Phase Space Entropy and Global Phase Space Structures of (Chaotic) Quantum Systems

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A quantum phase space entropy is defined, which directly reflects the global dynamical properties of the system similar to the synoptic view of several classical trajectories in a Poincaré section. The quantum results allow a direct comparison with a corresponding purely classical entropy. Numerical results for a periodically driven rotor illustrate the usefulness of phase space entropies for systems with mixed chaotic and regular dynamics.

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It is an ultimate aim in classical dynamics to understand the global properties of the flow in phase space. An indispensable tool for such an investigation is Poincaré's surface of section, where the time evolution of several carefully selected trajectories provides a synoptic picture of the system's dynamics. Here we will concentrate on the illustrative case of one-dimensional time-periodic systems (period T) often discussed in studies of the correspondence between quantum and classical dynamics. A stroboscopic Poincaré map can be obtained by displaying the phase space points (p,q) at times $t = nT$ $(n = 0,1,2,\ldots)$.

As an example we study the special case of a harmonically driven rotor [1,2]

$$H(t) = \frac{J^2}{2I} - f\cos\phi\,\cos\omega t \tag{1}$$

modeling, e.g., the rotational excitation of a molecule with a permanent dipole moment by an external force. We use units where the moment of inertia, I, and the excitation frequency, ω, are unity. In this case the classical angular momentum J and the rotor angle ϕ take the role of the canonical variables (p,q) used in the general discussion. The stroboscopic Poincaré map is shown in Fig. 1 for a field strength parameter $f = 0.45$. Because of symmetry only the upper half plane is shown. The central stability island is centered on a 1:1 resonance. It is surrounded by a chain of five islands centered on a stable period-five orbit. In addition, there are stable period-one orbits at $(J,\phi) = (0,0)$ and $(0,\pi)$. These islands are embedded in a chaotic region, which is sharply separated from the outer regular region.

A Poincaré map provides an accurate, however, qualitative picture of the dynamics. A more quantitative approach can be based on the entropy of the (coarse grained) classical phase space density. The phase space is partitioned into $i = 1,\ldots,M$ disjoint elements of area Δ. Starting a trajectory at (p,q) we can compute the probability $P_i(p,q)$ of finding the particle at partition i from the long-time average of the number of times partition i has been visited [3]. The Shannon entropy of the resulting density is $S_c(p,q) = -\sum_{i=1}^{M} P_i(p,q)\ln P_i(p,q)$.

Here we use a more sophisticated coarse graining based on a Gaussian smoothing of the classical phase space density [4], resulting in a density distribution $\bar{\varrho}_c(p',q',p,q)$ in (p',q') phase space, depending on the center (p,q) of an initial Gaussian distribution $\sim\exp\{-(p'-p)^2/2\Delta p^2 - (q'-q)^2/2\Delta q^2\}$. The relative widths of both Gaussians, the initial and the smoothing distribution, can be controlled by means of the squeezing parameter $s = \Delta p/\Delta q$. The distributions are normalized as $\int \bar{\varrho}_c(p',q',p,q)\,d\gamma' = 1$, where $d\gamma' = dp'\,dq'/\Delta$ with $\Delta = 4\pi\Delta p\Delta q$ is a dimensionless measure, i.e., the Gaussians cover a phase space area Δ. The entropy

$$S_c(p,q) = -\int \bar{\varrho}_c(p',q',p,q)\ln\bar{\varrho}_c(p',q',p,q)\,d\gamma' \tag{2}$$

measures the degree of phase space organization at (p,q): points in the regular region are expected to have low values of the entropy; points in the chaotic region are characterized by high values. This has been demonstrated for systems relevant in astrophysics [3] and also for a time-periodic anharmonic oscillator [4]. Moreover, this entropy is a dynamical invariant: *all* points belonging to the same minimal invariant set have the *same* entropy. On an invariant curve, the value of the entropy is roughly determined by the logarithm of the length L of the invariant curve: $S_c \sim \ln(L/\sqrt{\Delta})$. Invariant curves will hence appear as contour lines $S_c(p,q) = \text{const}$. All points in a connected

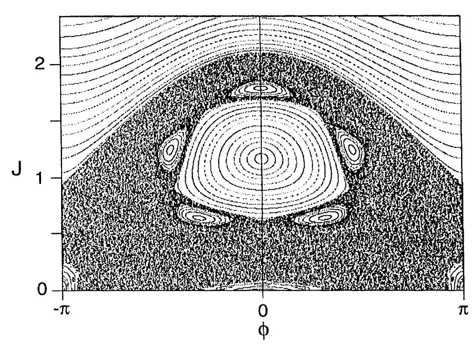

FIG. 1. Classical stroboscopic Poincaré section for a driven rotor with $f = 0.45$. The lower half plane is omitted because of symmetry.

