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LETTER TO THE EDITOR

The CTMC method as part of the study of classical chaotic Hamiltonian systems

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Abstract. Stability features of dynamical systems are frequently attributed to the implications of the Kolmogoroff–Arnold–Moser (KAM) theorem. However, application of this theorem requires compact phase-space regions. This is not the case in the hyperbolic Coulomb three-body problem encountered in most of the classical trajectory Monte Carlo (CTMC) applications. Therefore, the satisfactory results of the CTMC method in a wide energy region or its robustness with respect to perturbations cannot be interpreted in this way. We propose here a justification of the above properties based on the character of the space of initial conditions corresponding to the trajectory classes resulting in excitation, ionization and charge transfer. Numerical experiments are in progress in order to confirm that the algebraic dimension of the boundaries separating the three sets of trajectories is, indeed, fractal, so that the system could be at least partly classified as a chaotic dynamical system. The stability properties of the CTMC method can then be inferred straightforwardly, since chaotic dynamical systems are structurally stable.

The satisfactory accuracy by which the classical trajectory Monte Carlo (CTMC) method (Abrines and Percival 1966, Olson and Salop 1977, Peach *et al* 1985) approximates the experimentally measured effective cross sections for ionization (IN) and charge transfer (CT) in a wide energy region (McDowell and Janev 1985, Willis *et al* 1985, Olson *et al* 1993 (and references therein), Katsonis and Maynard 1991, 1995, Katsonis *et al* 1991, Maynard *et al* 1992, Katsonis *et al* 1995), is leading to a favourable comparison with the results of various quantum-mechanical calculations, at least for H targets.

Justifying the success of the CTMC method by theoretical arguments has been the aim of numerous investigators. Recently, Keller *et al* (1993) investigated the conditions of applicability of this method, especially in the case of energies lower than those corresponding to the classical orbital velocity of the hydrogen 1s electron. These authors also give improved ionization and electron-capture cross sections for protons colliding with H(1s), for collision energies down to 10 keV. As a matter of fact, an improved classical treatment, even with a simple Coulomb potential, is expected to be sufficient for the most common case of hydrogen targets. The alternative of treating the Coulomb three-body (CTB) problem within the quantum-mechanical formalism, which consists of resolving the three-particle Fadeev integral equations of motion with effective potentials (see Avakov *et al* 1990), seems a more involved task with less physical insight.

Keller *et al* used the Kolmogoroff–Arnold–Moser (KAM) theorem to specify quantum corrections by heuristically imposing a compactness condition in the initial state (model

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hydrogen atom), without addressing the more general problem of the full phase-space properties. As it is well known (see Lichtenberg and Lieberman 1983, pp 159–68), this theorem applies to bounded trajectories of dynamical systems, i.e. to a compact phase-space region. Moreover, it requires Hamiltonian perturbations which have at least $2N-2$ continuous derivatives (where N refers to the degrees of freedom of the system (Chirikov 1979)). In dynamical models currently used in the CMTC method e.g. as described in Peach *et al* (1985), the particles' trajectories come from and go to infinity, even if only a finite part of each trajectory is considered. Thus, the trajectories' behaviour is not described by the KAM theorem. It should be noted that in the modification of the standard CTMC method proposed in Keller *et al* (1993), the 'perturbation' of the Hamiltonian (a 'randomization' of momenta along the trajectory, at regular time intervals) belongs to the class C^0, i.e. it does not have continuous first-order derivatives. The continuity condition is not definitively restrictive, since in numerical studies concerning Hamiltonians with C^0 perturbations, indications have been found for the existence of invariant tori in accordance with the KAM theorem (Varvoglis 1985). Relaxation, however, of the compactness condition (i.e. extension to potentially unbounded motions) is a non-trivial task, although from the physical point of view it does not seem unreasonable.

Here we present an argument, interpreting the observed success of the CTMC method and probably the recent results of Keller *et al* (1993). Use is made here of a definition for the ordered and chaotic trajectories which differ from the common one, pertaining to the case where the trajectories have points at infinity. This definition, used previously by Bleher *et al* (1988), applies to dynamical systems with multiple modes of exit. It leads to a natural extension of the notion of chaotic regions of phase space whenever the trajectories are not confined in compact subsets of the phase space. In the simplest case, where there are *two* possible final evolutions of a trajectory, the problem may be modelled by the motion of a test particle in a two-dimensional box having two exit holes, A and B. In this case, the points of the set of initial conditions leading to one outcome (exit through hole A) are distributed among the points of the set of initial conditions leading to the other outcome (exit through hole B) in a way which characterizes the system. The boundary separating the two sets in initial-condition space contains fractal and non-fractal (smooth) regions intertwined. Whenever the boundaries of the two sets have fractal dimensions (as was the case in the study of Bleher *et al* (1988)) the system should be classified as chaotic.

