# Chaos in coplanar classical collisions with particles interacting through $r^{-2}$ forces

Fabio Sattin[1,*] and Luca Salasnich[2,†]
[1]Consorzio RFX and Istituto Nazionale per la Fisica della Materia, Unità di Padova, Corso Stati Uniti 4, I 35127 Padova, Italy
[2]Istituto Nazionale per la Fisica della Materia, Unità di Milano, Dipartimento di Fisica, Università di Milano, Via Celoria 16, I 20133 Milano, Italy
and Istituto Nazionale di Fisica Nucleare, Sezione di Padova, Via Marzolo 8, I 35131 Padova, Italy

(Received 24 August 1998)

The scattering among three particles interacting through $1/r^2$ forces, with opposite charges and widely different masses, is studied in a coplanar geometry. The present work shows that at low impact velocities the output of the collision presents typical characteristics of chaos. The details of the process are investigated. [S1063-651X(99)07701-6]

PACS number(s): 05.45.−a, 34.70.+e

Starting from the works of Gaspard and Rice [1], chaotic scattering was found to be ubiquitous. A large amount of work has been done on potential scattering (i.e., scattering of an elementary particle on fixed potential centers) [2–5], but also the scattering among at least three interacting bodies has received great attention (see the work of Petit and Hénon on the scattering between a planet and two satellites [6] or the system helium nucleus plus two electrons [7]). A monographic issue about this subject has been published in [8].

In all these studies the projectile and a target preserve their internal structure during the collision, but one can analyze also reactive collisions. Kovács and Wiesenfeld [9] studied, in a collinear geometry, the scattering between an atom and a diatomic molecule: $A+BC\leftrightarrow ABC\leftrightarrow AB+C$. More recently, we studied the chaotic behavior in the reaction between a hydrogen atom (proton plus electron) and a projectile proton interacting through Coulomb forces [10]. We analyzed the full three-dimensional problem at very low impact energies. We found that the transition from regular to chaotic scattering appears when impact velocity $v_p$ is reduced to a value below about 1/10 of the classical electron velocity $v_e$.

In this paper we present another investigation on the same subject: We think that it is worth consideration since collisions with rearrangement between electrically charged particles are one current topic in atomic physics, from both the theoretical and the experimental points of view [11]. The phase space of a system of three particles moving in three dimensions is too large to be easily handled; limiting to two dimensions will allow us to do a more detailed and accurate study. We will address the following topics. (a) Do features of chaotic scattering appear in two-dimensional collisions? (b) If so, do they appear in the form of a sharp order-chaos transition or as a smooth transition? (c) Is it possible to detect some traces of irregular behavior also in the heavy particles motion, instead of only when looking at the lightest one? (d) Finally, an investigation of the dynamics of the electron during the scattering is done. It gives insight into how the discontinuities on the output function appear.

The final state of the projectile may be defined through a set of parameters $\{A_f\}$ (e.g., the angle of deflection and final velocity), which are functions of the input quantities $\{A_i\}$ (e.g., the impact parameter and impact velocity). When the set of values $\{A_f\}$ depends sensitively by $\{A_i\}$, i.e., a finite variation of $\{A_f\}$ is caused by an infinitesimal variation of $\{A_i\}$, the system is chaotic.

Usually, one studies the so-called *scattering functions*, which are the output variables as a function of only one input variable, keeping the other input variables fixed. If a scattering function is fractal then the system is chaotic, but the converse is not necessarily true. In fact, Chen *et al.* [12] showed that time-independent Hamiltonian systems with more than two degrees of freedom can have chaotic sets with nonzero fractal dimension while at the same time the scattering functions do not show any fractal property. The scattering function has fractal behavior only if the Hausdorff dimension $D_c$ of the chaotic invariant set satisfies the inequality

$$D_c > 2N-(2+q), \tag{1}$$

where $N$ is the number of degrees of freedom and $q$ is the number of conserved quantities of the system (in our case $N=6$ and $q=4$). Therefore, a positive answer to the above question (a) will give us also a lower bound estimate of the Hausdorff dimension of the chaotic set of the system.

Our scattering problem has the alternative outcomes

$$\mathrm{H}+\mathrm{H}^+ \to \mathrm{H}^+ + \mathrm{H} \tag{2}$$

$$\to e+\mathrm{H}^+ + \mathrm{H}^+ \tag{3}$$

$$\to \mathrm{H}+\mathrm{H}^+. \tag{4}$$

At the end of the collision the electron may be captured by the projectile nucleus (charge transfer), it may be ionized (ionization), or it may remain bound to the target (excitation of the target). The values of the masses and charges are $m_{\mathrm{H}^+}=1836$, $m_e\equiv 1836$, and $Q_e=-Q_{\mathrm{H}^+}=-1$ (atomic units will be used throughout this paper).

