Semiclassical amplitudes: Supercaustics and the whisker map

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The semiclassical approximation for a quantum amplitude is given by the sum of contributions from intersections of the appropriate manifolds in classical phase space. The intersection overlaps are just the Van Vleck determinants multiplied by a phase given by a classical action. Here we consider two nonstandard instances of this semiclassical prescription which would appear to be on shaky ground, yet the corresponding physical situations are not unusual. The first case involves momentum-space WKB theory for scattering potentials; the second is a propagator for the whisker map that arises in generic two-dimensional systems. In the former case two manifolds become asymptotically tangent, and the semiclassical formula needs to be uniformized in order to give a meaningful wave function. We give a uniformization procedure. In the latter case, there are an infinite number of intersections in phase space within a zone with the area of Planck's constant (the limit of resolution for quantum mechanics), yet the semiclassical sum over all contributions is shown to be correct.

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I. INTRODUCTION

Semiclassical approximations to quantum mechanics are useful for physical insight as well as semiquantitative results. Consider the computation of a quantum amplitude of the form $\langle \phi_2 | \phi_1 \rangle$ (e.g., if $|\phi_2\rangle = |x\rangle$ and $|\phi_1\rangle = e^{-iHt/\hbar}|x'\rangle$; this is the coordinate space propagator). The semiclassical approximation for such a quantum amplitude is produced from classical objects and Planck's constant h: it has the form $\Sigma \sqrt{\rho}\, e^{iS/\hbar}$, where the sum goes over classical paths with boundary conditions determined by the two states in question. The phase S is the appropriate classical action for the classical path, and the weighting ρ is a classical probability density together with any Maslov factors arising from caustics encountered by the path [1]. This form emerges out of the stationary phase evaluation of Feynman path integrals where the stationary paths are classical trajectories; they dominate the path integral in the $\hbar \to 0$ limit. The validity of the semiclassical sum hinges on the differences in action between the different contributions being ''large'' compared with Planck's constant h. When this is not the case, the semiclassical approximation breaks down.

In this paper we study two situations which, to our knowledge, have not been discussed before in the literature, but the physical situations they represent arise quite generally. The first case (Sec. II) is the semiclassical energy eigenfunction (WKB) in momentum-space for potentials which are asymptotically constant, as in scattering systems. In phase space, the momentum manifold is asymptotically tangent to the energy manifold over an infinite range. A uniformization needs to be performed in order to give a reasonable approximation to the quantum amplitude. We call this a supercaustic to distinguish it from an ordinary caustic, which is the simple tangency of the manifolds that occurs when stationary phase points coalesce and the action difference becomes smaller than h. In the second case (Sec. III), there are an infinite number of semiclassical contributions converging together exponentially within an area of h in phase space. Planck's constant h sets a lower limit on the size of structure in classical phase space that quantum mechanics can resolve, yet the primitive semiclassics turn out to work very well with no corrections. We show why this is the case.

II. UNIFORMIZATION OF A SUPERCAUSTIC

When finding semiclassical energy eigenfunctions in a given representation (e.g., x or p), the sum discussed above goes over all the phase-space intersections of the constant energy manifold with the representation. This semiclassical (or WKB) wave function built on the Van Vleck determinants and classical actions in general provides a good approximation to exact wave functions, and solves Schrödinger's equation to order $\hbar$. An important exception occurs at caustics.

It is useful to consider classical phase-space diagrams, where the quantum states in question are represented by manifolds [2]. The quantum states are represented in phase space as lines of finite thickness, appropriate to the successive contours of fixed canonical variables (such as the action). The area of the intersections of two sets of such manifolds is then proportional to the Van Vleck prefactor in the semiclassical sum, which is just the classical probability density given the initial and final conditions; the action line integral along the manifold is in the phase S [3].

Consider the coordinate representation of a harmonic-oscillator eigenstate. Figure 1 shows a constant energy contour of energy E for a harmonic-oscillator potential in one dimension. The semiclassical coordinate space energy eigenfunction is the sum of contributions from each of the two intersections of the shaded vertical line representing x, with the circle corresponding to constant energy. These intersections represent the two classical ''roots'' with momenta $p(x) = \pm\sqrt{2m(E - V(x))}$. For x further to the right the intersections become closer, eventually coalescing (where the

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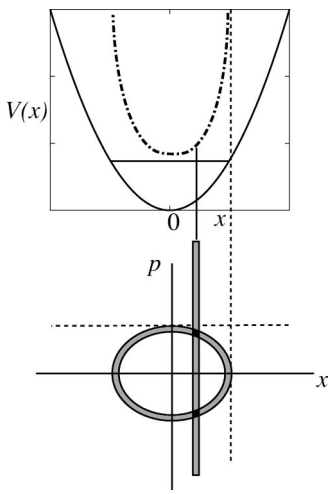

FIG. 1. Harmonic-oscillator potential $V(x)=x^2$ (above, solid line) and associated phase space (below). Caustics in coordinate space occur at the turning points of the motion (vertical dashed line), where the energy contour is parallel to an x state. There are also caustics in momentum space (horizontal dashed line), at the center of the well, and this is where the energy contour is parallel to a p state. The dot-dashed line shows the classical coordinate space density with a coordinate space caustic (infinity in the probability density). If we assign proper thickness variations to the areas representing the states, the intersections are proportional to Van Vleck determinants, in the limits that the thickness vanishes (see dark intersection zones).

manifolds are tangent) at the vertical dashed line shown. The classical probability diverges as $p(x)^{-1}$, and the semiclassical wave function as $p(x)^{-1/2}$. Such a coalesence of intersections (i.e., stationary phase points) is called a caustic, and it signals the breakdown of semiclassics. The difference in action between the two contributions goes to zero and the prefactor ρ goes to infinity. For coordinate space energy eigenfunctions, this occurs at the turning points of the motion, $p(x)=0$. If we apply $(H-E)$ to a WKB state, where H is the Hamiltonian, there results an error which goes to infinity as a turning point caustic is approached:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)-E\right)\psi^{\pm}_{wkb}(x)$$
$$=\hbar^2\left(\frac{-3p'(x)^2}{8mp(x)^2}+\frac{p''(x)}{4mp(x)}\right)\psi^{\pm}_{wkb}(x), \qquad (1)$$

where $\psi^{\pm}_{wkb}(x)=[1/\sqrt{p(x)}]e^{\pm(i/\hbar)\int^x p(x')dx'}$, $p(x')=\sqrt{2m(E-V(x'))}$, and one dimension has been assumed for simplicity.

