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Rainbow transition in chaotic scattering

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We study the effects of classical chaotic scattering on the differential cross section, which is the measurable quantity in most scattering experiments. We show that the fractal set of singularities in the deflection function is not, in general, reflected on the differential cross section. We show that there are systems in which, as the energy (or some other parameter) crosses a critical value, the system's differential cross-section changes from a singular function having an infinite set of rainbow singularities with structure in all scales to a smooth function with no singularities, the scattering being chaotic on both sides of the transition. We call this metamorphosis the *rainbow transition*. We exemplify this transition with a physically relevant class of systems. These results have important consequences for the problem of inverse scattering in chaotic systems and for the experimental observation of chaotic scattering.

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Chaotic scattering is one of the most important manifestations of chaos in open systems. The number of physical systems where chaotic scattering has been identified is far too many for an exhaustive list; notable examples include molecular dynamics [1], fluid dynamics [2], atomic physics [3], electronic conductance in mesoscopic systems [4], and scattering in smooth potentials [5], to name a few. Chaotic scattering is characterized by the presence of a Cantor set of singularities in *scattering functions* relating the final state of a scattered particle to its initial state, such as the deflection angle as a function of the impact parameter. This fractal set of singularities is the result of the existence of a fractal set of bounded unstable orbits in the scattering region. Systems with chaotic scattering have regions in the space of initial conditions where the outcome of the scattering is very sensitive to small changes in the initial state [6], which is a defining feature of chaos.

Most investigations of chaotic scattering so far have focused on the study of scattering functions, whose properties are determined by individual trajectories. Although sensitivity of individual trajectories to initial conditions may in principle be observable, in practice it is usually not possible to observe individual trajectories, and hence, this phenomenon is not accessible to direct observation. For this reason, the experimentally important quantities are those obtained from a beam of incident trajectories, spanning a large range of impact parameters. The scattering of a beam of incident particles is described by the *differential cross section* $d\sigma/d\Omega$, which measures the intensity of the scattered beam in a given direction, and is the measured quantity in most scattering experiments. A natural question arises: how does chaotic scattering manifest itself in the differential cross section $d\sigma/d\Omega$? In particular, does chaotic scattering imply a set of singularities with structure in all scales for $d\sigma/d\Omega$, as it does for the deflection angle? This paper addresses these questions.

Singularities in the differential cross section appear in the form of *rainbow singularities* [7], which arise as a result of the density of scattered trajectories being infinite for some directions, causing $d\sigma/d\Omega$ to diverge there. Rainbow singularities correspond to caustic directions, and are seen as sharp bright peaks in scattering experiments. They have been observed in many scattering experiments, including atomic scattering [8], optical systems [9], and nucleus-nucleus collisions [10]. The appearance of rainbow singularities in chaotic scattering systems has been investigated previously for particular potentials (usually superpositions of repulsive hills) [11,12]; in those studies, $d\sigma/d\Omega$ was shown to have an infinite set of rainbow singularities, which mirrored nicely the fractal set of singularities in the deflection function. Those results have led to the tacit belief [11] that all systems showing chaotic scattering have such a set of singularities in the differential cross section, related in a simple way to the set of singularities in the deflection function. In this paper, we address this issue in a general way, and we show that there are systems whose scattering is chaotic but have nevertheless a smooth differential cross section, with no rainbow singularities. This means that the presence of a fractal set of singularities in the deflection function, which characterizes chaotic scattering, is not necessarily reflected in the cross section. In fact, in this paper, we introduce a physically important class of potentials, which shows a kind of dynamical metamorphosis, namely, a transition from a differential cross section with an infinite set of rainbow singularities to a perfectly smooth cross section, even though the scattering is chaotic on both sides of the transition; we call this phenomenon a *rainbow transition*. We note that this phenomenon is not a pathology devoid of physical meaning; on the contrary, it is a common property shared by many important physical systems, such as the one we introduce below as an example. The reason why chaotic scattering systems do not necessarily have singularities in their differential cross sections is that rainbow singularities arise from extrema (maxima, minima, or saddle points) of the deflection function, which are not directly related to the deflection function's fractal set of singularities. In the previously studied systems, the potentials were such that the deflection function had a set of maxima and minima along with the fractal set of singularities, and as a consequence, $d\sigma/d\Omega$ also had a set of singularities mirroring those of the deflection function. However, this need not be the case: there are potentials whose deflection function has a Cantor set of singularities (which means that the system shows chaotic scattering) and has no maxima or minima, their differential cross section being smooth. We now proceed to illustrate the above points with a concrete system.

