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A trace formula for the semiclassical limit of some Hermitian operators

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Abstract
The aim of this paper is to provide an algorithm for calculating the leading order contributions for the semiclassical series of a functional of trace-class Hermitian operators. We base our study on the linear space structure of the space of bounded Hermitian operators on quantum Hilbert space. We work with a basis of operators with natural leading order Weyl symbols, performing stationary phase calculations with no assumption on their smoothness. The stationary points are tilted orbits near the periodic ones in phase space. We manage to get control of the error in the technique, which scales like some power a of $1/N$, with $1/2 < a \leqslant 1$. The calculations are directly applicable to quantum maps, and we provide some examples in finite dimension with quantum perturbed cat maps.

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1. Introduction and description of the results

We are interested in the problem of a semiclassical description of some dynamical properties of quantum Hermitian operators under a dynamics governed by a Hamiltonian whose classical counterpart is chaotic.

This problem dates back to the work of Wilkinson [25] who derived a sum rule for matrix elements of an arbitrary operator $\hat{A}$. Here we shall be concerned with the semiclassical limit of

$$\rho(E, \epsilon, N; \hat{A}) = \sum_{n=1}^{N} a_{nn}\delta_\epsilon(E - E_n) \tag{1}$$

the density of states with weight given by the operator $\hat{A}$. The meaning of the terms on the right-hand side of (1) is as follows: E_n are the eigenvalues of a Hamiltonian which specifies the quantum evolution in a finite-dimensional Hilbert space; $\delta_\epsilon(x)$ denotes a positive function with a single maximum at $x = 0$ which tends to the Dirac delta distribution when $\epsilon \to 0$.

We note that a comprehensive semiclassical understanding of (1) is just a first step towards the goals set by Wilkinson [25], which gave some information on the off-diagonal matrix elements, that is, transitions between quantum states promoted by a given operator $\hat{A}$ in terms of a classical correlation function, but only under the assumption of smoothness of $\hat{A}$, whose removal is precisely the focus of the present work.

A semiclassical analysis of ρ has been put forward by Eckhardt *et al* [11] with the assumption that A_W, the Weyl symbol of $\hat{A}$, is smooth on scales of the order of $\hbar$. The Weyl symbol of an operator $\hat{A}$ is the *dynamical variable* defined by the following integral,

$$A_W(q, p; \hbar) = \frac{1}{(2\pi\hbar)^l} \int \langle q - r/2| \hat{A} |q + r/2\rangle \, \mathrm{e}^{\mathrm{i}p\cdot r/\hbar} \, \mathrm{d}^l r \tag{2}$$

where l denotes the number of degrees of freedom. Note the possible dependence of the symbol on $\hbar$.

When one considers time evolved operators, even if their symbols are smooth on $O(\hbar)$, semiclassically they will develop structures finer than this scale [4, 5], because classical functions subject to chaotic evolution do so. This was illustrated for some states parametrized by curves in a two-dimensional phase space in [5]. The question of at what time scale this happens is another matter, and though Berry and Balazs predicted $t \sim O(\ln \hbar^{-1})$, the numerical investigations of O'Connor *et al* well surpassed this limit [18]. It should be mentioned that in [18], the states evolved are Gaussian wave packets.

However dangerous, relying on semiclassical evolution presently seems the only possible way of obtaining the semiclassical limit of Berry's phase in chaotic systems [22], since there appear traces of products of t-time-lagged operators for arbitrary t. In fact, this is yet another example of the non-commutation of the limits $\hbar \to 0$ and $t \to \infty$, ubiquitous in the semiclassics of chaotic systems. Another application of semiclassical long time evolution is to the capture of semiclassically single eigenstates [19]. This would be hopeless if one could show that the norm of the difference between the semiclassical and quantum propagators is of order unity after a sufficiently long time, though this does not preclude the appearance of scars, which would then necessarily be due to a family of eigenstates particularly concentrated on the trace of a subset of periodic orbits (using classical equipartition as well). We remark that this statement, if proved, would give more precise information about the relationship of the classical (periodic orbits) and quantum spectra, but we shall not deal with this difficult problem. Egorov-like theorems indicate that semiclassical evolution can be reliable, but some weak forms of this result might well be misleading, as Bouzouina and de Bièvre remarked (in [8], see proposition 4.1 and paragraph after theorem 4.2).

The present work departs from an elementary tool: the vector space structure of the space of Hermitian operators, of dimension N^2. The idea upon which this paper is based is to decompose an arbitrary $\hat{A}$ into a basis of operators whose principal symbols are natural and easily computable. We define the semiclassical asymptotic series of $\rho(\cdot; \hat{A})$ to be that of its decomposition on this basis. While it would be desirable that the semiclassical analysis of an operator does not depend on the choice of basis, we do not prove this. There is an analogous account of this decomposition in [21], section 4.2.

We mention the recent work of Campos *et al* [9] which uses the Lie algebraic structure of quantum and classical mechanics, besides formal power series, to develop a (non-periodic orbit) *classicalization* procedure for quantum operators.

Let us give an overview of our results. To evaluate (1) semiclassically, the first problem is to get a procedure to evaluate $\mathrm{Tr}(\hat{A}U^n)$ semiclassically, where U^n is the nth composition of the propagator. We decompose an arbitrary operator in a basis constructed from translation operators in phase space. The basis operators have phases which depend linearly on coordinates. After decomposition, the semiclassical trace is performed using the simple stationary phase technique, but here it is not the periodic orbits themselves that are the stationary points, because the phase of each component of the operator $\hat{A}$ is taken into account on evaluating the integrals similar to (2). The stationary phases are given by the action of stationary orbits, which are in one-to-one correspondence with the periodic ones and close to them in phase space. These orbits are here named *tilted orbits*. Their contributions have been mentioned in [7], and we make extensive computations using them. Thus we push to the last step in the calculations the use of the stationary method and this is the main difference of the present work with standard periodic orbit theory [11].

The final step is to sum the semiclassical traces of the N^2 components of the operator $\hat{A}$. This could entail a large error, as each component has an error of order $1/N$. We are able to restrict this error in a probabilistically large set of Hermitian operators. Here an interesting ingredient comes into play: the control of the Fourier coefficients of a distribution of extremal phases, which is a classical function. The estimate is a consequence of the continuity of this distribution. To our knowledge, this kind of analysis has not appeared in the literature of quantum chaos as yet. From this estimate, we can state that the difference between the exact quantum spectral weighted density of states (1) and the just described semiclassical approximation decreases like $O(1/N^a)$, for some $1/2 < a \leqslant 1$. The results are summarized in proposition 1 and equation (18).

An alternative path to the one we followed is worth mentioning: the semiclassical traces over phase space could be performed using semiclassical symbols of the operators using the Wigner function adapted to toral phase space, given by finite sums as explained by Agam and Brenner [1]. The necessary account of the fine structure of the operator involved would be obtained from its Fourier analysis: this step would correspond to the preliminary decomposition of the operator on a basis we derived in section 2.

As applications of the following analysis, we will compare some numerical computations of the weighted density of states quantally and semiclassically: when $\hat{A}$ is a random matrix and when it is a projection onto an eigenstate. Though the applications are for finite dimension, we found it worth working in a more general setting and consider infinite-dimensional Hilbert space, which we assume separable. In this case, $\hat{A}$ is assumed trace-class.

In the following section, we give details of the basis decomposition, and outline an extension of the results to infinite-dimensional separable Hilbert space. Section 3 is a preparation of a quantum propagator for the semiclassical analysis, in the spirit of Boasman and Keating's work [6]. The core of the argument is in section 4, a semiclassical algorithm for the operator weighted density of states (1) is developed and, more importantly, its error is estimated. In section 5 we illustrate the results numerically, including the behaviour of the error of the semiclassical approximation with respect to dimension N.