The momentum representation for p intersecting in the same region does so at a high angle, and does not suffer a caustic. However, momentum space has its own divergence problems elsewhere: not only may we have the type of caustic above, where the projection of the energy contour onto a line of constant momentum is parallel (dotted line in Fig. 1), but we may also encounter a contour which slowly *asymptotes* to a p state (Fig. 2) and remains almost parallel for an

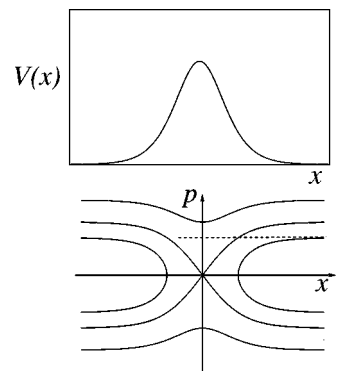

FIG. 2. Eckart barrier $V(x)=\mathrm{sech}^2 x$ (above) and associated phase space (below). As $x\pm\infty$ the potential flattens out. Here there is a ''supercaustic'' where the energy contour is asymptotic to a p state.

infinite extent along the contour. We shall call this more severe type of caustic a ''supercaustic.''

The WKB wave function in p space, obtained either by a stationary phase Fourier transform of the position space wave function to momentum space or by solving Schrödinger's equation to order $\hbar$ directly in momentum space, is

$$\phi_{wkb}(p)=\frac{1}{\sqrt{-V'(x(p))}}e^{(i/\hbar)\int^p x(p')dp'}, \qquad (2)$$

where

$$x(p')=V^{-1}(E-p'^2/2m), \qquad (3)$$

and V^{-1} is the inverse of the potential. (We note that V^{-1} is in general a multivalued function; the branch chosen in Eq. (3) is determined by the branch to which the classical contour corresponding to the semiclassical state we are describing belongs. For example, for a potential barrier centered at $x=0$ and for an energy below the barrier top, the positive (negative) branch choice of $x(p)$ gives a semiclassical state which lives on the right (left) side of the barrier (see Fig. 2). Caustics in momentum space, of the ordinary or super type, arise when the force is zero and the denominator in Eq. (2) vanishes. The exact solution in momentum space for a globally flat potential is a δ function, $\delta(p\pm\sqrt{2mE})$; this indicates that the exact eigenfunction for an asymptotically flat potential should also diverge. However, as we shall see shortly, the singularity in the WKB solution is quite incorrect.

Caustics of the simpler type have been well studied in position space. The potential may be approximated linearly near the turning point and there the (Airy function) solution found exactly; the WKB solution, valid further away, may then be ''glued'' smoothly to the exact solution near the turning point. Hence a uniformized semiclassical wave function valid everywhere may be obtained. More elaborately, there are uniformization techniques which involve a modification of the form of the WKB solution motivated by the exact solution near the turning point. Such methods give

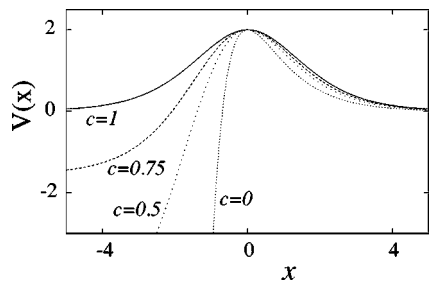

FIG. 3. The potential equation (4) with $Vo=2$ and $\alpha=1$. Uniformizing the p-space semiclassical wave function at the exponential tail ($x\rightarrow\infty$) is the subject of this section.

''connection formulas'' between classically allowed and forbidden regions. The reader is referred to the review by Berry and Mount for details of this [4] and references therein. The resulting uniformized wave function satisfies Schrödinger's equation to order $\hbar$, yet does not have the divergence problems of the WKB solution, i.e., it is *uniformly* valid in x. An analogous procedure in momentum representation can uniformize the ordinary type of caustic (Fig. 1) there.

The main result of this section is the uniformization of the momentum-space supercaustic associated with potentials which exponentially decrease asymptotically. In Sec. II A we introduce the potentials and demonstrate the incorrect divergence of the p-space WKB wave function at the supercaustic by calculating to order $\hbar^2$ the difference between the true Hamiltonian and the Hamiltonian for which ϕ_{wkb} is an exact eigenfunction. This is followed by the construction of a uniform semiclassical wave function for these potentials (Sec. II B). We show for the Eckart barrier how our uniformization compares to the exact eigenfunction, by calculating explicitly to order $\hbar^2$ the difference between the Hamiltonian for which the uniformized wave function is exact and the original wave function.

A. Supercaustic of an exponentially decreasing potential

Potentials of the form

$$V(x)=V_o\left(1-\left(\frac{1-e^{-\alpha x}}{1+c\ \ e^{-\alpha x}}\right)^2\right), \tag{4}$$

where $0\leqslant c\leqslant 1$, of which the Morse ($c=0$) and Eckart ($c=1$) potentials are special cases (Fig. 3), possess supercaustics in momentum space at $p\rightarrow\pm\sqrt{2mE}$. [We point out in passing that, for $E>V_o$, the simpler type of caustic also exists: at $p=\pm\sqrt{2m(E-V_o)}$, $V'(x(p))=0$ (the classical particle is at $x=0$) and the projection of the energy contour on to the p-axis is tangential].

We investigate the error in the WKB solution in momentum-space at the supercaustic. We need to compute the effect of the Hamiltonian on wave function (2),

$$\left[\frac{p^2}{2}+V\left(i\hbar\frac{d}{dp}\right)-E\right]\phi_{wkb}(p),$$

where we take mass 1. In momentum representation it is the kinetic term that is trivial (i.e., multiplicative) at the expense of the potential term which is now a differential operator. Momentum space is more complicated than coordinate space, where the kinetic term is only a second-order derivative (and the potential term is simply multiplicative). We evaluate the action of the potential term on the WKB wave function order by order in $\hbar$ in the following way. We first expand $V(i\hbar(d/dp))$ in a Taylor series of the form

$$V(0)+i\hbar V'(0)\frac{d}{dp}-\hbar^2\frac{V''(0)}{2}\frac{d^2}{dp^2}$$
$$-i\hbar^3\frac{V'''(0)}{6}\frac{d^3}{dp^3}+\hbar^4\frac{V''''(0)}{24}\frac{d^4}{dp^4}\cdots, \tag{5}$$

and operate with the series truncated say to four or five terms on wave function (2). Terms of the same order in $\hbar$ are collected; of course; typically each differential contributes to every order. At each order we find we have the first few terms of a Taylor series of a certain function; these functions are then taken to represent the result of $V(i\hbar(d/dp))\phi_{wkb}(p)$ at the corresponding order in $\hbar$. We find

$$V\left(i\hbar\frac{d}{dp}\right)\phi_{wkb}(p)=[V(x(p))+\hbar^2h(p)+O(\hbar^3)]\phi_{wkb}(p), \tag{6}$$

where

$$h(p)=-\frac{x'(p)^2V''''(x(p))}{8}-\frac{x''(p)V'''(x(p))}{6}$$
$$-\frac{3V''(x(p))^3x'(p)^2}{8V'(x(p))^2}+\frac{V''(x(p))^2x''(p)}{4V'(x(p))}$$
$$+\frac{V''(x(p))V'''(x(p))x'(p)^2}{2V'(x(p))}. \tag{7}$$

