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On the Fractal Character of the Planar Coulomb Classical Scattering

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Abstract

Numerical evidence is presented, indicating that the Coulomb three-body scattering problem possesses chaotic phase space regions for collision energies corresponding to the common classical approximation regime. Consequently, the stochasticity threshold of 100 eV, reported previously by Sattin and Salasnich, is extended by two orders of magnitude up to 20 keV. The underestimated stochasticity threshold reported by these authors was probably due to an inappropriate application of the specific numerical technique they used.

1 Introduction

The Classical Trajectory Monte Carlo (CTMC) method [1,2] is extensively used in modelling simple collisions between atoms, ions and electrons. The so calculated total and partial cross sections are satisfactory in a large energy interval, depending on the colliding constituents (atomic and mass numbers of the colliding particles as well as their state of ionization) and the refinements used in the exit tests for the classification of the trajectories [3].

The method consists essentially in the statistical study of a classical (or semi-classical) scattering problem, which, in the simplest possible case [4], is nothing more than a specific realisation of the Coulomb Three-Body (CTB) problem: a completely stripped ion as projectile (first body, typically a proton), coming practically from infinity, interacts with a hydrogen atom as target (composed by a nucleus and an electron, constituting the second and third body, respectively). Given the excess of available energy, the system may end up, after the interaction, in essentially three generic possible *exit channels*: either the electron remains bounded to the original nucleus (excitation, E), or the electron is orbiting around the incoming ion (charge transfer, C) or, finally, the electron is ejected from the target atom and the three particles move independently afterwards (ionization, I). Initial conditions for the three particles are selected at random and, after numerical integration, each trajectory is assigned an exit channel, according to the imposed exit tests. After the calculation of a large number of trajectories, it is expected that the fraction of them leading to E, C or I will give, approximately, the corresponding effective cross section.

Traditionally, the results of the CTMC method were considered to be reliable, provided that the system can be treated classically, presumably as long as the velocity of the impacting ion is larger than the classical velocity of the electron around the nucleus of the target. Otherwise, quantum-mechanical effects may become significant and the notion of a particle's trajectory looses its classical meaning. In the simplest case of a proton impacting on a hydrogen atom in the ground level, the threshold corresponds to a typical collision energy of, approximately, 25 keV. Consequently, it came as a surprise when the effective cross sections calculated through the CTMC method for collision energies in the keV region were shown far more reliable than the above simple theoretical arguments could predict [5]. Moreover the CTMC method turned out to be more stable than other quantum-mechanical methods, which have been shown to depend strongly on the number of states taken into account in the numerical calculations (see e.g. [6]).

The regime of validity of the CTMC method has been investigated by Keller *et al.* [7], who, based on the Kolmogorov-Arnold-Moser (KAM) theorem, specified quantum corrections to the classical trajectories consisting of small random perturbations, added during the numerical integration of the differential equations. For a simplified presentation of the KAM theorem see [8]. Using the CTMC method, in conjunction with the above technique, these authors found empirically that their final results (i.e. the calculated cross-sections) were independent of the nature of the perturbations, in particular both of the method of their introduction as well as of their statistical distribution. Moreover they found that this "modified" CTMC method was producing improved results, at least for the ionization of H by protons.

Subsequently, Katsonis and Varvoglis [9] conjectured, on theoretical grounds, that the CTB interaction is a scattering system exhibiting chaotic properties at least in some phase space regions, a fact that may explain the robusteness of the method, as discussed in what follows. It should be noted that the notion of chaos in the case of a scattering system is quite different from the one usually encountered in dynamical flows defined on compact phase space regions: it does not refer directly to the exponential divergence of nearby trajectories (according to the well known Lyapunov exponents), but rather to the intricate mixing of initial conditions leading to any one of the possible exit channels of the interaction (in the present case E, C or I). The set of initial conditions leading to a specific exit channel may be considered as its "basin" (designated here by the same symbols E, C or I). This is reminiscent of the relation between attractors and their basins in dissipative dynamical systems. In a scattering system we are not primarily interested in the properties of the exit channels (which cor-

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respond to the attractors in a loose analogy) but rather in the properties of their basins and on the dimensionality of their boundaries.

