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Semiclassical Wigner functions for quantum maps on a torus

Oded Agam and Naama Brenner
Department of Physics, Technion, Haifa 32000, Israel

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Abstract. A semiclassical formula is derived for the Wigner representation of the quasi-energy states of a quantum map on a torus. It is expressed as a finite sum over the classical fixed points of the map. A criterion for the appearance of 'scars' is presented. Semiclassical Wigner functions of the cat map are calculated and shown to reproduce the exact quantum mechanical results.

1. Introduction

Semiclassical studies of chaotic systems have focused mainly on properties of the spectrum. Central to this approach is the Gutzwiller trace formula [1], which expresses the density of states as a sum over classical periodic orbits. This sum suffers from divergence problems, which were recently resolved by introducing several resummation methods [2–6]. A semiclassical description of the dynamics of a system also requires understanding of the structure of the wavefunctions. One of the imprints of classical chaotic dynamics on the corresponding quantum eigenfunctions is the phenomenon of scars [7], which are the enhancement of the probability density near classical unstable periodic orbits. Scars have important consequences on the thermodynamic properties of quantum systems [8]. They were also suggested as a mechanism for the inhibition of ionization of atoms in a microwave field [9]. Heller found scars in the stadium billiard, and argued that they are generic for systems with a chaotic classical limit [7]. Later on, theoretical explanations within the framework of semiclassical periodic orbit theory were suggested by Bogomolny [10] and Berry [11]. The formulae in this theory express the probability density and the Wigner function as sums over all the classical periodic orbits. However, these sums suffer from the same divergence problem as the Gutzwiller trace formula for the density of states, and in order to get a meaningful result, the functions had to be smeared over a finite range of energy. The resummation method introduced by Berry and Keating for the spectral determinant [6], was used by Agam and Fishman to express individual Wigner functions as sums over an effectively finite number of periodic orbits [12].

In studying the quantum dynamics of chaotic systems, it is particularly convenient to consider discrete area-preserving mappings. These are obtained naturally as stroboscopic samplings of time-periodic systems, and also from the reduction of degrees of freedom in time-independent systems. Such reductions appear, for example, when there are some integrals of motion; then each constant of motion can be used to integrate out one degree of freedom, and the reduced dynamics is described by a map on the remaining degrees of freedom. Another example is a general Poincaré surface of section, such as the bounce map on the boundary of a billiard.

Early semiclassical studies of chaotic maps were performed by Berry and Balazs [13], and Berry *et al* [14]. They mainly considered the evolution of Wigner functions under the action of the map. Hannay and Berry [15] considered the specific case of linear maps on a torus (cat maps). They used number theory to calculate the exact propagator, and to investigate the quasi-energy spectrum and the dynamics. Eckhardt [16] used these results to derive an exact formula for the quasi-energy states of the cat map, and showed that they are related to the fixed points of the classical map. The periodic orbit approach to mappings was first introduced by Tabor [17]. He derived an analogue of the Gutzwiller trace formula for maps, which expresses the density of quasi-energy states in terms of the classical fixed points of the map. A treatment of cat maps within the periodic orbit theory was performed by Keating [18], who derived expressions for the propagator and the Wigner functions as sums over periodic orbits. Other systems which were investigated include the kicked rotor [19], the Baker's map [20, 21], the kicked top [22], the linearized standard map [23] and the kicked Harper map [24]. For maps with a finite phase space, the finiteness implies that the quasi-energy spectrum can be related to a finite sum over the fixed points of the map [3, 21]. Recently, this result was obtained by Smilansky [25] using a resummation method similar to that of Berry and Keating [6].

The purpose of this paper is to derive a semiclassical formula for the quasi-energy Wigner functions of quantum maps on a torus which are chaotic in the classical limit. In section 2, some general properties of quantum maps on a finite phase space will be discussed, the main results concerning the semiclassical spectral determinant for maps will be summarized, and the Wigner function will be defined. In section 3, the periodic orbit approach will be applied, in a manner similar to [12], in order to calculate the Wigner representation of the quasi-energy states, and to derive a semiclassical criterion for scars. A resummation technique suitable for maps will be used, as in [25]. In section 4, a specific example of the cat map will be discussed. It will be shown that for this system the semiclassical Wigner functions coincide with the exact ones. A summary and discussion of the main results will be presented in section 5.

2. Quantum maps

In this section some known results are summarized, and the nomenclature is set for subsequent discussion. It includes three subjects: some general properties of quantum mechanics for a system with a finite phase space, the semiclassical spectral determinant for maps, and the definition of the Wigner function.

Quantum maps arise naturally from time periodic systems. The evolution of such a system can be described by a unitary operator, which is the propagator for one time period:

$$|\psi_{k+1}\rangle = \hat{\mathcal{U}}|\psi_k\rangle \tag{2.1}$$

where $|\psi_k\rangle$ is the state of the system at the kth time step, and $\hat{\mathcal{U}}$ is the one-step evolution operator. The eigenfunctions $|\alpha\rangle$ of $\hat{\mathcal{U}}$ are called the quasi-energy states. They satisfy

$$\hat{\mathcal{U}}|\alpha\rangle = \mathrm{e}^{-\mathrm{i}\omega_\alpha}|\alpha\rangle \tag{2.2}$$

where ω_α is the corresponding quasi-energy.

When the phase space of the corresponding classical system is a two-dimensional torus, both coordinate and momentum are quantized. The Hilbert space reduces to functions defined on a discrete lattice, therefore, $\hat{q}$ and $\hat{p}$ are not well defined operators [26]. One defines the two basic operators, $\widehat{\mathrm{e}^{\mathrm{i}\alpha q}}$ and $\widehat{\mathrm{e}^{\mathrm{i}\beta p}}$, as the translation operators on the quantum lattice, with α and β chosen such that these operators have the symmetry of the phase space. An additional consequence of the finiteness of phase space is that the value of Planck's constant h is restricted to be $\mathcal{A}/N$, where $\mathcal{A}$ is the symplectic area of the phase space and N is an integer. The quantum lattice will consist of N^2 equally spaced points, and the semiclassical limit, $\hbar \to 0$, corresponds to the limit $N \to \infty$. We will assume that the torus is of unit symplectic area, and designate the lattice points $(q_n, p_m) = (n/N, m/N)$ by their indices (n, m). Then, the position eigenstates $|n\rangle$ correspond to eigenvalues q_n, and satisfy periodic boundary conditions: $|n + N\rangle = |n\rangle$. Similarly, for the momentum eigenstates $|m\rangle$ with the eigenvalues p_m, $|m + N\rangle = |m\rangle$. The transformation between the two representations is through the discrete Fourier transform

$$\langle m|\psi\rangle = \frac{1}{\sqrt{N}}\sum_{n=0}^{N-1} \mathrm{e}^{-\mathrm{i}2\pi nm/N}\langle n|\psi\rangle . \tag{2.3}$$

The operators acting on this Hilbert space, and, in particular, the evolution operator $\mathcal{U}$, are finite $N \times N$ matrices.

