Multiplicative semiclassical dynamics and the quantization time

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We study smooth, caustic-free, chaotic semiclassical dynamics on two-dimensional phase space and find that the dynamics can be approached by an iterative procedure that constructs an approximation to the exact long-time semiclassical propagator. Semiclassical propagation all the way to the Heisenberg time, where individual eigenstates are resolved, can be computed in polynomial time, obviating the need to sum over an exponentially large number of classical paths. At long times, the dynamics becomes quantumlike, given by a matrix of the same dimension as the quantum propagator. This matrix, however, differs both from the quantum and the one-step semiclassical propagators, allowing for the study of the breakdown of the semiclassical approximation. The results shed light on the accuracy of the Gutzwiller trace formula in two dimensions, and on the source of long-time periodic orbit correlations. [S1063-651X(98)12208-0]

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I. INTRODUCTION

Semiclassical methods have a long history dating back to the very beginnings of quantum mechanics, and have provided insight into many properties of quantum-mechanical systems. These methods provide a bridge, expressing quantum behavior in terms of classical paths and their corresponding actions. In integrable systems, the connection between quantum and classical behavior is well understood through Einstein-Brillouin-Keller (EBK) quantization techniques, which lead to an intuitive understanding of the quantum properties of these systems. For a nonintegrable system, it is not nearly as clear how much of the quantum behavior (e.g., spectrum, eigenstates, long-time dynamics, transport) can be understood via semiclassical methods. One would like to be able to separate out those features of the quantum behavior that can thus be explained in terms of interference between classical paths from the ''hard quantum effects,'' such as diffraction and tunneling.

Although the Van-Vleck formula describing short-time quantum behavior in terms of classical paths has been around for many years, it is only starting with the work of Gutzwiller [1] that it has been possible to try to understand long-time quantum properties in terms of classical behavior. Much insight is given by the Gutzwiller trace formula in the energy domain, which relates the quantum spectrum to a sum over classical periodic orbits. However, the formula is a formal expression, which needs to be resummed to get convergence in the limit where more and more orbits are included [2]. Furthermore, in practice summing over long orbits (ones with period comparable to $\hbar$ times the density of states of the system, so that individual eigenstates can be resolved) is not feasible, because the number of classical orbits grows exponentially with time in a chaotic system. Special cases are known for which the long-time semiclassical dynamics can be computed exactly, e.g., the cat map and geodesic flows on surfaces of constant negative curvature. However, the semiclassical evolution for these systems is in fact the same as the quantum evolution because of their linearity (or homogeneity in the case of constant negative curvature), making them less interesting as a testing ground for the general applicability of semiclassical methods. Cycle expansion methods, which use the symbolic dynamics of the underlying classical system to express long periodic orbits in terms of shorter ones, have been very important in this regard [3].

However, this still leaves open the question of the properties of the semiclassical dynamics in the time domain. Much important work here has been done in systems like the stadium billiard and the baker's map [4]. Numerical evidence was produced, and theoretical arguments given, showing clearly that the semiclassical approximation works well past the mixing time of the system, where multiple stationary paths contribute to the quantum propagator, and where the purely classical approximation (without interference effects) breaks down completely. This was initially somewhat surprising, because after the mixing time the classical dynamics begins generating structures in phase space on scales smaller than Planck's constant, while the quantum dynamics washes out any information on these scales. Thus the semiclassical approximation tries to follow the quantum propagator by summing over an exponentially large number of paths. This exponential proliferation of classical paths prevents one from performing meaningful long-time quantum-semiclassical comparisons for small values of $\hbar$ (large Heisenberg time). The fact that the quantum propagator effectively smears out all of the sub-$\hbar$ structure in phase pace, and thus contains an amount of information that scales only as a power law in $\hbar$, suggests that some such reduction may also be possible in the semiclassical calculation. This is important because *a priori* it is not at all obvious (i) that the long-time semiclassical dynamics converges in the sense of having well defined stationary states at the Heisenberg time, or for that matter (ii) that in those cases where the semiclassical dynamics does converge, what it converges to actually approximates the quantum dynamics, stationary states, etc. The breakdown of semiclassical validity, in particular in the presence of diffraction, discontinuities, and caustics, is also a somewhat controversial issue that has been difficult to address in practice because of the computational obstacles.

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A key reason for the finiteness of long-time information in the quantum case is the multiplicativity of the quantum propagator. In other words, the long-time dynamics can be obtained by simply iterating the short-time propagation (matrix multiplication in the case of a finite-dimensional Hilbert space). The semiclassical dynamics does not share this property because concatenations of classical paths in general produce paths that are *not* classical. Stationary phase integrals must be performed to obtain the long-time semiclassical propagator from shorter steps, and the number of stationary phase points grows exponentially with time. An interesting way to make the semiclassical dynamics multiplicative by extending the space on which the multiplicative operator acts has been described by Cvitanović and Vattay [5]. It has also been seen that in the special case of the baker's map, the long-time dynamics can be computed with good accuracy in polynomial time using the Heisenberg uncertainty principle and the exponential decay of time correlations in chaotic systems [6]. These methods (of which three are known to the author) effectively collect together all contributions from classical paths that come together on scales much smaller than $\hbar$. Semiclassical amplitude thus collected can then be propagated again, thus making the resulting dynamics multiplicative. All the methods, however, made use of the simple symbolic dynamics of the baker's map and its very special structure in position and momentum space. Some of the ideas of consolidation on sub-$\hbar$ scales, however, may yet turn out to be fruitful in analyzing more generic systems, with no such special structure.