The exit tests for deciding which exit channel will be assigned to each trajectory include the comparison of the energies of the electron with respect to each one of the two protons. Let us denote by $E_p := E(e - p_p)$ the energy of the electron with respect to the incoming proton, p_p, and by $E_t := E(e - p_t)$ the energy of the electron with respect to the target proton, p_t. Then the channel followed by each trajectory corresponds to one of the four quadrants of the plane E_p, E_t. The quadrant($E_p > 0, E_t < 0$) corresponds to the exit channel E, the quadrant ($E_p < 0, E_t > 0$) to the exit channel C and the quadrant ($E_p > 0, E_t > 0$) to the exit channel I. The fourth quadrant ($E_p < 0, E_t < 0$), corresponding to the formation of a ''molecule'', is usually taken to be of negligible probability with respect to the probabilities of the channels E, C or I. The sets of initial conditions (in phase space) corresponding to the special cases where either E_p or E_t are zero constitute the boundaries between the basins. In particular the set corresponding to the half-line ($E_p = 0, E_t > 0$) is the boundary between the basins of C and I and the set corresponding to the half-line ($E_p > 0, E_t = 0$) is the boundary between the basins of I and E. The intersection of the above two boundaries in phase space corresponds to the point ($E_p = 0, E_t = 0$). In the neighborhood of this point are mapped trajectories that follow any of the three exit channels. Since the trajectories of Hamiltonian dynamical systems are continuous functions of their initial conditions, there should be open regions in the initial conditions space with the same property: in a small open disk there are points belonging to all three basins. The above condition is possible in a 2-D space, only if the boundaries of the basins are fractal curves; the basins themselves are then similar to multifractal Julia sets on the complex plane [10].

In the planar case of the CTB problem, which is usually taken in order to avoid the complexity of additional degrees of freedom and in order to obtain better insight, the incoming ion moves on the same plane as the electron of the target atom. For a constant value of the collision energy, the space of initial conditions is two-dimensional (usually parametrised by the impact parameter, b, and the initial phase of the electron on its orbit, θ). Therefore the boundaries of the basins should be fractal curves, at least in some regions of the initial conditions space. It should be noted that, although the boundaries are fractals, the basins themselves are of *complete measure*, i.e. their dimension is equal to the dimension of the initial conditions' space. This is due to Liouville's theorem, which applies to all conservative dynamical systems (e.g. see [11]). Any set of initial conditions with a volume $V_0 = V(t = 0)$ in phase space has the same volume, $V(t)$, with the set of the points of the trajectories at any other time t. Since the CTB problem is a conservative Hamiltonian system, the Hausdorff dimension of any non empty basin of any one of the three exit channels is equal to the Hausdorff dimension of the set of initial conditions, which in the CTMC method is of complete measure.

Katsonis and Varvoglis [9], suggested on this ground that the robustness of the CTMC method in the low energy region, as well as its insensitivity to the nature of the induced perturbations reported in [7], might be attributed to the chaotic nature of the scattering problem through the following ''conjecture''. If the scattering CTB problem is indeed a chaotic system (at least in some phase space regions), then the quantum-mechanical effects, which are simulated in [7] by small statistical ''perturbations'' during the numerical integration of, otherwise, deterministic trajectories, do not affect statistically the calculation of effective cross-sections. The reason is that, for any initial condition leading to one exit channel, there is always in its neighbourhood another initial condition leading to a different channel. Therefore, a small uncertainty in the initial conditions of a trajectory, which is in any case introduced by the finite accuracy of the representation of the numbers in a computer, has the same effect as the addition of a small noise during the phase of its numerical integration. However without calculating the size of the chaotic regions it is impossible to estimate their importance. Therefore in [9] it was concluded that numerical experiments were necessary in order to corroborate their ''conjecture''.