In our geometry the scattering plane is the plane $(x,y)$. The target proton is initially fixed at the origin $\mathbf{r}_t=(0,0)$ and at rest $\mathbf{v}_t=(0,0)$. The position of the electron is $\mathbf{r}_e$

*Electronic address: sattin@igi.pd.cnr.it
†Electronic address: salasnich@hpmire.mi.infm.it

 

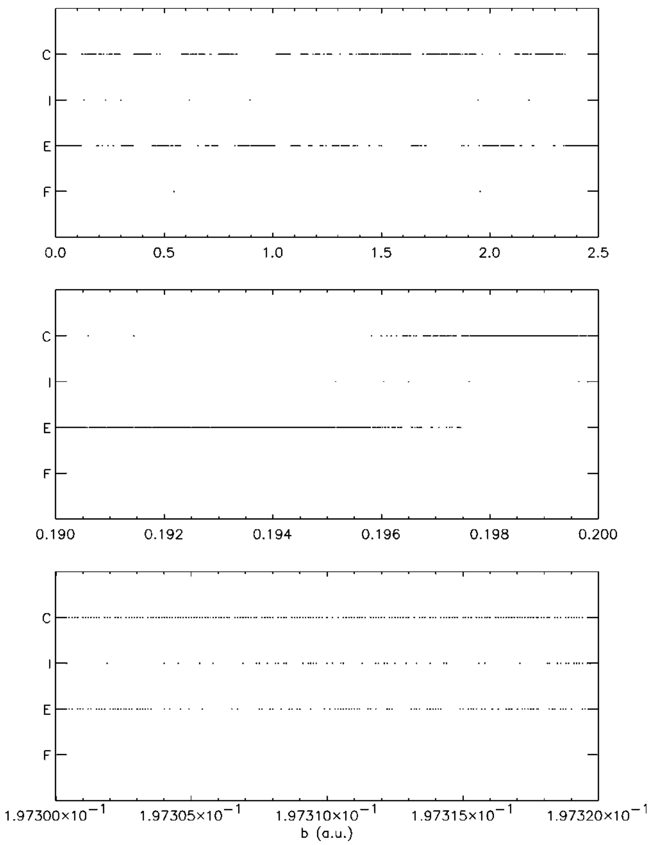


FIG. 1. Scattering function versus impact parameter $b$. $C$ denotes electron capture, $I$ ionization, $E$ electronic excitation, and $F$ undetermined. Here $v=0.10$ and $\theta=5.825\,12$ rad. From top to bottom successive enlargements are shown with respect to $b$. The number of runs is about 500 for each plot.

$=(r_e\cos\theta+\omega_e t,\, r_e\sin\theta+\omega_e t)$, where $r_e$ is the radius, $\theta$ is the initial phase, and $\omega_e=v_e/r_e$ is the angular velocity. Both $v_e$ and $r_e$ are equal to 1 in our units. The projectile proton is prepared with velocity $v_p$ in the positive direction of the $y$ axis and at the position $\mathbf{r}_p=(b,-a)$, where $b$ is the impact parameter and $a>0$ must be chosen so large that the target and the projectile may be considered initially as noninteracting. In these simulations $a\simeq 10$ was found to be a good choice.

The total energy of the system is given by

$$E=\frac{1}{2}m_{\mathrm{H}^+}v_t^2+\frac{1}{2}m_{\mathrm{H}^+}v_p^2+\frac{1}{2}m_e v_e^2 +\frac{1}{|\mathbf{r}_t-\mathbf{r}_p|}-\frac{1}{|\mathbf{r}_t-\mathbf{r}_e|}-\frac{1}{|\mathbf{r}_p-\mathbf{r}_e|}. \tag{5}$$

The classical equations of motion are numerically integrated by using a variable-order variable-step Adams algorithm (routine NAG D02CJF).

Note that the choice of the outcome is done on the basis of the energy of the electron with respect to the two bodies. An algorithm to identify all the possible outcomes is given in Ref. [13]. In particular, in our system three parameters remain free: $\theta$, $v_p$, and $b$. Numerical simulations have been carried out varying all of them. The output variables $\{A_f\}$ defined above reduce to just one element: the final state of the electron. It is a discrete function of its energy. Discrete variables are usually not employed in these studies but are not a novelty: Bleher *et al.* [14] have already investigated a chaotic system with a finite number of possible outcomes.

