Convergence of the Semiclassical Approximation for Chaotic Scattering

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The series that arises from the semiclassical approximation for scattering amplitudes is studied when the scattering is chaotic. It is argued that the terms of the series decay with an exponent equal to $1/2d$, where d is the capacity dimension of one of the classical scattering functions. The result applies to one-dimensional inelastic and two-dimensional elastic scattering, and it is verified numerically for a one-dimensional model. An estimate of how rapidly the semiclassical series converges is given.

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The standard semiclassical approximation, based on the Van Vleck formula [1], has proven to be a powerful tool for calculating quantum effects for systems that have chaotic classical dynamics. For example, it can be used to propagate wave packets with remarkable accuracy [2], and it leads to the Gutzwiller trace formula which gives approximate values for quantum energy levels [3]. Recent work has also applied Van Vleck's formula to systems that scatter chaotically [4], yielding approximations for scattering amplitudes [5], resonances [6], and correlation functions [7].

In this paper, we focus on the semiclassical expression for scattering amplitudes, which has the form of a series where each term corresponds to a particular classical scattering trajectory. When the scattering is chaotic, the terms of the series typically decrease algebraically, and the series' convergence properties may be nontrivial. In particular, the series may or may not be absolutely convergent, and the series may either converge rapidly or extremely slowly.

Our main result is that the exponent, β, characterizing the decay of the series' terms can, in many cases, be determined from the capacity dimension, d, of the fractal set of points on which one of the classical scattering functions is singular. The value of this relation is that it is usually much easier to calculate d than to find β directly from the semiclassical series. Once β is known, one can determine whether the series is absolutely convergent and estimate the series' convergence rate. Thus considerable information about the semiclassical approximation may be obtained from a simple classical calculation. The discussion in this paper is restricted to one-dimensional inelastic and two-dimensional elastic scattering, although we expect similar results to hold in higher dimensions. We also assume that the classical phase space contains no Kolomogorov-Arnol'd-Moser (KAM) tori, since these complicate the fractal properties of the classical scattering functions.

As an example, we consider first scattering for the one-dimensional system governed by the time-dependent Hamiltonian

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

where x is the position, p is the momentum, and t is the time. The spatial variation of the potential is taken to be $V(x) = V_0(1-|x|)^2$, if $-1 < x < 1$, and $V(x) = 0$, if $|x| \geq 1$. This system is an example of a kicked particle model, similar to many others that have been used to investigate chaos [8–10]. The classical scattering distribution $P_{\rm cl}(p,p_0)$ is defined so that a particle with an initial momentum $p_0 > 0$ and an initial position x_0, chosen at random with the constraint $x_0 < -1$, has a probability $P_{\rm cl}(p,p_0)dp$ of having a final (i.e., $t \to +\infty$) momentum between p and $p+dp$. $P_{\rm cl}(p,p_0)$ can be expressed in terms of the scattering function $p_f(x_0,p_0)$, which gives the final momentum for a trajectory beginning with the initial conditions (x_0,p_0):

$$P_{\rm cl}(p,p_0) = \frac{1}{p_0} \sum_j \left| \frac{\partial p_f(x_{0j},p_0)}{\partial x_{0j}} \right|^{-1}, \qquad (2)$$

where $\{x_{0j}\}$ is the set of initial positions between -1 and $-1-p_0$ satisfying $p_f(x_{0j},p_0) = p$ [9]. Only a finite range of initial positions need be considered, since the periodicity in time of H implies $p_f(x_0,p_0) = p_f(x_0 - p_0, p_0)$ for all $x_0 < -1$.

If $V_0 < 0$, the scattering process is chaotic for a range of values of p_0. The hallmark of chaotic scattering is that the scattering function $p_f(x_0,p_0)$ is fractal [4], as illustrated in Fig. 1. In particular, p_f as a function of x_0 is singular on a set of points having a capacity (or box-counting) dimension d, with each singularity corresponding to a trajectory that becomes trapped in the scattering region $(-1 < x < 1)$. These singularities are said to lie on the stable manifold of a chaotic repeller. In an arbitrarily small neighborhood about such a singular point, the variation of p_f is highly complicated, justifying the term chaotic. The dimension d, which can vary from 0 to 1, may be easily obtained by determining the uncertainty exponent α and using the identity $d = 1 - \alpha$ [11]. To find α, one calculates (numerically, in practice) the probability $f(\epsilon)$ that the signs of $p_f(x_0,p_0)$ and $p_f(x_0+\epsilon,p_0)$ are different for a randomly chosen x_0. The uncertainty exponent is then defined by $\alpha = \lim_{\epsilon\to 0}[\log f(\epsilon)/\log \epsilon]$.