For simplicity, we restrict ourselves in this paper to classical Hamiltonian systems whose (three-dimensional) potentials are symmetric with respect to the z axis; in this case, the dynamics is effectively two dimensional. We further restrict the incident particles to have initial velocities parallel to z. In this case, the motion of the particles is restricted to a plane containing z. These conditions being satisfied, the output direction of the particle depends only on the angle θ determined by the particle's velocity after the scattering and the z axis, with $0 \leqslant \theta < \pi$. The differential cross section depends thus on θ only. For a given θ, $d\sigma/d\Omega$ is the sum of the contributions from all trajectories scattered in the direction θ [7],

$$\frac{d\sigma}{d\Omega}(\theta) = \sum_i \frac{b_i}{\sin\theta}\left|\frac{d\phi(b_i)}{db}\right|^{-1}, \tag{1}$$

where $\phi(b)$ denotes the deflection suffered by an incident particle with impact-parameter b (b is measured with respect to the symmetry axis z). The sum is over all impact-parameters b_i satisfying $\phi(b_i) + 2n\pi = \theta$ for some integer n. Note that contrary to θ, ϕ can take either positive or negative values. The above formula relates the scattering function $\phi(b)$, which gives information about individual trajectories, to the differential cross-section $d\sigma/d\Omega$ that gives information about a beam of trajectories. In systems with chaotic scattering, there is a Cantor set of values of b for which $\phi(b)$ is singular. From Eq. (1), we see that $d\sigma/d\Omega$ can diverge in two ways [7]: (1) for $\theta = 0$ or $\theta = \pi$ (forward and backward glory), or (2) for $d\phi/db = 0$ (rainbow singularity). We focus our attention on the rainbow singularities, since the glory singularities are a purely kinematic effect that are not related to the scattering dynamics.

As an example, we introduce a class of potentials $U(x,y)$ defined on the planes containing the symmetry axis. U is defined to be the sum of two localized potential hills,

$$U(x,y) = V(x,y-a) + V(x,y+a), \tag{2}$$

where $V(x,y)$ is a spherically symmetric potential that decays rapidly for large distances, and it is attractive beyond a certain distance from the center. This attractive character is fundamental for the appearance of chaotic orbits: the dynamics in the field of two purely repulsive hills is always regular. We further impose the additional condition that the distance $2a$ which separates the center of the two hills is large enough so that the overlap of the two potentials is small, and the motion of a particle in the vicinity of one of the hills can be considered to be influenced by the potential of that hill alone, the effect of the other one being negligible. This latter condition allows the dynamics of the system to be understood as a sequence of scatterings from each individual hill, as we will see.

Examples of physical systems that could be modeled by Eq. (2) include the elastic interaction of an atom with a diatomic molecule whose atoms can be considered to be fixed [1], the electronic scattering by a diatomic molecule [13], the interaction of an electron or a hole with a pair of quantum dots in a semiconductor [14], and the scattering of light by a pair of transparent spheres with a refraction index which depends on their radius [7]. For definiteness, we choose V to be the Morse potential [15], given in appropriate units by

$$V(x,y) = \frac{1}{2}\{1 - \exp[\alpha(r - r_e)]\}^2 - \frac{1}{2}, \tag{3}$$

where $r^2 = x^2 + y^2$, and the parameters α and r_e are related to the range of the potential and the size of the repulsive core. The potential (3) is repulsive for $r < r_e$ and attractive for $r > r_e$, and approaches zero exponentially for $r \gg r_e$. The large separation condition spelled out in the previous paragraph means in this case $2\alpha(a - r_e) \gg r_e$. We choose the values $\alpha = 6$, $r_e = 0.68$, and $a = 2$ in what follows. The Morse potential describes approximately the interaction of two atoms due to their dipole-dipole interaction [15]. We emphasize that our results are not dependent on the particular, form of V, and in particular we show explicitly below that the rainbow transition in the differential cross section is a generic property for a large class of potentials V.

Because of the large separation condition, the scattering by the full potential U can be (approximately) described as being a succession of isolated scatterings by each of the hills $V(x,y-a)$ and $V(x,y+a)$. Since each hill is spherically symmetric, one single scattering on such a hill is not chaotic; but the composition of many individual scatterings by a pair of hills may be chaotic, as we will see. The scattering on an isolated hill is described by the deflection function $\phi_0(b)$. Remember that we allow ϕ_0 to assume arbitrary values, so the number of "turns" a particle makes during scattering is taken into account. Let ϕ_{max} be the maximum value (in module) assumed by ϕ_0. For $\phi_{max} \lesssim \pi$, the attractive part of the potential is not capable of bending an incident particle's trajectory enough for it to reach the other hill. Even though the repulsive core can deflect a particle towards the other hill, the attractive part does not participate in this "swinging" process. In this case, there is no fractal set of unstable orbits and no chaotic scattering, for the same reason that the scattering by two purely repulsive hills is not chaotic. For $\phi_{max} \lesssim \pi$, therefore, the scattering is regular, but for $\phi_{max} \gtrsim \pi$ it is chaotic, because the particle is now able to reach the other hill. ϕ_{max} is a function of the energy of the incoming particles: $\phi_{max} = \phi_{max}(E)$, and ϕ_{max} increases as the energy decreases. The transition point between chaotic and nonchaotic scattering, given by $\phi_{max} \approx \pi$, is found numerically to be $E = E_c \approx 0.39$, for the parameters chosen by us. Thus, the scattering, which is regular for $E > E_c$, becomes chaotic for $E < E_c$. This can be seen clearly in Fig. 1(a), which shows the deflection angle $\phi(b)$ (for the whole potential U, not for an isolated hill) as a function of the impact

