Semiclassical Propagation: How Long Can It Last?

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The Van Vleck–Gutzwiller propagator is a fundamental quantity in semiclassical theory whose validity was recently demonstrated to extend beyond the time previously thought feasible, i.e., well past the time after which classical chaos has mixed the phase space on a scale smaller than Planck's constant. Little justification was given for this seeming contradiction of the usual vision of semiclassical errors. Though perhaps nonintuitive, we find that standard arguments, properly applied to chaotic dynamics, do explain the long-time accuracy.

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Semiclassical approximations to the Schrödinger equation remain important in a large variety of contexts. They play the dual role of computational tools (when exact calculations are too difficult or unnecessary) and sources of insight and intuition, even if numerical solutions are available. However, classical chaos often spoils the utility of semiclassical methods. Gutzwiller [1] gave a formal connection between periodic orbits (embedded in chaos) and eigenvalues (the trace formula). Although the trace formula is not a practical tool and even divergent, it has been the guiding light in the search for more servicable approaches. A large effort to "quantize chaos," over many years, has begun to come to fruition. Recent progress has been dramatic, in both the time domain [2–4] and the energy domain [5–8]. Historically, however, the great bulk of the effort in semiclassical methods has taken place in the energy representation.

In 1928, Van Vleck [9] gave the time-dependent coordinate space propagator which was later modified by Gutzwiller to extend beyond caustics [1]. The Van Vleck–Gutzwiller expression is arguably the progenitor of all other semiclassical formulas: WKB wave functions, the Gutzwiller trace formula, and other energy domain quantities are obtained from it by a stationary phase Fourier transform from time into energy. It is therefore manifestly important to understand the accuracy of the semiclassical propagator and the time scale and mechanism for breakdown. In two rather different chaotic systems, the baker's map [4] and the stadium billiard [3], the semiclassical time propagation of localized initial states was shown to yield accurate dynamics for a much longer time than had been anticipated, based on simple (too simple it turns out) arguments about the classical time for mixing on the scale of Planck's constant. The mixing time for the exponentially unstable dynamics, such that most cells of size h in phase space are accessed by a typical initial state, goes as $\ln(1/h)$. The reasons for the good results well beyond the "logarithmic time" were suggested in the simple, locally linear structures which develop in the evolving phase space Lagrangian manifolds (this was actually exploited in the numerical method used to evaluate the semiclassical expressions). In the stadium case, some 30000 branches [30000 terms in the sum over contributions in Eq. (1) below] of the manifold passed through the region of the initial state. The distance between separate branches of the manifolds was vastly smaller than the distance across a circular phase space cell, yet the semiclassical correlation function was accurate.

The often quoted "truth" that structures on a scale finer than Planck's constant cannot have quantal significance was thus found to be only half true: Such fine structures cannot be seen individually in the quantum amplitudes but collectively they *can* yield accurate and usable semiclassical amplitudes.

How is it that the fine structures contain elements of the correct quantum amplitudes? Here we show that proper consideration of the evolving classical phase space structure, together with standard rules for the domain of accuracy of semiclassical methods, explains the observed long time accuracy. It is unnecessary to average the semiclassical and quantal results to obtain useful comparisons, as was done in Refs. [10,11].

The Van Vleck–Gutzwiller formula is [1,9,12]

$$G(\mathbf{q},\mathbf{q}_0;t) \approx G_{\rm sc}(\mathbf{q},\mathbf{q}_0;t) = \left(\frac{1}{2\pi i\hbar}\right)^{d/2} \sum_j \left|\mathrm{Det}\left(\frac{\partial^2 S_j(\mathbf{q},\mathbf{q}_0;t)}{\partial \mathbf{q}\,\partial \mathbf{q}_0}\right)\right|^{1/2} \times \exp[iS_j(\mathbf{q},\mathbf{q}_0;t)/\hbar - \tfrac{1}{2} i\pi\nu_j]\,. \quad (1)$$

In this expression, the sum over j is for all trajectories connecting $\mathbf{q}_0$ to $\mathbf{q}$ in time t, d is the number of degrees of freedom; the determinantal prefactor is the square root of the classical probability for the $\mathbf{q}_0 \to \mathbf{q}$ process, and the phase is the classical action $S_j(\mathbf{q},\mathbf{q}_0;t)$. An index ν_j based on the caustic structure of the evolving manifold $\mathbf{q}(t)$ is due to Gutzwiller [1]; see also Maslov and Fedoriuk [12] and a very recent and concise discussion by Littlejohn [13]. The action $S_j(\mathbf{q},\mathbf{q}_0;t)$ is the time integral of the Lagrangian

$$S_j(\mathbf{q},\mathbf{q}_0;t) = \int_0^t dt' \{\mathbf{p}(t')\cdot\dot{\mathbf{q}}(t') - H(\mathbf{p}(t'),\mathbf{q}(t'))\} \quad (2)$$

along the jth classical path (H is the classical Hamiltonian).

