Classical-trajectory Monte Carlo calculations for energetic electron-capture processes

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Electron-capture processes of a proton from a hydrogen atom are studied at a collision energy of 5 MeV by the classical-trajectory Monte Carlo method. Thomas double-scattering processes and knock-on captures, which are characteristic of high-energy ion-atom collisions, are *detected* in a two-dimensional treatment. Another type of capture that takes place through a momentum-matching mechanism is also investigated. Three-body effects modify these processes considerably in some cases from the idealized pictures given in a simplified treatment of successive two-body collisions published before [see, e.g., R. Shakeshaft and L. Spruch, Rev. Mod. Phys. **51**, 369 (1979)]. Three-dimensional calculations designed for knock-on captures are also performed, and the cross section, 1.9×10^{-29} cm^2, is in good agreement with quantum-mechanical calculations.

The classical-trajectory Monte Carlo (CTMC) method[1] has been widely used for ion-atom collisions. In this method classical equations of motion of a three (in some cases more) -body system are solved rigorously by numerical computations under randomly generated initial conditions that simulate quantum-mechanical distribution of initial states. Though the CTMC is based on purely classical mechanics, it has been proven to be a powerful method that gives reliable cross sections for a variety of ionization and charge-transfer processes. However, its application to high-energy collisions, particularly for charge transfers, is rather difficult since the sharp decline of the transition probabilities increases the necessary number of trajectories for sufficiently good statistics rapidly, and hence the computational time becomes extremely long.

In 1927 Thomas[2] pointed out, within a framework of classical mechanics, that a double-scattering mechanism becomes a dominant process of charge transfer at high impact velocities. At first the electron is kicked by the projectile toward the target nucleus, making an angle of 60° with the incident direction of the projectile. The electron then collides with the target nucleus and is deflected by 60° again. Finally, the electron achieves nearly the same velocity as the projectile and they make a bound state with a certain probability. A few decades later Drisko[3] found that the second-order Born term contains the contribution in a quantum-mechanical treatment, and it also overcomes the first-order Born [Oppenheimer, Brinkman, and Kramers[4] (OBK)] term in the high-energy region. After his work, many theoretical papers have been devoted to the study of this double-scattering mechanism. However, all the relevant quantum-mechanical theories are based on the perturbation theory, and nevertheless, the convergence of the perturbation series is an open question even at present. On the other hand, the two collisions are treated separately as independent two-body encounters in classical mechanics.[2,5] Nobody has confirmed that this process really occurs in a rigorous solution of a three-body problem.

The purpose of the present CTMC calculations is to *detect* the Thomas double scattering and other electron-capture processes that are peculiar to high-energy ion-atom collisions and to show how they are influenced by three-body effects that are absent in existing theoretical works.

We study charge transfer from a hydrogen atom to a proton at a collision energy of 5 MeV:

$$\mathrm{H}(1s)+p\rightarrow p+\mathrm{H}\ , \tag{1}$$

where the final bound state of the formed hydrogen atom need not be discriminated. The probability of charge transfer is extremely small at this energy. In fact, the cross section of the Thomas double scattering is of the order of 5×10^{-27} cm^2. We need to calculate 10^{12} trajectories for this detection at least. This number is too large even for the fastest vector processors in the world. We need a special design in order to make the calculation practically possible.

We simplify the problem dealing with two-dimensional collisions only. Since the Thomas double scattering occurs selectively in coplanar collisions, this simplification drastically enhances its probability. However, this restriction does not spoil the reality of the calculations at all. It gives a particular section of real three-dimensional collisions since the motion in a central force is essentially two dimensional in classical mechanics. We can always make the interacting three particles confined on a plane simply by choosing the initial conditions appropriately without imposing any restriction upon the equations of motion.