$x(p)$ is given by Eq. (3), $V(x(p))=E-p^2/2$, and the prime indicates differentiation with respect to the argument. Then, with $H=p^2/2+V(i\hbar d/dp)$, we have

$$(H-E)\phi_{wkb}(p)=\hbar^2h(p)\phi_{wkb}(p)+O(\hbar^3).$$

$h(p)$ is thus, to lowest order in $\hbar$, the error in the momentum-space WKB approximation of an energy eigenfunction.

Let us consider this function for potentials which, at large x, go like $W_oe^{-\alpha x}$ [e.g., for potentials (4), $W_o=2V_o(c+1)$]. Then, as $p\rightarrow\pm\sqrt{2E}$, $h(p)$ diverges. This is the momentum which a classical particle has asymptotically, that is, in the region where the potential becomes flat (and zero). The exact p-space wave function does indeed approach δ-function behavior here; although the WKB wave function also blows up, it very poorly represents this divergence as is evident in the blow-up of the difference Hamiltonian $h(p)$. In classical phase space this is where the constant energy

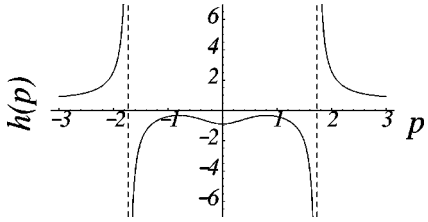

FIG. 4. The WKB wave function in p space differs from an eigenfunction of the Hamiltonian by $\hbar^2 h(p)+O(\hbar^3)$. Here we show $h(p)$ for the Eckart barrier, $V(x)=2\,\mathrm{sech}^2 x$, for $\phi_{wkb}(p)$ at energy $E=1.5$. The dashed lines indicate the $p=\pm\sqrt{2E}$ asymptotes. This corresponds to the dashed line in Fig. 2, and is where the potential becomes flat.

manifold asymptotes to a p eigenstate, and this is what we refer to as a supercaustic. In Fig. 4 we plot $h(p)$ for an Eckart barrier.

B. Uniformization

We saw above that momentum-space WKB theory fails in the asymptotic region of the potential (i.e., where the potential flattens out). The first step in uniformization is to find the exact energy eigenfunction in momentum representation of the Hamiltonian in this region:

$$H_{asy}=p^2/2+W_o e^{-\alpha x}.$$

We shall first find its exact eigenstates in configuration space, and then calculate the exact Fourier transform to momentum space. Performing the change of variable $z=(i2\sqrt{2W_o}/\hbar a)e^{-\alpha x/2}$ in Schrödinger's equation

$$\left(-\frac{\hbar^2}{2}\frac{d^2}{dx^2}+W_o e^{-\alpha x}-E\right)\psi_{asy}(x)=0$$

yields Bessel's equation of order $\nu=i2\sqrt{2E}/\hbar\alpha$:

$$\left(\frac{d^2}{dz^2}+\frac{1}{z}\frac{d}{dz}+\left(1-\frac{\nu^2}{z^2}\right)\right)\tilde{\psi}_{asy}(z)=0,$$

with solution

$$\psi_{asy}(x)=\mathcal{N}K_{(i/\hbar)(2/\alpha)\sqrt{2E}}\left(\frac{2\sqrt{2W_o}}{\hbar\alpha}e^{-\alpha x/2}\right). \tag{8}$$

$K_\nu(z)$ is MacDonald's function of order ν [5]. This has the correct behavior for $x\to-\infty$, where ψ exponentially decays. $\mathcal{N}$ is a normalization constant; choosing

$$\mathcal{N}=\frac{2}{\pi}\left(\frac{1}{2E}\right)^{1/4}\sinh\left(\frac{2\sqrt{2E}\pi}{\alpha\hbar}\right)\Gamma\left(1+\frac{i}{\hbar}\frac{2\sqrt{2E}}{\alpha}\right) \tag{9}$$

gives unit incoming flux from the right; that is,

$$\psi_{asy}(x\to\infty)\to\left(\frac{1}{2E}\right)^{1/4}(e^{-i\sqrt{2E}x/\hbar}+re^{i\sqrt{2E}x/\hbar}),$$

where $|r|=1$. This can be readily verified by the property (see Ref. [5])

$$K_\nu(z)\overset{z\to 0}{\to}\frac{\pi}{2}\left(\left(\frac{z}{2}\right)^{-\nu}\frac{1}{\Gamma(1-\nu)}+\left(\frac{z}{2}\right)^{\nu}\frac{1}{\Gamma(1+\nu)}\right).$$

$\Gamma(\omega)$ is the γ function:

$$\Gamma(\omega)=\int_0^\infty e^{-t}t^{\omega-1}\,dt, \tag{10}$$

By Fourier transform we obtain the solution in momentum space,

$$\begin{aligned}\phi_{asy}(p)&=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{-ipx/\hbar}\psi_{asy}(x)dx\\&=\frac{\mathcal{N}}{4\sqrt{2\pi\hbar}}e^{(-ip/\hbar\alpha)ln(2W_o/\alpha^2\hbar^2)}\\&\quad\times\Gamma\left(\frac{i}{\hbar\alpha}(p+\sqrt{2E})\right)\Gamma\left(\frac{i}{\hbar\alpha}(p-\sqrt{2E})\right),\end{aligned} \tag{11}$$

where we used the integral expression (see Ref. [5]) $K_\nu(z)=\frac{1}{2}(z/2)^\nu\int_0^\infty e^{-t-z^2/4t}t^{-\nu-1}\,dt$ for $|\arg(z)|<\pi/4$. This is the exact momentum-space eigenfunction for the Hamiltonian $p^2/2+W_o e^{-\alpha x}$. As expected, the semiclassical limit of the exact solution (11) yields the p-space WKB solution for this Hamiltonian: noting that