The classical dynamics is described by a continuous area-preserving map $\mathcal{M}$ from the unit torus onto itself. Denoting by (q, p) the coordinate and momentum on the torus, the map is defined by the generating function $S(q(k+1), q(k))$ such that

$$p(k+1) = \frac{\partial S(q(k+1), q(k))}{\partial q(k+1)} \qquad p(k) = -\frac{\partial S(q(k+1), q(k))}{\partial q(k)} \tag{2.4}$$

where k is an integer that represents the discrete time, and S is the one-step action of the trajectory from $(q(k), p(k))$ to $(q(k+1), p(k+1))$. A fixed point of order l of the mapping $\mathcal{M}$ satisfies $q(k+l) = q(k)$, $p(k+l) = p(k)$. We shall also refer to it as a periodic orbit of period l.

Similar to Gutzwiller's trace formula in which the semiclassical approximation for the density of states of autonomous systems is expressed in terms of the classical periodic orbits, Tabor [17] has shown that, in the semiclassical limit, the density of quasi-energies,

$$d(\omega) = \sum_{\alpha=1}^{N} \delta(\omega - \omega_\alpha) \tag{2.5}$$

may be expressed as a some over all the classical fixed points of the mapping:

$$d(\omega) = \frac{N}{2\pi} + \frac{1}{\pi}\mathrm{Re}\sum_{l=1}^{\infty} \mathrm{e}^{\mathrm{i}\omega l} \sum_{r_p n_p = l} \frac{n_p}{\sqrt{\det(M_p^{r_p} - I)}} \mathrm{e}^{\mathrm{i}S_p r_p/\hbar - \mathrm{i}\gamma_p r_p} . \tag{2.6}$$

Here p labels the primitive periodic orbits, which are orbits that do not trace themselves more than once, and r_p is the repetition number, S_p is the action of the pth primitive orbit, n_p is its period (the order of the fixed point), M_p is the monodromy matrix, which characterizes the linearized motion in the vicinity of the fixed point, and γ_p is the Maslov phase.

A non-singular function which is related to the quasi-energy spectrum is the spectral determinant $\Delta(\omega)$, defined as

$$\Delta(\omega) = \mathrm{e}^{-\mathrm{i}\pi\bar{N}(\omega)} \det\left(1 - \mathrm{e}^{\mathrm{i}\omega}\hat{\mathcal{U}}\right) \tag{2.7}$$

where

$$\bar{N}(\omega) = N\omega/2\pi + c(N) \tag{2.8}$$

is the mean quasi-energy staircase. The constant $c(N)$ in this formula accounts for the deviation of the quasi-energy density from a uniform distribution. For a generic chaotic systems which exhibits level repulsion, this constant vanishes in the semiclassical limit

$N \to \infty$ [25]. Therefore, in what follows, we shall approximate $\bar{N}(\omega) \simeq N\omega/2\pi$. The spectral determinant, $\Delta(\omega)$, is a real function, whose zeros coincide with the quasi-energy spectrum of the system. It is related to the density of states by

$$d(\omega) = -\frac{1}{\pi}\mathrm{Im}\frac{\mathrm{d}}{\mathrm{d}\omega}\log\Delta(\omega) \tag{2.9}$$

and may be expressed semiclassically as a product over the fixed points. Assuming that all the fixed points are hyperbolic, it has the form

$$\Delta(\omega) = \mathrm{e}^{-\mathrm{i}\omega N/2}\prod_p\prod_{j=0}^{\infty}\left(1 - \mathrm{e}^{\mathrm{i}\omega n_p + iS_p/\hbar - \mathrm{i}\gamma_p - u_p(j+\frac{1}{2})}\right) \tag{2.10}$$

where u_p is the instability exponent of the pth fixed point. The difficulty in using this product is that it is not absolutely convergent for any real ω. This is due to the exponential proliferation of the number of periodic orbits as their period increases. Several resummation methods were recently introduced in order to overcome this problem [2–6]. In many of them, a first step is to expand the product (2.10) as a Dirichlet sum over pseudo-orbits [27], which are linear combinations of primitive periodic orbits. The expansion takes the following form [25]:

$$\Delta(\omega) = \mathrm{e}^{-\mathrm{i}\omega N/2}\sum_{l=0}^{\infty} A_l\,\mathrm{e}^{\mathrm{i}\omega l} \tag{2.11}$$

where l is the period of the pseudo-orbit, and

$$A_l = \sum_{\mu(l)} c_\mu\,\mathrm{e}^{\mathrm{i}S_\mu/\hbar} \qquad A_0 = 1\,. \tag{2.12}$$

Here, $\mu(l)$ labels a pseudo-orbit defined by the set of repetition numbers $\{r_p\}_\mu$, satisfying $\sum_p n_p r_p = l$, and

$$S_\mu = \sum_p r_p S_p\,. \tag{2.13}$$

The pseudo-orbit amplitudes c_μ were calculated in [27]. Apparently, the infinite sum (2.11) is absolutely convergent only for values of ω with a sufficiently large imaginary part. However, it can be shown [21, 25] that due to the finiteness of $\mathcal{U}$, the contributions from pseudo-orbits with period larger than N vanish. This is related to the fact that for a matrix of dimensionality N, traces of powers higher than N can be expressed as linear combinations of traces of powers N or less. Moreover, the unitarity of $\mathcal{U}$ enables an additional reduction of the length of the required orbits. For odd N only pseudo-orbits of period $l \leqslant (N-1)/2$ are needed [25], and

$$\Delta(\omega) = 2\,\mathrm{Re}\,\mathrm{e}^{-\mathrm{i}\omega N/2}\sum_{l=0}^{(N-1)/2} A_l\,\mathrm{e}^{\mathrm{i}\omega l}\,. \tag{2.14}$$

This result can also be derived by assuming the analyticity of the spectral determinant and analytically continuing it to the real ω line [25]. In section 3, this method will be shown in detail for the case of the Wigner function.

We now define and summarize some properties of the Wigner function of maps on a torus. Consider first a one-dimensional system with continuous coordinate and momentum. For this system the Wigner function corresponding to the state $|\psi\rangle$ is defined as [28, 29]

$$W(q,p) = \frac{1}{h}\int \mathrm{d}q'\,\mathrm{e}^{-\mathrm{i}q'p/\hbar}\langle q - \tfrac{1}{2}q'|\psi\rangle\langle\psi|q + \tfrac{1}{2}q'\rangle \tag{2.15}$$

where (q, p) are the coordinate and conjugate momentum. This is a real function, containing all the quantum information about the state $|\psi\rangle$. In particular, its projection onto q is equal to the probability density $|\langle q|\psi\rangle|^2$, and the projection onto p is $|\langle p|\psi\rangle|^2$. In general, the Wigner function is an oscillating function with many details, and is not necessarily positive. However, a Gaussian smearing of it over a phase-space region on the order of $\hbar$ yields a Husimi-type distribution, which is an everywhere positive function and therefore may be interpreted as a probability density function.