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chaotic region will have a (high) entropy given by the phase space area A of the chaotic region $S_c = \ln(A/\Delta)$. In particular, this implies that the entropy shows a different scaling behavior with Δ in the chaotic and regular regions.

Here it will be demonstrated that an entropy can be constructed in a similar manner for quantum dynamics, which is ideally suited to elucidate the global features of the quantum system and to investigate the classical-quantum correspondence. We base our treatment on the Husimi phase space density (see [4–7] for recent related applications to chaotic systems)

$$\varrho\,(p',q';t) = |\langle p',q'|\Psi(t)\rangle|^2, \tag{3}$$

which is the overlap of the wave function $|\Psi(t)\rangle$ with a minimum uncertainty ($\Delta p \Delta q = \hbar/2$) wave packet (also denoted as a coherent state)

$$\langle x|p,q\rangle = \left(\frac{s}{\pi\hbar}\right)^{1/4} \exp\!\left(-\frac{s(x-q)^2}{2\hbar} + \frac{i}{\hbar}px\right) \tag{4}$$

in the coordinate representation with expectation values $\langle\hat{p}\rangle = p$ and $\langle\hat{q}\rangle = q$, and uncertainties $\Delta p = \sqrt{\hbar s/2}$ and $\Delta q = \sqrt{\hbar/2s}$. The distribution (3) is normalized with respect to the measure $d\gamma' = dp'\,dq'/2\pi\hbar$.

The Husimi density (3) of a coherent state (4) is

$$\varrho\,(p',q'|p,q) = |\langle p',q'|p,q\rangle|^2 = e^{-(p'-p)^2/s2\hbar - s(q'-q)^2/2\hbar}, \tag{5}$$

i.e., a Gaussian density centered at (p,q) in phase space. The squeezing parameter $s = \Delta p/\Delta q$ can be adapted to the problem under investigation [note that the harmonic oscillator (unit mass, frequency ω) coherent states have $s = \omega$].

One can now explore the quantum phase space dynamics starting an initial wave packet $|\Psi_{p,q}(t=0)\rangle = |p,q\rangle$ localized at (p,q) and compute from (3) its Husimi density

$$\varrho\,(p',q';p,q;t) = |\langle p',q'|\Psi_{p,q}(t)\rangle|^2. \tag{6}$$

In particular, one can compute the stroboscopic snapshots $\varrho\,(p',q';p,q;t_n)$ at times $t_n = nT$, $n = 0, 1, 2, \ldots$.

Contrary to the classical case, the quantum phase space distribution does *not* converge towards an invariant distribution. It shows fluctuations for all times, which can be described within the framework of random vector theory (see, e.g., the discussion in [1,8]). The long-time average of this fluctuating distribution converges:

$$\bar{\varrho}\,(p',q';p,q) = \frac{1}{N+1}\sum_{n=0}^{N} \varrho(p',q';p,q;t_n). \tag{7}$$

$\bar{\varrho}\,(p',q';p,q)$ is normalized with respect to the measure $d\gamma'$ and symmetric: $\bar{\varrho}\,(p',q';p,q) = \bar{\varrho}\,(p,q;p',q')$.

The quantum densities $\bar{\varrho}\,(p',q';p,q)$ could now be compared with the classical ones as a function on phase space (p',q') for special initial distributions centered at selected values of (p,q). Here, however, we are *not* interested in the quantum-classical correspondence for such selected cases. Instead, we will provide a measure of the localization of these phase space distributions as provided by the phase space entropy

$$S(p,q) = -\int \bar{\varrho}\,(p',q';p,q)\ln\bar{\varrho}\,(p',q';p,q)\,d\gamma' \tag{8}$$

as a function on phase space (p,q) which measures the (time averaged) spreading of a minimum uncertainty wave packet initially centered at (p,q). The map $(p,q) \to S(p,q)$, which can be easily plotted as a function on phase space, yields a *global* phase space picture of the dynamical localization properties of the quantum system, which clearly reflects the classical phase space structure, as will be demonstrated in the following example. It should be noted that the entropy (8) satisfies $S(p,q) \le 1$, with an equality only if $\bar{\varrho}$ agrees with the coherent state density (5) [9].