2. Basis decomposition

We begin with finite-dimensional Hilbert spaces with the 2-torus classical phase space. Let us recall the quantum kinematics set-up on the 2-torus with periodic boundary conditions [2, 12]. More general (quasi-periodic) boundary conditions can be considered [16]. There is a pair of canonical conjugate variables in classical phase space, p and q, called momentum and position respectively. Define the canonically conjugate operators: $\hat{p}$ and $\hat{q}$, as generators of translation operators acting on each other's eigenstates, for instance,

$$e^{-i\hat{p}/N\hbar}\,|\mathsf{n}\rangle = |\mathsf{n}+1\rangle$$

where $|\mathsf{n}\rangle$ denotes an eigenstate of $\hat{q}$. From a unitary boundary condition, which we took simply as periodic $|\mathsf{N}\rangle \equiv |0\rangle$, one gets the quantization condition $h = 1/N$ [8]. Furthermore to change from the eigenstates of $\hat{p}$ to those of $\hat{q}$, say $|\mathsf{k}\rangle$ and $|\mathsf{n}\rangle$, we have a discrete Fourier transform matrix

$$\langle \mathsf{k} | \mathsf{n} \rangle = \frac{1}{\sqrt{N}} \mathrm{e}^{-2\pi \mathrm{i} \frac{kn}{N}} =: \mathcal{F}_N. \tag{3}$$

We fix the coordinate representation to write all matrices, but the results do not depend on this choice. For ease of notation, the indices run through 0 to $N-1$. Given an $N \times N$ Hermitian matrix, we decompose it into the main diagonal, a real N-dimensional vector, and other $(N-1)N$-dimensional vectors, each formed by the concatenation of the jth upper diagonal with the $(N-j)$th lower diagonal. We agree to denote these as d_0 and d_j *diagonal matrices* respectively.

The set of periodic vectors $j = 0, \ldots, N-1$, $\bar{N} = \lceil \frac{N-1}{2} \rceil$,

$$v_\mu(j) = \begin{cases} \cos \frac{2\pi \mu j}{N} & \text{if} \quad 0 \leqslant \mu \leqslant \bar{N} \\ \sin \frac{2\pi(\mu - \bar{N}) j}{N} & \text{if} \quad \bar{N} < \mu < N \end{cases}$$

is a basis of real vectors and therefore the diagonal operators can be expressed uniquely in terms of diagonal matrices A whose entries are proportional to $v_\mu(j)$. We denote these matrices by $D_0(v_\mu)$, meaning they are 0th diagonal operators with vector v_μ along the diagonal, and sometimes refer to them as A_μ. They have as semiclassical correspondents, or Weyl symbols, A_k^W: $\cos 2\pi kq$ for $k \leqslant \bar{N}$ or $\sin 2\pi kq$ if $k > \bar{N}$. Here and in what follows we adopt the Weyl symbols of the covering space, though there is a procedure due to Rivas and Ozorio de Almeida [21] adapted to the torus (for operators that do not involve products, it is rather clear that both calculations give the same answer, provided that, when deriving the symbol on the torus, one extends it from a discretized phase space smoothly to the whole classical torus).

Given a diagonal operator of the type above, the Fourier transformed operator $B_n = \mathcal{F}_N^{-1} A_n \mathcal{F}_N$ has one of the forms

$$\tfrac{1}{2}\big(D_n(1) + D_n^\dagger(1)\big) \qquad \text{if} \quad n \leqslant \bar{N}$$

or

$$\frac{1}{2\mathrm{i}}\big(D_{n-\bar{N}}(1) - D_{n-\bar{N}}^\dagger(1)\big) \qquad \text{if} \quad n > \bar{N}.$$

(The notation $D_n(w_k)$ means a d_n diagonal matrix with the vector $w_k, k = 0, \ldots, N-1$ disposed orderly along its entries. Note that $D_1(1)$ is the elementary matrix which shifts the lines upwards once.) Since Fourier transformation exchanges coordinate and momentum representations, the operators above have semiclassical correspondents, Weyl symbols, B_n^W: $\cos 2\pi np$ and $\sin 2\pi np$, respectively.

In general, A_m and B_n do not commute. However, if N divides mn, $[A_m, B_n] = 0$. If N is a prime number we can construct the $(N-1)^2$ commutators

$$C_{mn} = \frac{1}{\mathrm{i}\sin(\pi\mu\nu/N)}[A_m, B_n]. \tag{4}$$

where $\mu = m$ if $m \leqslant \bar{N}$, $\mu = m - \bar{N}$ if $m > \bar{N}$ and similarly for ν in terms of n. For example, if $n \leqslant \bar{N} < m$, they have the form

$$C_{mn} = -\frac{1}{\mathrm{i}}\left[D_\nu\left(\cos\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right) - D_\nu^\dagger\left(\cos\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right)\right].$$

The other cases are given in the appendices. The Weyl symbol of the above commutators is the series (see, for instance, theorem 3.4.2 of [24]),

$$\frac{1}{s_{mn}} f(q) 2\sin\left(\frac{\hbar(\overleftarrow{\partial}_q\overrightarrow{\partial}_p - \overleftarrow{\partial}_p\overrightarrow{\partial}_q)}{2}\right) g(p) = \frac{\hbar}{s_{mn}}\left[f'(q)g'(p) - \frac{\hbar^2}{4\cdot 3!} f'''(q)g'''(p) + \cdots\right]$$

where $f(q) = A_m^W(q)$, $g(p) = B_n^W(p)$ and $s_{mn} = \sin(\pi mn/N)$. The leading order term is the *principal symbol*. We only mention this series, but in our semiclassical analysis, we work directly with the operators A_n, B_n and C_{mn}, which together with the identity $N \times N$ matrix are here called *periodic operators*.

If N is not prime, we define

$$C_{mn} = \begin{cases} A_m B_n & \text{if } N \text{ divides } mn \\ \frac{1}{\mathrm{i}\sin(\pi mn/N)}[A_m, B_n] & \text{otherwise.} \end{cases}$$

This completes a basis for the N^2 Hermitian matrices. Let us gather what we have constructed in the lemma:

Lemma 1. *The set of periodic operators*

$$\mathcal{B}_N = \{I, A_k, B_k, C_{km}, 1 \leqslant k, m < N\}$$

is a basis of $N \times N$ Hermitian matrices with coefficients in the real field.

We will study the limit of the operator weighted density of states when $N \to \infty$. For maps, this corresponds to the semiclassical limit. We fix an infinite-dimensional separable Hilbert space $\mathcal{H}$ and let $Q : \mathcal{H} \to \mathcal{H}$ be a trace-class operator. Though the argument is independent of the choice of basis, this is fixed so that the matrix elements q_{ij} do not change with N. We consider the projections $Q^{(N)} = P_N Q P_N$, where P_N is a family of projections satisfying $P_N P_{N'} = P_N$, for $N' \geqslant N$.

As N varies, the operator $Q^{(N)}$ varies as well, but we have $\lim_{N\to\infty} Q^{(N)} = Q$ in the operator norm topology if Q is compact, and in particular if it is trace-class. $Q^{(N)}$ may be viewed as an infinite matrix with entries $q_{jk}^{(N)}$, with $q_{jk}^{(N)} = 0$ for j or $k > N$. By the same token, we view the periodic operators as infinite matrices completed with zeros. We get a bound on the coefficients of the expansion of $Q^{(N)}$ in the periodic operators basis:

Lemma 2. *If $\hat{Q}$ is trace-class Hermitian and $Q^{(N)} = P_N Q P_N$, then the coefficients in the expansion*

$$Q^{(N)} = a_0 I + \sum_{i=1}^{N-1}\left(a_i A_i + b_i B_i + \sum_{j=1}^{N-1} c_{ij} C_{ij}\right) \tag{5}$$

are real and have upper bounds

$$|a_i| \leqslant \frac{K}{N} \qquad |b_i| \leqslant \frac{K}{N} \qquad |c_{ij}| \leqslant \frac{1}{\sin\left(\frac{ij\pi}{N}\right)}\frac{K}{N}$$

where K does not depend on N.