The Wigner function is a special case of a more general family of phase-space distributions, $\rho(q, p)$, defined as [30]

$$\rho(q, p) = \mathrm{tr}\,[\delta(\hat{\boldsymbol{x}} - \boldsymbol{x})|\psi\rangle\langle\psi|] \tag{2.16}$$

where $\boldsymbol{x} = (q, p)$ is the vector of coordinate and momentum in phase space. The different distributions are obtained from different orderings of the operators $\hat{q}$ and $\hat{p}$ in the δ-function [31]. The Wigner function is obtained from the ordering

$$\begin{aligned}\delta(\hat{\boldsymbol{x}} - \boldsymbol{x}) &= \frac{1}{h^2}\int \mathrm{d}q'\,\mathrm{d}p' \exp\left\{\frac{\mathrm{i}}{\hbar}[p'(\hat{q} - q) + q'(\hat{p} - p)]\right\} \\ &= \frac{1}{h^2}\int \mathrm{d}q'\,\mathrm{d}p'\, \mathrm{e}^{\mathrm{i}p'(\hat{q}-q)/\hbar}\, \mathrm{e}^{\mathrm{i}q'(\hat{p}-p)/\hbar}\, \mathrm{e}^{\mathrm{i}q'p'/(2\hbar)}\,. \end{aligned} \tag{2.17}$$

Other forms of phase-space distributions resulting from different orderings were discussed by Berry, and were shown to be inadequate for investigating the semiclassical limit [30].

In analogy to the definition (2.15), one would like to define a discrete version of the Wigner function corresponding to the state $|\psi\rangle$. Therefore, an appropriate definition of the delta function for this case is required. The natural discrete version of the second expression of (2.17), which is appropriate for odd N, is

$$\delta[(\hat{n}, \hat{m}) - (n, m)] = \frac{1}{N^2}\sum_{n',m'} \mathrm{e}^{\mathrm{i}m'(\hat{n}-n)2\pi/N}\, \mathrm{e}^{\mathrm{i}n'(\hat{m}-m)2\pi/N}\, \mathrm{e}^{\mathrm{i}m'n'\pi/N} \tag{2.18}$$

where the sums over n' and m' range from $-(N-1)/2$ to $(N-1)/2$ to ensure the reality of this function. A slightly different definition is also available for even N. In this work only the case of odd N will be considered. The Wigner function that results from the above definition and (2.16) is

$$W_\psi(n, m) = \frac{1}{N}\sum_{n',l} \mathrm{e}^{-\mathrm{i}2\pi n'm/N}\, \tilde{\delta}(2l - 2n + n')\, \langle l + n'|\psi\rangle\langle\psi|l\rangle \tag{2.19}$$

where

$$\tilde{\delta}(k) = \frac{1}{N}\sum_{m'} \mathrm{e}^{\mathrm{i}\pi m'k/N} = \frac{1}{N}\frac{\sin(\pi k/2)}{\sin(\pi k/2N)}\,. \tag{2.20}$$

The function $\tilde{\delta}(k)$ reduces to the Kronecker delta $\delta_{k,0}$ for even values of k, and satisfies $\sum_{-N}^{N-1}\tilde{\delta}(k) = 2$. The above definition of the Wigner function has the following properties: (i) it is real; (ii) a projection onto the q space yields $\sum_m W_\psi(n, m) = |\langle n|\psi\rangle|^2$, i.e. the probability to occupy the site q_n; and (iii) the projection onto p space yields $\sum_n W_\psi(n, m) = |\langle m|\psi\rangle|^2$ which is the probability to be with momentum p_m. These properties are proved in appendix A. Note that by construction the continuous Wigner function is recovered from (2.19) in the semiclassical limit $N \to \infty$.

3. Semiclassical Wigner functions for quantum maps

In this section we shall calculate the semiclassical approximation for the Wigner representation (2.19) of the quasi-energy functions $|\alpha)$ as defined in (2.2). The starting point is the formula for the resolvent

$$\hat{\mathcal{R}}(\omega) = \frac{1}{1 - e^{i\omega}\hat{\mathcal{U}}} = \sum_\alpha \frac{|\alpha)(\alpha|}{1 - e^{i(\omega - \omega_\alpha)}} \tag{3.1}$$

where ω is an arbitrary complex number. $\hat{\mathcal{R}}(\omega)$ may be expanded as a convergent power series. In the upper half plane it is of the form

$$\hat{\mathcal{R}}^+(\omega) = \sum_{k=0}^{\infty} e^{i\omega k}\hat{\mathcal{U}}^k \qquad \operatorname{Im}\omega > 0 \tag{3.2}$$

while for in the lower half plane

$$\hat{\mathcal{R}}^-(\omega) = -\sum_{k=1}^{\infty} e^{-i\omega k}(\hat{\mathcal{U}}^\dagger)^k \qquad \operatorname{Im}\omega < 0\,. \tag{3.3}$$

Consider first the case of ω in the upper half plane. We define the resolvent Wigner function as the Wigner representation of $\hat{\mathcal{R}}^+$,

$$\mathcal{R}_W^+(n,m) = \sum_{k=0}^{\infty} e^{i\omega k}\mathcal{U}_W^k(n,m) \tag{3.4}$$

where

$$\mathcal{U}_W^k(n,m) = \frac{1}{N}\sum_{n',l} e^{-i2\pi n'm/N}\tilde{\delta}(2l - 2n + n')(l + n'|\hat{\mathcal{U}}^k|l)\,. \tag{3.5}$$