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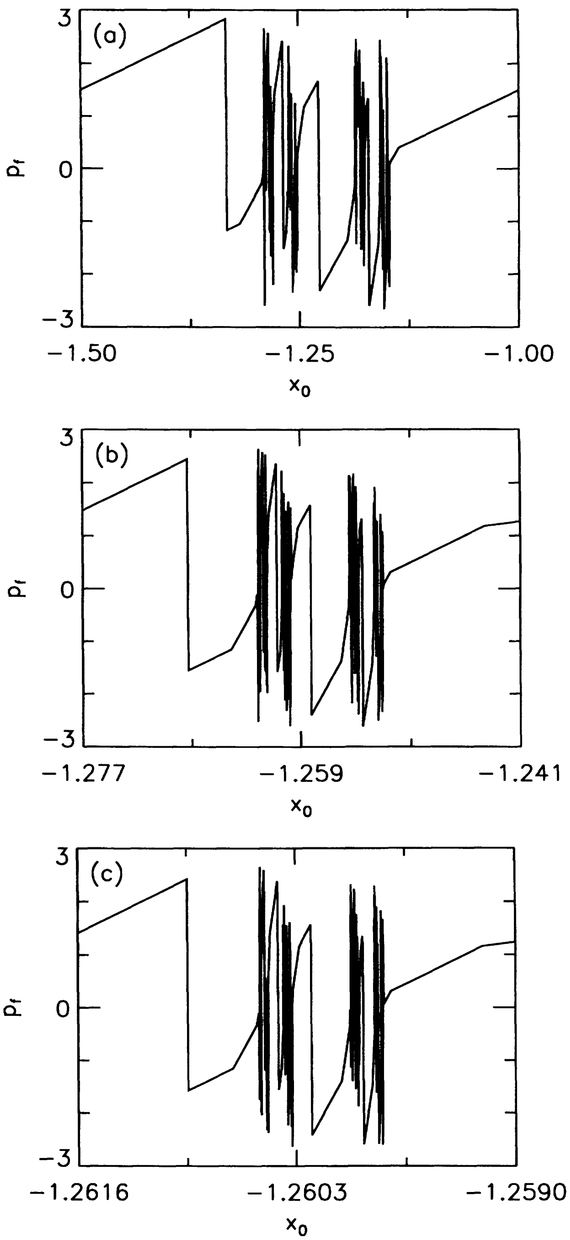

FIG. 1. (a) The classical scattering function $p_f(x_0, p_0)$ vs x_0 for $V_0 = -1.0$ and $p_0 = 0.5$. (b) and (c) are successive enlargements of (a) showing the self-similarity characteristic of fractals.

The Van Vleck formula gives a semiclassical approximation for the quantum mechanical propagator [1]. Applying it to scattering governed by H, one arrives, after some conventional manipulations [12], at the expression

$$P(p, p_0) = \frac{2\pi\hbar}{|p|p_0} |T(p, p_0)|^2 \sum_n \delta(p - q_n) \tag{3}$$

for the quantum scattering distribution. Here $T(p, p_0)$ may be interpreted as the scattering amplitude and the $\{q_n\}$ are the real solutions of $q_n^2/2 = p_0^2/2 + 2\pi\hbar m$, for all integer m. The appearance of δ functions in Eq. (3) is a consequence of quasienergy conservation that follows from the periodicity of H. The scattering amplitude is given by

$$T(p, p_0) = \sum_j \left| \frac{\partial p_f(x_{0j}, p_0)}{\partial x_{0j}} \right|^{-1/2} \times \exp\left[\frac{i}{\hbar} F_j(p, p_0) - \frac{i\pi}{2} \nu_j(p, p_0) \right], \tag{4}$$

where

$$F_j(p, p_0) = \lim_{t_f \to +\infty} \left\{ \frac{[p_f(x_{0j}, p_0)]^2}{2} t_f - \int_{t_0}^{t_f} dt\, [x(t)\dot{p}(t) + H(t)] \right\}, \tag{5}$$

with the integral being evaluated for the trajectory beginning at (x_{0j}, p_0). The index ν_j is simply equal to -1 if $V_0 < 0$ and 0 if $V_0 > 0$.