It is instructive and convenient for numerical computations to rewrite the expressions above in terms of the quasienergy states of the time-periodic system, i.e., solutions of the time-dependent Schrödinger equation of Floquet form $|\Psi_\alpha(t)\rangle = e^{-i\epsilon_\alpha t/\hbar}|\psi_\alpha(t)\rangle$ with T-periodic state $|\psi_\alpha(t+T)\rangle = |\psi_\alpha(t)\rangle$. The ϵ_α are the quasienergies.

For an initially coherent state $|\Psi_{p,q}(t=0)\rangle = |p,q\rangle$, the Husimi distribution (6) of the time-evolved state at times $t_n = nT$, $n = 0, 1, \ldots$ can be written as

$$\varrho\,(p',q';p,q;t_n) = \sum_\alpha |\langle\alpha|p',q'\rangle|^2\,|\langle\alpha|p,q\rangle|^2 + \sum_{\alpha\neq\beta} e^{-(i/\hbar)(\epsilon_\beta-\epsilon_\alpha)nT}\langle p,q|\beta\rangle\langle\beta|p',q'\rangle\langle p',q'|\alpha\rangle\langle\alpha|p,q\rangle, \tag{9}$$

with $|\alpha\rangle = |\psi_\alpha(0)\rangle$, because of the periodicity of $|\psi(t)\rangle$. The terms appearing in the first sum can be identified with the Husimi densities $\varrho_\alpha(p,q) = |\langle p,q|\alpha\rangle|^2$ of the quasienergy states at time zero, and the second sum vanishes in the long-time limit yielding

$$\bar{\varrho}\,(p',q';p,q) = \lim_{N\to\infty}\frac{1}{N+1}\sum_{n=0}^{N}\varrho\,(p',q';p,q;nT) = \sum_\alpha \varrho_\alpha(p',q')\,\varrho_\alpha(p,q). \tag{10}$$

This is a doubly stochastic distribution based on the initial and final Husimi distributions of the quasienergy states α. The entropy (8) can then be studied as a function on phase space when the individual Husimi distributions $\varrho_\alpha(p,q) = |\langle p,q|\alpha\rangle|^2$ of the quasienergy states are known. *Individual* distributions of this type have been investigated by various authors [6,7], and in some cases close correspondence with individual classical orbits has been observed. Some overall features could be elucidated by summing over certain subclasses, for example, the extended (or irregular) states [6]. Summing over *all* states yields no information because of the normalization $\sum_\alpha \varrho_\alpha(p,q) = 1$ satisfied in each phase space point. The entropy $S(p,q)$ allows us, however, to analyze *global* phase space structures without the need to distinguish between regular and irregular states.

In case of the rotor (1) the coherent states must be redefined because of the 2π periodicity of the angle coordinate ϕ following [10]. The quasienergy states for the rotor [1] as well as their projections onto the rotor coherent states are computed in the present study using the efficient (t,t') method [11] in the free rotor basis. The phase space distributions $\bar{\varrho}\,(J',\phi';J,\phi)$ in (10) are integrated over J' and ϕ' [compare (8)], which finally yields the entropy $S(J,\phi)$ as a function on phase space. The squeezing parameter s is chosen as the frequency of the harmonic oscillator approximation to the motion in the central island, i.e., $s = \sqrt{f/2}$ [2].