$$\Gamma(z\to\infty)\to e^{zlnz-z-(1/2)lnz+(1/2)ln2\pi},$$

we find that, as $\hbar\to 0$,

$$\phi_{asy}(p)\to\frac{\mathcal{N}\alpha}{4}\sqrt{\pi\alpha\hbar}\,e^{-\pi\sqrt{2E}/\hbar a}\phi_{asy,wkb}(p), \tag{12}$$

where

$$\begin{aligned}\phi_{asy,wkb}(p)&=\frac{1}{\sqrt{-V'(x(p))}}\exp\left(\frac{-i}{\hbar}\int_0^p x(p')dp'\right)\\&=\sqrt{\frac{1}{\alpha(E-p^2/2)}}\\&\quad\times\exp\left[\frac{-2i}{\hbar\alpha}\left(p-\sqrt{\frac{E}{2}}\ln\left(\frac{p+\sqrt{2E}}{p-\sqrt{2E}}\right)\right.\right.\\&\quad\left.\left.+\sqrt{\frac{E}{2}}\pi i-\frac{p}{2}\ln\left(\frac{E-p^2/2}{W_o}\right)\right)\right].\end{aligned} \tag{13}$$

Equation (11) is an exact solution in the region where the WKB solution for potentials of the form of Eq. (4) diverges. This exact solution for the exponentially decreasing potential is what we need for the uniformization of the supercaustic of these potentials. We would like our uniform semiclassical wave function to satisfy Schrödinger's equation up to order

$\hbar$, and have the correct blow-up behavior near $p=\pm\sqrt{2E}$, so that the error in being an exact energy eigenfunction is everywhere finite and of order $\hbar^2$ (and higher). Below, we shall show that this can be achieved by multiplying Eq. (11) by well-behaved WKB factors which correct for the difference between the original potential and the exponentially decreasing one on which the uniformization is based. This accounts for the behavior away from the supercaustic. We hope the following will clarify what is meant by this.

The general potential (4) has the exponential asymptotic behavior

$$V(x\to\infty)\to 2V_o(c+1)e^{-\alpha x}:=V_{asy}(x). \tag{14}$$

We observe that the classical position for the exponentially decaying potential $V_{asy}(x)$ may be written

$$x^{asy}(p)=-\frac{1}{\alpha}\ln\left(\frac{E-p^2/2}{2V_o(c+1)}\right),$$

and, for this potential,

$$V'_{asy}(x(p))=-\alpha(E-p^2/2).$$

Now, the classical position as a function of momentum for the *general* potential (4) is

$$x(p)=-\frac{1}{\alpha}\ln\left(\frac{E-p^2/2}{2V_o(c+1)}\right)-\frac{1}{\alpha}\ln\left(\frac{2(c+1)\left(1-c\sqrt{1-\frac{E-p^2/2}{V_o}}\right)}{\left(1-c^2\left(1-\frac{E-p^2/2}{V_o}\right)\right)\left(1+\sqrt{1-\frac{E-p^2/2}{V_o}}\right)}\right)\equiv x^{asy}(p)+x_{extra}(p), \tag{15}$$

and the derivative of the potential is

$$V'(x(p))=-\alpha(E-p^2/2)\left(\frac{2(c+1)\left(1-c\sqrt{1-\frac{E-p^2/2}{V_o}}\right)}{\left(1-c^2\left(1-\frac{E-p^2/2}{V_o}\right)\right)\left(1+\sqrt{1-\frac{E-p^2/2}{V_o}}\right)\left(\frac{1-e^{-\alpha x(p)}}{1+ce^{-\alpha x(p)}}\right)}\right)\equiv V'_{asy}(x(p))\times V'_{extra}(p). \tag{16}$$

The sum and factorization properties in Eqs. (15) and (16) respectively, enable us to write the p-space WKB wave function for the general potential as the product

$$\phi_{wkb}(p)=\phi_{asy,wkb}(p)\times\frac{1}{\sqrt{V'_{extra}(p)}}e^{-(i/\hbar)\int^p x_{extra}(p')dp'}, \tag{17}$$

where $\phi_{asy,wkb}(p)$ is as in Eq. (13) with $W_o=2V_o(c+1)$. We can now assert the uniformization for potentials of form of Eq. (4) is

$$\begin{aligned}\phi_{unif}(p)=\mathcal{N}'\exp&\left[\frac{-ip}{\hbar\alpha}\ln\left(\frac{4V_o(c+1)}{\alpha^2\hbar^2}\right)\right]\\&\times\Gamma\left(\frac{i}{\alpha\hbar}(p+\sqrt{2E})\right)\Gamma\left(\frac{i}{\alpha\hbar}(p-\sqrt{2E})\right)\\&\times\frac{1}{\sqrt{V'_{extra}(p)}}e^{-(i/\hbar)\int^p x_{extra}(p')dp'},\end{aligned} \tag{18}$$

where we have replaced the WKB solution for the exponential potential with the exact solution there from Eq. (11). This wave function has the correct blow-up behavior as $p\to\pm\sqrt{2E}$ [the extra WKB factors tend to 1 (up to a phase) in this limit] and, as $\hbar\to 0$, this reduces, by construction, to the WKB wave function. The WKB factors are well-behaved semiclassical objects: the divergent part of the semiclassics has already been extracted and replaced by an exact solution for the asymptotic region. This solution is then modified by benign WKB factors accounting for the difference between the true potential and the exponential.

The final check, of course, is to calculate the deficit of ϕ_{unif} as an eigenfunction [following the procedure as in obtaining Eq. (6)]. That it is now finite is clear, from the above comments. As an example, we consider the Eckart barrier $V(x)=V_o\,\mathrm{sech}^2(x)$. Equation (19) gives

$$\begin{aligned}\phi^R_{unif}(p)=\exp&\left[\frac{-ip}{2\hbar}\ln\left(\frac{2V_o}{\hbar^2}\right)\right]\Gamma\left(\frac{i}{2\hbar}(p+\sqrt{2E})\right)\\&\times\Gamma\left(\frac{i}{2\hbar}(p-\sqrt{2E})\right)\left(\frac{1}{1-\frac{E-p^2/2}{V_o}}\right)^{1/4}\\&\times\exp\left[-\frac{i}{\hbar}\int_0^p\ln\left(\frac{1}{2}\left(1+\sqrt{1-\frac{E-p'^2/2}{V_o}}\right)\right)dp'\right],\end{aligned} \tag{19}$$

where the R superscript denotes the state at energy E that

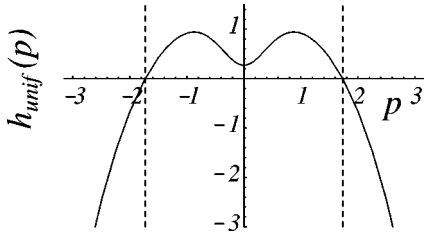

FIG. 5. This plot of $h_{unif}(p)$ shows how much the uniformized semiclassical wave function at energy $E=1.5$ for the Eckart barrier $2\,\mathrm{sech}^2\,x$ misses being an energy eigenfunction to order $\hbar^2$. Notice that the function is finite and ''small'' in the physical domain $|p| \leqslant \sqrt{2E}$ (between the dashed lines), unlike the case for the WKB wave function (Fig. 4).