The semiclassical analysis begins by replacing the exact propagator $\hat{\mathcal{U}}^k$ by its semiclassical approximation. The matrix elements of the latter between two lattice points $|q_a)$ and $|q_b)$ are given in terms of the classical trajectories which connect q_a and q_b in time k

$$(q_b|\hat{\mathcal{U}}^k|q_a) = \sum_\nu \left(\frac{i}{h}\frac{\partial^2 S_\nu(q_b, q_a; k)}{\partial q_a \partial q_b}\right)^{1/2} \exp\left\{\frac{i}{\hbar}S_\nu(q_b, q_a; k) - i\gamma_\nu\right\} \tag{3.6}$$

where ν labels the various classical paths, $S_\nu(q_b, q_a; k)$ is the corresponding action of k time steps, which is the sum of the one-step action as defined in (2.4), and γ_ν is the Maslov phase of the νth orbit. Now we substitute this expression into (3.5), use the Poisson summation formula for evaluating the sums over n' and l, and perform the integral in the stationary phase approximation. In this semiclassical calculation it is consistent to replace the function $\tilde{\delta}(k)$ by a delta function with the appropriate weight. (This replacement simplifies the calculation considerably, but the final result is obtained also by direct calculation). The leading contribution in this stationary phase approximation comes from trajectories which satisfy the midpoint rule

$$q_n = \tfrac{1}{2}(q_a + q_b) \qquad p_m = \tfrac{1}{2}(p_a + p_b) \tag{3.7}$$

where p_a and p_b are the classical momenta corresponding to the points q_a and q_b. The distance between the endpoints, $|q_a - q_b|$, of such a trajectory is smaller than half the torus size, therefore its midpoint (3.7) is uniquely defined on the torus. The result one obtains is

$$\mathcal{U}_W^k(n,m) = \frac{1}{N}\sum_\nu \frac{2}{\sqrt{\det(M_\nu + I)}} e^{(i/\hbar)\phi_\nu(q_n, p_m; k) - i\gamma_\nu} \tag{3.8}$$

where

$$\phi_\nu(q_a, q_b; k) = S(q_a, q_b; k) - p_m(q_b - q_a)\,. \tag{3.9}$$

Here ν labels the mid-point trajectories, and M_ν is the monodromy matrix, which is associated with the linearized motion in the vicinity of the νth trajectory. It may be expressed as

$$M_\nu = \frac{1}{S_{ab}} \begin{pmatrix} -S_{aa} & S_{ab}^2 - S_{aa}S_{bb} \\ -1 & S_{ab} - S_{bb} \end{pmatrix} \tag{3.10}$$

where $S_{ij} = \partial^2 S/\partial q_i \partial q_j$. For the special case of $k = 0$, only zero-length orbits contribute; for these, $M = I$, the action and the Maslov index vanish and $\mathcal{U}_W^0(n, m) = 1/N$. We now introduce an averaging $\langle \cdots \rangle$ over a small region in phase space, both in q and in p. This average involves a number of lattice points N_A such that $N \ll N_A \ll N^2$, which is well defined in the semiclassical limit. Applying the averaging to $\mathcal{R}_W^+(n, m)$ leaves only the contribution of classical trajectories which are close to periodic ones. Note that this procedure is unnecessary when calculating the resolvent Wigner function of time-independent systems [11]. The reason is that in these systems the midpoint rule is satisfied by a continuum of points on periodic orbits. This degeneracy implies that the most important contribution comes from the vicinity of periodic orbits. Such a situation does not exist for one-dimensional maps, therefore in order to express the resolvent in terms of periodic orbits the averaging procedure is required.

The phase (3.9) can, therefore, be expanded around the periodic orbits. Let $X = (q, p)$ be a fixed point of order l of the classical mapping, and let ξ denote the displacement in phase space from X such that $X + \xi$ is a vector on the quantum lattice, see figure 1. Then the expansion of the phase is [32]

$$\phi(X + \xi; l) = \phi(X; l) + \xi \frac{\partial \phi}{\partial \xi} + \frac{1}{2} \xi \frac{\partial^2 \phi}{\partial \xi^2} \xi\,. \tag{3.11}$$

The derivatives are given by

$$\frac{\partial \phi}{\partial \xi} = J(X_b - X_a) \qquad \frac{\partial^2 \phi}{\partial \xi^2} = J\left(\frac{\partial X_b}{\partial \xi} - \frac{\partial X_a}{\partial \xi}\right) \tag{3.12}$$

where J is the unit symplectic matrix

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{3.13}$$

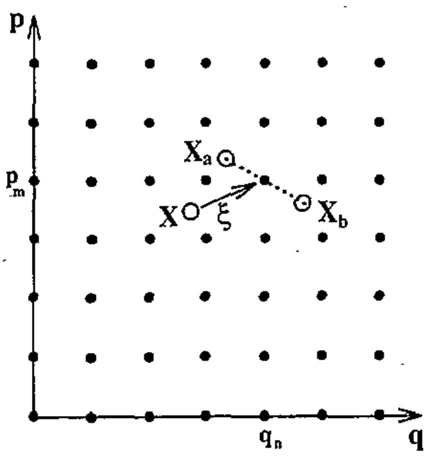

Figure 1. An illustration of the notations used in expanding the phase (3.9) around a periodic orbit. X is a classical fixed point, ξ is a vector representing the displacement from the fixed point to a nearby lattice site. X_a and X_b satisfy the midpoint rule for this site.

and $X_{a(b)} = (q_{a(b)}, p_{a(b)})$. The expansion (3.11) is shown in some detail in appendix B. Since the derivatives are evaluated at the fixed point, $X_a = X_b$, the linear contribution to (3.11) vanishes. This results from the fact that only midpoint trajectories whose length is less than half the torus size contribute; otherwise, one would have to consider cases where $X_b - X_a$ is an integer vector. The expansion of (3.9) around the periodic orbit labelled by p is thus

$$\phi_p = S_p + \xi J \frac{M_p - I}{M_p + I} \xi \tag{3.14}$$

where S_p is the action of the periodic orbit and M_p is the monodromy matrix. The resulting smoothed Wigner resolvent is therefore

$$\langle \mathcal{R}_{\mathrm{W}}^{+}(n,m)\rangle = \frac{1}{N} + \frac{1}{N} \sum_{\mathrm{ppo}} \sum_{r=1}^{\infty} \mathrm{e}^{\mathrm{i}\omega n_p r} \frac{2}{\sqrt{\det(M_p^r + I)}} \exp\left\{ \frac{\mathrm{i}}{\hbar} \left[S_p r + \xi J \frac{M_p^r - I}{M_p^r + I} \xi \right] - \mathrm{i}\gamma_p r \right\}. \tag{3.15}$$