It is well known that chaotic Hamiltonian dynamical systems are *structurally stable*, i.e. small perturbations of the Hamiltonian function of the system (in the form appearing in the KAM theorem above) leave the system chaotic (Lichtenberg and Lieberman 1983, p 271). Note that the corresponding Kolmogoroff–Sinai metric entropy of the system (Gutzwiller 1990) is expected to vary smoothly, as in bounded systems. According to the CTMC method, what is identified as a target ionization (or charge transfer) cross section is calculated through an averaging process over the distribution of the projectile–target initial conditions leading to the removal of the electron from the target (and final settling into the projectile region). It is, therefore, natural to postulate that this average would not change considerably through a slight perturbation in the case when the system is chaotic.

The CTB dynamical system, which we have used in our CTMC code for H targets (one negative–two positive charges), may be modelled, following Bleher *et al* (1988), by a box in a three-dimensional space with three holes, representing the three possible inelastic outcomes of a collision (excitation, ionization or charge transfer). We conjecture that the behaviour of this system should be *qualitatively* similar to that of the system studied by Bleher *et al*, i.e. that it should possess chaotic regions in phase space. If this conjecture is true, then, for similar reasons presented subsequently, one would expect the two-negative–

one-positive charge CTB system to exhibit chaotic properties as well. A general study of the planar CTB system is given in Gu and Yuan (1993), who have investigated the e^-–He^+ scattering and the general features of the trajectories. They found that this dynamical system shows, indeed, chaotic behaviour, a fact that corroborates our conjecture about the chaotic character of the former.

Most of our CTMC calculations for atomic collisions pertain to the study of the effective cross sections in collisions of a stripped ion $A^{q+}(q = Z)$ with a hydrogen atom composed of an electron e^- and a proton p^+, which is part of the dynamic study of the CTB system (e^-, p^+, A^{q+}); in the case of $Z = 1$ it simplifies to (e^-, p^+, p^+). An interesting special case of the latter system is the one where the two protons are fixed, which corresponds to the H_2^+ molecule, successfully studied with the canonically invariant quantization method of Maslov by Strand and Reinhardt (1979). This system is integrable, so that the motion of the electron is not chaotic; the stability of H_2^+ has been proved classically to come from the tunnelling e^- trajectories confined between an ellipse and either one of two hyperbolae. Aside from this exceptional case and for similar reasons, the system (e^-, p^+, p^+) should exhibit, as mentioned before, dynamical features analogous to those of the system (e^-, e^-, α^{2+}), where α^{2+} stands for the alpha particle. In the (e^-, p^+, p^+) case each of the two protons is about 2000 times heavier than each of the electrons of the (e^-, e^-, α^{2+}) case. Inversely, the sole e^- is about 4×2000 times lighter than the corresponding α^{2+} and the attractive e^-–α^{2+} potential coefficient is the double of the e^-–p^+ case. In accordance with the dynamical system invariance under $T^2/L^3 = 1$ transformations, T and L being the time and length units respectively, the distance scale is clearly smaller in the (e^-, e^-, α^{2+}) case than in the (e^-, p^+, p^+) one. Moreover, existing (e^-, e^-, α^{2+}) dynamical studies may have different aims (e.g. Yamamoto and Kaneko 1993), therefore the initial conditions used and the classes of the CTB trajectories which are studied are not necessarily the same as with the (p^+, p^+, e^-) case. It is still possible to gain significant insight by comparison of the results pertaining to both cases. The importance of the Kepler-like two-body problem is inherent in various categories of trajectories of both systems, the T^2/L^3 invariance corresponding to the third Kepler law.

In systems having only chaotic trajectories, the calculated effective cross section should not depend on the selection of the phase-space region where the average is calculated, or on any slight perturbation of the dynamical system itself. On the contrary, whenever ordered regions exist in the phase space, the calculated effective cross section should depend on the specific region of the phase space (containing only ordered, only chaotic or both types of trajectories) as well as on any perturbation destroying invariant tori of the system (and, therefore, converting ordered trajectories to chaotic). Note that the numerical procedure applied to Keller *et al* (1993) can be thought of as doing exactly the latter task: randomization of momenta destroys any region of ordered motion, thus rendering the calculation of the averages more robust and independent of the specific selection of initial conditions.

The same argument applies for the interpretation of CTMC successful calculations of effective cross sections. Since, by our conjecture the classical dynamical system is already chaotic to some extent, additional quantum mechanical 'perturbations' are not expected to alter significantly its phase-space structure portrait, apart, perhaps, from the elimination of the remaining ordered regions. This should be the case in the energy region within which intrinsic quantum processes are not prevailing. However, calculations corresponding also to collision energies lower than 10 keV amu^{-1} have been given and discussed, both for charge transfer (Katsonis and Maynard 1995) and for ionization (Katsonis *et al* 1995). A quasi-classical approximation through a trace formula pertaining to non-bounded systems

(Hejhal 1983, Gutzwiller 1990) might be of help otherwise.

Finally, it should be noted that the above considerations could be verified numerically, by calculating the regions of initial conditions in phase space leading, respectively, to ionization, charge transfer or excitation, and measuring the dimension of the boundaries separating exit and capture modes in phase space. Results indicating a non-integer algebraic (Renyi) dimension for this boundary would corroborate our conjecture. We are presently working towards this direction.

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