Accuracy of the semiclassical approximation for chaotic scattering

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The semiclassical approximation for scattering probabilities is tested for a simple chaotic system consisting of a particle in one dimension scattering from a localized potential that varies periodically in time. Good agrement between semiclassical and exact quantum mechanical results is found even for relatively large de Broglie wavelengths.

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Although the standard semiclassical approximation for scattering probabilities [1,2] has been widely applied to chaotic systems [3], the evidence for its validity is largely indirect. In particular, it leads to successful predictions for S-matrix correlation functions [4,5], and closely related approximations can accurately propagate wave packets [6] and give the location scattering resonances [7]. The purpose of this paper is to present a more direct test of the semiclassical approximation by comparing semiclassical scattering probabilities for individual states with exact quantum mechanical results.

As a model, we consider a particle in one dimension scattering from a spatially localized, time varying potential. The Hamiltonian is

$$H=\frac{p^2}{2}+V_0e^{-x^2}\sum_{n=-\infty}^{+\infty}\delta(t-n)\ , \tag{1}$$

where t is the time and (x,p) are the position and momentum coordinates. This corresponds to a particle receiving periodically spaced "kicks." Models of this type show many of the generic features of chaotic dynamics and have been employed frequently [8-10]. One of their advantages is that their dynamical behavior, both classical and quantum, can be found by iterating maps, which greatly simplifies numerical calculations.

The scattering process governed by (1) is chaotic if $V_0<0$ and the initial momentum is not too large. When V_0 is between 0 and about -6, the series that gives the semiclassical scattering amplitude converges slowly and is difficult to evaluate in practice. However, as V_0 is decreased the convergence improves considerably, and the scattering amplitude may be calculated in a straightforward manner. Here we choose $V_0=-12$; for this case, the semiclassical series converges after roughly 100 terms. A detailed discussion of the convergence properties of the semiclassical approximation is given elsewhere [11].

Our main conclusion is that the semiclassical approximation can be remarkably accurate even for relatively large de Broglie wavelengths. The approximation does fail, as is well known, near classical singularities such as caustics. This problem can presumably be remedied with conventional techniques [2,12], but this is not attempted here. Below we present our calculational methods followed by our numerical results.

The classical probability that a particle, with an initial momentum $p_0>0$ and a randomly chosen initial position $x_0\ll-1$, scatters to a final momentum between p and $p+dp$, is given by $D_{\rm cl}(p,p_0)dp$, where $D_{\rm cl}(p,p_0)$ is the classical scattering distribution. The scattering distribution is most easily found by calculating a large number of trajectories with initial positions distributed uniformly on an interval $\bar{x}-p_0<x_0\le\bar{x}$, where $\bar{x}\ll-1$. Only a finite range of initial positions is needed, since a trajectory beginning at x_0-p_0 scatters to the same final momentum as one beginning at x_0, in the limit $x_0\to-\infty$. The trajectories are obtained by iterating the map

$$\begin{aligned} x_{n+1}&=x_n+p_{n+1}\ ,\\ p_{n+1}&=p_n-V'(x_n)\ , \end{aligned} \tag{2}$$

which follows from the equations of motion derived from (1), with $V'(x)$ denoting the derivative of $V(x)\equiv V_0\exp(-x^2)$ and (x_n,p_n) denoting the position and momentum just prior to the time $t=n$ [8-10].

The classical scattering distribution also has the expression

$$D_{\rm cl}(p,p_0)=\frac{1}{p_0}\sum_j\left|\frac{\partial p_f(x_{0j},p_0)}{\partial x_{0j}}\right|^{-1}\ , \tag{3}$$

where the scattering function $p_f(x_0,p_0)$ gives the final momentum as a function of the initial conditions and $\{x_{0j}\}$ is the set of initial positions between $\bar{x}$ and $\bar{x}-p_0$ satisfying $p_f(x_{0j},p_0)=p$ [9]. While (3) is not convenient for direct computation, it shows that the classical scattering distribution is infinite whenever $\partial p_f/\partial x_{0j}$ vanishes for at least one value of j. Such an infinity is referred to as a rainbow singularity or a caustic.

The quantum scattering distribution $D(p,p_0)$ can be found by propagating a state $|\psi_n\rangle$ with the quantum map

$$|\psi_{n+1}\rangle=e^{-i\hat{p}^2/2\hbar}e^{-iV(\hat{x})/\hbar}|\psi_n\rangle\ , \tag{4}$$

where $(\hat{x},\hat{p})$ are the position and momentum operators

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[8,9]. In the position representation, (4) takes the form

$$\langle x|\psi_{n+1}\rangle=(2\pi i\hbar)^{-1/2}e^{ix^2/2\hbar}\times\int_{-\infty}^{+\infty}dx'\langle x'|\psi_n\rangle\exp\left[-\frac{i}{\hbar}xx'+\frac{i}{2\hbar}x'^2-\frac{i}{\hbar}V(x')\right]. \quad (5)$$