In this paper, we take a somewhat different approach to the problem, inspired by the fact that in the baker's map we have found that a good approximation to the long-time semiclassical dynamics could be obtained even if one periodically projects the higher-dimensional semiclassical vector onto the N-dimensional quantum space. In other words, the true semiclassical dynamics is evaluated exactly for T_Q steps. (T_Q is called the quantization time, and can be thought of as the time domain analog of the T^* parameter in the spectral theory of Bogomolny and Keating [7]. One should note, however, that in periodic orbit theory, the critical time T^* should scale as the mixing time, logarithmically with $\hbar$, whereas our scale T_Q is of order 1 in units of the shortest periodic orbit. See the discussion in Sec. V.) Matrix elements are then taken between quantum states, producing a matrix of the same dimension as the quantum propagator. This matrix is then iterated to produce an approximation to the long-time semiclassical behavior. Now for $T_Q=1$ this is very reminiscent of Bogomolny's approach to quantization [8]. It should be noted, however, that for $T_Q=1$, this procedure does *not* produce anything at all resembling the long-time semiclassical dynamics. In fact, for small T_Q one gets closer and closer to the exact *quantum* dynamics, as can be seen by taking the limit $T_Q\rightarrow 0$ and recovering the Feynman form of the quantum propagator. This is good if one just wants to know the quantum answer, but not if one is interested in understanding how quantum dynamics is affected by classical properties, in the sense, for example, of the Gutzwiller trace formula. What is interesting here is that for $T_Q\gg 1$, but still much smaller than the Heisenberg time, one can obtain a good approximation to the actual long-time *semiclassical* dynamics, and thus study the validity (and breakdown) of the semiclassical propagation. Detailed comparisons become easily possible between quantum and semiclassical spectra, eigenstates, long-time transport, and other properties.

Here we apply these ideas to a somewhat different class of systems, ones that lack the somewhat unpleasant ''cut and paste'' discontinuities of the baker's map, which are not piecewise linear, and which are also more generic in the sense of constituting a large family and allowing for continuous perturbations. These systems, namely smooth automorphisms of the torus (e.g., kicked maps and perturbed cat maps) lack a special symbolic dynamics and have no preferred basis, making them a good test case for the ideas outlined above. An important constraint is that we shall be looking exclusively here at caustic-free, purely chaotic systems. Caustics, discontinuities, and mixed phase space are all important subjects of inquiry and will be looked at in a future paper. It should be pointed out that the procedure presented in what follows does not make use of detailed knowledge about the system at hand. In this way, it may be more robust than, for example, the cycle expansion methods in periodic orbit theory. Because no explicit use is made of periodic orbits, it need not be the case here that long periodic orbits can be expressed in terms of short periodic orbits, for example. All that is needed is that long paths can be constructed out of short paths, something that is true in all but the most pathological cases.

The rest of this paper is organized as follows: we first briefly review the classical, quantum, and semiclassical dynamics of the systems under consideration. The iteration of semiclassical propagators is discussed, and error estimates are given as a function of propagation time, quantization time, and $\hbar$, with particular emphasis on Heisenberg-time propagation. Numerical tests follow, showing the convergence of the iterative approximation as well as measuring the deviation from exact quantum and one-step iterative results. Then the ''effective one-step semiclassical propagator'' is discussed, which with exponential accuracy describes long-time semiclassical propagation, and which differs from the quantum and one-step semiclassical matrices. Again, numerical findings are presented. Finally, the conclusion treats some general questions and addresses possible applications and extensions of the results obtained.

In a companion paper to this article [9], the methods are extended and applied to the study of semiclassical dynamical localization in classically diffusive systems, showing that in fact interference between classical paths is sufficient to understand the end of quantum diffusion in these systems.

II. THEORETICAL ANALYSIS

A. Hard chaotic dynamics on a torus

We will consider smooth, chaotic classical dynamics on a compact phase space, satisfying the Anosov property and free from caustics in the coordinate system of interest. (The Anosov property means that at each phase space point the tangent space can be decomposed into an exponentially expanding linear subspace and an exponentially contracting linear subspace. For two-dimensional phase spaces, there is one expanding and one contracting direction at each point.) To be specific, let us take the following family of discrete area-preserving maps on a torus:

$$p \to \tilde{p} = p + mq - V'(q) \bmod 1,$$

$$q \to \tilde{q} = q + n\tilde{p} + T'(\tilde{p}) \bmod 1. \quad (1)$$

The above dynamics can be obtained from the stroboscopic discretization of a kicked system [10] with a kick potential $-\frac{1}{2}mq^2 + V(q)$ applied once every time step and a free evolution governed by the kinetic term $\frac{1}{2}np^2 + T(p)$. Here m,n are arbitrary integers, while V,T are smooth periodic functions. The system can also be thought of as a continuous perturbation of the linear system (cat map) [11]

$$p \to \tilde{p} = p + mq \bmod 1,$$

$$q \to \tilde{q} = np + (mn+1)q \bmod 1. \quad (2)$$

The Jacobian of the transformation in Eq. (1) is given by

$$J = \begin{bmatrix} 1 & m - V''(q) \\ n + T''(\tilde{p}) & 1 + [n + T''(\tilde{p})][m - V''(q)] \end{bmatrix}. \quad (3)$$

We notice that for given integers m,n we can choose the functions V and T such that the quantity $m - V''(q)$ is strictly greater than 0 for all q and similarly for $n + T''(\tilde{p})$. (In words, we ensure that the system everywhere looks locally like an inverted harmonic oscillator.) This implies strict positivity of all four entries in the Jacobian matrix, a property that is of course preserved under iteration of the dynamics. Furthermore, positivity of both off-diagonal entries implies hyperbolicity, because it ensures $\det J > 2$. All such systems therefore provide examples of hard chaos, being free of integrable regions. To see that they are free of caustics in either position or momentum space, it is sufficient to note that the two off-diagonal entries of the Jacobian, $\partial p(t)/\partial q(0)$ and $\partial q(t)/\partial p(0)$, always remain nonzero.