Accuracy of semiclassical propagation revolves around the stationary phase approximation. The key to understanding the errors is to regard the initial Lagrangian manifold as primal [12], representing the semiclassical Green's function as an integral over all initial momenta [2,14] corresponding to the initial state $|\mathbf{q}_0\rangle$ at $t=0$ for fixed $\mathbf{q}_0$. For the Van Vleck-Gutzwiller expression, one can derive an alternative formulation

$$G_{\rm sc}(\mathbf{q},\mathbf{q}_0;t)=\left(-\frac{i}{4\pi^2\hbar^2}\right)^{d/2}\int d\mathbf{p}_0\left|\mathrm{Det}\left(\frac{\partial \mathbf{p}_t}{\partial \mathbf{p}_0}\right)\right|^{1/2} \times\exp[i\mathbf{p}_t\cdot\mathbf{q}/\hbar+i\tilde{S}(\mathbf{p}_0,\mathbf{q}_0;t)/\hbar-\tfrac{1}{2}i\pi\nu(\mathbf{p}_0)]\,, \tag{3}$$

where $\tilde{S}(\mathbf{p}_0,\mathbf{q}_0;t)=S(\mathbf{q}_t,\mathbf{q}_0;t)-\mathbf{p}_t\mathbf{q}_t$ and $S(\mathbf{q}_t,\mathbf{q}_0;t)$ is the usual coordinate space action and $\mathbf{q}_t$ is considered to be a function of $\mathbf{p}_0,\mathbf{q}_0$. Note that the sum over separate contributions to the amplitude from $|\mathbf{q}_0\rangle$ to $|\mathbf{q}\rangle$ is absent, since all the stationary phase contributions are included in the integral over initial values of momentum. After some time t, the current values of the position and momentum are given parametrically (in $\mathbf{p}_0$ for fixed $\mathbf{q}_0$) as

$$\mathbf{q}_t=\mathbf{q}_t(\mathbf{q}_0,\mathbf{p}_0),\quad \mathbf{p}_t=\mathbf{p}_t(\mathbf{q}_0,\mathbf{p}_0)\,. \tag{4}$$

For convenience we specialize to a two-dimensional phase space. For a chaotic system, the path traced out by the parametric equations grows exceedingly complicated as time increases. The Lagrangian manifold τ_t $(=\{q_t,p_t\})$ begins to track the homoclinic and heteroclinic oscillations of pieces of unstable manifolds, following further along their winding arms as time increases. Nonetheless, we conduct our analysis in terms of standard results for the accuracy of stationary phase integrals. The integral, Eq. (3), has stationary phase points in p_0 whenever $q_t(q_0,p_0)=q$. Near a fold in the Lagrangian manifold, two such stationary phase points coalesce, and in the usual manner the stationary phase integral becomes inaccurate if the stationary phase points are close enough together that an area less than h is enclosed in the sector between the line q and τ_t.

Figure 1 shows the shape of a segment of the $q_0=0$ manifold near $p_0=0$ after several iterations of the standard map [15], except that we have unfolded the map by not applying the 2π modulo condition in angle. This has the advantage of simplifying the structure locally in phase space; the overlap with a localized state is now obtained by replicating that state periodically, as is shown by the shaded disk. We consider the Green's function first, i.e., $\langle q|q_t\rangle$. The figure has regions blackened out that violate the area h rule for a particular value of h. Some of the blackened areas are standard textbook caustics; others are thin "tendrils" [10]. However, no matter how thin a tendril has become nor how many folds upon folds have been generated by the dynamics, the sole criterion for accuracy of a given pair of coalescing stationary phase points in the integration variable p_0 is their distance as measured by the phase accumulation of the exponent between the points in question; this accumulation should be 2π or greater, which translates into the area h in the phase plane. Thus, even though the points marked C,D in Fig. 1 are not separated by 2π, and are generating inaccuracies if $|q\rangle$ should happen to cut through those regions, the contribution from A and B encloses area greater than h and is accurate even though the distance between A and B is minuscule on the scale of $h^{1/2}$. Note that subsequent evolution will fold the Lagrangian manifold further but cannot reduce the area enclosed between A and B (which have been chosen to lie on a stable manifold and will move exponentially closer together). The Poincaré-Cartan theorem of dynamics also guarantees that the area preservation and phase difference between A and B hold even if the phase plane is a surface of section. We emphasize that developing folds, once formed, remain and collapse upon themselves with further evolution while preserving their h area. This has the effect that caustic behavior becomes increasingly nonlocal.