Proof. First $a_0 = (\mathrm{Tr}\, Q^{(N)})/N$. Since Q is trace-class $\mathrm{Tr}\, Q^{(N)} = \sum_{i=1}^{N} q_{ii} \leqslant \sum_{i=1}^{\infty} |q_{ii}| < \infty$. Note that $\alpha \stackrel{\text{def}}{=} \sum_i |q_{ii}|$ is also an upper bound for $\sum_i |\tilde{Q}_{ii}|$ where $\tilde{Q} = \mathcal{F}_N Q \mathcal{F}_N^{-1}$. The trace defines an inner product on Hermitian operators. Subject to this inner product $\mathcal{B}_N$

is orthogonal. Now $\left|a_i \frac{N}{2}\right| = |\operatorname{Tr}(QA_i)| \leqslant \alpha$, since A_i is diagonal and its elements have absolute value less than 1:

$$\left|b_i \frac{N}{2}\right| = \left|\operatorname{Tr}\left(Q\mathcal{F}_N^{-1} A_i \mathcal{F}_N\right)\right| = |\operatorname{Tr}(\tilde{Q} A_i)| \leqslant \alpha.$$

For C_{ij} we have

$$\left|c_{ij} \frac{N}{2}\right| = \frac{1}{\sin\frac{ij\pi}{N}} |\operatorname{Tr}(QAB) - \operatorname{Tr}(QBA)| = \frac{1}{\sin\frac{ij\pi}{N}} |\operatorname{Tr}([Q, B]A)|$$

and this is less than the sum of absolute values of diagonal elements in $[Q, B]$. But by the triangle inequality, the sum of absolute values of diagonal elements of $[Q, B]$ is bounded by 2α. □

Remark 1. For small i, j, the bound on c_{ij} can be improved to $O(1/\sqrt{N})$ using the Cauchy–Schwarz inequality, but this bound suits our needs, since the factor $\sin\frac{ij\pi}{N}$ is cancelled after we perform the stationary phase integrals.

We point out some extensions of this discussion. The case of kicked maps [5] is already contained in the above. First, for a finite-dimensional Hilbert space not necessarily obtained from an l-torus, the quantization condition need not have the form $h = 1/N$. However, using some translation group structure within phase space, one observes that finite dimensionality of Hilbert space implies compactness of phase space (this is more stringent than compactness of an energy surface). In each model, the idea is to use some sort of periodicity of a shift or translation operator having a classical counterpart.

Now the extension to the infinite-dimensional case, at least when phase space is $\mathbb{R}^{2l}$, can be accomplished using Heisenberg-like translation operators,

$$\hat{T}_\xi = \mathrm{e}^{2\pi \mathrm{i} N(p\hat{q} - q\hat{p})} \qquad \xi = (q, p)$$

whose combinations like $\frac{1}{2}\left(T_{(n,0)}^\dagger + T_{(n,0)}\right)$ give rise to the periodic operators $D_0(V_n)$ defined above. These operators form a basis of N^2 Hermitian matrices. We work only in separable Hilbert spaces. In this case, we further assume, as required by lemma 2, that the operator $\hat{A}$ is trace-class: $\sum_n |\langle\phi_n| \hat{A} |\phi_n\rangle| < \infty$ for any orthonormal basis $\{|\phi_n\rangle\}$. This hypothesis assures that the manipulations in the beginning of the next section make sense mathematically. Thus $\hat{A}$ is in particular compact, and we can find N sufficiently large such that its projection $\hat{A}^{(N)}$ in the basis of periodic operators $\mathcal{B}_N$ satisfies $\|\hat{A} - \hat{A}^{(N)}\| < \delta$, where $\|\cdot\|$ is the operator norm. Note that δ does not depend on $\hbar$, but it may depend on N.

3. Quantum propagators

In this section, we write the lth power of the propagator in a form suitable for later application of the saddle point method. The expression is exact, and we make no approximations. We chose to work with hyperbolic cat maps without time-reversal symmetry. However, the semiclassical analysis can be applied to any quantum map which can be written in the form given in equation (10), for which it suffices to have a smooth generating function (twice differentiable classical generating function).

We begin by recalling somewhat briefly the stationary phase techniques for traces on the torus derived by Keating [15] and applied in a non-quadratic phase by Boasman and Keating [6]. The technique permits us to write an exact expression for the propagator in terms of infinite sums of integrals over the torus which will be later arranged in a finite sum of integrals over $\mathbb{R}$, thereby excluding edge effects when the stationary phase method is finally applied. A semiclassical trace formula for the density of states for quantum maps was first studied by Tabor [23].

The lth power of the propagator appears in the operator weighted density of states:

$$\begin{aligned}\rho(\theta,\epsilon,N;\hat{A}) &= \sum_n a_{nn}\delta_\epsilon(\theta-\theta_n)\\ &= \sum_n a_{nn}\sum_{l\in\mathbb{Z}} \mathrm{e}^{\mathrm{i}l(\theta-\theta_n)-\epsilon|l|}\\ &= \sum_{l\in\mathbb{Z}} \mathrm{e}^{\mathrm{i}\theta l-\epsilon|l|}\,\mathrm{Tr}(\hat{A}U^l).\end{aligned} \tag{6}$$

In the second equality we used Lorentzians for the smeared Dirac deltas, and U^l denotes the lth power of the propagator. The strategy now is to express the finite sums into a sum of integrals over $\mathbb{R}^{\nu(l)}$, using the Poisson summation formula.

Only in the following section shall we devise a semiclassical method for evaluating the traces in equation (6).

The unit step propagator $U(q',q)$ is the composition of a shear in momentum followed by the propagator of the cat map and then composed with a shear in position [10]:

$$U(q',q) = \mathcal{F}^\dagger U_{S_p}\mathcal{F}U_c U_{S_q}.$$

The shear in position is diagonal in momentum representation; let $G(p)$ denote its time-one Hamiltonian function (cf equation (3.8) in [3]). On the other hand, the shear in momentum is diagonal in the position representation and we denote by $-F(q)$ its time-one Hamiltonian function. All variables are discrete, ranging in $0, 1/N, \ldots, (N-1)/N$. $U(q',q)$ is an N^2 matrix, and we view q', q as its indices. We will have the opportunity to use the Poisson summation formula

$$\sum_{t\in\mathbb{Z}}\delta(x-t) = \sum_{k\in\mathbb{Z}} \mathrm{e}^{2\pi\mathrm{i}kx}. \tag{7}$$

The propagator is given by the product

$$U = U_1U_2$$

with

$$\begin{aligned}U_1 &= \mathcal{F}^\dagger\,\mathrm{e}^{-2\pi\mathrm{i}NG(p)}\delta_{p,p'}\mathcal{F}\\ U_2 &= \left(\frac{1}{\mathrm{i}N}\right)^{1/2}\exp\left[2\pi\mathrm{i}N\left(\frac{1}{2}(t_{11}q^2-2qq'+t_{22}q'^2)+F(q)\right)\right].\end{aligned}$$

Here U_2 is the propagator considered by Basilio de Matos and Ozorio de Almeida in [3]. The coefficients t_{11} and t_{22} come from the 2×2 cat map matrix, integer and unimodular: $g = \begin{bmatrix} t_{11} & t_{12}\\ t_{21} & t_{22}\end{bmatrix}$, which we take hyperbolic: $t_{11}+t_{22} > 2$.

Now

$$\begin{aligned}U_1(q',q) &= \frac{1}{N}\sum_{p=0}^{(N-1)/N}\exp[2\pi\mathrm{i}N(q'p-G(p)-qp)]\\ &= \int_0^1 \mathrm{d}p\sum_{k\in\mathbb{Z}}\delta(Np-k)\,\exp[2\pi\mathrm{i}N(q'p-G(p)-qp)]\\ &= \int_0^1 \mathrm{d}p\sum_{k\in\mathbb{Z}}\exp[2\pi\mathrm{i}N(p(q'-q-k)-G(p))]\end{aligned}$$

the second equality is true because $G(p+1) = G(p)$ and we used (7) in the last step.

Repeating the same steps as in the derivation of U_1, we get

$$U(q', q) = \sum_{r=0}^{(N-1)/N} U_1(q', r) U_2(r, q)$$
$$= N^{1/2}\, \mathrm{e}^{-\mathrm{i}\pi/4} \int_0^1 \mathrm{d}p \int_0^1 \mathrm{d}r \sum_{k,m\in\mathbb{Z}} \exp[2\pi \mathrm{i} N(S(q, r, p, q') - kp - mr)]$$

where

$$S(x_1, x_2, x_3, x_4) = x_3(x_4 - x_2) - G(x_3) + \tfrac{1}{2}\left(t_{11}x_1^2 - 2x_1x_2 + t_{22}x_2^2\right) + F(x_1) \tag{8}$$

$S(x_1, x_2, x_3, x_4)$ is the action of a unit step classical orbit. We define

$$\mathsf{x}_l = (x_1, \ldots, x_{3l+1}) \qquad l \geqslant 1$$
$$S_l(\mathsf{x}_l) = \sum_{i=1}^{l} S(x_{3i-2}, x_{3i-1}, x_{3i}, x_{3i+1}) \qquad l \geqslant 1 \tag{9}$$

and $S_1(\mathsf{x}_1)$ is also given by (8). This way the total action along the orbit is written as the sum of actions of steps in which x_{3i-2} is the initial position, x_{3i-1} the position before the shear in position, x_{3i} the final momentum, and x_{3i+1} the final position after the ith step.