In the above sum, p denotes a primitive periodic orbit, r counts the repetitions, and n_p is the length of the primitive orbit in discrete time units, i.e. the order of the primitive fixed point. The next step is to sum over all the repetitions r. This is done in the same manner as in [12]. We restrict ourselves to the case where all fixed points are hyperbolic, namely the eigenvalues of the monodromy matrix are $\mathrm{e}^{\pm u_p}$. Each term in the sum (3.15) is expanded as a power series in e^{-u_p}, and then the sum over r becomes a simple geometric series that can be summed to yield

$$\langle \mathcal{R}_{\mathrm{W}}^{+}(n,m)\rangle = \frac{1}{N} + \frac{2}{N} \sum_{\mathrm{ppo}} \sum_{j=0}^{\infty} \frac{\mathrm{e}^{\mathrm{i}\omega n_p} g^{(j)}(\mathrm{i}b_p)\, \mathrm{e}^{(\mathrm{i}/\hbar)S_p + \mathrm{i}b_p \mathrm{i}\gamma_p} \mathrm{e}^{-u_p(j+\frac{1}{2})}}{1 - \mathrm{e}^{\mathrm{i}\omega n_p}\, \mathrm{e}^{(\mathrm{i}/\hbar)S_p - \mathrm{i}\gamma_p}\, \mathrm{e}^{-u_p(j+\frac{1}{2})}} \tag{3.16}$$

where

$$b_p = \frac{1}{\hbar} \xi R_p \xi \tag{3.17}$$

while

$$R_p = J \frac{M_p - I}{M_p + I} \left| \det J \frac{M_p - I}{M_p + I} \right|^{-1/2} \tag{3.18}$$

and $g^{(j)}$ are polynomials in the variable $\mathrm{i}b_p$, given by

$$g^{(j)}(\eta) = \sum_{l=0}^{j} (-1)^{j-l} \mathrm{e}^{-\eta} \frac{1}{l!} \left(\frac{\partial}{\partial z} \right)^{l} \mathrm{e}^{\eta(1-z)/(1+z)} \bigg|_{z=0}. \tag{3.19}$$

The first few of them are

$$g^{(0)}(\eta) = 1 \qquad g^{(1)}(\eta) = -1 - 2\eta \qquad g^{(2)}(\eta) = 1 + 4\eta + 2\eta^2 \tag{3.20}$$

(see [12] for details). The common denominator of the terms in the sum (3.16) is, up to a phase factor, the spectral determinant (2.10). In its region of convergence in the upper half plane, we will denote this function by $\Delta_+(\omega)$. Equation (3.16) can therefore be written in the form $\mathcal{N}_+/\Delta_+(\omega)$, where

$$\mathcal{N}_+ = \frac{\Delta_+(\omega)}{N} + \frac{2}{N} \sum_{\mathrm{ppo}} \sum_{j=0}^{\infty} \Delta_+^{(p,j)}(\omega) g^{(j)}(\mathrm{i}b_p)\, \mathrm{e}^{\mathrm{i}b_p} \tag{3.21}$$

and

$$\Delta_+^{(p,j)}(\omega) = \mathrm{e}^{-\mathrm{i}\omega N/2} \exp\left\{\mathrm{i}\omega n_p + \mathrm{i}S_p/\hbar - \mathrm{i}\gamma_p - u_p\left(j+\tfrac{1}{2}\right)\right\}$$
$$\times \prod_{(p',j')\neq(p,j)} \left(1 - \exp\left\{\mathrm{i}\omega n_{p'} + \mathrm{i}S_{p'}/\hbar - \mathrm{i}\gamma_{p'} - u_{p'}\left(j'+\tfrac{1}{2}\right)\right\}\right). \tag{3.22}$$

A similar derivation can be made for the lower half plane. The corresponding functions will be labelled by a subscript $(-)$. In this case, $\langle \mathcal{R}_{\mathrm{W}}^{-}(n,m)\rangle = \mathcal{N}_-/\Delta_-(\omega)$, where

$$\mathcal{N}_- = -\frac{2}{N}\sum_{\mathrm{ppo}}\sum_{j=0}^{\infty} \Delta_-^{(p,j)}(\omega) g^{(j)}(-\mathrm{i}b_p)\,\mathrm{e}^{-\mathrm{i}b_p} \tag{3.23}$$

while $\Delta_-^{(p,j)}(\omega)$ is defined similar to (3.22), and satisfies $\Delta_-^{(p,j)}(\omega) = [\Delta_+^{(p,j)}(\omega^*)]^*$.

The two expressions for the Wigner resolvent, in terms of periodic orbits, converge only far away from the real ω-axis. In order to get a convergent expression for this function on the real line, an analytic continuation is required. This is done for the numerator and the denominator separately, using the Cauchy integral formula. The analytic-continued denominator is the spectral determinant $\Delta(\omega)$ (equation (2.14)) discussed in section 2. We are left, therefore, only with the analytic continuation of the numerator. For this purpose, the functions $\Delta_\pm^{(p,j)}(\omega)$ are expanded as sums of pseudo-orbits, as explained in [12]:

$$\Delta_+^{(p,j)}(\omega) = \mathrm{e}^{-\mathrm{i}\omega N/2}\sum_{l=1}^{\infty} A_l^{(p,j)}\,\mathrm{e}^{\mathrm{i}\omega l} \tag{3.24}$$

where

$$A_l^{(p,j)} = \sum_{\mu(l)} c_\mu^{(p,j)}\,\mathrm{e}^{\mathrm{i}S_\mu/\hbar}. \tag{3.25}$$

Here, the pseudo-orbits μ have been arranged in groups labelled by l. In each group, the pseudo-orbits are composed of r_p repetitions of the primitive orbit p, and $r_{p'}$ repetitions of the other orbits, such that

$$\sum_{p'\neq p} r_{p'}n_{p'} + (r_p+1)n_p = l \tag{3.26}$$

where n_p labels, as usual, the length of the primitive orbit in discrete time units. $\mathcal{S}_\mu$ is the composed action of the pseudo-orbit

$$\mathcal{S}_\mu = \sum_{p'\neq p} r_{p'}S_{p'} + (r_p+1)S_p. \tag{3.27}$$

We assume that there exists an analytic function $\mathcal{N}(\omega)$ defined in a strip around the real axis, which sufficiently far from the axis is represented by the expansions $\mathcal{N}_\pm(\omega)$. By Cauchy's integral formula,

$$\mathcal{N}(\omega) = \frac{1}{2\pi\mathrm{i}}\oint \mathrm{d}t\,\frac{\mathcal{N}(t)}{(t-\omega)}. \tag{3.28}$$

The contour of integration will be chosen as shown in figure 2. The contribution from the segments C_{L} and C_{R} vanish in the limit $\Omega\to\infty$. On each of the integration segments $C_\pm$, the corresponding series representations $\mathcal{N}_\pm$ can be used, and therefore

$$\mathcal{N}(\omega) = \frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathcal{N}_+(t'+\mathrm{i}t'')}{t'+\mathrm{i}t''-\omega}\,\mathrm{d}t' - \frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathcal{N}_-(t'-\mathrm{i}t'')}{t'-\mathrm{i}t''-\omega}\,\mathrm{d}t'. \tag{3.29}$$

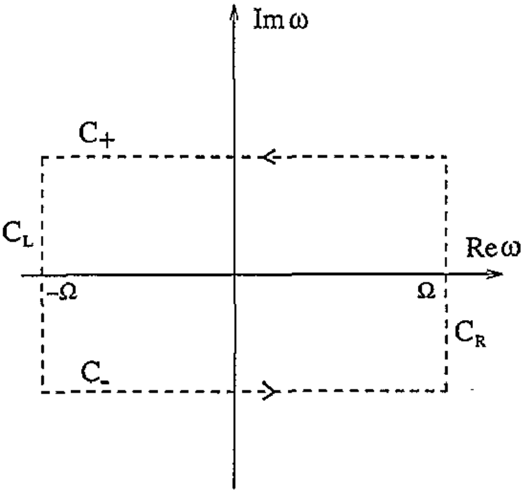

Figure 2. The contour of integration in ω plane used for the analytic continuation of the function $\mathcal{N}(\omega)$.