We solve the Hamilton equations of motion[1] ($i=1$ or 2);

$$\frac{d\mathbf{r}_i}{dt}=\frac{\partial H}{\partial \mathbf{p}_i}\ , \tag{2}$$

$$\frac{d\mathbf{p}_i}{dt}=-\frac{\partial H}{\partial \mathbf{r}_i}\ , \tag{3}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are a set of Jacobi coordinates that describes the relative motion of the three particles and $\mathbf{p}_1$

and $\mathbf{p}_2$ are their conjugate momenta. In the present calculations, we take $\mathbf{r}_1$ as the vector from the target nucleus to the electron and $\mathbf{r}_2$ as the vector from the center of mass of the target atom to the projectile. H is the classical Hamiltonian of the three particles in an inertia frame, where the center of mass of the whole system is at rest. The Kepler orbit of the initial state is set on the collision plane containing the impact-parameter vector and the initial projectile position. Then it is evident that the components of Eqs. (2) and (3) that are perpendicular to this plane are decoupled and are zero at any time because the force vectors are always on the collision plane. We solve the equations of motion from the moment at which the projectile is located 10 a.u. from the target atom before the collision till the moment at which the two nuclei are separated more than 10 a.u. again after the collision.

We have calculated 109 million trajectories generating the initial bound states by the microcanonical distributions.[1] Three hundred hours of CPU time is required for this calculation on FACOM 780. Among this enormous number of samplings, only 82 events induced charge transfer. They are classified into three types, analyzing the trajectories, although some of them are difficult to classify because of their complexity.

The first one is the Thomas double scattering that we are searching for. This process shows the characteristic that the scattering angles are peaked around the critical angle, 1 mrad in the c.m. frame. This critical angle is determined by the combined effects of the deflection of the projectile and the recoil of the target nucleus caused by the collisions with the electron. In contrast with the other two types, only this process can occur, even at large impact parameters. Thirty-nine events are identified as the Thomas double scattering and we give some examples in Fig. 1. In each figure, the projectile is approaching from the left-hand side and the electron is orbiting the target nucleus counterclockwise before the collision. The symbols on each line show the positions of the particles at the moments located with equal time intervals of 0.1 a.u. around the closest-approach point. These are helpful for the reader to trace the trajectories as a function of time. Figures 1(a) and 1(b) are typical examples of the Thomas double scattering. In these cases the impact parameters are relatively large and each collision is little affected by the third particle. Figures 1(c) and 1(d) give examples for small impact parameters. We see a large difference from the idealized picture[5] of the double scattering. The scattering angles of the two-body collisions are closer to 90° rather than to 60°. The assumption made in the simplified treatment that the projectile collides with a free electron does not hold any longer at these small impact parameters, since the electron is situated in the neighborhood of the target nucleus before the collision.

The second category is of the "OBK type," which means that the electron is captured by the projectile through a mechanism of momentum matching as in the OBK approximation. This process occurs only for the combination of a very small impact parameter and a high eccentricity of the initial atomic state. The three particles come closer to one another near the origin at the