In Figs. 1 and 2 some consecutive blowups of the scattering function are presented as a function of $b$, for two different choices of $v_p$ and $\theta$. There are regions where the outcome is a regular function of $b$, alternated with other regions where an irregular behavior appears. One recognizes a kind of self-similarity, the same pattern repeating at smaller and smaller scales. This is the distinctive aspect of fractal behavior. The same results appear varying $\theta$, with $v_p$ and $b$ fixed.

A clear picture is obtained by studying the scattering function versus the proton velocity $v_p$. In Fig. 3 this is shown for one couple of values $(b,\theta)$. The great degree of irregularity at small $v_p$'s is visible. For higher $v_p$'s the zones where the electron is captured and those where it remains close to the target proton are more clear-cut. Ionization is by far the least probable process. One may judge that the order-chaos transition does appear quite smooth and the scattering at $v\simeq 0.2,0.3$ is not yet entirely regular.

In order to quantify the amount of chaos one can compute the fractal dimension of the scattering function. Given a reference trajectory with initial impact parameter $b$, we slightly modify the impact parameter to $b+\epsilon$ and make another run. The results of the two runs are compared. The starting trajectory is said to be uncertain if the two final states are different. The fraction $f(\epsilon)$ of uncertain trajectories as a function of the parameter $\epsilon$ scales as

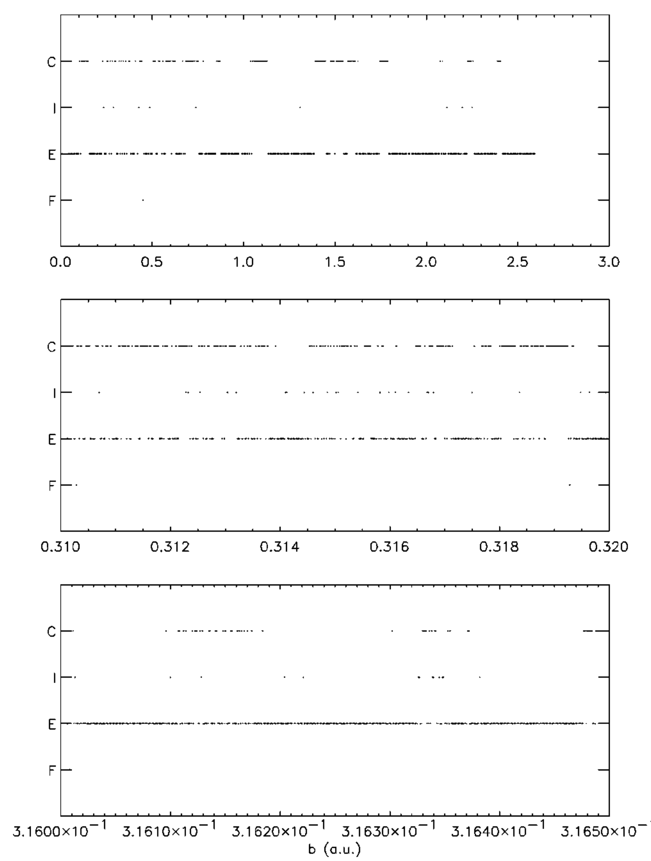


FIG. 2. Same as Fig. 1, but now $v=0.120$ and $\theta=0.252\,62$ rad. The number of runs is about 500 for each plot.