Then $S_l(\mathsf{x}_l)$ denote the action for a classical orbit o of time length l. The vector x_l is such that its component x_{3j-2} is the jth position of the orbit o, x_{3j} is its jth momentum and x_{3j-1} are intermediate positions, before the jth shear in position, but x_{3j-1} will not be relevant for the main discussion.

Finally U^l can be written compactly as

$$U^l(q', q) = N^{3l/2-1}\, \mathrm{e}^{-\mathrm{i}l\pi/4} \sum_{\mathbf{k}\in\mathbb{Z}^{3l-1}} \int_{I^{3l-1}} \mathrm{d}\bar{\mathbf{x}}_l \exp\left[2\pi \mathrm{i} N(S_l(\mathsf{x}_l) - \mathbf{k}\cdot\bar{\mathbf{x}}_l)\right] \tag{10}$$

where $\bar{\mathbf{x}}_l = (x_2, \ldots, x_{3l})$, $I = [0, 1]$ and I^{3l-1} denotes the $(3l - 1)$-dimensional cube, and $q' = x_{3l+1}$ and $q = x_1$.

We have thus shown that U^l involves integration on the unit cube in $\mathbb{R}^{3l-1}$. The extra $2l$ integrations (compared with [6]) come exactly from the shear in position which introduces at each time step a pair of Fourier transforms. The shear in position breaks time-reversal symmetry.

Grouping the quadratic terms of the action we get the following expression for it,

$$S_l(\mathsf{x}_l) = \frac{1}{2}\mathsf{x}_l \cdot (Q_l \mathsf{x}_l) + \sum_{i=1}^{l} [F(x_{3i-2}) - G(x_{3i})]$$

where Q_l is a square matrix and the other nonlinear terms are sufficiently small so that Anosov's theorem applies. We recall that F is the perturbation associated with the shear in momentum while G is the perturbation coming from the shear in position. Both are periodic functions.

The reasoning below requires that the action S_l be twice differentiable and have isolated stationary points, but it need not be the generating function of a perturbed cat map.

4. Semiclassical analysis

The method we now explain for the semiclassical approximation of (1) is for large, but finite, dimension N. We fix an operator $\hat{A}$ acting on a Hilbert space, which can be infinite dimensional, in which case $\hat{A}$ is assumed trace-class. Under some mild conditions, we get a sequence of approximations of $\rho(\theta, \epsilon, N; \hat{A})$, with error decreasing as some power of $1/N$. These approximations are based on three ingredients: the decomposition of the operator $\hat{A}$ on $\mathcal{B}_N$, a stationary phase method which takes into account the operator phases and a control of the Fourier coefficients of the distribution of extremal actions of the dynamics.

We divide this section into two parts: in the first we show how to incorporate in the phase of the propagator the contribution of each separate component of the $N \times N$ matrix $\hat{A}$ and finally we use the stationary phase method in a conveniently defined subset of operators to obtain the leading order term in the asymptotic semiclassical series for $\rho(\theta, \epsilon, N; \hat{A})$. The dependence on N is to be understood as coming from different projections of the same fixed operator $\hat{A}$ (with some abuse in notation) acting on an infinite-dimensional separable Hilbert space $\mathcal{H}$, as discussed before lemma 2.

4.1. Accounts of the operator's phases

When evaluating the trace $\mathrm{Tr}(\hat{A}U^l)$, we first decompose $\hat{A}$ into the basis $\mathcal{B}_N$:

$$\mathrm{Tr}(\hat{A}U^l) = a_0\,\mathrm{Tr}(U^l) + \sum_{i=1}^{N-1}\left(a_i\,\mathrm{Tr}(U^l A_i) + b_i\,\mathrm{Tr}(U^l B_i) + \sum_{j=1}^{N-1} c_{ij}\,\mathrm{Tr}(U^l C_{ij})\right).$$

The phase of each periodic operator is linear in x_l.

Altogether we have four types of terms to consider: $\mathrm{Tr}(A_m U^l)$, $\mathrm{Tr}(B_n U^l)$, $\mathrm{Tr}(A_m B_n U^l)$ and $\mathrm{Tr}(B_n A_m U^l)$, where A_m is diagonal in position and B_n is diagonal in momentum (the identity term is included in the discussion of the first type).

Since we are to consider the phase of each operator, we have in fact a pair of stationary phase calculations for $\mathrm{Tr}(A_m U^l)$ and $\mathrm{Tr}(B_n U^l)$ and four stationary phase calculations for $\mathrm{Tr}(A_m B_n U^l)$ and $\mathrm{Tr}(B_n A_m U^l)$. For instance, $\mathrm{Tr}(A_m U^l)$ gives rise to terms of the form

$$N^{3l/2}\,\mathrm{e}^{-\mathrm{i}l\pi/4} \sum_{\mathbf{k}\in\mathbb{Z}^{3l}} \int_{I^{3l}} \mathrm{d}\mathbf{y}\,\exp\left[2\pi\mathrm{i}N\left(S_l(\mathsf{x}_l) - \mathbf{k}\cdot\mathbf{y} \pm \frac{m}{N}x_{3l}\right)\right]$$

where $\mathbf{y} = (x_1, \ldots, x_{3l})$, and $x_{3l+1} = x_1$ in x_l. In the terms containing B_n the extra Fourier transforms force the introduction of other two integrals. For instance, $\mathrm{Tr}(A_m B_n U^l)$ gives rise to the four terms

$$N^{3l/2+1}\mathrm{e}^{-\mathrm{i}\pi l/4} \sum_{\mathbf{k}\in\mathbb{Z}^{3l+2}} \int_{I^{3l+2}} \mathrm{d}\mathbf{y}\,\exp\left[2\pi\mathrm{i}N\left(S_l(\mathsf{x}_l) + x_{3l+2}(x_1 - x_{3l+1}) - \mathbf{k}\cdot\mathbf{y} \pm \frac{m}{N}x_1 \pm \frac{n}{N}x_{3l+2}\right)\right]$$

where $\mathbf{y} = (x_1, \ldots, x_{3l}, x_{3l+1}, x_{3l+2})$. The other two cases containing B_n give rise to integrals similar to this.

We note that the phases of A_m and B_n modify the total phase by adding to it a linear term in the initial position and final momentum respectively. Indeed, we have

Lemma 3. *For each periodic operator P, $\mathrm{Tr}\,PU^l$ is given by*

$$N^{\nu(l)}\,\mathrm{e}^{-\mathrm{i}l\pi/4} \sum_{\mathbf{k}\in\mathbb{Z}^{\nu(l)}} \int_{I^{\nu(l)}} \mathrm{d}\mathbf{y}\,\exp\left[2\pi\mathrm{i}N\Phi_l(\mathbf{k},\mathbf{y})\right]$$

where the total phase Φ_l is

$$\Phi_l(\mathbf{k},\mathbf{y}) = \frac{1}{2}\mathbf{y}\cdot Q_l\mathbf{y} - \mathbf{k}\cdot\mathbf{y} + \sum_{i=1}^{l}(F(x_{3i-2}) - G(x_{3i})) + \phi_A(\mathbf{y}) + \phi_B(\mathbf{y})$$

and $\nu(l) = 3l$ *if P is diagonal in position, and* $\nu(l) = 3l + 2$ *otherwise. Moreover* $\phi_{A,B}$ *are linear functionals with* rational coefficients*:* j/N*, and* Q_l *is a* $\nu(l) \times \nu(l)$ *matrix with integer coefficients.*

Now the periodicity of the non-quadratic terms implies, for any $\mathbf{M} \in \mathbb{Z}^{\nu(l)}$,

$$\Phi_l(\mathbf{k}, \mathbf{y} + \mathbf{M}) = \frac{m}{N} + (Q_l\mathbf{M}) \cdot \mathbf{y} + \Phi_l(\mathbf{k}, \mathbf{y}) \pmod 1 \tag{11}$$

for some $m \in \mathbb{Z}$ that depends on $\mathbf{M}$. Therefore the function $\psi = \mathrm{e}^{2\pi \mathrm{i} N \Phi_l(\mathbf{k},\mathbf{y})}$ is periodic in $\mathbb{R}^{\nu(l)}$. The infinite sum on $\mathbb{Z}^{\nu(l)}$ of the integral over cubes $I^{\nu(l)}$ can be decomposed into a finite sum over a parallelopiped $\square$—defined as the fundamental period of ψ—of integrals over $\mathbb{R}^{\nu(l)}$ (exactly as in Boasman and Keating [6]).