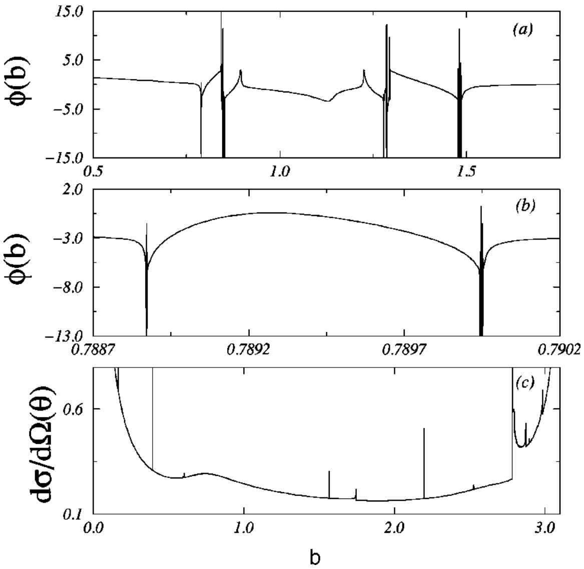

FIG. 1. (a) Deflection angle ϕ as a function of the impact parameter b, for $E=0.38$. ϕ is calculated by numerically integrating the equations of motion for initial conditions $y_0=-10$ and $x=b$. (b) is an enlargement of (a). The scattering is clearly chaotic, and $\phi(b)$ has an infinite set of maxima and minima in all scales. (c) Differential cross section $d\sigma/d\Omega$ as a function of the scattering angle θ for $E=0.38$. $d\sigma/d\Omega$ has an infinite set of rainbow singularities.

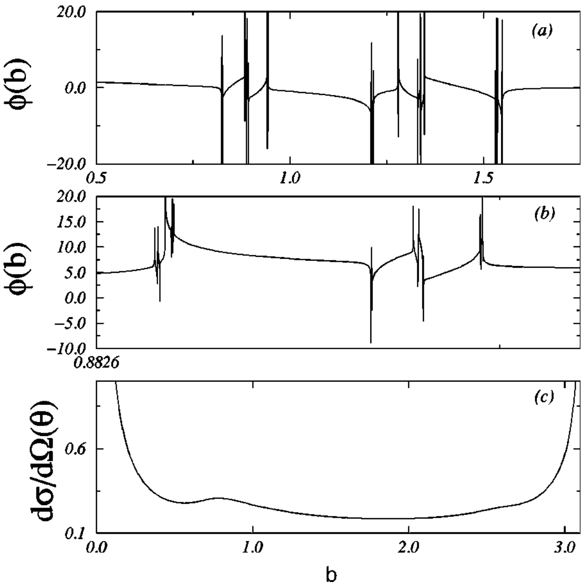

FIG. 2. Same as Fig. 1, for $E=0.28$. Although the scattering is still chaotic, $\phi(b)$ no longer has any smooth maximum or minimum, and $d\sigma/d\Omega$ is smooth.

parameter for $E=0.38$. Magnifications of Fig. 1(a) [one of them is shown in Fig. 1(b)] show that $\phi(b)$ has structure on all scales, and the calculation of the box-counting dimension of the set of singularities on the one-dimensional segment parametrized by b, using the uncertainty method [16], gives $d=0.26\pm0.02$. We note that every time ϕ_{max} crosses an odd multiple of π, a set of unstable orbits is created in a homoclinic bifurcation, corresponding to particles being able to make multiple turns around a hill.