The integration yields

$$\mathcal{N}(\omega) = \frac{1}{2N}[\Delta(\omega) + \mathrm{i}\Delta_i(\omega)] + \frac{4\mathrm{i}}{N}\,\mathrm{Im}\left\{\sum_{p,j} g^{(j)}(\mathrm{i}b_p)\,\mathrm{e}^{\mathrm{i}b_p}\sum_{l=1}^{(N-1)/2} A_l^{(p,j)}\,\mathrm{e}^{\mathrm{i}\omega(l-N/2)}\right\} \tag{3.30}$$

where

$$\Delta_i(\omega) = 2\,\mathrm{Im}\,\mathrm{e}^{-\mathrm{i}\omega N/2}\sum_{l=0}^{(N-1)/2} A_l\,\mathrm{e}^{\mathrm{i}\omega l}\,. \tag{3.31}$$

The residue of the Wigner resolvent $\langle\mathcal{R}_{\mathrm{W}}(n,m)\rangle$ at the quasi-energy ω_α is the Wigner representation of the quasi-energy state $|\alpha\rangle$. Thus

$$\langle W_\alpha(n,m)\rangle = \frac{1}{N\Delta'(\omega_\alpha)}\left[\tfrac{1}{2}\Delta_i(\omega_\alpha) + 4\,\mathrm{Im}\left\{\sum_{p,j} g^{(j)}(\mathrm{i}b_p)\,\mathrm{e}^{\mathrm{i}b_p}\sum_{l=1}^{(N-1)/2} A_l^{(p,j)}\,\mathrm{e}^{\mathrm{i}\omega(l-N/2)}\right\}\right] \tag{3.32}$$

where $\Delta'(\omega)$ is the derivative of $\Delta(\omega)$ with respect to ω. Equation (3.32) is the principal result of this paper. It describes the Wigner representation of the quasi-energy state smoothed over a small region in phase space, in terms of a finite sum over the classical periodic orbits of the map. To the leading order in $1/N$ this function is normalized. Due to the smoothing, which is over a phase-space region large compared to $1/N$, the sum over phase points can be approximated by an integral. Then, the normalization is a result of the sum rule

$$\Delta'(\omega) = \tfrac{1}{2}N\Delta_i(\omega) + \sum_{(p,j)} n_p\bar{\Delta}^{(p,j)}(\omega) \tag{3.33}$$

where

$$\bar{\Delta}^{(p,j)}(\omega) = 2\,\mathrm{Im}\,\mathrm{e}^{-\mathrm{i}\omega N/2}\sum_{l=1}^{(N-1)/2} A_l^{(p,j)}\,\mathrm{e}^{\mathrm{i}\omega l}\,. \tag{3.34}$$

This sum rule may be obtained by direct analytic continuation of $\Delta'_\pm(\omega)$.

A semiclassical criterion for scars can be obtained as in [12]. Let $Y_p(\omega_\alpha)$ be the excess probability (relative to the smooth background term $\Delta_i(\omega_\alpha)/2N\Delta'(\omega_\alpha)$) of the particle in the state $|\alpha\rangle$ to be in the vicinity of the periodic orbit p. It is equal to the integral of the

Wigner function over a small region around the fixed point, minus the contribution from the background. This function may be expressed in terms of classical fixed points as

$$Y_p(\omega_\alpha) = \frac{n_p}{\Delta'(\omega_\alpha)} \sum_j \bar{\Delta}^{(p,j)}(\omega_\alpha)\,. \tag{3.35}$$

When $Y_p(\omega_\alpha)$ is of order of unity, one expects $W_\alpha(n, m)$ to be scarred around the pth periodic orbit.

4. An example: the cat map

The semiclassical expression for the Wigner function, (3.32), was obtained by a formal procedure involving an analytic continuation in ω. It is instructive to work out a specific example in which the outcome of this procedure can be compared to an exact result. A model in which the semiclassical approximation is expected to be exact is the family of hyperbolic linear maps on the torus, known as the cat maps. The purpose of this section is to calculate the semiclassical Wigner functions corresponding to the cat map, and to show that they do indeed coincide with the exact ones. The main practical difficulty in calculating semiclassical quantities of chaotic systems, such as the Wigner function (3.32), is the exponential proliferation in the number of periodic orbits needed for the calculation. Even though a finite number of orbits appears in the sum (3.32), in the semiclassical limit $N \to \infty$, this number is exponentially large. The advantage of using a model in which the semiclassical approximation is exact, is that it may be tested for a small value of N.

The cat map is defined by the following classical transformation on the torus:

$$\begin{pmatrix} q_{k+1} \\ p_{k+1} \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} q_k \\ p_k \end{pmatrix} \bmod 1\,. \tag{4.1}$$

The action which generates this map is [18]

$$S(q_{k+1}, q_k; n_w, m_w) = qk^2 - q_k(q_{k+1} + n_w) + (q_{k+1} + n_w)^2 - m_w q_{k+1} \tag{4.2}$$

where n_w and m_w are the winding numbers in q and in p, respectively. For a given value of N, the corresponding quantum evolution over one time step is generated by the propagator [15]

$$\langle q_b|\hat{\mathcal{U}}|q_b\rangle = \left(\frac{-\mathrm{i}}{N}\right)^{1/2} \exp\left[\mathrm{i}2\pi N\left(q_a^2 - q_a q_b + q_b^2\right)\right] \tag{4.3}$$

where q_a and q_b are points on the lattice of size N. (Note that the propagator is defined up to an overall phase factor; for convenience, our definition differs by a factor of i from that of Hannay and Berry).

In the following calculation, we shall chose $N = 3$. This is clearly not compatible with the semiclassical limit, $N \to \infty$. However, for the cat map there exists a suitable definition of the Wigner function for which the stationary phase integrals turn out to be exact for all values of N. This is the definition introduced by Hannay and Berry [15] and used by Keating [18]. Restricted only to the integer lattice points, it is

$$W_\psi(n, m) = \frac{1}{N} \sum_{n'=0}^{2N-1} \left\langle n + \tfrac{1}{2}n' \middle|\psi\right\rangle\left\langle\psi\middle| n - \tfrac{1}{2}n'\right\rangle \mathrm{e}^{-\mathrm{i}2\pi mn'/N} \tag{4.4}$$

where ψ is understood to be zero at half-integer points. Like our definition (2.19), this function can be shown to satisfy all properties required from a phase-space distribution.