lives on the right-hand side of the barrier, corresponding to the positive branch of the V^{-1} function (see also Fig. 2). The state on the left, is given by the complex conjugate

$$\phi^L_{unif}(p)=\overline{\phi^R_{unif}(p)}.$$

$\phi^L_{unif}(p)$ stems from uniformization based on the $e^{+\alpha x}$ potential. To calculate the action of the Hamiltonian on Eq. (19), we proceed as in Eq. (5). It is easiest, however, to perform the differentiation operations on the Γ functions within the integral expression for the Γ function [Eq. (10)], and then integrate the result at the final stage. In particular,

$$(i\hbar)^n \frac{d^n}{dp^n}\Gamma\left(\frac{i}{2\hbar}(p\pm\sqrt{2E})\right) = \int_0^\infty \left(-\frac{1}{2}\ln t\right)^n e^{-t} t^{(i/2\hbar)(p\pm\sqrt{2E})-1}\, dt$$

We used MATHEMATICA to operate with the first few terms of Eq. (5) on ϕ_{unif}, but with the $\Gamma((i/2\hbar)(p+\sqrt{2E}))\Gamma((i/2\hbar)(p-\sqrt{2E}))$ replaced by $t^{(i/2\hbar)(p+\sqrt{2E})}\tilde{t}^{(i/2\hbar)(p-\sqrt{2E})}$. At the expense of simplifying the differentiation operations we have complicated the resumming at each order in $\hbar$. We obtain, after much algebra,

$$V\left(i\hbar\frac{d}{dp}\right)\phi_{unif}(p) = [V(x(p)+\hbar^2 h_{unif}(p)+O(\hbar^3))]\phi_{unif}(p), \tag{20}$$

where $h_{unif}(p)$ is a long expression (a sum of about 50 terms) depending on V_o, E, and p. $\hbar^2 h_{unif}(p)$ is the perturbation which turns off the quantum phenomenon of barrier tunneling (to order $\hbar^2$): the semiclassical wave function $\phi^{R(L)}_{unif}$ lives only on the right (left) side of the barrier and is an eigenstate of $H-\hbar^2 h_{unif}$ to order $\hbar^2$. In this sense the effect of h_{unif} is to suppress tunneling to the left (right) up to order $\hbar^2$. We note that a complementary concept of turning off above-barrier reflection was discussed in Ref. [6]. In Fig. 5 we plot $h_{unif}(p)$ for energy $E=1.5$ in the Eckart barrier $2\,\mathrm{sech}^2\,x$ (cf. the corresponding quantity for the WKB function, Fig. 4).

III. SEMICLASSICAL QUANTIZATIONS OF THE WHISKER MAP

We continue our investigation of semiclassical amplitudes with the whisker map. Arnold first coined the term ''whisker'' for branches of the separatrix [7]. The separatrix is one of the most common structures in the phase space of generic systems, and it is the birthplace of chaos in near-integrable systems. Near a resonance in a two-degrees-of-freedom near-integrable system, one can transform to a pair of approximate ''slow'' action-angle variables and a pair of approximate ''fast'' action-angle variables. To first order, the Hamiltonian in the slow variables is a pendulum, and a closer look reveals a chaotic layer around the pendulum separatrix. The whisker map describes the motion in this chaotic layer.

Zaslavskii and Filonenko [8] originated this mapping; it was later extensively studied by Chirikov [9]. Specifically, it is the mapping of the fast action and angle when they pass through a surface of section erected at the hyperbolic point of the (slow variable's) pendulum. One obtains

$$I' = I - k\sin\theta,$$
$$\theta' = \theta + \lambda \ln\left|\frac{c}{I'-I_o}\right| \quad (\mathrm{mod}\, 2\pi). \tag{21}$$

We refer the reader to the literature [9,10] for details and for the identification of the parameters k and λ in terms of the original parameters of the two-dimensional Hamiltonian. There are essentially two independent parameters in the classical whisker map: λ, which shears the angle before it is wrapped back to the domain $[0,2\pi)$, and k, which determines the jumps in action. I_o simply translates in action space, and c can be absorbed into a scaled action. In our numerical work c is taken to be 1.

A particularly interesting feature of this mapping, arising from choosing an $I-\theta$ surface of section at fixed slow angle, is that much occurs in just one iteration: in the infinite time it may take to return to the surface of section erected at the hyperbolic point of the slow variable pendulum, the fast angle θ may undergo an infinite number of oscillations. The slightest perturbation throws the system even after just one iteration, since even the smallest perturbation can have a large effect in the nearly infinite time it takes to come back to the pendulum's hyperbolic point.

In this section we compute matrix elements of the quantum and semiclassical one-step evolution operator U in the angle and action bases. We note that in Ref. [11] a full quantization in the action representation was given. Here our interest is in a semiclassical study where we find a remarkable classical phase-space structure. For example, in an angle representation the infinite number of oscillations alluded to above gives rise to an infinite number of intersections of the relevant phase-space manifolds, which approach each other exponentially closely in classical phase space. Semiclassically we know we must add the infinitely many contributions; Quantum mechanics smears over structure below the

scale of Planck's constant h, so the question might arise as to the relevance of all the terms, or whether they are semiclassically legitimate, well-separated stationary phase points. We shall discuss these and other semiclassical issues shortly; first, we discuss the full quantization in angle representation and in action representation.