The quantization of kicked systems is straightforward and well-covered in the literature [10]. We take $\hbar$ so that $N = 1/2\pi\hbar$ has an integer value. Then an N-dimensional position basis for the Hilbert space is given by $|q_i\rangle$, where $q_i = (i + \epsilon_0)/N$, $i = 0 \cdots N-1$. Similarly, the momentum space basis is given by $|p_j\rangle$, with allowed values $p_j = (j + \epsilon_1)/N$, $j = 0 \cdots N-1$. $\epsilon_{0,1}$ form a family of possible quantization conditions (they correspond to phases associated with circling the torus in the p and q directions, respectively). The two bases are related by a discrete Fourier transform. The dynamics is now defined by the unitary $N \times N$ matrix

$$U = \exp\left[-i \left(\frac{1}{2} n\hat{p}^2 + T(\hat{p}) \right) \Big/ \hbar \right] \times \exp\left[i \left(\frac{1}{2} m\hat{q}^2 - V(\hat{q}) \right) \Big/ \hbar \right], \quad (4)$$

where each factor is evaluated in the appropriate basis, and an implicit forward and backward Fourier transform has been performed. As in the linear (cat map) case, continuity of the potential and kinetic terms (mod $\hbar$) requires that N be chosen even, unless both m and n are even. The key point is that U here is just a matrix, and the long-time quantum evolution of the system is given by matrix multiplication. Alternatively, the matrix U can be diagonalized to find the stationary properties (eigenstates and eigenvalues) of the system. All this can be performed in polynomial time, and the total amount of information contained in the quantum system is of order N^2. In particular, all of the information is present in the one-step quantum propagator.

B. Semiclassical dynamics

We now consider the long-time semiclassical dynamics as given by the Gutzwiller–Van-Vleck propagator [1] evaluated between quantum mechanically allowed states. In position space, the propagator has the form

$$G_{\mathrm{sc}}(q,q',t) = \left[\frac{1}{2\pi i\hbar} \right]^{d/2} \sum_j \left| \det \frac{\partial^2 S_j(q,q',t)}{\partial q \partial q'} \right|^{1/2} \times \exp\left[\frac{i S_j(q,q',t)}{\hbar} - \frac{i\pi\nu_j}{2} \right], \quad (5)$$

where S_j is the action for classical path j, the determinant corresponds to the classical probability density for going between q and q' via this path, and the phase is given by the action, corrected by the count of conjugate points ν_j. For any given time t, this produces an $N \times N$ matrix A_t. The semiclassical evolution must of course be evaluated in some coordinate system, such as position or momentum, but once the matrix has been constructed it can be rotated into any quantum basis that one finds convenient. Being a matrix connecting quantum in and out states, A_t looks like a quantum object, but it is not unitary ($A_t A_{-t} \neq I$) and does not satisfy multiplicativity ($A_{t+t'} \neq A_t A_{t'}$). Thus it is not *a priori* obvious, for example, that the semiclassical evolution at long times converges to a well-defined set of eigenstates and eigenvalues, i.e., $A_t \psi_n \approx e_n^t \psi_n$, or whether such eigenvalues and eigenstates e_n, ψ_n have any connection with those of the quantum dynamics.

Let us study the deviation from multiplicativity of the semiclassical dynamics in a smooth chaotic system. We note first that for semiclassical propagators in the time domain,

$$A_{2t}(q'',q) = \int_{\mathrm{sp}} dq' A_t(q'',q') A_t(q',q), \quad (6)$$

where $\int_{\mathrm{sp}}$ indicates that the equality holds only if the intermediate integration is performed by stationary phase [12]. If the integration is performed exactly instead of in the stationary phase approximation, we obtain a relative error of order $\hbar$ in the answer. Of course, for large t, many stationary paths are summed over on the right-hand side of Eq. (6). The relative error in ignoring subleading terms in the stationary phase expansion for *each* such path is $O(\hbar)$. So the fractional error in the full answer is also $O(\hbar)$, provided that the errors add no more coherently than the leading terms themselves. This error comes from higher-order terms in the stationary phase expansion. [In the presence of caustics, the coefficient of the $O(\hbar)$ term can blow up in certain regions of space, eventually dominating the semiclassical evolution. Possibilities for handling this problem include uniformization or choosing a different basis (e.g., a Gaussian basis) for performing the semiclassical calculation. To avoid these se-

rious difficulties we will deal throughout this paper with systems that are caustic-free in the chosen basis.]

For systems on a compact classical phase space, position and momentum values are of course labeled by discrete integers, so strictly speaking the notion of stationary phase integration is not well defined. To make sense of the semiclassical dynamics, one must rewrite the sums over topological classes (winding numbers) using the Poisson summation formula, and evaluate the resulting integrals by stationary phase [11]. This produces a semiclassical propagator defined only on a discrete position (or momentum) grid. However, in the limit of small $\hbar$ (large N), the spacing between quantum basis states vanishes, and the discreteness of the quantum basis ceases to be physically significant. This is true as long as all quantum structures in phase space are ''generic,'' scaling as $\sqrt{\hbar}$ in both the q and p directions, while the spacings Δq and Δp scale as $\hbar$. The error analogous to Eq. (6) that we are interested in for a compact phase space is the difference between performing a sum over intermediate channels q' and performing the corresponding *integral* by stationary phase. We can then write

$$A_{2t}(i,k)=\sum_{j=0}^{N-1} A_t(i,j)A_t(j,k)+O(N^{-3/2}). \tag{7}$$

Note that the error scales as $N^{-3/2}\sim\hbar^{3/2}$ because normalization (probability conservation) requires that the actual matrix elements of A_t and A_{2t} scale as $N^{-1/2}\sim\hbar^{1/2}$. The relative error is scaling as $N^{-1}\sim\hbar$. We now define a natural norm for measuring the difference between two matrices (under which a unitary matrix has norm 1),

$$\|A-B\|^2\equiv\frac{1}{N}\,\mathrm{tr}(A-B)^{\dagger}(A-B)=\frac{1}{N}\sum_{ij}\,|(A-B)_{ij}|^2. \tag{8}$$

We then have

$$\|A_{2t}-(A_t)^2\|^2=O(\hbar^2), \tag{9}$$

whereas the matrices A_t individually have norm of order unity. Of course, the coefficient in front of the $O(\hbar^2)$ depends on the amount of nonlinearity in the underlying classical dynamics. For example, the cat map given by Eq. (2) is exactly linear, and produces a semiclassical dynamics A_t that is exactly multiplicative. This, however, is not very interesting because in that case A_t is also equal to the exact quantum dynamics U^t. For generic perturbing potentials $V(q)$ or $T(p)$, the semiclassical answer differs from the quantum, and in that case the number multiplying $\hbar^2$ will indeed be of order unity.