The resulting quantum mechanical phase space entropies $S(J,\phi)$ are shown in Fig. 2 as contour plots over the (J,ϕ) plane for the parameter $f = 0.45$ and three values of $\hbar$ ($\hbar = 0.1$, 0.0316, 0.01, e.g., equidistant steps in $\ln \hbar$). First, we observe a surprisingly clear image of the global dynamical long-time properties of the quantum system. Wave packets placed at the high entropy regions spread over extended regions of phase space, those started in the low entropy valleys remain localized on smaller regions. The overall impression is remarkably similar to the classical phase space structure in the Poincaré section in Fig. 1, in particular, for the small value of $\hbar = 0.01$. The stability zones appearing as islands in the Poincaré section are clearly detected as pronounced minima. When the wave packet localizes at a single island the value of the entropy at its center can be estimated to be close to 1 (the entropy of a minimum uncertainty wave packet is exactly equal to 1). A localization at a chain of n islands leads to $S \approx 1 + \ln n$ at the center of the islands. Wave packets placed in the extended plateau spread over the classically chaotic region with area A, and the value of the entropy is approximately given by $S = \ln(A/2\pi\hbar)$.

For a large value of $\hbar$, details of the phase space structure are washed out as expected. When $\hbar$ is decreased, finer phase space details are resolved and additionally the difference between the entropy in the regular and chaotic region increases due to the different scaling behavior with $\hbar$. This also applies to the classical entropy $S_c(J,\phi)$, which is shown for the case $\hbar = 0.01$ in Fig. 3 (the squeezing parameter s is the same as in the quantum case). It is important to note that in the presence of phase space symmetries quantum and classical systems show characteristic differences, which can be removed, however, by desymmetrizing the system. This means that phase space points related by a symmetry transformation are identified. In practice, the phase space density is generated by summing over all trajectories belonging to the same symmetry class. With this modification, the classical entropies in

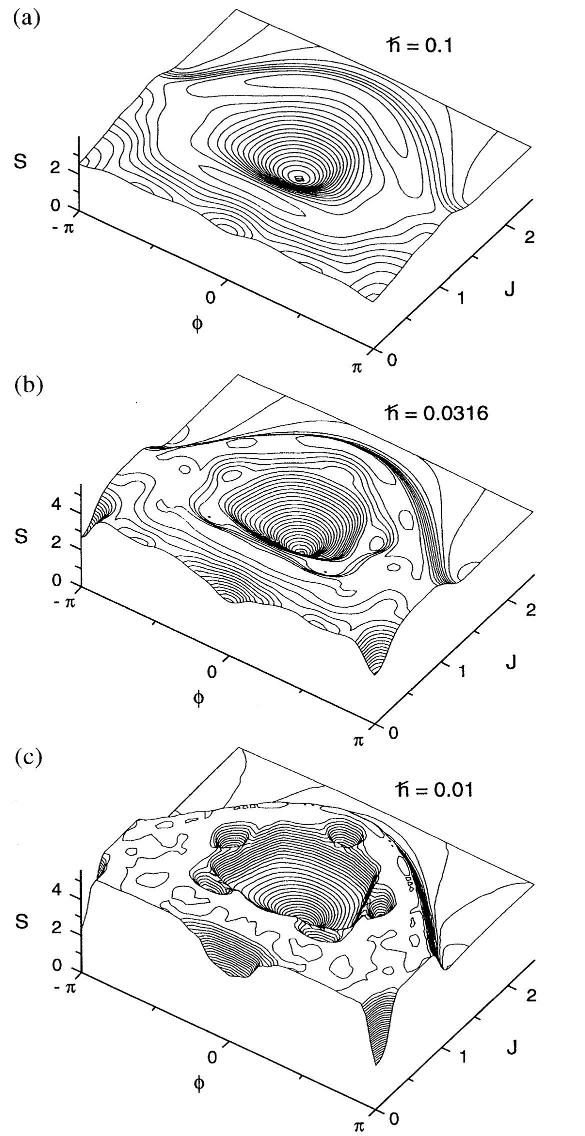

FIG. 2. Quantum phase space entropy $S(J,\phi)$ shown as a contour plot over phase space for a driven rotor with $f = 0.45$ and $\hbar = 0.1$, 0.0316, and 0.01.