Lemma 4. *For each periodic operator* P, Tr PU^l *is given by*

$$N^{\nu(l)}\, \mathrm{e}^{-\mathrm{i}l\pi/4} \sum_{\mathbf{k}\in\square} \int_{\mathbb{R}^{\nu(l)}} \mathrm{d}\mathbf{y} \exp[2\pi \mathrm{i} N(\tilde{S}_l(\mathbf{y}) - \mathbf{k}\cdot\mathbf{y} + \phi_A(\mathbf{y}) + \phi_B(\mathbf{y}))] \tag{12}$$

where $\tilde{S}_l(\mathbf{y}) = \frac{1}{2}\mathbf{y}\cdot Q_l\mathbf{y} + \sum_{i=1}^{l}(F(x_{3i-2}) - G(x_{3i}))$ *contains the phase nonlinear terms.*

So far, we have not made any approximation to perform the trace. Now we are ready to use the stationary phase method.

Remark 2. It is clear that $\mathrm{Tr}(A_m B_n U^l)$ and $\mathrm{Tr}(B_n A_m U^l)$ need not be equal. However, their real stationary points are related so that their corresponding phases differ by $\frac{nm}{N^2}\pi$ (modulo some other $\pi/2$ phases) cancelling out the sine that we divided $[A_m, B_n]$ to define C_{mn}. This calculation is in appendix B.

From the numerical point of view, the phases $\phi_{A,B}$ can be considered as perturbations of the action of the cat map, therefore we can safely use the unperturbed orbits as initial guesses in Newton's method to determine the stationary *tilted orbit* for each term in the outer sum of (12). Note also that, since $\phi_A = \pm\frac{m}{N}x_1$, an orbit repetition will not give rise to a stationary tilted orbit equal to the repetition of the corresponding shorter stationary tilted orbit. This makes the calculations even longer; yet another difference of formula (12) and standard periodic orbit sums. It is obvious, but worth stressing, that the stationary phases are close, but are not equal to the periodic orbit actions (plus some Maslov index).

The steps made up to now obtained N^2 integrals, each coming from a different component of the operator $\hat{A}$, whose phases will influence the coordinates of the stationary phase points. Thus we shall not write a formula for the sum over stationary phase points, which only in the identity component are the periodic orbits.

4.2. Conclusion of the algorithm and error estimate

Note that the number of points with integer coordinates in the parallelopiped $\square$ is given by $\det Q_l$ (see lemma 3), which can be shown to be the number of fixed points of g^l, where g is the unperturbed hyperbolic map [6, 15]. Hence the real stationary points $\nabla_{\mathbf{y}}\Phi_l = 0$ are in one-to-one correspondence with those of the unperturbed case. In particular, the number of stationary points of the phase does not change if we add linear terms, independent of their size. This last remark is important since the phases of the periodic operators are, by construction, linear functionals of $\mathbf{y}$.

We use the stationary phase method for the integrals in lemma 4 as in [17], and take only the leading order term. To derive an estimate for the error in using the decomposition (5) keeping, for each periodic operator, only the leading order term in the asymptotic series in $\frac{1}{N}$, we resort to a probabilistic approach. From remark 1, we know that each coefficient in the expansion for the *trace* of a Hermitian matrix is a real number in an interval whose length does not exceed $\frac{k}{\sqrt{N}}$, for some constant k. Now an $N \times N$ Hermitian matrix is determined by such N^2 coefficients.

We use the Chebyshev inequality [13],

Lemma 5. *If $X_1, \ldots, X_{N^2}$ are independent random variables uniformly distributed in $\left[-\frac{1}{\sqrt{N}}, \frac{1}{\sqrt{N}}\right]$, then*

$$P\left(\left|\sum_i X_i\right| \geqslant 1\right) \leqslant \frac{2}{3\sqrt{N}}.$$

Let $Y(\alpha)$ denote the set of Hermitian operators $\hat{A}$ in a separable Hilbert space such that $\sum_i |\langle e_i| |e_i\rangle| \leqslant \alpha$. Let a_i, b_j, c_{ij} be the coefficients of the projection $O^{(N)}$ of some $\hat{A} \in Y(\alpha)$ according to equation (5). In $Y(\alpha)$, for each N, we have a product probability measure, which we denote by P, with support contained in $\prod_{i=0}^{N^2-1}[-\alpha_i, \alpha_i]$, with $\alpha_0 = \frac{\alpha}{N}, \alpha_i = \frac{2\alpha}{N}, i = 1, \ldots, 2N-1$ and $\alpha_i = \frac{C}{\sqrt{N}}$ for $i \geqslant 2N$, for some constant C, as given in lemma 2 and remark 1.

Every trace-class operator is compact, therefore $\|\hat{A} - A^{(N)}\| \to 0$. Moreover, since $\hat{A}$ is also Hermitian, the spectral radius equals the operator norm. The spectrum of $\hat{A} - A^{(N)}$ is summable therefore

$$\|\hat{A} - A^{(N)}\| < \frac{C}{N^{1+\delta}} \qquad \text{for some} \qquad \delta > 0$$

for every $\hat{A} \in Y(\alpha)$. Thus, for sufficiently large $N \geqslant N_0$, $\|\hat{A} - A^{(N)}\| < \frac{1}{N}$. Since we obtain only the leading order term for $A^{(N)}$, the requirement that N is sufficiently large gives an upper bound on the interference between the difference between different projections $A^{(N)} - A^{(N')}$ and the semiclassical approximation.

Let

$$\mathring{Y}(\alpha) = \left\{ \hat{A} \in Y(\alpha) \text{ and } \left| a_0 + \sum_i \left(a_i + b_i + \sum_j c_{ij} \right) \right| < \alpha \right\}.$$

Applying Chebyshev's inequality, we note that $\mathring{Y}(\alpha)$ is a subset of $Y(\alpha)$ probability measure $1 - C(\alpha)/\sqrt{N_0}$, where C depends only on α and N_0 may depend on $\hat{A}$.

We assume that there is a single real stationary phase point $\nabla\Phi_l = 0$ for each $\mathbf{k} \in \Box$. This implies the condition that each periodic orbit is isolated in phase space, and the so-called hyperbolic systems—among which are the hyperbolic cat maps—fulfil this condition. Observe that sometimes the term *chaotic* refers to systems where this assumption does not hold.

Proposition 1. *If $\hat{A} \in \mathring{Y}(\alpha)$ and $A^{(N)}$ is its projection on the basis $\mathcal{B}_N$, then for large enough N*

$$|\mathrm{Tr}(A^{(N)}U^l) - \mathrm{Tr}_{sc}(A^{(N)}U^l)| \leqslant \frac{K}{N}$$

for some constant K, and where

$$\mathrm{Tr}_{sc}(A^{(N)}U^l) = \sum_{P \in \mathcal{B}_N} a_p \,\mathrm{Tr}_{sc}(PU^l) \qquad a_p = \mathrm{Tr}(PA^{(N)})$$

i.e., it denotes the linear combination of the stationary phase method applied to the traces of the periodic operators composed with U^l. $\mathrm{Tr}_{sc}(PU^l)$ *denotes the leading order term in the semiclassical asymptotic series on powers of* $1/N$ *of the integral in equation (12).*

Proof. We just have to note that the difference $\mathrm{Tr}(A^{(N)}U^l) - \mathrm{Tr}_{sc}(A^{(N)}U^l)$ is a sum of the form

$$\sum_p a_p R_p$$

where R_p is $O(1/N)$ according to the stationary phase method. Using Hölder's inequality, since $\hat{A} \in \mathring{Y}(\alpha)$, $\left|\sum_p a_p R_p\right| \leqslant \alpha \max_p |R_p| \leqslant \frac{K(\alpha)}{N}$. □

To truncate the sum over periods, we will need a property of the distribution of the actions of periodic orbits. For each $\mathbf{k} \in \Box$, the leading order term is approximately

$$\mathrm{e}^{-\mathsf{h}_\mu l/2}\, \mathrm{e}^{2\pi \mathrm{i} N \Phi_l(\mathbf{k},\mathbf{y}_k)}$$

where h_μ denotes the *metric entropy* and $\Phi_l(\mathbf{k}, \mathbf{y}_k)$ the stationary phase.