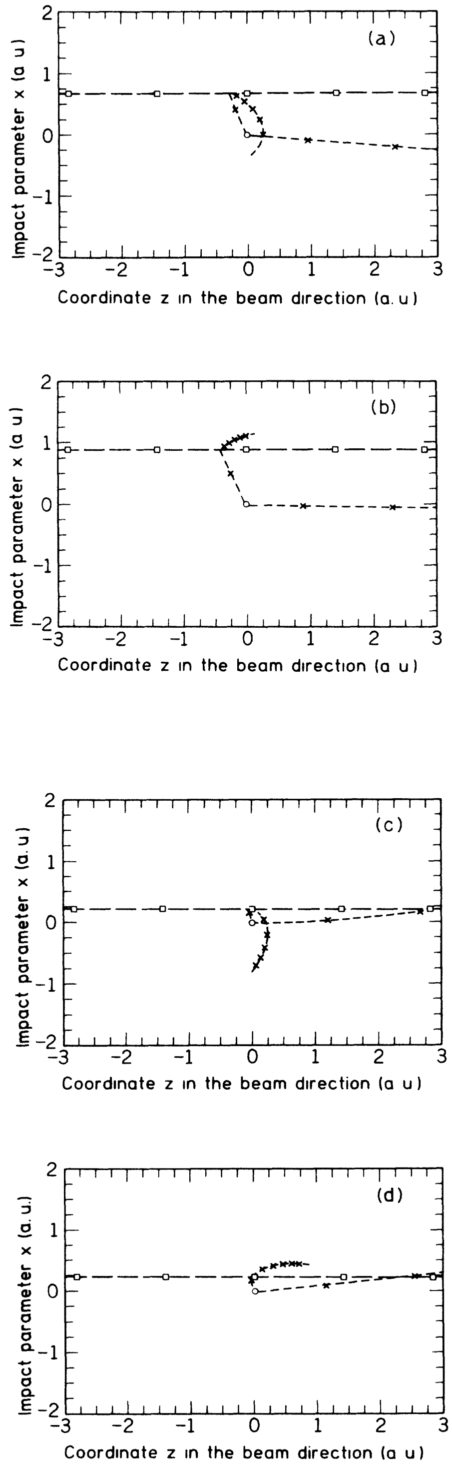

FIG. 1. Trajectories of Thomas double scatterings detected in the two-dimensional CTMC calculations. Long-dash lines and short-dash lines denote the trajectories of the projectile and the electron, respectively. Open squares and crosses are plotted for helping the readers to imagine the time evolution of the collision processes (see text). The target nucleus is initially located at the coordinates ($x=0$, $z=0$) (denoted by a circle). Since the recoil is very small its position is unchanged within the scale given in the figure. The coordinates are given in atomic units.

same time, and the electron is accelerated to a high velocity by the strong attractive forces of the nuclei. The electron then transfers to a bound state of the projectile and, together, they move away. Since the electron is located in the neighborhood of the projectile nucleus after the collision, the final state also has a high eccentricity. A classical orbit with a high eccentricity corresponds to the s ($l=0$) state of quantum mechanics. This preference of high eccentricities coincides with the trend of the OBK approximation that electron captures between s states become dominant at high energies. Only eight events are identified as OBK-type captures. Figure 2 shows examples of this process.

The third process is the knock-on capture predicted by Mapleton,[6] in which the projectile has a head-on collision with the target nucleus. This process occurs only for the case in which the masses of the nuclei are nearly equal. In the idealized picture[5] of knock-on capture, the projectile stops a moment after the collision and the target begins to move away abruptly with the same velocity that the projectile had before the collision. The electron continues to move along its initial orbit as if the replacement of the nucleus had not taken place. This process can be easily distinguished from the others since only this corresponds to a backscattering in the c.m. frame. Figure 3 shows some examples among the 25 identified events. Figure 3(a) is the most typical knock-on capture in which the projectile almost stops after the collision. In most cases the projectile does not stop as in the examples 3(b), 3(c), and 3(d). In the cases of 3(c) and 3(d) the motion of the electron is influenced by the other particles, and its orbit is considerably changed during the collision. The electron encounters the ejected target nucleus after the nuclear collision in Fig. 3(c); the electron is kicked back by the projectile before the nuclear collision in Fig. 3(d). These two figures show that higher-order effects are also important for knock-on captures.

A comment should be given on the impact-parameter

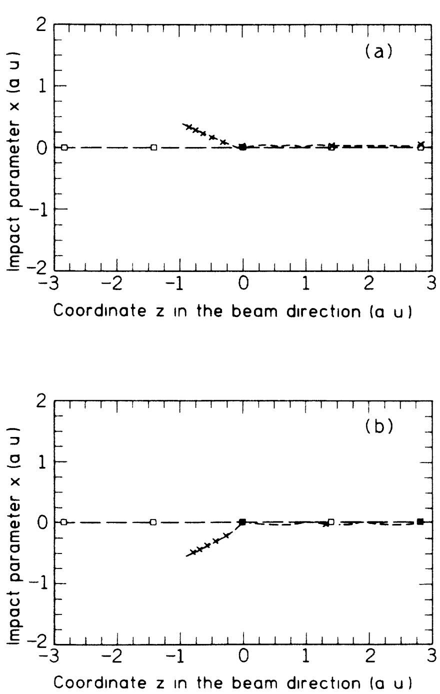

FIG. 2. The same as Fig. 1, but for OBK-type captures. At the origins, the three particles are overlapping.