From Figs. 1(a) and 1(b), we see that there is an infinite number of maxima and minima in the deflection function ϕ, occurring on the smooth intervals of ϕ in between the singularities. This is a consequence of the fact that the deflection function $\phi_0(b)$ of one isolated hill has one maximum ϕ_{max} and one minimum $-\phi_{max}$; remember that the scattering by the total potential U can be regarded as a sequence of scatterings by individual hills. From our earlier discussion, this means that the differential cross section has an infinite set of rainbow singularities. This is also confirmed by a direct numerical calculation of the cross section using Eq. (1) [17]. The result is shown in Fig. 1(c), where the rainbow singularities are seen as sharp spikes. We thus find that for energies close to the critical energy E_c (but lower than E_c), the differential cross section has a set of rainbow singularities mirroring the singularities in ϕ, just as in the systems studied previously [11,12]. Since the maxima and minima of ϕ lie on the complement of the Cantor set of singularities, the rainbow singularities form a countable set, with structure on all scales, which reflects the fractal structure of the set of singularities of ϕ.

This is not the whole story, however. As E is further lowered, ϕ_{max} grows, and the maximum (and minimum) in ϕ_0 becomes sharper and sharper. For a second critical energy $E_t<E_c$, ϕ_{max} diverges: $\phi_{max}(E)\to\infty$ for $E\to E_t$ from above. For $E\leqslant E_t$, $\phi_0(b)$ has no maxima or minima, and consequently, the deflection function $\phi(b)$ of the full potential U also has no maxima or minima. We find numerically $E_t\approx0.30$ for our parameters. The deflection function $\phi(b)$ for $E=0.28$ is plotted in Figs. 2(a) and 2(b), and we see clearly that although it has a fractal structure, it has no maxima or minima. As a result, there are no rainbow singularities for $E<E_t$, and the differential cross section is perfectly smooth, as shown in Fig. 2(c), although the scattering is still chaotic for $E<E_t$, as is evident from Figs. 2(a) and 2(b), and from a numerical calculation of the box-counting dimension of the set of singularities, which gives $d=0.34\pm0.02$. As E crosses E_t from above, there is a transition from a differential cross section with an infinite number of rainbow singularities to a smooth one, with the scattering being chaotic on both sides of the transition; this is the rainbow transition. Since every time ϕ_{max} crosses an odd multiple of π, a set of unstable orbits is created, and since $\phi_{max}\to\infty$ as E approaches E_t, the transition at energy E_t is the accumulation point of an infinite number of (homoclinic) bifurcations.

Although for convenience of explanation we illustrated this transition with a particular choice of potential (3), our result is general. To show this, let us consider the effective potential of one hill V(r)

$$V_{eff}(r)=V(r)+\frac{L^2}{2mr^2}, \tag{4}$$

where L is the angular momentum of the particle with respect to the center of the hill, and m is the reduced mass. ϕ_{max} diverges for some energy whenever V_{eff} has a positivevalued maximum, which corresponds to the existence of a circular unstable periodic orbit C with positive energy, thus enabling an incoming particle to approach C asymptotically. Those are the orbits with diverging ϕ_0 (that is, they lie on the stable manifold of C). Since V is by assumption attractive for large enough r, V approaches zero from negative values for $r\rightarrow\infty$. If V decays fast enough so that $r^2V(r)\rightarrow 0$ as $r\rightarrow\infty$, the positive term $L^2/2mr^2$ in Eq. (4) eventually becomes larger in module than the negative term $V(r)$, for large r. Since $V_{eff}\rightarrow 0$ for $r\rightarrow\infty$, this means that V_{eff} has a maximum V_{max}, with $V_{max}>0$. This proves that all potentials of the form (2) where V is spherically symmetric with a rapid enough decay for large r (faster that r^{-2}) display the rainbow transition from a singular to a smooth cross section studied above (as long as the separation $2a$ is large enough). In fact, we expect this transition to be found in many other systems, not just in those described by Eq. (2).

To sum up, we have shown that the differential cross section of a scattering system may be smooth even when the scattering is chaotic, and we have studied a class of systems which show a rainbow transition from a cross section with an infinite set of rainbow singularities to a smooth one, the system showing chaotic scattering on both sides of the transition. This is important because the differential cross section is in many cases the most accessible quantity in a scattering experiment, and the possibility of a smooth cross section in chaotic scattering systems may pose new challenges for the observation of chaotic scattering. Our results also have important consequences to the theory of inverse chaotic scattering, since it does not appear to be possible to infer the fractal structure of the invariant set of a chaotic scattering system from a smooth cross section. As a final note, even though we have limited ourselves to classical scattering, our results should also hold for wave scattering in the short-wavelength limit.

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[17] In the numerical calculation of $d\sigma/d\Omega$ from Eq. (1), we compute $\phi(b)$ in the interval $-2<b<2$ with high resolution (10^{-7} for the example presented here); we also use an additional routine for finding zeros of $d\phi/db$, in order to be able to locate the very narrow rainbow peaks).