Quite independently from the above authors, Homan *et al.* [12] studied the coplanar interaction of Na^+ with an excited Rydberg Li* atom for various initial phase angles and impact parameters and presented their results graphically, by color-coding the initial conditions corresponding to each basin. The intricate patterns and the tangled interwinding of the basins which appear in their results may be considered as a clear indication for the fractality of the basins' boundaries. However, since these authors neither tested their reslults for self-similar behaviour nor calculated the dimension of the boundary curves, the problem of the chaotic nature of the three body Coulomb scattering was far from being considered as settled.

2. Fractal nature of the system

Following the aforementioned conjecture, Sattin and Salasnich [13, 14] had undertaken the direct investigation of the fractal nature of the basins' boundaries of the proton-hydrogen scattering problem in its simplest case: monoenergetic co-planar orbits with the target's electron in the ground state. For the numerical evaluation of fractality, these authors followed the uncertainty exponent technique, introduced in [15] for scattering problems. Their conclusion was that the interaction is indeed chaotic but the chaos becomes prominent only for collision energies of the order of 100 eV or lower, well below the regime of validity of the classical approximation needed for CTMC applications.

Unfortunately, in calculating fractal dimensions, Sattin and Salasnich departed from the method of [15], since they kept fixed all other initial conditions but the impact parameter. Consequently their results pertain only to a 1-D section of the 2-D initial condition's space. Therefore, although these authors detected the existence of self-similar structures in the space of initial conditions, they were not able to estimate the ''size'' of the corresponding regions, especially in the keV energy region, nor to calculate the fractal dimension of the basins' boundaries. What they really calculated was the capacity dimension of the basins themselves. Therefore figure 4 of [14], which represents the main result of the paper, shows, essentially, the fact that, for low interac-

tion energies, the capacity dimension of the basin of a specific exit channel is 1 (i.e. equal to the dimension of the initial conditions' space). On the other side, as the initial velocity of the projectile was increased, the existence of a threshold energy value was correctly detected, above which the calculated dimension of the basin becomes zero, simply because almost all trajectories end up in the other two exit channels and, therefore, the specific basin is practically empty.

In this context it is worth to mention that the result presented in [13] and [14], pertaining to the appearance of chaos in a scattering problem, is analogous to the well known result of Hénon and Heiles [16] for the case of classical chaos. In the case of classical chaos the measure of the phase space region filled by ordered trajectories drops from complete to zero within a very narrow strip of energy values. In the same way, in the case of a scattering problem the measure of the basin of a specific exit channel, in a fixed region of phase space, drops from complete to zero within a very narrow strip of collision energies. Since the results of [13] and [14] do not address the crucial problem of the fractality of the basins' boundaries, in particular in the keV energy region, we decided to extend their calculations in the full 2-D initial conditions space.

3. Calculations and results

For the numerical integration of the equations of motion a standard numerical code of the Laboratory of Plasma Physics at Orsay has been used, which follows the formulation described in [2]. For the present study, the space of the initial conditions was restricted to the case of co-planar trajectories with fixed impact energy. The incoming ions are launched from a fixed distance, r_0, towards the atom target, which is at rest. Since the electron of the target is assumed, in the present work, to be on a circular orbit with radius equal to the *Bohr radius*, it has only one degree of freedom, namely its initial phase, θ. The incoming ion has one degree of freedom as well, the impact parameter, b. We used both positive and negative values for the impact parameter, the negative ones representing the side of r_0 where the angular momentum of the ion has the same sign as that of the electron. The two initial conditions were chosen at random within a $[b, \theta]$ box, whose sides were selected each time according to the desired resolution, while r_0 was taken equal to 40 times the Bohr radius. In each case 56700 trajectories were calculated and the exit channel they followed (E, C or I) was recorded. Then the initial conditions of the trajectories that ended up in E, C or I were plotted as dots in three separate plots, one for each exit channel. In this way we were able to get a rough representation of the three basins.