Fig. 3 show a striking similarity with the corresponding quantum entropy in Fig. 2. Figure 4 finally shows the entropy as a function of the angular momentum J at $\phi = 0$, i.e., a vertical cut through the plots shown in Fig. 2, for all three values of $\hbar$. Also shown are the classical entropies. In the center of the 1:1 resonance island all entropies agree with the estimate $S \approx 1 + \ln n = 1 + \ln 2 = 1.69$ (note that this resonance island has a symmetric partner at negative J values, i.e., $n = 2$). The period-five islands can only be resolved when $2\pi\hbar$ is smaller than the classical phase space area (i.e., for $\hbar = 0.01$) and the entropy approaches $S \approx 1 + \ln n = 1 + \ln 10 = 4.16$. In the chaotic region, one clearly recognizes the scaling of

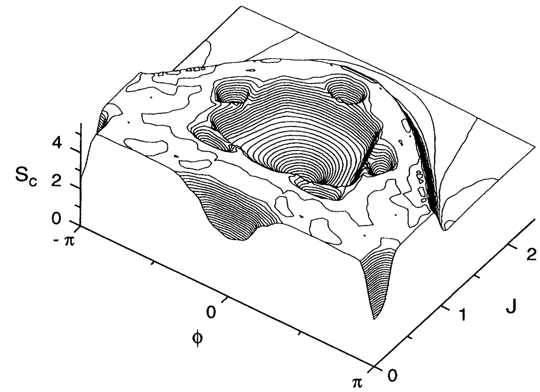

FIG. 3. Classical phase space entropy $S_c(J, \phi)$ shown as a contour plot over phase space for a driven rotor with $f = 0.45$. The Gaussian smoothing width is $\Delta = 2\pi\hbar$ with $\hbar = 0.01$.

$S(p,q)$ with $\ln \hbar$, whereas in the regime of invariant curves it scales as $\frac{1}{2} \ln \hbar$.

Finally, it should be pointed out that the quantum system can also exhibit localization on regions different from the obvious cases of classical stability islands or bounded chaotic regions. Examples of such cases are unstable orbits, "ghost" orbits [12], or regions surrounded by cantori in chaotic phase space [13]. This will be analyzed in detail in a forthcoming study for different parameter values. In the present case, one might recognize an additional chain of six minima surrounding the chain of five minima which is visible for $\hbar = 0.0316$. A corresponding stable classical orbit exists for smaller values of f, but no longer for $f = 0.45$ used in the present study. These localization properties may also be responsible for the differences still existing between quantum and classical entropies in the chaotic region for the smallest values of $\hbar$ in Fig. 4.

The basic quantity of interest in the present study, the quantum phase space entropy $S(p,q)$ defined in (8), shows some similarity to the entropy in the quasienergy basis $\{\alpha\}$

$$S_{(\alpha)}(p,q) = -\sum_{\alpha} \varrho_\alpha(p,q) \ln \varrho_\alpha(p,q), \qquad (11)$$

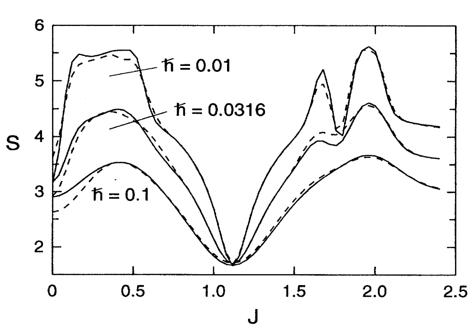

FIG. 4. Classical (——) and quantum (- - -) phase space entropies as a function of J for $\phi = 0$ for $\hbar = 0.1$, 0.0316, and 0.01.

which has been considered previously [1,4,8]. Such a phase space entropy has, however, no direct classical analog. Furthermore, $S_{(\alpha)}(p,q)$ shows random fluctuations of order $\hbar^{1/2}$ [14], which are in general not negligible and which do *not* appear in $S(p,q)$. Moreover, it can be shown that $S_{(\alpha)}(p,q) \leq S(p,q)$. In addition, the entropy $S(p,q)$ turns out to be the Wehrl entropy [9,15] for the statistical operator $\hat{\rho} = \sum_\alpha g_\alpha |\alpha\rangle\langle\alpha|$ with weights $g_\alpha = |\langle p,q|\alpha\rangle|^2$.

In conclusion, we have demonstrated that the dynamical phase space entropies for quantum systems provide a useful *quantitative* measure of the phase space localization properties on (classically) regular and chaotic regions. Additional more detailed applications and more material on the relation to other entropylike measures will be reported elsewhere.

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