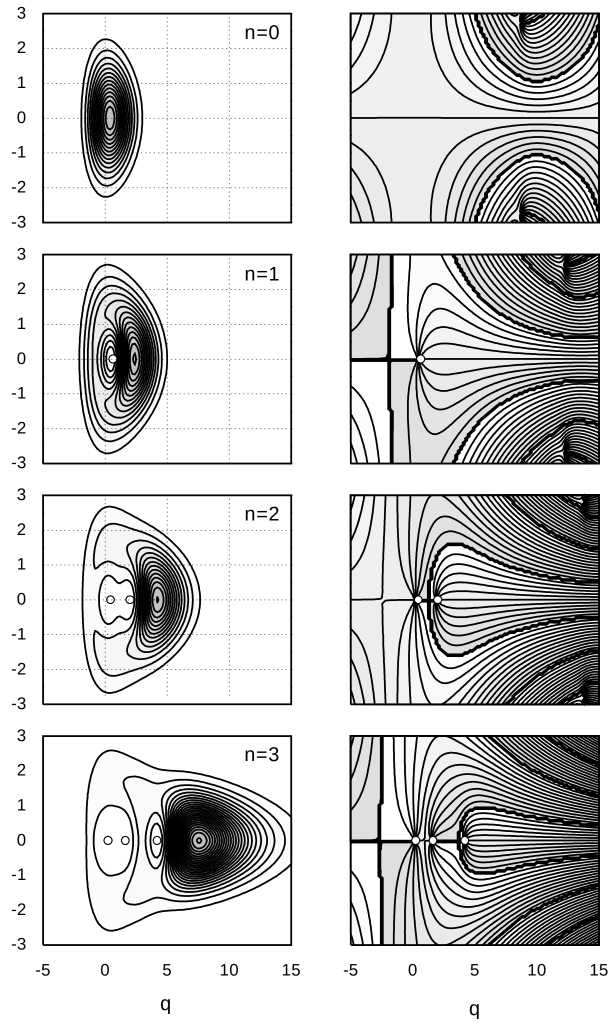

Figure 2. Husimi distributions for a Morse oscillator with four bound states E_n, $n = 0, \ldots, 3$ as a contour diagram of ϱ (left) and of the lines of constant phase (right) for a squeezing parameter $s = 1$.

For the case of a Morse potential, this behaviour can be studied analytically, at least approximately. In order to evaluate the Husimi integral in (1) approximately, we observe that the Morse ground state is close to a harmonic oscillator state for large values of D, i.e.

$$\psi_0(q) = A_0\,\mathrm{e}^{-\zeta/2}\zeta^{\sigma_0} \approx \frac{1}{\sqrt[4]{\pi}}\,\mathrm{e}^{-q^2/2}. \tag{11}$$

Using (11), we can approximate the Gaussian $\mathrm{e}^{-q^2} \approx \sqrt{\pi}\,A_0^2\,\mathrm{e}^{-\zeta}\,\zeta^{2\sigma_0}$ and the Husimi density is

$$\varrho^{(s)}(p,q) \approx \left| \frac{A_n}{a} (\sqrt[4]{\pi}\,A_0)^s\,\mathrm{e}^{-sq^2/2}(4D)^{(sq-\mathrm{i}p)/a} \int_0^\infty \mathrm{d}\zeta\,\mathrm{e}^{-(s+1)\zeta/2}\zeta^b\,{}_1\mathrm{F}_1(-n; 2\sigma_n+1; \zeta) \right|^2 \tag{12}$$

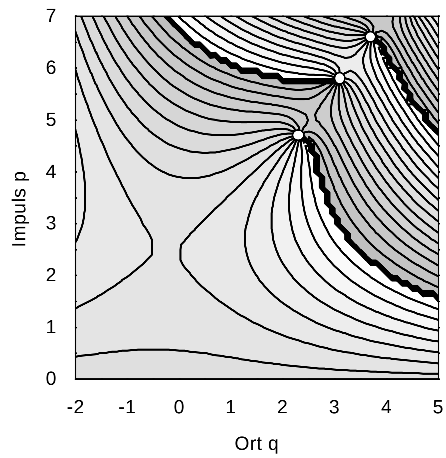

Figure 3. Phases of the Husimi distribution for the ground state of a strongly anharmonic Morse oscillator ($D = 1/2$) demonstrating the existence of zeros.

with $b = s\sigma_0 + \sigma_n - (sq - \mathrm{i}p)/a - 1$, i.e. a Laplace transform of ${}_1F_1$, which can be evaluated in closed form [20, (3.2.16)]:

$$\varrho(p,q) \approx \left| \frac{A_n}{a} (\sqrt[4]{\pi}\, A_0)^s \mathrm{e}^{-sq^2/2} \times \left(\frac{1}{2}(s+1)\right)^{-s\sigma_0+\sigma_n} ((s+1)2D)^{(sq-\mathrm{i}p)/a}\, \Gamma(b)\, {}_2F_1\left(-n, b; 2\sigma_n + 1; \frac{2}{s+1}\right) \right|^2 . \tag{13}$$

The zeros of (13) are given by the zeros of the hypergeometric function

$${}_2F_1\left(-n, b; 2\sigma_n + 1; \frac{2}{s+1}\right) = \sum_{j=0}^{n} \frac{(-n)_j (b)_j}{(2\sigma_n + 1)_j\, j!} \left(\frac{2}{s+1}\right)^j \tag{14}$$

which is a polynomial of nth degree in $(sq - \mathrm{i}p)$. For the state $n = 2$, in particular, the zeros are given by

$$\frac{1}{a}(sq - \mathrm{i}p) = \frac{1}{2}(3s - 1) \pm \sqrt{\left(D - \frac{3}{4}\right)s^2 - D + 1}. \tag{15}$$