Several hundred sets, of 56700 trajectories each, were calculated. In the beginning we selected as collision energy 100 eV, which is the threshold energy for the onset of chaotic motion calculated in [13]. It was very easy to see, even by simple inspection, that in this regime the initial conditions space presented a clear fractal structure. Since, however, this is a known result, we decided to focus our simulations on the energy level of 20 keV, which is close to the classical approximation regime.

In the lower order resolution ($0 < \theta < 2\pi$, $-2.5 < b < +2.5$) we first identified regions with signs of possible self-similarity. In a second step we selected small boxes centered on the regions of interest identified in the first step and with sides approximately ten times smaller and we repeated the calculations selecting the initial conditions inside these boxes. After repeating this process in successive steps, we were able to find self-similar structures in many regions. In figures 1–3 we give a typical example, where one can see that the basin of the I exit channel is self-similar for at least three successive scalings, which span two orders of magnitude in the b axis and four orders of magnitude in the θ axis. This can be considered as a clear indication of fractality, as discussed in [17]. Even more, there are indications in our results that the basins have the *Wada property*, which is stronger than simple fractality. This property refers to the fact that any initial condition, which is on the boundary of one basin, is also simultaneously on the boundary of all other basins [18].

We measure the dimension of a basin's boundary by the well known algorithm introduced in [15]. In each b, θ box, as the ones presented in Figs. 1–3, we select at random 2700 "central I trajectories, b_i, θ_i, $i = 1, 2700$. For each central trajectory we integrate twenty "side" trajectories, which have the same initial θ_i but initial impact parameters equal to $b_i \pm \varepsilon_j$, $j = 1, 10$. We calculate the fraction, f, of pairs

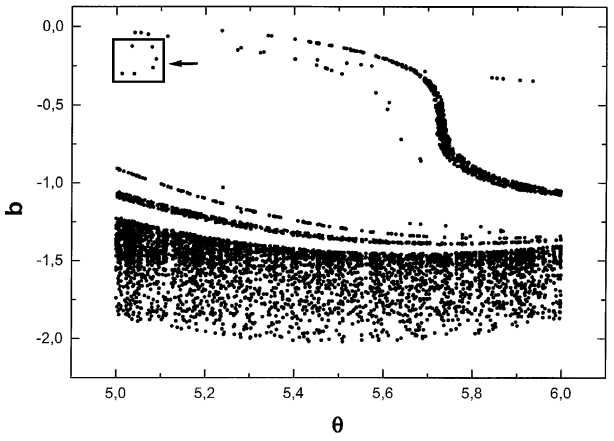

Fig. 1. Basin of the ionization exit channel at the lowest resolution. The small strucutre in the box on the upper left part was considered worth of a more detailed study.

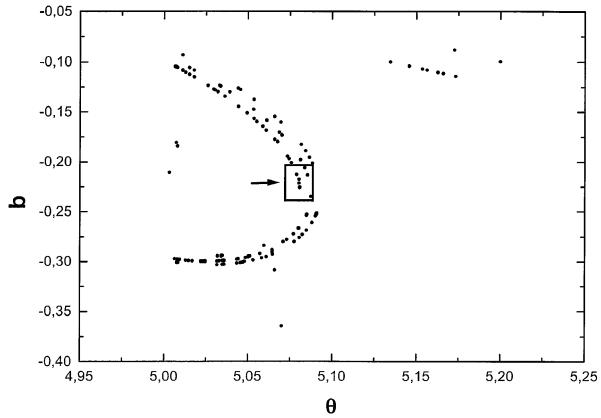

Fig. 2. The area in the square on the upper left part of figure 1 in higher resolution. The single line in figure 1 is decomposed in three lines.