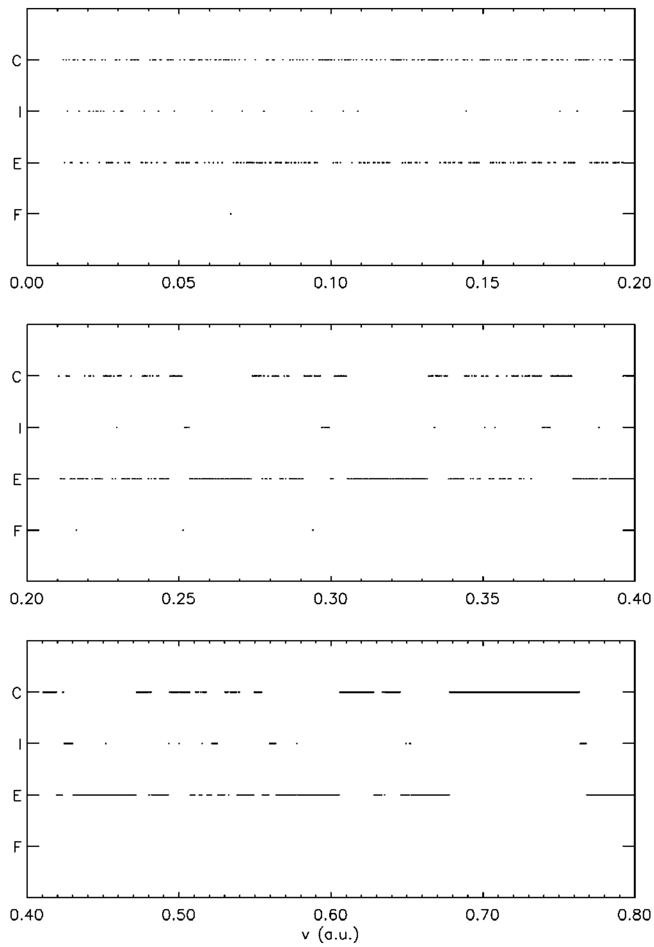


FIG. 3. Scattering function versus impact velocity $v$. $b = 0.2893$ and $\theta = 5.825\,12$ rad. The number of runs is about 400 for each plot.

$$f(\epsilon) \sim \epsilon^{1-d}, \quad \text{for} \quad \epsilon \rightarrow 0, \tag{6}$$

where $d$ is the capacity dimension [3]. In Fig. 4 we plot the capacity dimension $d$ as a function of $v_p$. There is a regular decrease of $d$ for $v_p < 0.3$ and then $d$ is nearly constant but positive.

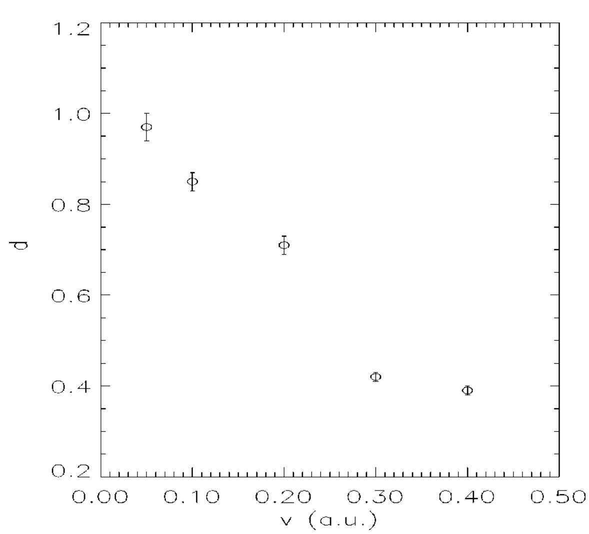


FIG. 4. Capacity dimension $d$ versus impact velocity $v$. Statistical errors are shown.

One of the main purposes of this work is to analyze in detail the behavior of the electron in correspondence with a singularity of the scattering function. In Fig. 5 the trajectories of the particles are shown for two almost identical runs, differing only by a very small value of the impact parameter. We see that initially the electron trajectories in the two cases nearly overlap. The two paths begin to differ when the nuclei reach the point of closest approach. The potential experienced by the electron may be sketched as two wells located around the nuclei divided by a symmetrical ridge. Obviously, the location of the ridge dynamically evolves in time as the nuclei move. The electron initially lies in one of the two potential wells and it is able to escape to the other well only if at some time during the collision it passes near the ridge with enough velocity to cross it. Note that we are referring to the component of the velocity orthogonal to the potential ridge. Once the electron has fallen into the other potential well it is very unlikely that it can cross the ridge the opposite way and return to the former nucleus. Two electrons differing by an infinitesimal value of the velocity, $u$ and $u + \epsilon$, will undergo entirely different fates provided $u + \epsilon$ is not enough to cross the potential barrier while $u$ is.