Thus the state can be propagated by one unit of time by doing a single Fourier transform. In order to obtain $D(p,p_0)$, the initial state $|\psi_0\rangle$ is chosen to have an average momentum p_0 with a small uncertainty δp. $D(p,p_0)$ is then simply the momentum distribution for $|\psi_n\rangle$ in the limit of large n. More precisely, we take $|\psi_0\rangle$ to be the Gaussian wave packet

$$\langle x|\psi_0\rangle=\left[\frac{2(\delta p)^2}{\pi\hbar^2}\right]^{1/4}\times\exp\left[\frac{ip_0x}{\hbar}-\frac{(\delta p)^2}{\hbar^2}(x-x_0)^2\right]. \quad (6)$$

In the limits that $n\rightarrow+\infty$, $x_0\rightarrow-\infty$, and $\delta p\rightarrow 0$, we have

$$D(p,p_0)=\frac{1}{2\pi\hbar}\left|\int_{-\infty}^{+\infty}dx\langle x|\psi_n\rangle e^{-ipx/\hbar}\right|^2. \quad (7)$$

Because of quasienergy conservation, the quantum scattering distribution consists of a sum of δ functions located at values of p satisfying $p^2/2=p_0^2/2+2\pi\hbar m$, for integer m [9,10]. In practice, the distribution obtained by wave packet propagation has sharp peaks instead of δ functions, since the ideal limits are not realized. Hence to obtain the probability $P(p,p_0)$ to scatter to an allowed sate p, one integrates over the corresponding peak of $D(p,p_0)$.

The standard semiclassical approximation for the scattering probability is [1,2]

$$P(p,p_0)\approx\frac{2\pi\hbar}{|p|p_0}|T(p,p_0)|^2. \quad (8)$$

Here $T(p,p_0)$ is the scattering amplitude given by

$$T(p,p_0)=\sum_j\left|\frac{\partial p_f(x_{0j},p_0)}{\partial x_{0j}}\right|^{-1/2}\times\exp\left[\frac{i}{\hbar}F_j(p,p_0)-\frac{i\pi}{2}\nu_j(p,p_0)\right], \quad (9)$$

where

$$F_j(p,p_0)=\lim_{t_f\rightarrow+\infty}\left\{\frac{[p_f(x_{0j},p_0)]^2}{2}t_f-\int_{t_0}^{t_f}dt[x(t)\dot{p}(t)+H(t)]\right\}, \quad (10)$$

with the integral being evaluated for the trajectory beginning at (x_{0j},p_0). The Maslov index ν_j is obtained by counting the number of times $\partial p(t)/\partial x_{0j}$ changes sign, along the trajectory, when $V''(x(t))$ is positive and subtracting the number of times $\partial p(t)/\partial x_{0j}$ changes sign when $V''(x(t))$ is negative [13].

The most difficult part of evaluating (9) is finding the set of initial positions $\{x_{0j}\}$, which requires locating the roots of $p_f(x_{0j},p_0)=p$. When the scattering is chaotic, this equation has an infinite number of solutions and (9) is an infinite series. If the series converges sufficiently rapidly (when its terms are ordered according to their absolute magnitudes) then enough terms can be found by a straightforward bisection algorithm to obtain a good approximation for the semiclassical amplitude; fortunately, the largest terms are generally the easiest to find.

As is discussed in Ref. [11], one can relate the convergence properties of the semiclassical series to the capacity dimension d of the fractal set of points on which the scattering function $p_f(x_0,p_0)$ is singular (for fixed p_0). Near these singularities, which lie on the stable manifold of a chaotic repeller, p_f varies in a highly complicated fashion, exhibiting the sensitive dependence on initial conditions characteristic of chaos (see Fig. 1) [3]. If the dynamics is hyperbolic, the terms in (9) decay algebraically, on average, with an exponent $-1/2d$. Making a random phase assumption, one can then estimate the

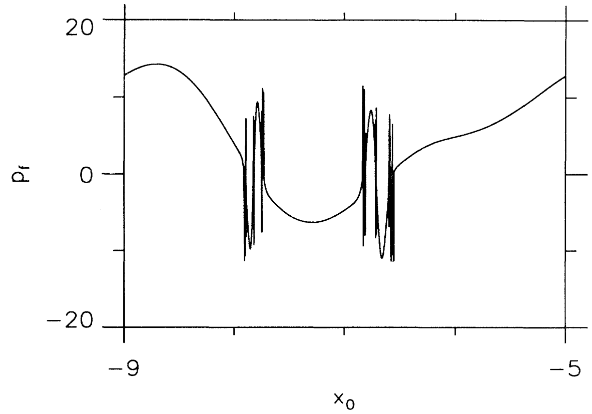

FIG. 1. The scattering function $p_f(x_0,p_0)$ vs x_0 for $p_0=4.0$ and $V_0=-12.0$. p_f varies erratically near points on the stable manifold of a chaotic repeller.