The result in Eq. (9) is already quite promising. It tells us that for small $\hbar$, it is a very good approximation to compute the semiclassical dynamics exactly for 10 steps and then square the matrix instead of trying to do the exact calculation for 20 steps. The former is a much easier problem to solve because the number of classical paths needed to compute A_t scales exponentially with t. Inspired by this, we ask to what extent we may approximate the exact time-t semiclassical propagator for large t by dividing t into more and more shorter time intervals. Replacing A_t by $(A_{t/M})^M$ involves making an error $M-1$ times, each time approximating a stationary phase integration by exact multiplication. Assuming these errors add incoherently, and taking M to be large, we then have

$$\|A_t-(A_{t/M})^M\|^2=O(M\hbar^2). \tag{10}$$

One can also obtain this result by iterating the procedure indicated by Eq. (9) for M that is a power of 2. (In other words, we express A_t in terms of $A_{t/2}$ plus an error term, then $A_{t/2}$ in terms of $A_{t/4}$ plus another error term, etc.) However, we need to be careful about the assumption of incoherent accumulation of errors. Because the Hilbert space is finite-dimensional, eventually we must consider interference between different error terms. To see this in our formalism, let $B=A_{t/M}$ and $C=(A_t)^{1/M}$. (Although the Mth root of a matrix is in general an ambiguous quantity, here there is no ambiguity in what we mean by the matrix C: we simply choose that root which is closest to B.) Now the quantity that we are interested in is $\|C^M-B^M\|^2$. Let $\epsilon\equiv C-B$. To lowest order in ϵ,

$$\|C^M-B^M\|^2=\|\epsilon B^{M-1}+B\epsilon B^{M-2}+\cdots+B^{M-1}\epsilon+O(\epsilon^2)\|^2. \tag{11}$$

Now we work in the basis in which B is diagonal, and write ϵ as the sum of its diagonal and off-diagonal parts in that basis. The diagonal part of ϵ commutes through B, giving a coherent contribution from the M terms in the sum. The off-diagonal part leads to an incoherent contribution because the eigenphases of B are generic. So we obtain for the basis-independent norm

$$\|C^M-B^M\|^2=O(M\|\epsilon_{\text{off-diag}}\|^2)+O(M^2\|\epsilon_{\text{diag}}\|^2)+O(M^2\|\epsilon^2\|^2)+\cdots. \tag{12}$$

Now as long as the errors in the stationary phase approximation are not *preferentially* diagonal (i.e., not in general tending to multiply the exact answer), the weight of the matrix ϵ that is on the diagonal is a fraction $1/N\sim\hbar$ of the total weight of ϵ. Noting from Eq. (9) that $\|\epsilon\|^2=O(\hbar^2)$, we see that $\|\epsilon_{\text{diag}}\|^2=O(\hbar^3)$. Furthermore, for the values of M that we are going to consider (up to the Heisenberg time $T_H\sim\hbar^{-1}$), terms higher order in ϵ [e.g., $O(M^2\hbar^4)$] can be ignored. So we obtain

$$\|A_t-(A_{t/M})^M\|^2=O(M\hbar^2)+O(M^2\hbar^3), \tag{13}$$

valid for $M\leqslant O(\hbar^{-1})$.

C. Heisenberg time dynamics

In particular, let us consider what happens at the Heisenberg time $t=T_H\sim O(\hbar^{-1})$ (computing the semiclassical dynamics to times longer than this will not produce interesting new information because individual eigenstates and eigenvalues will already have been resolved). Let T_Q be the ''quantization time,'' the time for which we will compute the semiclassical propagator A_{T_Q} exactly. First, letting $M=t/T_Q$, we can rewrite Eq. (13) as

$$\|A_t - A_{T_Q}^{t/T_Q}\|^2 = O\left(\frac{t\hbar^2}{T_Q}\right) + O\left(\frac{t^2\hbar^3}{T_Q^2}\right). \tag{14}$$

Then by the Heisenberg time $t = O(\hbar^{-1})$, we accumulate an error

$$\|A_{T_H} - (A_{T_Q})^{T_H/T_Q}\|^2 = O\left(\frac{\hbar}{T_Q}\right) + O\left(\frac{\hbar}{T_Q^2}\right). \tag{15}$$

The above formula is expected to hold for all $T_Q \geqslant 1$, where classical paths exist connecting any two coordinate points. If we apply the result to the case $T_Q = 1$, which characterizes the one-step Bogomolny propagator, we find

$$\|A_{T_H} - (A_1)^{T_H}\|^2 = O(\hbar). \tag{16}$$

So one result of the above calculation is that for smooth one-dimensional kicked systems (or for two-dimensional Hamiltonian systems, where the scaling of the density of states works identically), in the absence of caustics the exact semiclassical propagator deviates from the iteration of the one-step dynamics only by an error term of order $\sqrt{\hbar}$, by the Heisenberg time. How does this propagation relate to the exact quantum dynamics? For a single time step we know that the relative error between semiclassical and quantum amplitudes scales as $\hbar$, so

$$\|A_1 - U\|^2 = O(\hbar^2). \tag{17}$$

Following a line of reasoning completely analogous to the one that took us from Eq. (9) to Eq. (16) (i.e., noticing that off-diagonal terms in the error add incoherently, etc.), we find

$$\|(A_1)^{T_H} - U^{T_H}\|^2 = O(\hbar). \tag{18}$$

Now combining this with Eq. (16) we obtain a relation between the exact semiclassical and exact quantum answers:

$$\|A_{T_H} - U^{T_H}\|^2 = O(\hbar). \tag{19}$$

Thus, in the absence of discontinuities and caustics, the semiclassical approximation is expected to do quite a good job in approximating the quantum dynamics all the way out to the Heisenberg time (in two dimensions, that is—in three dimensions the same analysis leads to the conclusion that the semiclassical approximation is marginal at the Heisenberg time).