We first estimate a related sum. Let us write

$$\Phi_l(\mathbf{k}, \mathbf{y}) = \Psi_l(\mathbf{k}, \mathbf{y}) + \phi(\mathbf{y})$$

where ϕ contains the phase coming from a periodic operator. We know that Ψ_l contains the action coming from an orbit of length l and, when $\phi \equiv 0$, the stationary phase points $\mathbf{y}_k$ are the periodic orbits of period l. Ψ_l is the sum of the generating function S of the map lifted to $\mathbb{R}^2$, cf equation (9). The sum

$$\sum_{\mathbf{k}\in\Box} \mathrm{e}^{2\pi \mathrm{i} N \Psi_l(\mathbf{k},\mathbf{y}_k)} \tag{13}$$

is asymptotically for large l given by

$$\frac{\mathrm{e}^{\mathsf{h}l}}{l} \int \mathrm{e}^{2\pi \mathrm{i} N S(p,q)}\, \mathrm{d}q\, \mathrm{d}p \tag{14}$$

with h denoting the *topological entropy*, using the equipartition of orbits [20]. For large N, this scales like $1/N$.

It is not immediately clear if a similar scaling should be valid when $\phi \neq 0$. Partition the interval $[0, 1)$ into intervals $I_0 = [0, \phi_1)$, $I_k = [\phi_k, \phi_{k+1})$, where $\phi_k = \frac{k}{M}$. If $\varphi \in I_i$, we put

$$r_M(\varphi, l) = \#\{\mathbf{k} \in \Box \mid \{\Psi_l(\mathbf{k}, \mathbf{y}_k)\} \in I_i\}$$

where $\{\cdot\}$ denotes the fractional part, and

$$r_M(\varphi, M) = \limsup_{l\to\infty} \frac{r_M(\varphi, l)}{\mathrm{e}^{\mathsf{h}l}/l}. \tag{15}$$

We note that $r_M(\varphi)$ is positive, bounded and defined as a sup-limit of simple functions. Since the intervals on which $r_M(\varphi, l)l\, \mathrm{e}^{-\mathsf{h}l}$ is constant depend only on M, $r_M(\varphi)$ is simple too. The sequence of functions $r_M(\varphi)$ satisfies for every M:

$$\sum_{i=1}^{M} r_M(\varphi_i) = 1 \quad \Leftrightarrow \quad \int_0^1 (M\, r_M(\varphi))\, \mathrm{d}\varphi = 1. \tag{16}$$

Here $r_M(\varphi)$ counts the proportion of phases falling on an interval of length $1/M$. These phases are, by transversality of $\Psi_l(\mathbf{k}, \mathbf{y})$, for different $\mathbf{k}$, different for each orbit. We put

$$r(\varphi) = \liminf_{M\to\infty} M\, r_M(\varphi)$$

which, by Fatou's lemma, is in $L^1([0,1])$. r is a probability measure. From property (16) it follows that $r(\varphi)$ is almost everywhere bounded. Indeed, if $\varphi \in E \subset [0,1)$ is such that $r(\varphi) \to \infty$, then $m(E) = 0$. Otherwise for M sufficiently large, there are $I_1, \ldots, I_k$ covering E, with $I_i \cap E \neq \emptyset$ such that

$$r_M(\varphi) > \frac{2}{Mm(E)} \geqslant \frac{2}{k} \Rightarrow \sum_{i=0}^{M} r_M(\varphi_i) > 2.$$

Now note that

$$\sum_{\mathbf{k}\in\Box} \cos(2\pi N \Psi_l(\mathbf{k}, \mathbf{y}_k)) = \frac{\mathrm{e}^{\mathsf{h}l}}{l} \sum_i r_M(\varphi_i) \cos(2\pi N \varphi_i) + C_1 \frac{N\,\mathrm{e}^{\mathsf{h}l}}{lM}$$

where the last term is the error coming from approximating $\cos(2\pi N \Psi_l(\mathbf{k}, \mathbf{y}_k))$ by $\cos 2\pi N\varphi_i$. We take M sufficiently larger than N, namely $M/N = o(1)$. Approximating the first sum by an integral (this trapezoidal rule produces an error of the order of $1/M$, hence negligible), the scaling equation (14) yields

$$\hat{r}(N) = \int_0^1 r(\varphi)\, \mathrm{e}^{2\pi \mathrm{i} N\varphi}\, \mathrm{d}\varphi = O(1/N)$$

which, by Wiener's theorem, implies that r is a continuous measure (with no discrete part).

Define $p_M(\varphi, l) = \#\{\mathbf{k} \in \Box \,|\, \{\Phi_l(\mathbf{k}, \mathbf{y}_k)\} \in I_i\}$ and $p(\varphi)$ analogously. The stationary phase points $\mathbf{y}_k$ for $\Phi_l(\mathbf{k}, \mathbf{y})$ are linked to those of $\Psi_l(\mathbf{k}, \mathbf{y})$ by the convergence of Newton's method, when one *turns on* the linear term $\phi(\mathbf{y})$. Thus $\mathbf{y}_k$ remain approximately equidistributed, and thus $\phi(\mathbf{y})$ mod 1 is approximately equidistributed as well. Therefore $p(\varphi)$, being the density of phases Φ_l, remains continuous. However, this gives us the bound $\hat{p}(n) = o(1/n^{1/2})$. What is essential again is the transversality of the various $\Phi_l(\mathbf{k}, \mathbf{y})$, and this is enough to imply that $p(\varphi)$ is bounded almost everywhere and a continuous measure.

The above sum may be written as an integral over [0, 1),

$$\frac{\mathrm{e}^{\mathsf{h}l}}{l} \int_0^1 \mathrm{e}^{2\pi \mathrm{i} N\varphi}\, \mathrm{d}\mu_l$$

where

$$\mathrm{d}\mu_l = \frac{l}{\mathrm{e}^{\mathsf{h}l}} \sum_{\mathbf{k}\in\Box} \delta(\varphi - \varphi_k)\, \mathrm{d}\varphi$$

and $\varphi_k = \Psi_l(\mathbf{k}, \mathbf{y}_k)$ are the stationary phases modulo 1. If μ is a weak-star limit of μ_l, the scaling (14) is translated to $\hat{\mu}(N) = O(1/N)$, which by Wiener's theorem implies that μ is a continuous measure. A side remark is that for each period l, the stationary phases are different for different $\mathbf{k}$, by transversality. Since μ_l tends to continuous measures, one has a stronger property that for any φ,

$$\lim_{\epsilon\downarrow 0} \int_{\varphi-\epsilon}^{\varphi+\epsilon} \mathrm{d}\mu = 0$$

which implies that the count of phases near an arbitrary point,

$$\#\{\mathbf{k} \in \Box : \varphi - \epsilon < \varphi_k < \varphi + \epsilon\} = o(\mathrm{e}^{\mathsf{h}l}/l) \tag{17}$$

for ϵ small enough.

The stationary phase points $\mathbf{y}_k$ for $\Phi_l(\mathbf{k}, \mathbf{y})$ are linked to those of $\Psi_l(\mathbf{k}, \mathbf{y})$ by the convergence of Newton's method, when one *turns on* the linear term $\phi(\mathbf{y})$. Thus the set $\{\mathbf{y}_k, \mathbf{k} \in \Box\}$ remain approximately equidistributed, and thus $\phi(\mathbf{y})$ mod 1 is approximately equidistributed as well. Hence, defining ν as the density of stationary phases coming from Φ_l, (17) remains valid, and using Wiener's theorem the other way around, $\hat{\nu}(N) = o(1/N^{1/2})$.

Proposition 2. *ν is a probability measure with no discrete component.*

Note that $d\nu$ is a classical function: it is the probability density of the extremal actions (modulo 1).

Remark 3. If one could prove, for instance, that μ is absolutely continuous, then ν could be expected to inherit the same property.