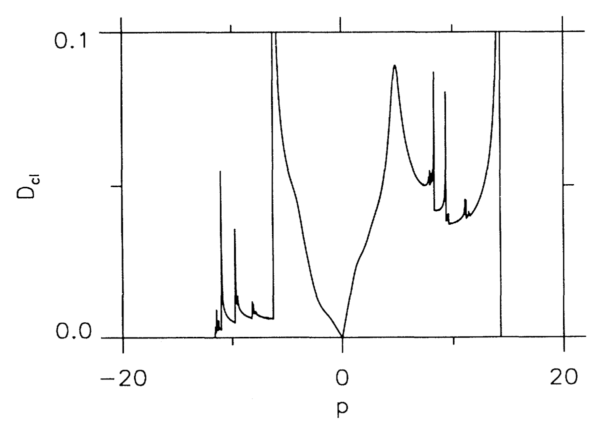

FIG. 2. The classical scattering distribution $D_{cl}(p,p_0)$ for $p_0=4.0$ and $V_0=-12.0$, showing many rainbow singularities.

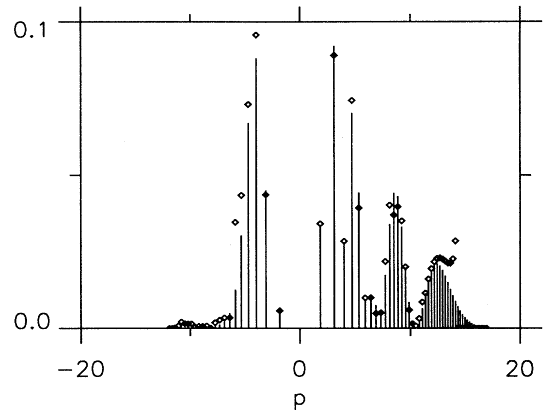

FIG. 3. The scattering probability $P(p,p_0)$ vs p for $p_0=4.0$, $V_0=-12.0$, and $\hbar=0.5$. The lines indicate exact quantum results, while the diamonds give the semiclassical approximation.

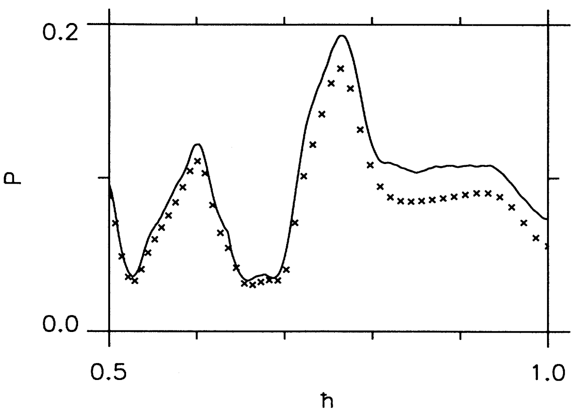

FIG. 4. The scattering probability $P(p,p_0)$ vs $\hbar$ for $p_0=4.0$, $V_0=-12.0$, and $p=-4.0$. The solid line is the semiclassical approximation and the $\times$'s are exact quantum results.

number of terms required to evaluate (9). To achieve 1% accuracy, one finds that one needs roughly the $100^{d/(1-d)}$ largest terms.

This estimate applies only for V_0 less than about -4, since for greater values the dynamics may not be hyperbolic due to the presence of stability islands [10]. When $V_0<-4$, numerical evidence suggests the dynamics is hyperbolic, at least for practical purposes. In this paper, we use $V_0=-12$, in which case $d=0.49\pm0.01$. Thus to find a good approximation to (9), we require about the 100 biggest terms. In general, the convergence rate of the semiclassical a series improves as V_0 is reduced.

The classical scattering distribution is shown in Fig. 2 for $p_0=4$. The sharp peaks are rainbow singularities; the distribution is infinite at these points, although they appear finite in Fig. 2 due to numerical limitations. In Fig. 3, the corresponding quantum scattering probabilities for $\hbar=0.5$ are given as obtained from an exact quantum calculation (lines) and from the semiclassical approximation (8) (diamonds). The exact quantum results are for a wave packet that initially has $\delta p/p_0=0.004$. The semiclassical approximation is reasonably accurate, except for some values of p that lie near rainbow singularities. These defects should be correctable by using some type of uniform approximation [2,12]. The overall good agreement between the exact and semiclassical results is remarkable considering that the initial de Broglie wavelength, $2\pi\hbar/p_0\approx0.79$, is comparable to the width of the potential. A comparison of the exact and semiclassical elastic backscattering probabilities is plotted in Fig. 4 as a function of $\hbar$, again confirming the validity of Eq. (8).

These results support previous work [4–7] that indicates that the semiclassical approximation works well even for relatively large values of $\hbar$. When the semiclassical series converges rapidly, it can be used as a practical computational method; the semiclassical results presented in this paper required far less computational time than their quantum counterparts. This is particularly true for one-dimensional inelastic scattering (as considered here) and two-dimensional elastic scattering, since in both these cases the required root search is on a one-dimensional manifold. A physical application of the method would be to the calculation conductances for two-dimensional microstructures [5]. In cases where the semiclassical series converges slowly, some refinement of the series appears needed to make it a useful computational tool.

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