But there still is a difference between the long-time semiclassical and quantum behavior, implying also a difference between the corresponding eigenvalues and eigenstates. These corrections arise from ''hard quantum'' effects, those beyond the stationary phase approximation. To be able to separate these from those effects that are purely semiclassical, one needs to be able to compute A_t explicitly for $t \sim T_H$, to a better approximation than that given by the exact quantum mechanics, Eq. (19). Iteration of the one-step semiclassical propagator A_1 will not do, since it differs from the true semiclassical propagation as much as from the quantum. So we proceed to consider a quantization time $T_Q \gg 1$. From Eq. (15) we see that iteration of A_{T_Q} comes much closer to the exact semiclassics than the difference between the latter and quantum mechanics.

$$\|(A_{T_Q})^{t/T_Q} - A_t\|^2 \ll \|A_t - U^t\|^2 \tag{20}$$

for $t \sim T_H$. This implies

$$\|(A_{T_Q})^{t/T_Q} - A_t\|^2 \ll \|(A_{T_Q})^{t/T_Q} - U^t\|^2, \tag{21}$$

and thus iteration of A_{T_Q} gives us an answer much closer to A_t than to U^t, allowing us to see how the long-time semiclassical dynamics differs from the quantum dynamics, without the need for doing an exponentially large amount of work. The approximation is a controlled one, and one can keep increasing T_Q until the desired level of convergence to the exact semiclassics is reached.

These ideas, extended properly to quantization of noncompact phase spaces, can be used for example to see dynamic semiclassical localization without having to sum explicitly over a number of classical paths that is exponential in the localization time. The results are presented in a companion paper [9], and address a long-standing question in the literature over whether dynamic localization is a semiclassical or hard quantum phenomenon.

III. NUMERICAL TESTS

We proceed now to justify numerically the power-counting arguments presented in the preceding section. The system we will use is the kicked system of Eq. (1), with $m = n = 1$, and $V(q) = -(K/(2\pi)^2)\sin 2\pi q$. This can be thought of as a standard map (kicked rotor) with an extra inverted harmonic oscillator potential $-\frac{1}{2}q^2$, or as a sinusoidal perturbation of the $\left[\begin{smallmatrix}1 & 1\\ 1 & 2\end{smallmatrix}\right]$ cat map. $T(p)$, the perturbation of the quadratic kinetic term, is set to zero for simplicity. Also for simplicity, periodic boundary conditions, with no phases, are imposed, i.e., $\epsilon_0 = \epsilon_1 = 0$. The caustic-free condition requires kick strength $|K| < 1$. The system is then guaranteed to satisfy the Anosov property, as explained in the discussion following Eq. (3). We choose $N = 256$ to be the dimension of the Hilbert space. This is well in the semiclassical regime, and large enough so that a direct summation of classical paths to the Heisenberg time (there are 3^{256} of them) is clearly not practical.

We then fix a value of K, at $K = 0.5$, and compute the matrix elements of the semiclassical propagator between quantum states in the momentum basis (using p is natural because we are thinking of this as a kicked system; also working in momentum space leads naturally into the study of dynamical localization). Exact semiclassical matrices A_{T_Q} are computed for quantization times $T_Q = 1 \cdots 8$, using the Gutzwiller–Van-Vleck expression, Eq. (5). The convergence of the iterative approximation can then be investigated. We first compute the quantity $\|(A_{T_Q})^{t/T_Q} - (A_8)^{t/8}\|^2$ for $T_Q = 1,3,5,7$, and for a range of times t that extends beyond the Heisenberg time $T_H = 256$. As explained above, the exact semiclassical propagator for times of order T_H cannot be computed exactly, so we use the difference between approximations at different values of T_Q as a measure of conver-

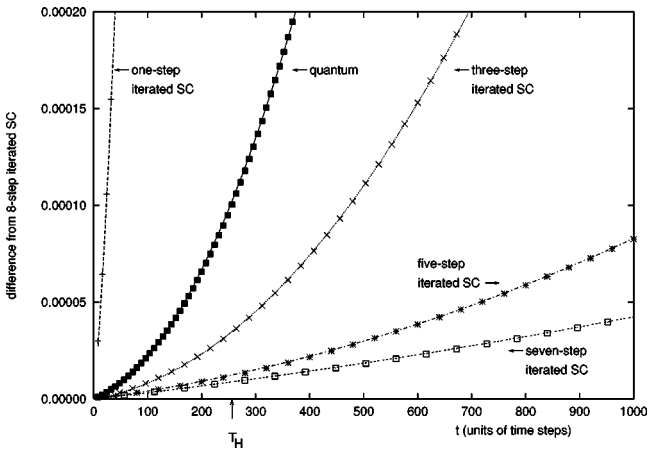

FIG. 1. Convergence to long-time semiclassical behavior with increasing quantization time T_Q. A long-time calculation with $T_Q=8$ is used as the reference. From top to bottom, the five sets of data represent the squared difference between this calculation and (i) the iterated one-step semiclassics, (ii) the quantum mechanics, (iii) the three-step iterated semiclassics, (iv) the five-step iterated semiclassics, and (v) the seven-step iterated semiclassics. The Heisenberg time is $T_H=256$. Each curve is fit to the sum of a linear and quadratic function of time, in accordance with Eq. (14).