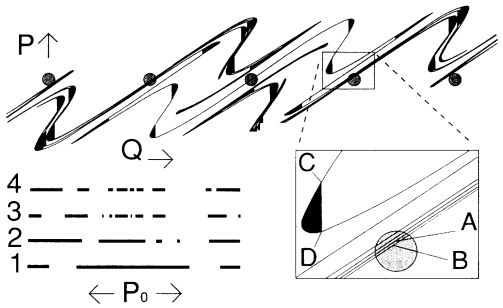

FIG. 1. Upper: Part of the $q_0=0$ manifold unfolded in the angle variable after several iterations. Left: Fragment of the initial q-manifold after removing "bad" segments for times 1, 2, 3, and 4. Right: Detail of the upper diagram showing the coherent state and the semiclassically inaccurate region in dark.

As a global measure of the accuracy of the semiclassical propagator, we adopt the following criterion: Ranges of p_0 which contribute to such caustic zones are eliminated, and the fraction F_p of initial p_0 remaining good constitutes a figure of merit. This is a reasonable measure, because all "good" regions translate into pieces of the evolving Lagrangian manifold which yield accurate amplitudes.

At first it would seem that the good regions of initial p_0 would disappear exponentially fast, since the folds and thus the caustics will proliferate exponentially. However, since the length of the manifold is increasing exponentially in tandem with the folds (typically with the same exponent), folds which develop later each correspond to an exponentially smaller piece of the initial range of p_0. Figure 1 illustrates how the ranges of good initial p_0 become more and more like a Cantor set.

In coordinate space, the inaccurate regions of overlap are almost everywhere if one considers (1) the black re-

gions showing violation of the area h rule in the coordinate space amplitude, and (2) the modulo 2π condition, which folds Fig. 1 over on itself. Also, it should be noted that diffraction errors on the "dark side" of the black regions extend the region of inaccuracy. Still, the Van Vleck-Gutzwiller Green's function can accurately propagate states: In spite of its failure in coordinate space, Fig. 2 shows that a coherent state, represented by the disk, is faring quite well. Propagation of an extended state in amplitude space by explicitly integrating over the badly behaved semiclassical Green's function thus works. The major part of the correlation function $\langle\alpha|q_t\rangle$, where $|\alpha\rangle$ is the coherent state is coming from the replicas on either side of the center, and these are entirely in "safe" zones. The zones of poor amplitude for a "circular $\Delta p=\Delta q$" coherent state are reasonably estimated by a superposition of the p and the q error zones. If a coherent state comes too close or enters such a zone, it will yield somewhat inaccurate amplitudes, although the magnitude of the error cannot climb to very large values as it does in coordinate or momentum space because of singularities in the Van Vleck-Gutzwiller determinant.

From the phase space, Lagrangian manifold analysis it is quite clear that the accuracy of semiclassical amplitudes is very nonuniform; it would be possible to find inaccurate regions almost immediately, while other zones are well behaved far past the logarithmic time. Very often, smooth state correlation functions are physically the desired quantity; other times, as when determining energy eigenvalues, for example (by Fourier transform of a correlation function [3]), one has a choice of states. This makes the present results of far-reaching consequence for applications.

We turn to the dependence of the fraction F_p on h. At a fixed time, a finite number of folds will have developed. As $h\to 0$, $F_p\to 1$. For a given fold, suppose we transform canonically to the coordinate system p',q' so that the fold is aligned along the q' axis. This gives, to second order in p_0, $q'=\gamma+\alpha p_0+\beta p_0^2$, $p'=\alpha' p_0$. The line corresponding to $|q_0\rangle$ is now rotated by the transformation, and cuts the fold at an angle. If the area enclosed is h, the range of p_0 corresponding to "bad" parts of the fold is easily shown to go as $h^{1/3}$, at least for sufficiently small h, where the folds are isolated and the quadratic expansion in p_0 holds. This dependence has been checked for the standard map; see Fig. 3.