A. Quantization

A ''Hamiltonian'' which gives rise to the whisker map is

$$H=\lambda(I-I_o)\left(\ln\left|\frac{c}{I-I_o}\right|+1\right)-k\cos\theta\sum_n\ \delta(t-nT). \tag{22}$$

Integrating the equations of motion $\dot{\theta}=\partial H/\partial I$, $\dot{I}=-\partial H/\partial\theta$ over a period T yields the whisker map [Eq. (21)]. As for any map, the choice of Hamiltonian is not unique. For example, having the ''potential'' term acting first for a finite fraction of period T and then the ''kinetic'' term for the remaining fraction also results in the whisker map equations. This nonuniqueness is not surprising considering that the map only ''sees'' the system once each period, and not in between. The quantum evolution operator over one period (Floquet operator), $U=\mathcal{T}\exp(-i\int_0^T H\,dt/\hbar)$ (with $\mathcal{T}$ denoting positive time ordering) *is* unique as we would expect: all choices of H give the operator

$$U=\exp\left(-i\lambda(I-I_o)\left(\ln\left|\frac{c}{I-I_o}\right|+1\right)\Big/\ \hbar\right)e^{ik\cos\theta/\hbar}, \tag{23}$$

where θ and I are now of course quantum operators. The phases ν of the eigenvalues $e^{-i\nu}$ of the unitary operator U are called quasienergies and are defined mod 2π. The corresponding quasienergy eigenstates are also called Floquet states.

The quantum probability amplitude for being at angle θ_f after one iteration of the whisker map, having started at θ_i, is given by the propagator

$$\begin{aligned}K(\theta_i,\theta_f)&=\sum_n\ \langle\theta_f+2\pi n|U|\theta_i\rangle\\&=\sum_n\ \int dI\frac{1}{2\pi i\hbar}e^{iI(\theta_f-\theta_i+2\pi n)/\hbar}\\&\quad\times\exp\left(-i\lambda(I-I_o)\left(\ln\left|\frac{c}{I-I_o}\right|+1\right)\Big/\ \hbar\right.\\&\quad\left.+ik\cos\theta_i/\hbar\right),\end{aligned} \tag{24}$$

where the sum over n is a sum over domains in angle resulting from taking mod 2π in the map. We have used the closure relation $\int dI|I\rangle\langle I|=\mathbf{1}$ and the bracket $\langle I|\theta\rangle=\exp(iI\theta/\hbar)/\sqrt{2\pi i\hbar}$ which follows from action and angle being canonically conjugate variables with commutator $[\theta,I]=i\hbar$.

The sum over domains may be transformed into a sum in action space (Poisson's summation formula): $\Sigma_n e^{iI2\pi n/\hbar}=\Sigma_j\hbar\,\delta(I-j\hbar)$. This yields the quantization rule for allowed actions and ensures periodic boundary conditions in angle. Inserting this into Eq. (24) would give an infinite sum over I-matrix elements of oscillating exponentials. To avoid this divergence, we truncate the phase space to a finite cylinder symmetric about I_o:

$$\theta\in[0,2\pi),\quad I\in[-I_c+I_o,I_c+I_o).$$

The number of quantum states is $N=2I_c/\hbar$ which allows each state an area of Planck's constant h in phase space. The closure relation in action becomes $\mathbf{1}=\Sigma_{j=-N/2}^{N/2-1}|I_j\rangle\langle I_j|$ where $I_j=j\hbar$ for example (or $j\hbar+\text{integer}\hbar$). Finally, we replace $\sqrt{1/(2\pi i\hbar)}$ with $\sqrt{\hbar/(2I_c)}$ as the normalization factor, and $\int dI$ with $\hbar\Sigma_j$, to obtain

$$\begin{aligned}K(\theta_i,\theta_f)&=\left(\frac{\hbar}{2I_c}\right)e^{ik\cos\theta_i/\hbar}\\&\quad\times\sum_{j=[(-I_c+I_o)/\hbar]_+}^{[(I_c+I_o)/\hbar]_-}\exp\left(ij(\theta_f-\theta_i)-i\lambda(j-I_o/\hbar)\right.\\&\quad\left.\times\left(\ln\left|\frac{c}{j\hbar-I_o}\right|+1\right)\Big/\ \hbar+ik\cos\theta_i/\hbar\right),\end{aligned} \tag{25}$$

where $[\ ]_{-(+)}$ rounds down (up) to the nearest integer. θ_f and θ_i also take on quantized values: only N angle states may fit into 2π, so each allowed state has support integer$\times\pi\hbar/I_c$. Choosing states θ_p to be centered at $p\pi\hbar/I_c$ gives periodic boundary conditions in action. [Note that in Eq. (25) and in any following equations, i, which does not appear as a subscript, is $\sqrt{-1}$.]

We observed in the classical map that I_o acts only as a translation in action, shifting the entire phase space by a constant. Indeed, I_o plays the same role here: if we rotate our basis to $|\tilde{\theta}\rangle=e^{-iI_o\theta/\hbar}|\theta\rangle$, then the propagator $K(\tilde{\theta}_i,\tilde{\theta}_f)$ has no I_o dependence. The quantization changes since the δ function is now $\delta(I-I_o-j\hbar)$. I_o is much like a gauge variable: any choice of I_o leads to the same quantum mechanics *provided* the basis is rotated.

The propagator in action is

$$\begin{aligned}K(I_f,I_i)&=\langle I_f|\exp\left(-i\lambda(I-I_o)\left(\ln\left|\frac{c}{I-I_o}\right|+1\right)\Big/\ \hbar\right)\\&\quad\times e^{ik\cos\theta/\hbar}|I_i\rangle\\&=\frac{\hbar}{2I_c}\exp\left(-i\lambda(I_f-I_o)\left(\ln\left|\frac{c}{I_f-I_o}\right|+1\right)\right)\\&\quad\times\sum_{p=0}^{2(I_c/\hbar)-1}\exp\left(-i\pi(I_f-I_i)p/I_c\right.\\&\quad\left.+ik\cos\left(\frac{p\pi\hbar}{I_c}\right)\Big/\ \hbar\right),\end{aligned} \tag{26}$$

where we inserted the identity in the form of a complete set of angles in the middle of the factorized propagator. This result was also obtained in Ref. [11]. Again, we see the

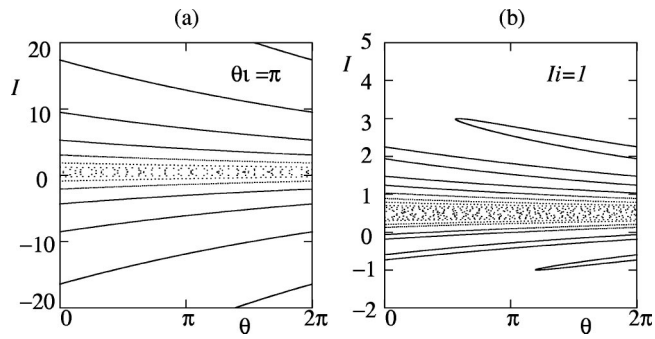

FIG. 6. Classical one-time step evolution of the whisker map, $\lambda=10$, $k=2$, and $I_o=0.5$. (a) Initial distribution at $\theta=\pi$. (b) Initial distribution at $I=1$.

gauge nature of I_o: if we define $|\tilde{I}\rangle=|I-I_o\rangle$, then I_o drops out of $K(\tilde{I}_f,\tilde{I}_i)$ i.e., the propagator is the same for all gauge choices provided we translate the basis (cf. the classical case).