In some cases, the sum appearing in Eq. (4) is not absolutely convergent and is thus meaningful only if an order for the terms is specified. Henceforth we assume the terms to be ordered according to their absolute magnitudes. Defining weights $w_j(p, p_0) = |\partial p_f/\partial x_{0j}|^{-1/2}$ and phases $\delta_j(p, p_0) = F_j/\hbar - \pi\nu_j/2$, Eq. (4) can be written as

$$T(p, p_0) = \sum_{j=1}^{+\infty} w_j(p, p_0) e^{i\delta_j(p, p_0)}, \tag{6}$$

with $w_j \geq w_{j+1}$. Numerically, we find the weights to decay, on the average, proportionally to $j^{-\beta}$, as shown in Fig. 2, if p_0 and $|p|$ are less than a critical value p_c. Inside this critical range, β is independent of p and p_0, while outside the series truncates after a finite number of terms.

The evaluation of the weights is greatly facilitated by exploiting the fact that their associated trajectories can be assigned binary symbols. Consider the positions at times $t = n$ (i.e., when the particle is kicked), and indicate with a $-$ each time the position is between -1 and 0 and with $+$ each time the position is between 0 and $+1$. Thus every scattering trajectory is labeled by a finite sequence of $+$'s and $-$'s. Moreover, it is easy to show, using the piecewise linearity of the equations of motion that follow from H, that for given (p, p_0) there is at most one trajectory for each sequence. This allows the weights to be found in a systematic and efficient manner. A further simplification is that the weights depend only on the symbolic lengths of the sequences (e.g., the weights associated with $- + - - +$ and $- + + - +$ are the same), which accounts for the steps in Fig. 2.

The central result of this paper is that

$$\beta = 1/2d. \tag{7}$$

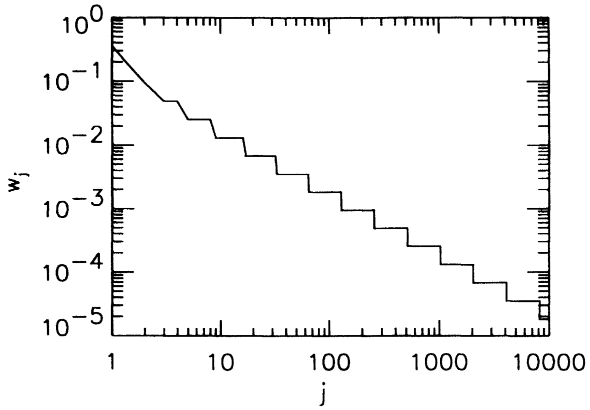

FIG. 2. Log-log plot of the weights $w_j(p, p_0)$ vs j for $V_0 = -1.0$, $p = 1.0$, and $p_0 = 0.5$. The weights decay, on the average, as $j^{-\beta}$, where in this case $\beta \approx 0.950$.

A comparison of β with $1/2d$ is given in Table I for several values of V_0, indicating good agreement. The values for β were found by calculating all the scattering trajectories up to a symbolic length of 20, while the values for d were obtained from the corresponding uncertainty exponents.

To understand why this relationship holds consider $p_f(x_0, p_0)$ for fixed p_0 on the interval $-1 - p_0 \leq x_0 < -1$. This interval is divided into an infinite number of subintervals by the singularities associated with trapped trajectories (symbolically these are represented by infinite sequences of $+$'s and $-$'s). If these intervals are ordered according to their lengths, the length of the jth interval is $\sim j^{-1/d}$. Since the variation of p_f is about the same for each subinterval, a "typical" derivative, $\partial p_f / \partial x_0$, for a subinterval scales inversely with the subinterval's length or as $j^{1/d}$, suggesting that the weights scale as $j^{-1/2d}$. One may object that the subintervals and weights are not in one to one correspondence; indeed most subintervals contribute an infinite number of weights for particular values of p. However, for a given subinterval the weights decay roughly exponentially, and it can be shown that this is sufficiently rapid to justify Eq. (7). When $|p|$ or p_0 is larger than p_c, Eq. (7) does not apply, because none of the allowed scattering trajectories come near the chaotic repeller.