Summing up, we have to leading order in N

$$e^{-\mathsf{h}_\mu l/2} \sum_{\mathbf{k}\in\square} \cos(2\pi N \Phi_l(\mathbf{k})) = \frac{\tilde{C}\, e^{(\mathsf{h}-\mathsf{h}_\mu/2)l}}{l N^a} \qquad a > 1/2$$

Recall that Tr_{sc} is defined in proposition 1. We can now state our result

Theorem 1. *For N large enough, consider the operator weighted density of states*

$$\rho(\theta, \epsilon, N; \hat{A}) = \sum_{l\in\mathbb{Z}} e^{i\theta l - \epsilon|l|} \mathrm{Tr}(A^{(N)} U^l)$$

for trace-class operators $\hat{A}$ in a set $\mathring{Y}(\alpha)$ of probability $1 - C/\sqrt{N}$. Then for $\epsilon > \mathsf{h} - \mathsf{h}_\mu/2$, the semiclassical operator weighted density of states

$$\rho_{sc}(\theta, \epsilon, N; \hat{A}) = \sum_{l=-L}^{L} e^{i\theta l - \epsilon|l|}\, \mathrm{Tr}_{sc}(A^{(N)} U^l) \tag{18}$$

satisfies the error estimate

$$\Delta(N) \stackrel{\mathrm{def}}{=} \sup_\theta |\rho(\theta, \epsilon, N; \hat{A}) - \rho_{sc}(\theta, \epsilon, N; \hat{A})| \leqslant \frac{K}{N^a} \tag{19}$$

with $a \in (1/2, 1]$, for some constant K.

Proof. The neglected terms of order $1/N$ from the stationary phase applied to the traces $\mathrm{Tr}_{sc}(A^{(N)} U^l)$, up to period L, have their contribution to $\Delta(N)$ bounded by

$$d_1 = \frac{C_1}{N}\left(1 + 2e^{(\mathsf{h}-\mathsf{h}_\mu/2-\epsilon)} \frac{1 - e^{(\mathsf{h}-\mathsf{h}_\mu/2-\epsilon)L}}{1 - e^{\mathsf{h}-\mathsf{h}_\mu/2-\epsilon}}\right)$$

using that $\epsilon > \mathsf{h} - \mathsf{h}_\mu/2$.

For the late terms, the discussion before the statement gave the bound, for each periodic operator,

$$d_2 = 2C_2 \frac{e^{(\mathsf{h}-\mathsf{h}_\mu/2-\epsilon)(L+1)}}{(L+1)N^a}$$

with $a > 1/2$. The sum over the basis follows the same argument as in the proof of proposition 1. □

From formula (18) and proposition 1, we see that the operator intervenes in the classical spectrum contributing to the semiclassical approximation of the (smeared) weighted density of states. Indeed the Fourier transform of (18), with respect to $\hbar$, would not show peaks on the actions of short periodic orbits.

The numerical examples shown in the next section will leave some directions for further research. Since the Fourier analysis is over phase space, a question that arises is about families of operators localized in momentum and position, so defined by their components in the basis $\mathcal{B}_N$. Another interesting question would then try to probe contributions of chosen periodic orbits without so much smearing of the eigenvalues by adjusting the support of the operators.

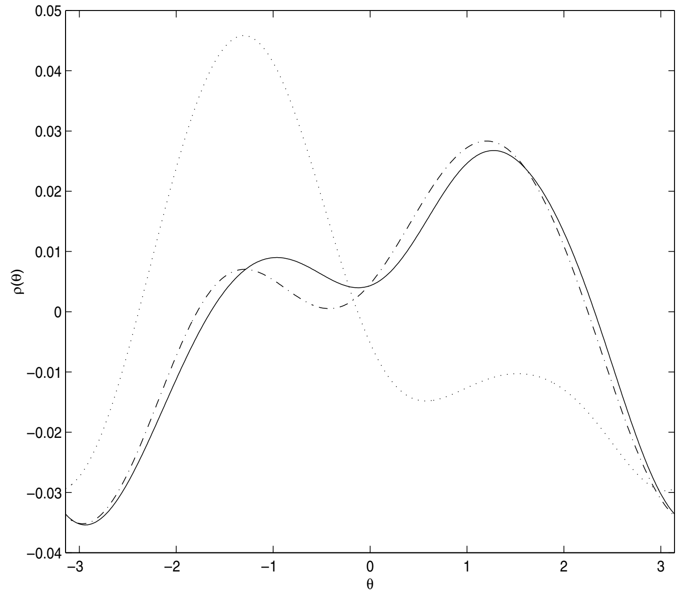

Figure 1. Comparison between quantum (solid line), semiclassical calculation given in (18) (dash-dotted curve) and semiclassical periodic orbit calculation as in [11] (dotted curve) for a diagonal operator with random entries, $N = 107$ and $\frac{\epsilon}{2\pi} = 0.25$. Orbits of period up to 3 were used.

5. Numerical illustrations

We give three kinds of examples comparing the quantum and semiclassical weighted density of states (1) and (18). A final example is shown comparing the predictions of the error of this semiclassical technique $\Delta(N)$, equation (19), with respect to N.

We work with the quantized cat map prescribed the choices:

$$g = \begin{bmatrix} 2 & 3 \\ 1 & 2 \end{bmatrix}$$
$$F(q) = \frac{\kappa_q}{4\pi^2} x(\sin(2\pi q) - 0.5\cos(4\pi q)) \qquad \kappa_q = 0.08$$
$$G(p) = \frac{\kappa_p}{4\pi^2} (\cos(2\pi p) - 0.5\sin(4\pi p)) \qquad \kappa_p = 0.03.$$

We considered $\hat{A}$ a diagonal matrix with random entries first, for a comparison with the periodic orbit series in [11]. It is verified that this semiclassical theory for (1) does not work, since one cannot expect the symbol of $\hat{A}$ to be smooth on small scales in phase space. We used as its symbol its Fourier decomposition, as explained in section 2. This prevented a totally independent comparison, but, to our knowledge, the symbol of a random matrix has no alternative definition than that outlined in section 2. We see in figure 1 a good agreement between (1) and (18).

The second example uses a full Hermitian random matrix: $C = (V + V^t) + \mathrm{i}(W - W^t)$, where V^t is the transpose of V; W and V are random matrices with real entries uniformly distributed in $(0, 1)$. Results displayed in figure 2 show a good agreement.

In the third example, we take a family of projections on some eigenstates of the propagator, see figure 3. The levels are sorted with increasing eigenvalue θ_k, ranging from $-\pi$ to π. A remarkable symmetry between the various semiclassical graphs was observed here, probably

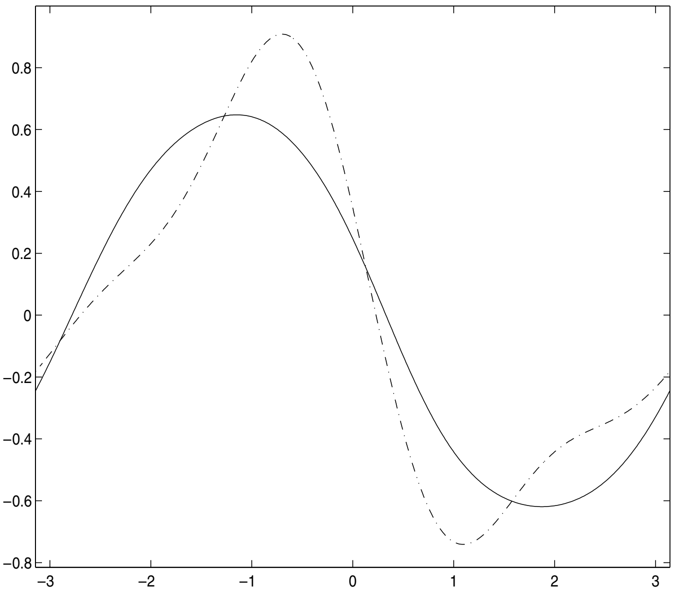

Figure 2. Comparison between quantum (solid line) and semiclassical calculation (18) given for a random Hermitian matrix; $N = 73$ and $\frac{\epsilon}{2\pi} = 0.25$. Orbits of period up to 3 were used.