B. Semiclassical approximation

Semiclassical quantization of maps proceeds much like that of continuous time systems: amplitudes are expressed as the square root of a classical probability times an exponential whose phase is the appropriate classical action. If more than one classical path links the two end points in question, then a sum of such terms, one for each classical path, is needed. Pictorially, the one-step semiclassical propagator from an initial state $|i\rangle$ to a final state $|f\rangle$ may be represented as summing, with appropriate complex weights, the intersections of two manifolds in classical phase space: one is the distribution corresponding to $|f\rangle$, the other the distribution obtained by evolving the manifold of points corresponding to $|i\rangle$ for one iteration. This yields a very interesting picture for the whisker propagator in angle representation [Fig. 6(a)]: there is an infinite number of intersections of the evolved initial angle state with any final angle state (a vertical line). The I value of the intersections converge toward I_o. This raises an interesting question for semiclassics: the full quantum mechanics smears over structure in phase space below the level of h, yet, within an $\hbar$ slice of I_o there is an infinite number of semiclassical contributions to be summed. Does the quantum mechanics ''see'' them all? In fact, as we shall see shortly, it does.

One may compute the semiclassical angle propagator from the type 1 classical generating function F_1:

$$K^{sc}(\theta_i,\theta_f)=\sum\sqrt{\frac{-1}{2\pi i\hbar}\frac{\partial^2 F_1}{\partial\theta_i\,\partial\theta_f}}e^{iF_1(\theta_f,\theta_i)/\hbar}, \tag{27}$$

where $I_i=-\partial F_1(\theta_f,\theta_i)/\partial\theta_i$ and $I_f=\partial F_1(\theta_f,\theta_i)/\partial\theta_f$ and the sum is over different classical paths that link θ_i with θ_f. For the whisker map, $F_1(\theta_f,\theta_i)=I_o(\theta_f-\theta_i)\mp c\lambda\exp(-(\theta_f-\theta_i)/\lambda)+k\cos\theta_i$, where the two signs represent the classical paths above and below I_o, respectively. This gives

$$\begin{aligned}K^{sc}(\theta_i,\theta_f)&=\frac{1}{I_c}\sqrt{\frac{i\pi c\hbar}{2\lambda}}\sum_{n=n_c}^{\infty}e^{-(\theta_f-\theta_i+2\pi n)/2\lambda}e^{iI_o(\theta_f-\theta_i+2\pi n)/\hbar}\\&\quad\times e^{ik\cos\theta_i/\hbar}(e^{-ic\lambda e^{-(\theta_f-\theta_i+2\pi n)/\lambda}/\hbar}\\&\quad-ie^{ic\lambda e^{-(\theta_f-\theta_i+2\pi n)/\lambda}/\hbar}),\end{aligned} \tag{28}$$

where the sum is over different domains in angle, arising from taking mod 2π after the shearing. (We note again the gauge role of I_o is manifest: using the rotated basis as described in Sec. III A the I_o dependence in the propagator drops out). The sum has a lower limit at

$$n_c=\left[\frac{1}{2\pi}\left(\lambda\ln\left|\frac{c}{I_c}\right|-(\theta_f-\theta_i)\right)\right]_+ \tag{29}$$

(where, as before, $[\ ]_+$ rounds up to the closest integer); this corresponds to the truncation of the cylinder in the action coordinate. The two terms for each n represent the two classical paths that have been sheared over to angle $\theta_f+2\pi n$ before taking mod 2π: one with actions staying above I_o, and one staying below I_o. The upper limit of the sum extends to infinity with the differences between the terms becoming exponentially small: in the phase-space picture, these contributions are at actions which converge together exponentially toward I_o. In particular, there is an infinite number of such contributions within a phase-space area h. The classical paths they represent shear farther and farther each to a different domain in angle. At the same time the part of the evolved manifold they lie on is becoming thinner and thinner as it stretches out, which is reflected in the exponential decay of the Van Vleck prefactor in Eq. (28). Each term thus represents a topologically distinct classical path, having traversed 2π in angle a different number of times, and is an independent and exponentially decreasing contribution to the semiclassical amplitude. This is why the semiclassical sum works so well despite there being an infinite number of contributions within an area h in classical phase space. Moreover, there are no caustics in the angle representation; the manifold in Fig. 6(a) is never tangent to an angle state. The semiclassical approximation is very good, as seen in Fig. 7, where the quantum and semiclassical one-step propagators are plotted. (One mild warning to the reader: diffraction at the cutoff introduced at large actions affects the quantum sum over action matrix elements and the semiclassical sum over angle domains in different ways. The consequence is that they differ more in certain ranges of final angle than in others.)

Equation (28) can also be obtained from a stationary phase Fourier transform of the action integral in Eq. (24), each stationary phase point being the classical action at a given stationary phase point, or intersection in phase space. We can also obtain a fully quantum propagator starting from semiclassics, if we write the map as an involution of two (noncommuting) maps $T=T_2\circ T_1$, where

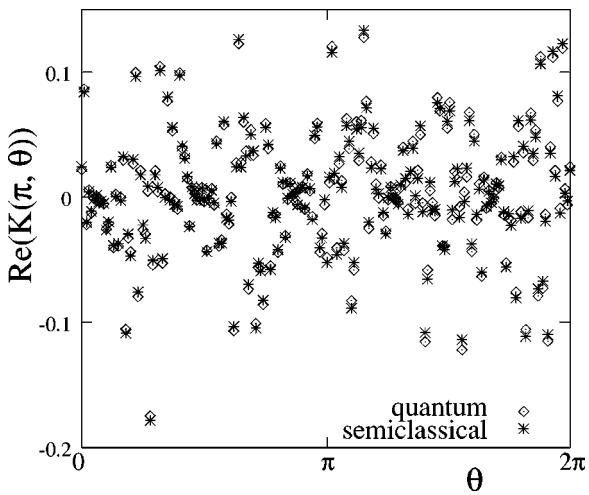

FIG. 7. Quantum and semiclassical one-step propagators for the whisker map: $\lambda=10$, $k=2$, $I_o=0.5$, $\hbar=0.2$, and $\theta_i=\pi$.

$$T_1: \quad \theta'=\theta, \quad I'=I-k\sin\theta,$$
$$T_2: \quad \theta'=\theta+\lambda\ln|c/(I-I_o)|, \quad I'=I. \tag{30}$$