Table 1. The quasi-energies and their corresponding Wigner functions for the cat map with $N = 3$. Each entry in the table corresponds to the value of the Wigner function on a lattice point $(n/3, m/3)$ with $n, m = 0, 1$ and 2. The bottom left entry corresponds to the point $(0, 0)$ and the bottom right entry to $(\frac{2}{3}, 0)$.

$\omega_1 = \frac{17}{12}\pi$			$\omega_2 = \frac{5}{12}\pi$			$\omega_3 = \frac{7}{4}\pi$		
$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	0	0	0
$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	0	0	0
$-\frac{1}{3}$	$\frac{1}{6}$	$\frac{1}{6}$	$-\frac{1}{3}$	$-\frac{1}{6}$	$-\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$

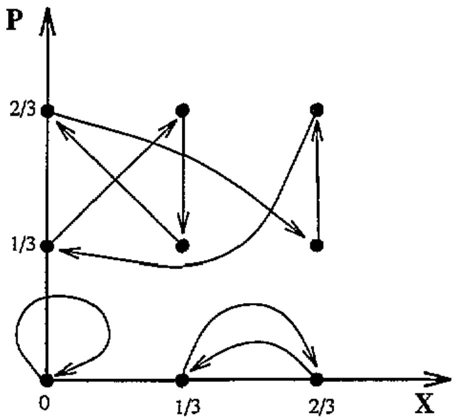

Figure 3. The cycles of the hyperbolic cat map on the 3×3 lattice. Arrows show the action of the classical transformation (4.1) on the lattice points. Note that all points in a cycle admit the same value of the Wigner function (see table 1).

The semiclassical formula corresponding to this definition is

$$W_\alpha(n, m) = \frac{1}{N\Delta'(\omega_\alpha)}\left[\frac{1}{2}\Delta_i(\omega_\alpha) + 2\,\mathrm{Im}\left\{\sum_{p,j} g^{(j)}(\mathrm{i}b_p)\,\mathrm{e}^{\mathrm{i}b_p}\sum_{l=1}^{(N-1)/2} A_l^{(p,j)}\,\mathrm{e}^{\mathrm{i}\omega(l-N/2)}\right\}\right]. \tag{4.5}$$

This expression differs from (3.32) in two respects. First, in the case of the cat map a phase-space averaging procedure is not needed, since the expansion of actions to second order is exact. Second, the midpoint trajectories can be of length up to the torus size, in contrast to (3.32), in which only trajectories of at most half the torus size contribute. This implies that in the semiclassical limit, contributions are not concentrated only near periodic orbits, but also near the antipode points. Consequently, this definition does not in general recover the expected classical behaviour in the limit $N \to \infty$. Still, it is a legitimate definition of the Wigner function, and since the stationary phase approximation for this case turns out to be exact it enables a direct testing of the resummation involved in deriving (4.5).

In table 1, we present the quasi-energies and the Wigner functions (4.5) obtained by direct diagonalization of the propagator (4.3) for $N = 3$. Each entry in the table corresponds to the value of the Wigner function on a lattice point $(n/3, m/3)$, with $n, m = 0, 1$ and 2. The bottom left entry of the table corresponds to the point $(0, 0)$, and the bottom right entry to $(\frac{2}{3}, 0)$. The three Wigner functions agree with the expected classical behaviour, namely points on the lattice which permute under the classical motion have the same value of the Wigner function [15]. Figure 3 shows these cycles on the 3×3 lattice.

For $N = 3$, only first order fixed points are required for the semiclassical resummed formulae. There are two such points, $(0, 0)$ and $\left(\frac{1}{2}, \frac{1}{2}\right)$, which we denote by $p = 0$ and

$p = 1$, respectively, with winding numbers $(n_w, m_w) = (0, 0)$ and $(1, 2)$. The torus actions corresponding to these fixed points are $S_0 = 0$ and $S_1 = \frac{3}{4}$. The monodromy matrix is in this case the linear transformation itself, and therefore all trajectories of the same length have the same amplitude, which in this case is $1/\sqrt{2}$. For the small value of N taken here, the constant $c(N)$ in (2.8) has to be specified exactly. In our case it is $c(3) = 7\pi/24$. The spectral determinant (2.14) can now be calculated from the contributions of the two fixed points, in which $A_0 = 1$ and $A_1 = -e^{i\pi/4}$. Using the resummed formula (2.14) one obtains

$$\Delta(\omega) = 4\sin\left(\tfrac{5}{12}\pi - \omega\right)\sin\left(\tfrac{1}{8}\pi + \tfrac{1}{2}\omega\right). \tag{4.6}$$

The three zeros of this function in the range $\omega \in [0, 2\pi]$ are equal to the three eigenvalues of the propagator (4.3), see table 1. A similar calculation for $\Delta_i(\omega)$, defined in (3.31), gives

$$\Delta_i(\omega) = 2\sin\left(\tfrac{7}{24}\pi - \tfrac{3}{2}\omega\right) - 2\sin\left(\tfrac{13}{24}\pi - \tfrac{1}{2}\omega\right). \tag{4.7}$$

With this information the Weyl term $\overline{W}_\alpha = \Delta_i(\omega_\alpha)/2N\Delta'(\omega_\alpha)$, which is the constant term in (4.5), can be calculated:

$$\overline{W}_1 = \tfrac{1}{6} \qquad \overline{W}_2 = \tfrac{1}{6} \qquad \overline{W}_3 = 0. \tag{4.8}$$

Next we calculate the functions $\bar{\Delta}^{(p,j)}(\omega)$ defined in (3.34). From the amplitudes $A_l^{(p,j)}$, only those with $l = 1$ contribute, and they are

$$A_1^{(0,j)} = e^{-u(j+\frac{1}{2})} \qquad A_1^{(1,j)} = e^{i\pi/2-u(j+\frac{1}{2})} \tag{4.9}$$

where u is the instability exponent satisfying $e^{-u} = 2 - \sqrt{3}$. The result is,

$$\bar{\Delta}^{(0,j)}(\omega) = 2\,e^{-u(j+\frac{1}{2})}\sin\left(\tfrac{7}{24}\pi - \tfrac{1}{2}w\right) \tag{4.10}$$

$$\bar{\Delta}^{(1,j)}(\omega) = 2\,e^{-u(j+\frac{1}{2})}\cos\left(\tfrac{7}{24}\pi - \tfrac{1}{2}w\right). \tag{4.11}$$

Using the expressions (4.6), (4.7) (4.10) and (4.11), one can easily verify that the sum rule (3.33) holds exactly.