Figure 4 shows the motion of the zeros of state $n = 2$ ($D = 8$, $a = 1/\sqrt{2D} = 1/4$) at

$$sq - \mathrm{i}p = \tfrac{1}{8}(3s - 1) \pm \tfrac{1}{4}\sqrt{29s^2 - 28} \tag{16}$$

when the squeezing parameter s is varied. For small values of s, the zeros are outside of the classical energy shell $H(p,q) = E_2$. The zeros are real for $s \leqslant s^* = 2\sqrt{7/29} \approx 0.98$. For $s < s^*$ there are two complex conjugate zeros, following the curve

$$p^2 = 7/16 - 29/(32 - 4q) \tag{17}$$

which approach the limit $p_{-\infty} = \pm\frac{1}{4}\sqrt{7} \approx \pm 0.66$ for $q \to -\infty$, respectively $s \to 0$. As shown in figure 4, the numerically determined zeros (circles) are in satisfactory agreement with these results (broken curve). For large squeezing, $s < 0.05$, the zeros are outside the classical energy shell. This 'disappearance' of the zeros could have been anticipated from

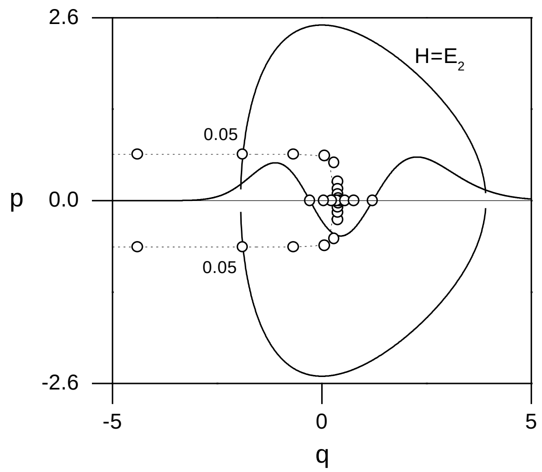

Figure 4. Zeros of the state $n = 2$ for a Morse potential ($D = 8$) as a function of the squeezing parameter s. For small values of s, the zeros are outside of the classical energy shell $H(p, q) = E_2$.

the non-existence of zeros in the momentum space wavefunction for the Morse oscillator [17, 21].

Furthermore, it should be stressed that in the approximate treatment above we found again exactly n zeros for state n, i.e. we missed the weak zeros far out in the complex plane. This is a consequence of the approximation (11), where special adapted 'Morse-like' minimum uncertainty wavepackets have been used representing a displaced and scaled Morse oscillator ground state (see [22] for a theory of generalized coherent states).

Let us now consider a two-dimensional case

$$H(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{2m}(p_x^2 + p_y^2) + V(q_x, q_y). \tag{18}$$

Here one can construct a quantum analogue of the classical Poincaré surface of section by looking at the Husimi distribution $\varrho(\boldsymbol{p}, \boldsymbol{q})$ of a quantum (eigen)state (which is a density in four-dimensional phase space) on a two-dimensional section. Typically, one considers the equivalent of a classical Poincaré section, the density for, for example,

$$q_y = 0 \qquad \text{and} \qquad p_y = p_y^{(E)} = +\sqrt{2m\{E - V(q_x, 0)\} - p_x^2} \tag{19}$$

where the energy E is in most cases taken as the energy E_n of the eigenstate ψ_n (see, e.g., [23, 11]). In this case, the Husimi density can reveal a quantum correspondence to the typically mixed regular and chaotic classical dynamics. In full phase space, the zeros of the Husimi function (a squared modulus of a analytic complex function) has nodal surfaces, which intersect the surface of section (19) in points, similar to the one-dimensional case. There are, however, important differences. First, as pointed out by Arrantz *et al* [11], the Husimi function is not a squared modulus of an analytic function on a complex (p_x, q_x)-plane. Secondly, in the one-dimensional case, the Husimi densities decay exponentially outside the classical energy shell $H(p_x, p_y^{(E)}, q_x, 0) = E_n$. In the case of a surface of section (19), the region outside the energy shell is inaccessible in classical and quantum mechanics, because there is no solution of (19) in this region, i.e. no intersection of the energy shell $H(\boldsymbol{p}, \boldsymbol{q}) = E_n$ with the (p_x, q_x)-plane. As a trivial consequence, all Husimi zeros on the surface of the section are located inside the energy shell. Moreover, their number is finite because of their limited density. The weak zeros are no longer detectable in such a plot. It should be pointed out, however, that the zeros move with the energy E and if a surface of section (19) is constructed for large values of the energy E the weak zeros will be found again. As a last remark, we note that clearly the number of zeros inside the energy shell will in general not be equal to the number of the quantum state. For systems where such an agreement has been observed (see, e.g., [11]), we conjecture that the number of zeros will decrease for a reduced squeezing parameter s. However, such a squeezing factor may be very small, so that the number and arrangement of the zeros still carry important information about the nature and even the ordering of the quantum states as reported in recent articles [3, 11, 12].

In conclusion, we have demonstrated for the case of a Morse oscillator that the behaviour of the zeros of the Husimi function differs in some important features from common folklore. We hope that this will help to establish a more adequate view, in particular because of the importance of the Husimi zeros in contemporary research in the field of quantum chaos.

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