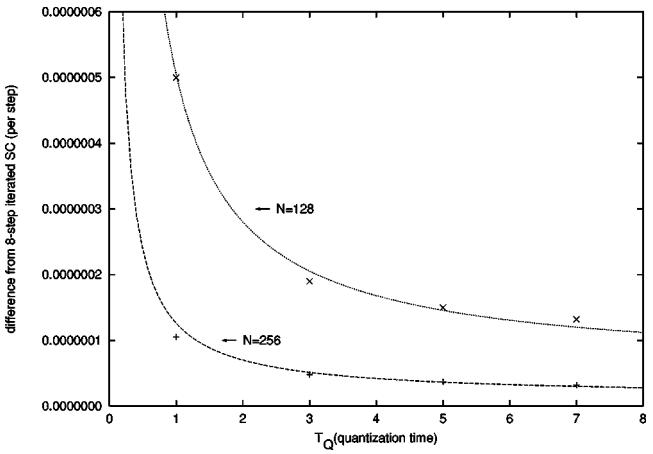

FIG. 2. Convergence of the linear coefficients in the previous figure (error per time step), with increasing quantization time T_Q. From left to right, the four data points measure the divergence per unit time of the $T_Q=8$ calculation from (i) the quantum mechanics, (ii) the three-step semiclassical approximation, (iii) the five-step approximation, and (iv) the seven-step approximation. The upper and lower sets of points correspond to Heisenberg times $N=128$ and $N=256$, respectively. Theoretical curves corresponding to Eq. (24), with $c=0.29$, are drawn through the data.

gence as $T_Q\to\infty$. At the end of the next section, we will see an example of a numerical test for moderate time t, where exact semiclassical calculation is in fact possible, though very time consuming. There, approximation techniques are explicitly shown to produce a very good answer with much less effort. We assume errors in successive approximations are uncorrelated, i.e.,

$$\|A_{T_Q}^{t/T_Q}-A_{T_Q'}^{t/T_Q'}\|^2\approx\|A_{T_Q}^{t/T_Q}-A_t\|^2+\|A_{T_Q'}^{t/T_Q'}-A_t\|^2. \quad (22)$$

For comparison purposes, the difference with the quantum dynamics $\|U_t-(A_8)^{t/8}\|^2$ is also computed. All these are plotted as a function of time t in Fig. 1. From top to bottom, the quantities plotted are the squared differences between the eight-step iterated semiclassics $A_8^{t/8}$ and (i) the one-step iterated semiclassics A_1^t, (ii) the quantum mechanics U^t, (iii) the three-step iterated semiclassics $A_3^{t/3}$, (iv) the five-step iterated semiclassics, and finally (v) the seven-step iterated semiclassics. Each set of points is also fitted to a function of the form $at+bt^2$, as suggested by Eq. (14).

We notice first of all that the three-step, five-step, and seven-step approximations come progressively closer to the eight-step approximation that is our basis of comparison. The differences between all these are significantly smaller than that between any of these and the quantum dynamics. Finally, the one-step iterated approximation does a (relatively) poor job of reproducing the long-time semiclassical behavior (however, the difference between it and the other calculations is still small, due to the smallness of $\hbar$). Consistent with the prediction of Eqs. (14) and (22), all the curves are well fitted by the sum of a linear and quadratic function of time. Furthermore, at least for $T_Q>3$, the linear term is seen to dominate for times up to the Heisenberg time ($T_H=N=256$ in this calculation). Thus, to understand the convergence of the iterative method for $T_Q\gg1$, it is sufficient to look at the behavior of the linear term in Fig. 1.

This is in fact done in Fig. 2. For each T_Q, we find the numerical value of $a(T_Q)$ that fits

$$\|A_{T_Q}^{t/T_Q}-A_8^{t/8}\|^2=a(T_Q)t+b(T_Q)t^2. \quad (23)$$

In Fig. 2, the quantity $a(T_Q)$ is plotted vs T_Q, using pluses for $N=256$ and crosses for $N=128$. However, for $T_Q=1$, the difference between the *quantum* dynamics and the eight-step iterated semiclassics is plotted, i.e., the linear coefficient of $\|U^t-A_8^{t/8}\|^2$, *not* $\|A_1^t-A_8^{t/8}\|^2$. The latter value is off the scale in the figure, being 30×10^{-7} for $N=256$ and 115×10^{-7} for $N=128$ (notice that this error, though relatively large compared to those obtained for bigger T_Q, still has the right $\hbar^2$ dependence). From Eqs. (14) and (22), we predict

$$a(T_Q)=c\hbar^2\left(\frac{1}{8}+\frac{1}{T_Q}\right), \quad (24)$$

for $T_Q\gg1$, where c is an undetermined constant of order unity. This predicted behavior fits the observed values of $a(T_Q)$ quite nicely, with $c=0.29$. The resulting curves, following Eq. (24), are plotted in Fig. 2. We see that the error in the iterative approximation indeed scales as $\hbar^2$ per time step, leading to an error of order $\hbar$ by the Heisenberg time. Furthermore, the error goes to zero as $T_Q\gg1$, in the predicted manner, and is already much smaller than the difference between the quantum mechanics and the semiclassics by $T_Q=3$.

IV. EFFECTIVE ONE-STEP LONG-TIME PROPAGATOR

We have seen in the preceding sections how to obtain convergent approximations to the semiclassical propagator

for long times, including times beyond the Heisenberg time. This dynamics can now be Fourier transformed to obtain local densities of states for various initial wave packets, and from these the eigenstates and eigenvalues could be extracted. In particular, the semiclassical spectrum can be obtained by tracing over the Fourier transformed semiclassical evolution. The quantization time T_Q can be increased until the desired level of convergence is reached, and the eigenstates and eigenvalues obtained in this way can finally be compared with those of the quantum matrix.

This, however, is a rather tedious process, requiring the approximate semiclassical propagator to be evaluated at many values of t, from short times to times well beyond T_H. Moreover, if we settle on a fixed quantization time T_Q, and computed all long-time dynamics using it, we will finally obtain nothing more than the eigenstates and eigenvalues of the matrix A_{T_Q}. So clearly the sensible thing to do is to diagonalize A_{T_Q} directly for a range of values of T_Q and check for convergence as $T_Q \gg 1$. Unfortunately, a technical difficulty arises here. Eigenstates of the true dynamics (quantum or semiclassical) with eigenphases separated approximately by an integer multiple of $2\pi/T_Q$ may get mixed with each other in the diagonalization of A_{T_Q}, preventing one from extracting the true eigenstates. This behavior appears to be generic (it does not happen in A_1 due to level repulsion in the presence of chaos). One can try to get around this difficulty by comparing the eigenstates of A_{T_Q} for a range of T_Q, and selecting those that come closest to agreeing for several values of T_Q. Such a procedure does in fact appear to converge to a reasonable set of N eigenstates, and it might be expected to produce results comparable to those that would be obtained by Fourier transforming long-time dynamics produced by using several matrices A_{T_Q}. (For example, we could approximate $A_{100} \approx A_9^4 A_8^8$, $A_{101} \approx A_9^5 A_8^7$, etc. This procedure is in fact useful for evaluating long-time propagators at arbitrary times t, including those that are not divisible by a suitable value of T_Q.)