TABLE I. Numerical results for several values of V_0. In all cases, $1/2d$ is very nearly equal to the exponent β, as predicted by Eq. (7).

V_0	β	p_c	d	$1/2d$
−0.5	0.750	1.62	0.67	0.75
−1.0	0.950	2.73	0.52	0.96
−1.5	1.130	3.79	0.44	1.14
−2.0	1.272	4.83	0.40	1.25
−2.5	1.388	5.85	0.36	1.39

The above argument is readily extended to other one-dimensional inelastic scattering models and to two-dimensional elastic scattering. The semiclassical amplitude is generally given by an expression similar to Eq. (6) with the weights being determined by the derivative of a classical scattering function. For two-dimensional elastic scattering, the relevant classical scattering function is the final scattered angle θ_f as a function of the impact parameter b, and the weights are simply $|\partial \theta_f / \partial b_j|^{-1/2}$ [5]. The exponent β should be equal to $1/2d$ for a range of final angles, and outside this range the weights should decay faster than $j^{-1/2d}$. One restriction on Eq. (7) is that it may fail when the scattering is nonhyperbolic, as is the case when KAM tori are present. For such systems, the fractal properties of the scattering function are somewhat different than have been assumed [10, 13].

When Eq. (7) holds, it can be used to relate the dimension d to the convergence properties of the series for a semiclassical scattering amplitude [14]. The series is absolutely convergent if $\beta > 1$, which according to Eq. (7) will be true if $d < \frac{1}{2}$. The number of terms that should be evaluated in order to obtain a reasonable approximation can be roughly estimated by considering the series

$$T_R = \sum_{j=1}^{+\infty} j^{-\beta} e^{i\delta_j^R}, \tag{8}$$

where the phases δ_j^R are taken to be random. The convergence rate of the sum in Eq. (8) is likely to be similar to that in Eq. (6), since the phases in (6) often behave in a pseudorandom manner. If T_R is approximated by the first N terms of (8), there will be an error $E_N = \sum_{j=N+1}^{+\infty} j^{-\beta} e^{i\delta_j^R}$. The average of the squared magnitude of T_R is

$$\langle |T_R|^2 \rangle = \sum_{j=1}^{+\infty} j^{-2\beta} \approx (2\beta - 1)^{-1}, \tag{9}$$

while $\langle |E_N|^2 \rangle \approx [(2\beta - 1)N^{2\beta-1}]^{-1}$. Demanding that $\langle |E_N|^2 \rangle$ be less than 1% of $\langle |T_R|^2 \rangle$ and using (7) leads to the condition

$$N > 100^{1/(2\beta-1)} = 100^{d/(1-d)}. \tag{10}$$

This inequality implies that the number of terms needed to accurately determine a semiclassical scattering amplitude depends sensitively on the dimension d. For example, if $d = \frac{1}{4}$ only a few terms would be needed, while $d = \frac{1}{2}$ requires about 100 terms and $d = \frac{3}{4}$ about 10^6 terms. As d approaches 1, the estimate (10) diverges, suggesting that a straightforward evaluation of the semiclassical series is not feasible.

In summary, the convergence properties of the series for the semiclassical scattering amplitude may be conveniently determined from the capacity dimension d. When $d < \frac{1}{2}$, the series converges absolutely and rapidly. When

$\frac{1}{2} < d < \frac{2}{3}$, the convergence is not absolute, but probably the first few thousand terms of the series are sufficient to obtain a good approximation for the scattering amplitude. Finally, when d is significantly bigger than $\frac{2}{3}$ a direct evaluation of series is likely to be extremely difficult. In such cases, more sophisticated summation techniques, perhaps similar to those applied to the Gutzwiller trace formula [15], appear to be called for.

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