The semiclassical propagator for each individual map is exact, since each map only changes either action or angle, not both. To construct the angle propagator for T we compose the θ to I propagator for T_1 with the I to θ propagator for T_2:

$$K(\theta_i,\theta_f)=\sum_n \int dI \frac{i}{2\pi\hbar} e^{iF_3^{(T_1)}(I,\theta_i)/\hbar} e^{iF_2^{(T_2)}(\theta_f+2\pi n,I)/\hbar}. \tag{31}$$

The generating functions F_3 and F_2 above are each bilinear in the mixed term, and the Van Vleck prefactor for each is just 1; this is consistent with the semiclassical construction so far, being exact. It is not difficult to calculate these and one exactly finds formula (24) which was derived purely quantum mechanically. Performing the sum over domains exactly as described there gives the quantum propagator [Eq. (25)], and performing the I integral by stationary phase gives the semiclassical equation (28).

We now turn to the semiclassical one-step action space propagator from I_i to I_f. Graphically, this is represented by the intersection of the horizontal I-state at I_f with the manifold in Fig. 6(b); the manifold was obtained by evolving initial conditions with action I_i and evenly space angle for one iteration of the whisker map. There are two ordinary caustics in this representation due to the curving created by k, and we expect that the action space semiclassics fails here. When both I_i and I_f are taken close to I_o, the manifold stretches out, becoming almost parallel to an action state, dangerously resembling the supercaustic of Sec. II. There the asymptotic tangency of the manifold with the representation caused a harsh divergence in the semiclassics. However, here there is no problem for the semiclassics considering the ''thickness'' or weight of the manifold in this region, which is exponentially thin, cancelling the tangency effect. The semiclassical action propagator is

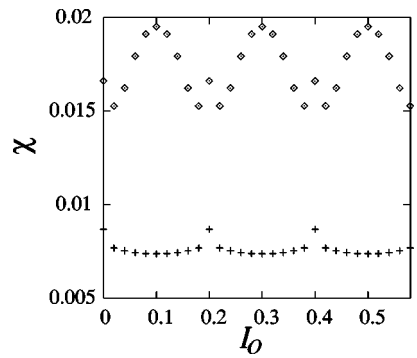

FIG. 8. Normalized difference between quantum and semiclassical propagators [Eq. (32)] as a function of $I_o(+)$. Also plotted is the difference between the quantum and the semiclassical sum cutoff within a value of $\hbar$ of $I_o(\diamond)$. Parameters are $\lambda=10$, $k=2$, and $\hbar=0.2$. The cutoff in action is 20.

$$\begin{aligned}K^{sc}(I_i,I_f)=&\sqrt{\frac{1}{2\pi i\hbar k}}\left(\frac{1}{1-\left(\frac{I_f-I_i}{k}\right)^2}\right)^{1/4}\\&\times\exp\left(-i\lambda(I_f-I_o)\left(\ln\left|\frac{c}{I_f-I_o}\right|+1\right)\Big/\hbar\right)\\&\times\left(\exp\left[i/\hbar\left(k\sqrt{1-\left(\frac{I_f-I_i}{k}\right)^2}\right.\right.\right.\\&\left.+(I_f-I_i)\sin^{-1}\left(\frac{I_f-I_i}{k}\right)\right]\\&+i\exp\left[-i/\hbar\left(k\sqrt{1-\left(\frac{I_f-I_i}{k}\right)^2}\right.\right.\\&\left.\left.\left.\left.+(I_f-I_i)\sin^{-1}\left(\frac{I_f-I_i}{k}\right)\right)\right]\right)\right).\end{aligned}$$

Finally, we consider a quantity independent of representation which shows the normalized difference between the semiclassical and quantum propagators,

$$\begin{aligned}\chi&\equiv\frac{1}{N}\mathrm{Tr}(U^{qm}-U^{sc})^\dagger(U^{qm}-U^{sc})\\&=\frac{1}{N}\sum_i\sum_j|K^{qm}(\theta_i,\theta_j)-K^{sc}(\theta_i,\theta_j)|^2,\end{aligned} \tag{32}$$

where U^{qm} is the quantum evolution operator and U^{sc} would be the evolution operator that gives the semiclassical propagator. In Fig. 8 we plot χ as a function of I_o, and notice that the difference is very small. (We also plot the difference between the quantum and the semiclassical sum cutoff within $\hbar$ of I_o, and find a larger difference—the contributions within $\hbar$ of I_o are indeed important). Notice also the $\hbar$ periodicity with I_o, as expected from its role as a gauge parameter: it is clear from the amount of rotation or shift needed to yield the same quantum mechanics for different I_o's that I_o's differing by $\hbar\times$(integer) are equivalent.

IV. SUMMARY AND CONCLUSIONS

In this paper we have considered two types of quantum amplitudes which might have been thought to be semiclassically troublesome. The first, a ''supercaustic,'' results from the *asymptotic* tangency of classical phase-space manifolds, a tangency which leads even the correct quantum amplitude to diverge. We showed that the semiclassical divergence is completely wrong, but were able to uniformize the semiclassical amplitude in a time tested manner, by comparison with the local behavior of known potentials. We did not treat all possible asymptotic forms; rather, we focused on those potentials which decay exponentially at large distance. However, our techniques point the way to uniformizing other asymptotic forms.

The second case treated was quite different. The whisker map, treated semiclassically in angle space representation, has an infinite number of contributions converging in a small region of phase space. It was shown that in fact the sum is finite, and very close to the exact quantum amplitude. In an action basis, a supercaustic seemed to arise, but the asymptotic tangency with the higher branches of the mapped manifolds was more than canceled by the exponential thinning of those manifolds.

In a sense the whisker map problem echoes the findings several years earlier regarding chaotic systems, for which the number of semiclassical contributions grow exponentially with time [12,13]. There is no intrinsic error associated with either a large number of terms in the semiclassical sum over contributions, nor in the proximity of the distinct contributions in phase space. Rather, as always, it is the enclosed *area* between successive contributions (obtained by following the manifolds in their intricate foldings from one intersection to another) that matters. In the chaotic case it was shown [13] that even though the proliferation of caustics is indeed exponential, the increase in the time for which the semiclassical result holds is a fractional power law in $\hbar$, not logarithmic in $\hbar$ as had been suggested. Here we have seen the appearance of an *infinite* number of terms in one iteration of the whisker map, and yet the semiclassical sum is accurate. In this case the validity of each term is due to its topological distinctness.

ACKNOWLEDGMENTS

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