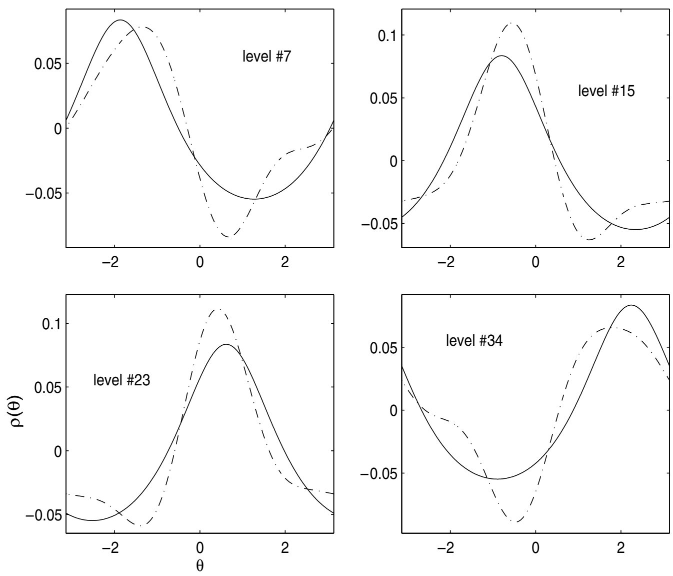

Figure 3. Comparison between equations (1) and (18) when the operator is a projection onto one eigenstate; the quantum curve is solid. Here $N = 37$ and $\frac{\epsilon}{2\pi} = 0.25$. Orbits of period up to 3 were used.

due to the small Hilbert space dimension: $N = 37$. If $19 - n = j - 19$, then $\rho_n(\theta) \approx \rho_j(-\theta)$, where ρ_k is the operator weighted density of states for $\hat{O}$ equals the projection onto eigenstate k.

The modest dimensions of the matrices $N = 107$, $N = 79$ or $N = 37$ are justified by computer limitations (a Pentium II was used). The same reason excuses the generous

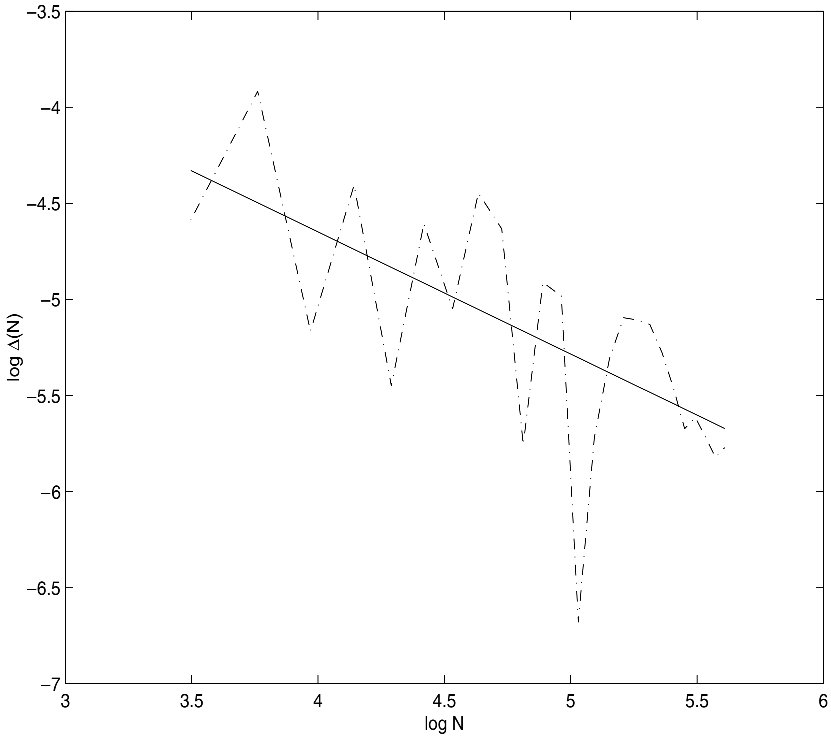

Figure 4. For N in the interval [33, 253] in steps of 10, the uniform difference of ρ and ρ_{sc}, with respect to θ, is evaluated numerically, showing an oscillatory decaying behaviour. The fitting line obtains the decaying rate $a = 0.63$ approximately, a as in equation (19). Here $\frac{\epsilon}{2\pi} = 0.25$ and orbits of period up to 3 were used to evaluate ρ_{sc}.

smearing $\frac{\epsilon}{2\pi} = 0.25$, about twice the lower bound given in theorem 1. For comparison of convergence, we considered orbits up to period 4, it took about 10 hours for the example with the random matrix, with $N = 37$ and $\frac{\epsilon}{2\pi} = 0.2$, but no significant convergence to the quantum curve was observed.

To check the behaviour of the difference of this semiclassical approximation to the quantum ρ, we produced figure 4. We used a random operator $\hat{A}$, a banded matrix of dimension 273, with off-diagonal elements a_{ij} different from zero only for $|i - j| < 25$. We further required that $\|\hat{A} - A^{(k)}\| < 1/k$ for each $N_j = 33 + 10j$, $j = 0, \ldots, 24$ and to achieve this, we modulated the random entries in each diagonal by the decaying function $1/k^{-1.2}$. Furthermore if $l = |i - j|$ is the distance from the diagonal, the random elements had the amplitude diminished by a factor $l^{-0.2}$. We made enough tests, with different choices of definition of $\hat{A}$, the exponent a appearing in equation (19) being less than 1, for small N.

Starting at such small values of N was necessary for a significant variation on $\log N$. A larger value of the decaying rate a is expected if longer orbits are used.

Acknowledgments

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Appendix A. Commutators

We list below all cases for the commutators $C_{mn} = \frac{1}{\mathrm{i}\sin(\pi\mu\nu/N)}[A_m, B_n]$,

$$C_{mn} = \begin{cases} \frac{1}{\mathrm{i}}\left[D_\nu\left(\sin\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right) - D_\nu^\dagger\left(\sin\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right)\right] & \text{if} \quad m, n \leqslant \bar{N} \\ -\frac{1}{\mathrm{i}}\left[D_\nu\left(\cos\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right) - D_\nu^\dagger\left(\cos\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right)\right] & \text{if} \quad n \leqslant \bar{N} < m \\ -\left[D_\nu\left(\sin\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right) + D_\nu^\dagger\left(\sin\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right)\right] & \text{if} \quad m \leqslant \bar{N} < n \\ \left[D_\nu\left(\cos\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right) + D_\nu^\dagger\left(\cos\left(\frac{2\pi\mu}{N}(k+\nu/2)\right)\right)\right] & \text{if} \quad \bar{N} < m, n \end{cases}$$

where $\bar{N} = \left\lceil \frac{N-1}{2} \right\rceil$, $\mu = \begin{cases} m & \text{if } m \leqslant \bar{N} \\ m - \bar{N} & \text{if } m > \bar{N} \end{cases}$ and analogously for ν in terms of n, and assuming N does not divide $\mu\nu$.

Appendix B. On the stationary phase of C_{mn} operators

It will be noted that it is sufficient to analyse the case $\mathrm{tr}\, C_{mn}U$. B_n contains two terms of the form

$$B_n(x, y) = \frac{1}{N} \sum_{p=0}^{(N-1)/N} \mathrm{e}^{2\pi\mathrm{i}N((y-x)p \pm \frac{n}{N})p}$$

hence the phase takes the form (for $\mathbf{k} = 0$)

$$\Phi_{AB} = x_5(x_1 - x_4) - \frac{n}{N}x_5 + \frac{m}{N}x_4 + \left[x_3(x_4 - x_2) - G(x_3) + \frac{1}{2}\left(t_{11}x_1^2 - 2x_1x_2 + t_{22}x_2^2\right) + F(x_1)\right]$$

whereas

$$\Phi_{BA} = x_5(x_1 - x_4) - \frac{n}{N}x_5 + \frac{m}{N}x_1 + \text{same}.$$

The following systems are obtained from the stationary phase condition:

$$\begin{array}{ll} \nabla\Phi_{BA} = 0 & \nabla\Phi_{AB} = 0 \\ x_5 + t_{11}x_1 - x_2 + f(x_1) = 0 & x_5 + t_{11}x_1 - x_2 + f(x_1) = -\frac{m}{N} \\ -x_3 - x_1 + t_{22}x_2 = 0 & -x_3 - x_1 + t_{22}x_2 = 0 \\ x_4 - g(x_3) = 0 & x_4 - g(x_3) = 0 \\ -x_5 + x_3 = -\frac{m}{N} & -x_5 + x_3 = 0 \\ x_1 - x_4 = \frac{n}{N} & x_1 - x_4 = \frac{n}{N} \end{array}$$

and eliminating x_5 we obtain two equivalent systems. The only difference is $x_5(BA) = x_5(AB) + \frac{m}{N}$. Hence the stationary phases for this pair of terms (there are four pairs of terms altogether) satisfy $\Phi_{BA} = \Phi_{AB} - \frac{nm}{N^2}$.

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