The time dependence of F_p is more problematical and system dependent, but we can make some headway by using the Smale-like horseshoe construction as a model of the tangles developing in the Lagrangian manifold. Consider a p-like (horizontal) Lagrangian manifold which folds once to a U shape, lying on its side, making one caustic in coordinate space. After compression by a factor of 2 and stretching by the same factor, it is folded again, making a total of three caustics. The nth cycle yields $2^{n+1}-1$ total caustics, but the stretching by the factor 2^n means that each successive caustic spans a smaller range of initial manifold, by a factor $\frac{1}{2}^n$. A constant fraction of the initial manifold therefore lands in caustics at each step, whether or not it has previously been part of another caustic. Thus the fraction removed is not confined just to the remaining good regions of the initial manifold, but is applied apparently at random to the whole of the initial manifold. The differential equation describing this removal procedure is

$$-\frac{dF_p}{dt}=\alpha\lambda\hbar^{1/3}F_p,\quad\Longrightarrow F_p(t)=\exp(-\alpha\lambda\hbar^{1/3}t)\,, \tag{5}$$

where λ is the Lyapunov exponent and α a system-dependent proportionality constant. Thus the good initial manifold disappears relatively slowly and the half-life for good semiclassical propagation scales as $\hbar^{-1/3}$.

The area rule leads to the remarkable conclusion that stronger chaos may actually *help* the semiclassical accuracy by producing larger folds with more area enclosed. This might lead to the worry that the generic "soft" chaos systems would be problematical, but some recent calculations show good agreement though much more study is required.

The present Letter reconciles the standard theories of semiclassical mechanics with the intriguing findings of unexpected long time accuracy for chaotic systems. The

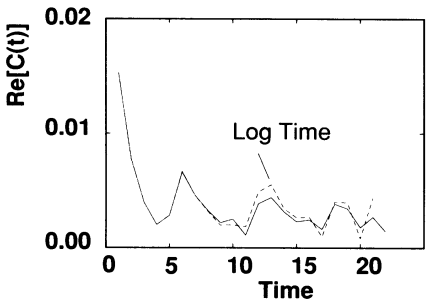

FIG. 2. Comparison of an exact quantum and semiclassical calculation of $C(t)=\langle\alpha|p_0(t)\rangle$ for the standard map ($K=2.14$). The semiclassical is the dashed line and the quantum is the solid line. The initial state is the p state at 0; the coherent state was localized at $x_0=\pi$, $p_0=0$, and $\hbar=0.00159$.

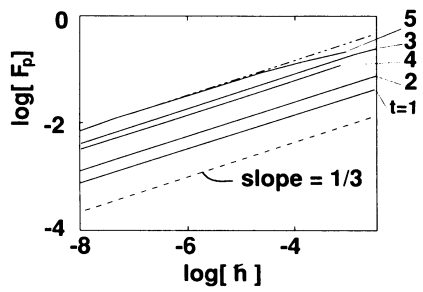

FIG. 3. The fraction F_p of the "good" manifold remaining in $|p_0\rangle$ is shown as a function of $\hbar$ for different iterations of the mapping ($t=1$ to 5).

understanding of the source of errors, in our case the "lack of errors," opens a new door in the field of applications of semiclassical techniques for classically chaotic systems. Perhaps of more importance is to realize that with so much research emphasis on semiclassical techniques in the energy domain, its fundamental precursor, the time Green's function, still deserves far more exploration.

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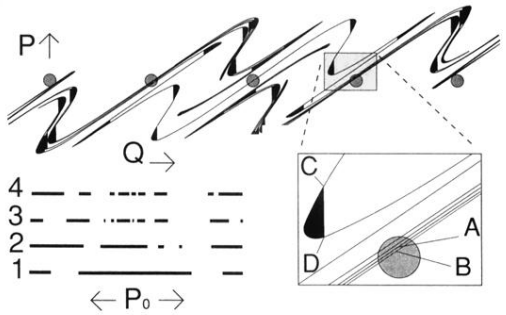
[15] The standard map is a 2D mapping of the cylinder onto itself defined by the following equations: $p_{n+1}=p_n+K\sin(x_n)$, $x_{n+1}=x_n+p_{n+1}$ (mod2π). The parameter K determines the chaoticity of the mapping. We selected $K=2.14$ in the calculations shown in this Letter. For information on the quantized version see Chirikov's contribution in *Chaos and Quantum Physics*, Proceedings of the Les Houches Summer School, Session LII, edited by M.-J. Giannonni, A. Voros, and J. Zinn-Justin (Elsevier, New York, 1991), and references therein.



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