In order to calculate the contributions of the periodic orbits to the Wigner function, the matrix R_p of (3.18) must be found. It is the same for the two fixed points, and is equal to

$$R_p = \sqrt{3}\begin{pmatrix} 1 & 0 \\ 0 & -\dfrac{1}{3} \end{pmatrix}. \tag{4.12}$$

Due to the fact that only first order fixed points contribute for the case $N = 3$, it is easy to sum over the index j in (4.5). The part of the sum which depends on j is

$$\sum_{j=0}^{\infty} g^{(j)}(ib_p)\,e^{ib_p}\,e^{-u(j+\frac{1}{2})} = \tfrac{1}{6}\,e^{ib_p/\sqrt{3}}. \tag{4.13}$$

This result was obtained by substituting (3.19) for the $g^{(j)}(ib_p)$ and changing the order of summation over l and j. A question which arises at this point, is what values of ξ in (3.17) should be taken in the sum (4.5). For a smoothed Wigner function, as defined in (3.32), only small values of ξ contribute effectively. However, in the case of the cat map no smoothing was introduced, therefore, also values of ξ which are larger than the torus size may contribute. Such situations correspond to expansions around images of the fixed points outside the fundamental torus, for which the linear term in (3.11) vanishes. The values of ξ must be such that for the points they define there exists a midpoint orbit. In the present case of $N = 3$, to each lattice point correspond six midpoint orbits, and therefore the contributions come effectively from the two fixed points in the fundamental torus and four of their images outside the torus. The result of such a calculation yields exactly the three Wigner functions presented in table 1.

5. Discussion

The main result of this paper is (3.32) for the semiclassical smoothed Wigner function of the quasi-energy state. This function is defined on a lattice of points in phase space, of size $N \times N$, and is expressed in terms of a finite sum over the fixed points of the classical mapping of order up to $(N-1)/2$. The semiclassical limit corresponds to $N \to \infty$. As this limit is approached, fixed points of higher order contribute to the sum, and the quantum lattice samples finer structures of the phase space. Projections of this formula onto the coordinate and momentum spaces yield the respective probability distributions of the quasi-energy state. This formula is the analogue of the formula for an energy Wigner function of a time independent chaotic system, and is derived by similar methods [12]. An important difference between the two cases is that here the finiteness of the sum is exact, whereas for the energy Wigner function the cutoff of the periodic orbit sum is smoothed by a complementary error function. The derivation assumes the analyticity of the Wigner function in the variable ω, while for the energy Wigner function analyticity in $1/\hbar$ was assumed. For the example of the cat map with $N = 3$, it was shown that the resummed semiclassical formula for the Wigner function is exact. This calculation suggests that the analytic continuation procedure used in order to truncate the infinite sum over fixed points, is exact in the case of the cat map, and may provide a good approximation for other systems.

Numerical computations for one-dimensional mappings are in general much simpler than for two-dimensional chaotic systems. Therefore a numerical verification of the formula (3.32) for the Wigner function is expected also to be simpler than its time independent counterpart. This may provide a tool for the numerical investigation of the validity of the semiclassical approximation for wavefunctions.

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Appendix A. Projections of the discrete Wigner function

In this appendix it is shown that the important properties of the Wigner function are satisfied by the expression (2.19). Changing the sum over n' to a sum over $-n'$, and the sum over l to a sum over $l - n'$, gives the complex conjugate of the function, therefore it is real. We shall now show that its projections onto the coordinate and momentum spaces give the corresponding probability distributions. Projecting onto q,

$$\sum_m W_\psi(n, m) = \frac{1}{N} \sum_{n',l} \left(\sum_m \mathrm{e}^{-\mathrm{i}2\pi n' m/N} \right) \tilde{\delta}(2l - 2n + n') \, \langle l + n' | \psi \rangle \langle \psi | l \rangle \, . \tag{A.1}$$

The sum over m in the brackets is $\delta_{n',0}$. This implies that only the value $n' = 0$ contributes, and therefore $\tilde{\delta}(2l - 2n) = \delta_{n,l}$. Summing now over l gives

$$\sum_m W_\psi(n, m) = |\langle n | \psi \rangle|^2 \, . \tag{A.2}$$

For the projection onto the coordinate q, it is convenient to substitute $\tilde{\delta}(2l - 2n + n')$ by the sum in (2.20). Then, summing over n yields $\delta_{m',0}$, thus only $m' = 0$ contributes. Changing variables $l + n' \to l$ gives

$$\sum_n W_\psi(n, m) = \frac{1}{N} \sum_{n',l} \langle n'|\psi\rangle\langle\psi|l\rangle\, \mathrm{e}^{-\mathrm{i}2\pi m(n'-l)/N} . \tag{A.3}$$

Identifying in this expression the discrete Fourier transform, (2.3) one finds that

$$\sum_n W_\psi(n, m) = |\langle m|\psi\rangle|^2 . \tag{A.4}$$

Appendix B. Expansion of the phase (3.9) near periodic orbits

In this appendix the phase in (3.9) is expanded to second order near a periodic orbit. The derivation follows closely [32], and is added only for completeness.

Differentiating (3.9) with respect to ξ and using the classical relations

$$\frac{\partial S}{\partial q_a} = -p_a \qquad \frac{\partial S}{\partial q_b} = p_b \tag{B.1}$$

one obtains

$$\frac{\partial \phi}{\partial \xi} = (p - p_a)\frac{\partial q_a}{\partial \xi} - (p - p_b)\frac{\partial q_b}{\partial \xi} + (q_a - q_b)\frac{\partial p}{\partial \xi} . \tag{B.2}$$

Now using the midpoint relation $2q = q_a + q_b$, which also implies

$$\frac{\partial q_b}{\partial \xi} = 2\frac{\partial q}{\partial \xi} - \frac{\partial q_a}{\partial \xi} \tag{B.3}$$

and also using $2p - p_a - p_b = 0$, leads to

$$\frac{\partial \phi}{\partial \xi} = -2(p - p_b)\frac{\partial q}{\partial \xi} + (q_a - q_b)\frac{\partial p}{\partial \xi} . \tag{B.4}$$

Substituting $\partial q_a/\partial \xi$ from (B.3) in (B.2), one similarly obtains

$$\frac{\partial \phi}{\partial \xi} = 2(p - p_a)\frac{\partial q}{\partial \xi} + (q_a - q_b)\frac{\partial p}{\partial \xi} . \tag{B.5}$$

Adding the two last equations and dividing by 2, yields

$$\frac{\partial \phi}{\partial \xi} = (p_b - p_a)\frac{\partial q}{\partial \xi} - (q_b - q_a)\frac{\partial p}{\partial \xi} = J(\mathbf{X}_b - X_a) . \tag{B.6}$$

An additional differentiation with respect to ξ gives (3.12).

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