However, a simpler solution now presents itself. Given that we believe A_{T_Q} have similar eigenstates for all values $T_Q \gg 1$, these must also be the eigenstates of

$$D_{T_Q} \equiv A_{T_Q} A_{T_Q-1}^{-1}, \tag{25}$$

for example. No mixing of eigenstates should arise in D_{T_Q} (because of level repulsion), and moreover this method has the advantage that the semiclassical eigenvalues can be read off directly, without having to decide which root of an eigenphase must be taken in each case. T_Q is then increased, and convergence to the ''true'' semiclassical eigenstates and eigenvalues is obtained (convergence is expected based on what we know about the convergence of the dynamics from the two previous sections).

In fact, it is sufficient to look at convergence of the D_{T_Q} matrix. In Fig. 3, the results of such an analysis are presented, for the same system as that studied numerically in Sec. III. Here a Heisenberg time (matrix size) $N=64$ is used. We plot the squared norm $\|D_{T_Q} - D_9\|^2$ for $2 \leqslant T_Q \leqslant 6$ (for $T_Q > 6$, numerical errors begin to play a role in the error analysis, however the downward trend continues to

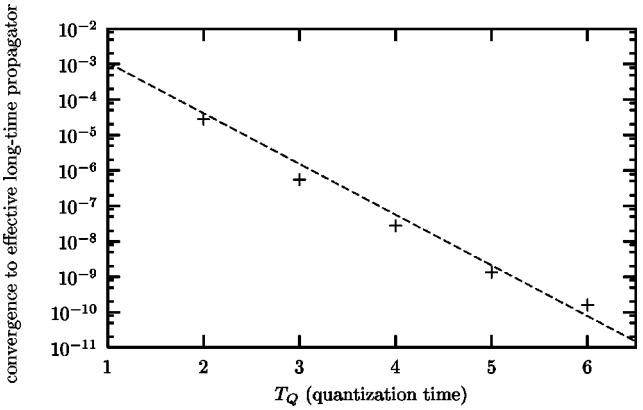

FIG. 3. Exponential convergence of the quantity $D_{T_Q} = A_{T_Q} A_{T_Q-1}^{-1}$ towards the *effective* one-step long-time semiclassical propagator $D_\star$ [Eq. (26)]. Data provided for $D_2 \cdots D_6$; D_9 is used as the reference.

5.4×10^{-12} for the difference between D_8 and D_9). For comparison, we also measure $\|A_1 - D_9\|^2 = 4.6 \times 10^{-5}$ and $\|U - D_9\|^2 = 6.2 \times 10^{-6}$.

Remarkably, we find exponentially fast convergence with the quantization time, in marked contrast with the power-law convergence obtained previously for the dynamics. The data agree well with the exponential form $\hbar^2 \exp(8.1 - 3.2 T_Q)$, which is also plotted in Fig. 3. This exponential behavior is consistent with analogous results seen in cycle expansion methods. How can it be reconciled with the power-law behavior seen in Eq. (13)? Let

$$D_\star \equiv \lim_{T_Q \to \infty} D_{T_Q}. \tag{26}$$

Now clearly $A_t = D_\star^t (1 + \epsilon_t)$, where ϵ_t is a correction falling off exponentially with t, would satisfy the finding [upon substitution into Eq. (25)] that D_{T_Q} converges exponentially quickly. However, it would not be consistent with Eq. (13), which requires power-law behavior for the dynamics, and which we have seen verified numerically. The two results can be reconciled if we notice that exponential convergence of D_{T_Q} to $D_\star$ only requires

$$A_t = D_\star^t (1 + \epsilon_\star + \epsilon_t). \tag{27}$$

Here $\|\epsilon_t\|^2 = O(\hbar^2 \exp(-\alpha t))$, while $\epsilon_\star$ is a t-independent matrix with norm $\|\epsilon_\star\|^2 = O(\hbar^2)$. α is a constant associated with the mixing time scale of the underlying classical dynamics. Now when taking the product $D_t \equiv A_t A_{t-1}^{-1}$, the $\epsilon_\star$ contribution cancels, producing $D_\star$ plus a time-dependent correction that goes as $O(\hbar^2 \exp(-\alpha t))$. However, if we compare A_t with $A_{t/M}^M$ using Eq. (27), where t and t/M are assumed for simplicity to be large, we notice that the latter quantity has an extra $M-1$ term of order $\epsilon_\star$ compared with the exact semiclassics A_t. This is consistent with what we found in Eq. (11), and leads to power-law errors as in Eq. (13). For example, from Eq. (27) we see $A_{2t} - A_t^2 = O(\epsilon_\star)$, in agreement with Eq. (9).

Our interpretation of Eq. (27) is that ϵ_t is an error that results from concatenating short classical paths to produce long ones. It is thus analogous to the errors obtained in ap-

proximating long periodic orbits by short ones in cycle expansion methods. $\epsilon_\star$, on the other hand, is an error in some way associated with projecting the full semiclassical dynamics for any time t onto quantum initial and final states. This error is therefore independent of the time after which such projection is performed. It should be possible to make a connection between this effect and what happens in the baker's map, for example, when a slightly higher-dimensional effective semiclassical space (in which the semiclassical dynamics is almost exactly iterative) must be projected onto N vectors to produce quantities that can be compared with quantum matrix elements [6]. One would also like to understand better the parametrization ambiguities in the definition of $D_\star$ and $\epsilon_\star$. For example, we could have written

$$A_t=(1+\tilde{\epsilon}_\star+\tilde{\epsilon}_t)\tilde{D}_\star^t \tag{28}$$

as an alternative to Eq. (27). This would be natural if we had looked at the quantity $A_{T_Q-1}^{-1}A_{T_Q}$ $[=(A_{-T_Q}A_{1-T_Q}^{-1})^\dagger]$ instead of D_{T_Q} as defined above.