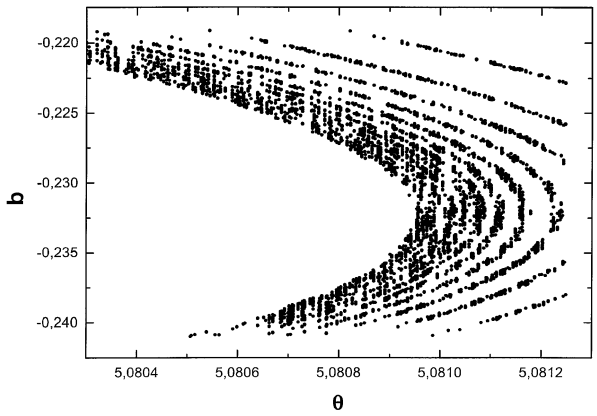

Fig. 3. The leftmost of the three lines in figure 2, if seen in higher resolution, is decmposed again in a set of higher order lines.

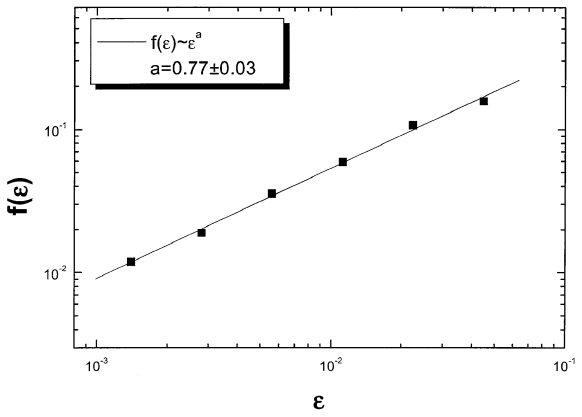

Fig. 4. A least square fit to the data $f(\epsilon)$ vs ϵ for figure 1. The co-dimension of the basin's boundary, 0.77 ± 0.03, is not a natural number, so that the boundary is a fractal curve.

of side trajectories that follow a different exit channel from that of the central trajectory and we plot the points $f_j - \varepsilon_j$ in log-log axes. According to the theory presented in [15], the points should lie on a straight line of the form $\log(f) = c + \alpha \log(\varepsilon)$ where the slope, α, is equal to the co-dimension of the basin's boundary. Therefore $d = D - \alpha$ is equal to the dimension of the boundary, where $D = 2$ is the dimension of the initial conditions phase space. In Fig. 4 we present the results for the basin appearing in Fig. 1. By a least square fitting of a straight line to the data we find $\alpha = 0.77 \pm 0.03$, from which it follows that $d = 1.23 \pm 0.03$, clearly a non-integer. Therefore the basin's boundary is fractal.

From the form of the algorithm it is clear that the calculated d is a sort of an "average" dimension of all "families" of boundaries appearing in each box, as discussed already in [15]. Since the dimension of non-fractal boundaries is always 1 while that of fractal boundaries is always larger than 1, this "average" is lower than the true dimension of the fractal boundaries. Therefore if one is willing to calculate the dimension of a *single* family, he should select a box with a finer resolution, such as the ones appearing in figures 2 or 3. A calculation for the box in figure 3 gives for the family shown there $d = 1.62 \pm 0.03$.

4. Discussion – Conclusions

How much confidence should we have on our calculations? First of all, the values of ε in figure 4 span two orders of magnitude, an interval that usually is considered as sufficient for reliable results. Moreover two specific tests were performed, in order to confirm the significance of our results. The first one was to calculate d in regions of the initial conditions space where there is not any apparent self-similar structure. The result was $d = 1$, i.e. a regular, non-fractal, line, as it should be expected. The second one was to calculate d for all three exit channels corresponding to the same set of initial conditions. Within the available accuracy the calculated values $d_i, i = 1, 3$ were equal. This shows that the non-integer value of d calculated in the present paper is not due to a numerical artifact, but it is a property of the true dynamical system of ion-atom collisions, as suggested in [9], which appears in a region of collision energies within the regime of validity of the classical approximation. Then we have to conclude that the scattering of protons by hydrogen atoms is indeed a chaotic dynamical system for values of collision energies where the classical approximation is valid.

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