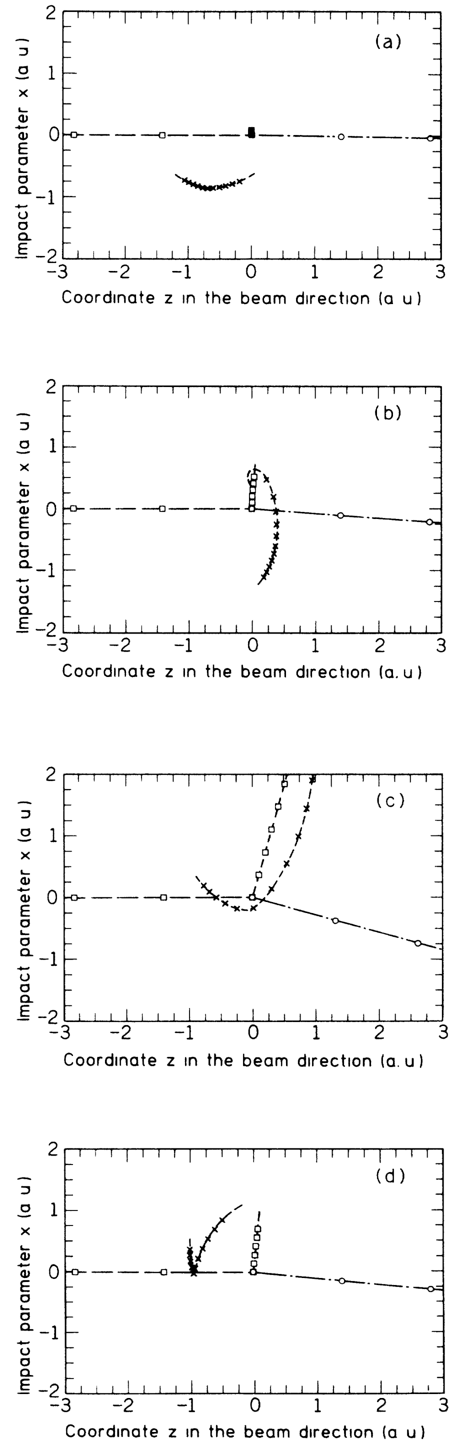

FIG. 3. The same as Fig. 1, but for knock-on captures. The trajectory of the ejected target nucleus is shown by a dot-dash line.

dependence of the knock-on capture processes. In the present calculations, the particles are treated as point charges and the scattering angles are essentially determined by the Rutherford scattering of the two nuclei. Nevertheless, the impact parameter that can induce knock-on captures extends up to 10^{-3} a.u., which is too large, though it is invisible in these figures, to bring about a two-body backscattering. This is not surprising if we realize that the origin of the laboratory frame is not situated on the target nucleus but on the center of mass of the target atom. The target nucleus itself moves around the center of mass with a radius of the order of 10^{-3} a.u.

Three-dimensional cross sections are not to be derived from the present two-dimensional calculations. In order to see the validity of the CTMC method for high-energy electron-capture processes, we have made three-dimensional CTMC calculations designed for knock-on capture exclusively. Only small impact parameters are generated to enhance its probability. Among 39 million trajectories, 314 events induced knock-on captures and we obtain a cross section of 1.9×10^{-29} cm^2 with a statistical uncertainty of $\pm15\%$, which is in good agreement with the value of 2.2×10^{-29} cm^2 of the quantum-mechanical calculations.[5]

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