In any case, we see that the matrix $D_\star$ is key to understanding the long-time semiclassical dynamics. This matrix is an effective one-step propagator that can be used to obtain the semiclassical propagator at time $t+1$ with exponential accuracy, given the propagator for time t. It thus gives to us in a trivial way the stationary properties of the long-time semiclassical evolution.

To show how the factorization given in Eq. (27) can be used in practice, we take the kicked map studied earlier in this section and compute an approximation to A_9 by evaluating

$$A_9\approx D_\star^9(1+\epsilon_\star)=D_\star^4D_\star^5(1+\epsilon_\star)\approx D_\star^4A_5\approx(A_5A_4^{-1})^4A_5. \tag{29}$$

All errors ϵ_t in Eq. (29) are exponentially small in the relevant times t: an error of size ϵ_9 is made in the first approximation, and errors of size ϵ_5,ϵ_4 in the third and fourth steps, the latter of course dominating the error in the final answer. Notice that we need to evaluate the semiclassical dynamics A_t exactly at two values of t to obtain the two matrices $D_\star$ and $\epsilon_\star$. After computing the semiclassical propagator A_9 exactly, we find (factoring out the $\hbar$ dependance) that the error $\|(A_5A_4^{-1})^4A_5-A_9\|^2$ is $0.000\,03\hbar^2$. In the same units, we find the error $\|A_5A_4-A_9\|^2$ to be $0.5\hbar^2$, still not bad, but lacking the exponential error suppression. For comparison, the difference between the exact semiclassical 9-step propagator A_9 and the quantum mechanics U_9 is $3.1\hbar^2$, while the difference from the 9-times iterated one-step propagator ($\|A_1^9-A_9\|^2$) is $89.5\hbar^2$. (It is interesting to note just how poorly iteration of the one-step semiclassical propagator A_1 does in reproducing the correct longer-time semiclassical behavior.)

Of course, this procedure can now be extended to times much longer than 9, where exact evaluation of the semiclassics is clearly not practical. Six digits of accuracy in long-time semiclassical propagation (beyond what is expected merely from the smallness of $\hbar$) are obtained with only a modest amount of work.

V. CONCLUSION

We have seen in the preceding section that long-time semiclassical behavior is given to exponentially good accuracy by iteration of an effective matrix $D_\star$ that is different from both the quantum evolution matrix U and the one-step semiclassical propagator A_1. In fact, the one-step semiclassical propagator contains essentially no information about long-time semiclassical dynamics, except of course for the similarity based on both being related to the quantum evolution. However, knowing the semiclassical dynamics for times $T_Q\gg 1$ (measured in units of the shortest periodic orbit time) enables one to deduce stationary semiclassical behavior, including dynamical information to the Heisenberg time and beyond. Why is long-time semiclassical information exhausted at $T_Q\gg 1$? In periodic orbit methods, one expects knowledge of long-time dynamics to be contained in orbits of length up to the mixing time ($\sim\ln N$), at which point phase space has been explored at the scale of Planck's constant. Longer orbits can be produced from these if we allow smearing over sub-Planck coordinates. The $O(N)$ periodic points at the mixing time contain $O(N^2)$ pieces of information if we record where each lies in relation to some quantum basis. Similarly, the full quantum theory can of course be described by an $N\times N$ matrix. The information required to obtain the semiclassical theory is only slightly bigger, scaling in the same way with N. We note that collecting and iterating semiclassical information after one time step on a scale of $1/N$ allows one to resolve periodic orbits up to the mixing time, while collecting after a slightly longer exact evolution is equivalent to having knowledge of periodic orbits longer than the mixing time, where exponential convergence is expected.

The results obtained here may shed light on the accuracy of the Gutzwiller trace formula in the energy domain. Though the relationship between the two approaches is a nontrivial one (the trace formula focusing on *periodic* orbits, and thus corresponding to a stationary phase integration of the dynamics), one may hope that further progress may be made in bringing together dynamical and periodic orbit methods. In any case, we have already seen that the stationary phase integration implicit in the trace formula is *not* necessary for obtaining sensible semiclassical eigenvalues and eigenstates, which compare well with those of an exact quantum calculation.

More work is also needed in bringing together the approximation methods discussed here with other semiclassical consolidation techniques, such as those that have been used quite successfully for the baker's map [6].

These iterative methods may in addition provide a new perspective on the long-standing questions of classical periodic orbit correlations and of how semiclassical dynamics can reproduce Heisenberg-time quantum behavior [13]. All such issues become much less mysterious once we realize that long orbits are given to a good approximation by concatenating shorter classical trajectories. Thus, long-time semiclassical evolution can produce δ-function peaks in the spectrum for essentially the same reason as the quantum-mechanical evolution, i.e., it is given (approximately) by iteration of an (almost) unitary finite matrix.

Many of the findings may be modified in the presence of

discontinuities, strong diffraction, and caustics, where classical-quantum correspondence is more poorly understood. In particular, the proliferation of caustics may be expected to cause a divergence between semiclassical and quantum dynamics well before the Heisenberg time is reached [4]. In these situations, a better understanding of iterative dynamical methods may still allow one to follow the semiclassical dynamics past the scale at which this divergence occurs, and to see explicitly when and in what way the semiclassical approximation breaks down (and what corrections to the semiclassical formulas may be necessary to restore long-time correspondence). In some cases, certain qualitative features of the quantum dynamics (e.g., dynamical localization [9] and level spacing statistics) may be well reproduced by the long-time semiclassical dynamics, even when detailed correspondence between the propagators has been lost.

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