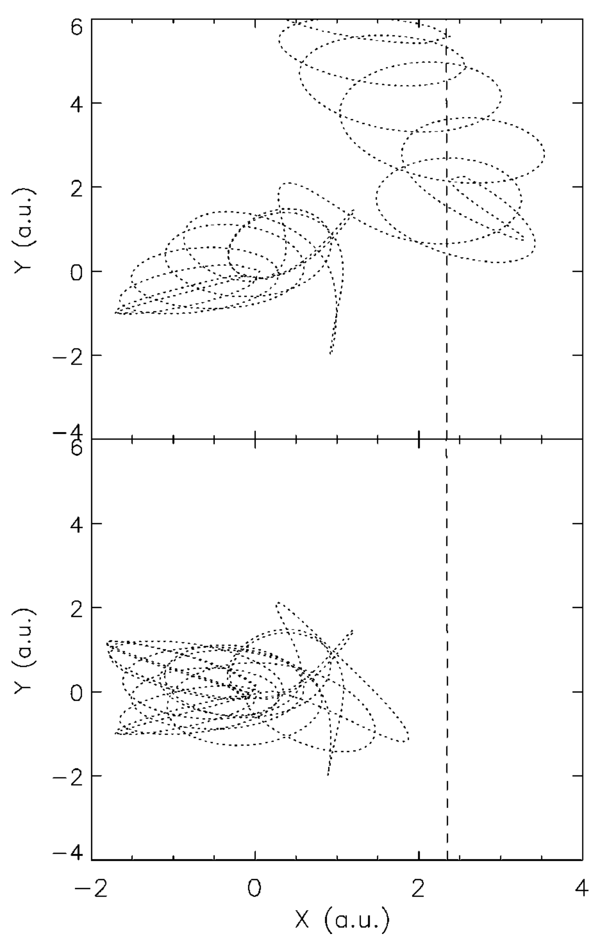


FIG. 5. The upper panel shows trajectories of the particles in the interaction region. $v = 0.10$, $\theta = 5.825\,12$ rad, and $b = 2.345$. The dashed line is the trajectory of the heavy projectile. The dotted line is the electron trajectory. The initial position of the electron is close to (0,0). The trajectory of the target nucleus is not shown since it is always close to the origin (0,0). The lower panel shows the same process, but now with $b = 2.350$.

It is interesting to note that chaotic features appear only as singularities of the scattering function: An analysis of the delay time (the time needed by the electron to quit the interaction region) reveals that it is not a sensitive function of the scattering. This is related to the fact that the electron does closely follow one of the nuclei and the trajectories of the heavy particles are always regular: No complicated patterns appear from a study of their behavior.

In summary, a study of the two-dimensional low-energy scattering between charged particles has been carried out. Simulations have been done using a larger number of runs than in our previous paper [10] thereby diminishing statistical errors. The results confirm the findings of Ref. [10] that the scattering becomes irregular when the energy is low enough. Insight as to why chaos appears has been given by looking at the detailed trajectories of the electron. Abrupt discontinuities in the output function are correlated with the structure of the potential experienced by the electron.

It is useful to discuss the validity of the model used. At very small impact velocities, it is not entirely justified to treat the heavy particles as classical objects and even less so for the light particle. The processes (2)–(4) should be studied within the framework of quantum mechanics. However, (i) one may imagine applying the same apparatus not to the ground state but to a Rydberg state, where using the classical mechanics is justified, and (ii) the use of classical or semiclassical models has recently been extended with satisfactory results in realms thought previously to be amenable only to quantum treatment; see, for example, the classical description of the helium atom [15] or the treatment of the hydrogen ionization by electron scattering at energies near threshold [16]. In that work, furthermore, the evidence for chaos was found, reminiscent of the results shown in this paper.


[1] P. Gaspard and S. A. Rice, J. Chem. Phys. **90**, 2225 (1989); **90**, 2242 (1989); **90**, 2255 (1989).

[2] S. Bleher, C. Grebogi, and E. Ott, Phys. Rev. Lett. **63**, 919 (1990).

[3] S. Bleher, C. Grebogi, and E. Ott, Physica D **46**, 87 (1990).

[4] G. Troll, Physica D **83**, 355 (1995).

[5] S. Brandis, Phys. Rev. E **51**, 3023 (1995).

[6] J. M. Petit and M. Hénon, Icarus **66**, 536 (1986).

[7] J.-M. Yuan and Y. Gu, Chaos **3**, 569 (1993).

[8] Chaos **3**, (4) (1993), special issue on chaotic scattering, edited by T. Tél and E. Ott.

[9] Z. Kovács and L. Wiesenfeld, Phys. Rev. E **51**, 5476 (1995).

[10] F. Sattin and L. Salasnich, J. Phys. B **29**, L699 (1996).

[11] B. H. Bransden and M. R. C. McDowell, *Charge Exchange and the Theory of Ion-Atom Collisions* (Oxford Science, New York, 1992).

[12] Q. Chen, M. Ding, and E. Ott, Phys. Lett. A **145**, 93 (1990).

[13] K. Tökesi and G. Hock, Nucl. Instrum. Methods Phys. Res. B **86**, 201 (1994).

[14] S. Bleher, C. Grebogi, E. Ott, and R. Brown, Phys. Rev. A **38**, 930 (1988).

[15] T. Yamamoto and K. Kaneko, Phys. Rev. Lett. **70**, 1928 (1993).

[16] J.-M. Rost, Phys. Rev. Lett. **72**, 1998 (1994); J. Phys. B **27**, 5923 (1994); **28**, 3003 (1995).