Impact-parameter treatment of classical trajectory Monte Carlo calculations for ion-atom collisions

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A simplified classical trajectory Monte Carlo (CTMC) method is proposed for ion-atom collisions. With the introduction of the prescribed classical trajectories for the internuclear motion, the electronic motion in the time-dependent interaction is solved classically. It gives almost identical integrated cross sections with the "exact" CTMC calculations. Differential cross sections are also calculated for $p+\mathrm{H}\rightarrow\mathrm{H}+p$. The results are in excellent agreement with the experiments.

INTRODUCTION

The classical trajectory Monte Carlo method (CTMC) has been successfully applied to ion-atom collisions.[1-5] It solves classical equations of motion of a few-body system rigorously by numerical calculations under randomly selected initial conditions that simulate the quantum-mechanical distribution of the initial atomic state. Though CTMC has been proven to give reliable cross sections in various processes, its application is limited to three- or four-body collisions at intermediate velocities. Computational time becomes enormous for a larger system or for higher velocities.

On the other hand, approximate calculations are inevitable in quantum-mechanical treatments.[6] The perturbation theory neglects higher-order couplings completely. Distorted-wave theories take account of only a part of interactions to infinite order. The close-coupling calculations cannot get rid of the inaccuracy caused by the truncation of the expansion, though full interactions are included in this subspace. The inaccuracy involved in these approximations is sometimes difficult to assess.

Most of these quantal treatments rely on the impact-parameter picture in the intermediate- to high-energy region. The motion of heavy nuclei is treated classically and the Schrödinger equation that describes the motion of electrons is solved as a time-dependent problem. Heavy nuclei are assumed in most cases to move along a straight-line trajectory with a constant velocity, irrespectively of the motion of electrons. In contrast with the aforementioned approximations for the electronic motion, the validity of the impact-parameter method has been well established.

In this Brief Report we apply the concept of the impact-parameter method to CTMC calculations. Since the CTMC is a classical theory, the only modification is the separation of nuclear motion from electronic motion.

THEORY

Consider the following processes of a three-body system with Coulomb interactions in which the masses M_A and M_B of particles A and B are much larger than the mass M_C of the third particle C:

$$A+(B+C)\rightarrow A+(B+C)\ , \tag{1}$$

$$\rightarrow(A+C)+B\ , \tag{2}$$

$$\rightarrow A+B+C\ . \tag{3}$$

Parentheses denote a bound state of two particles. Owing to the large mass ratios, it is a good approximation to assume that the motion of heavy particles A and B is insensitive to the details of the kinematic evolution of the light particle C. Therefore, we describe the relative motion between A and B by a given function of time for each impact parameter b. This assumption reduces the present three-body problem to a much simpler one-body problem in which a particle C is moving under a time-dependent two-center potential. The Hamilton-Jacobi equations of motion are written as[7]

$$\frac{d\mathbf{r}}{dt}=\frac{\partial H}{\partial\mathbf{p}}\ , \tag{4a}$$

$$\frac{d\mathbf{p}}{dt}=-\frac{\partial H}{\partial\mathbf{r}}\ , \tag{4b}$$

where $\mathbf{r}$ is the coordinate of the particle C measured from the center of mass of the particles A and B, and $\mathbf{p}$ is its conjugate momentum. The classical one-body Hamiltonian is given by

$$H=\frac{1}{2M_C}p^2+\frac{Z_BZ_C}{|\mathbf{r}+a\mathbf{R}|}+\frac{Z_AZ_C}{|\mathbf{r}-b\mathbf{R}|}\ , \tag{5}$$

with

$$a = M_A/(M_A+M_B)\ ,$$

$$b = M_B/(M_A+M_B)\ .$$

where $\mathbf{R}$ is the internuclear distance vector and Z_A, Z_B, and Z_C are the charges of particles A, B, and C, respectively. Equations (4a) and (4b) are solved numerically under randomly selected initial conditions generated by a microcanonical distribution of classical orbits.[1] Since we give $\mathbf{R}$ as an explicit function of time, we need not choose the impact parameter b randomly. Thus the number of randomly generated parameters is 5:[1-5] the eccentricity of the Kepler motion, its time-angle variable θ_n, and three Euler angles that determine the plane and the major axis of the Kepler motion. The final state of the particle C is classified into the three channels (1)–(3) in the same way as in usual CTMC calculations.[1-5]

The evolution of $\mathbf{R}$ and the scattering angle χ are determined by the motion of A and B interacting through a two-body potential $V(R)$ in the present treatment. The differential cross section is calculated by[7]

$$\frac{d\sigma}{d\Omega} = \frac{b(\chi)P(b)}{\sin\chi}\left|\frac{db}{d\chi}\right|\ , \tag{6}$$

where $P(b)$ is the transition probability of one of the processes (1)–(3).

RESULTS AND DISCUSSIONS

We have applied the present CTMC method to charge transfer and ionization processes of a hydrogen atom colliding with a proton and other multicharged ions at energies above a few tens of keV/amu. The transition probabilities $P(b)$ so obtained, and, consequently, the integrated cross sections, agree to within 0.01% with the results of the usual CTMC calculations[1-5] where the full three-body equations are solved. This fact demonstrates the usefulness of the present method. Furthermore, we have found that $P(b)$ depends very little on the choice of the two-body potential $V(R)$. In fact, we have seen almost no difference in the resultant $P(b)$ calculated by using a straight-line trajectory and that using curved trajectories determined by a realistic potential $V(R)$. This is reasonable because, at these energies, the collision is confined within the scattering angle of the order of 10^{-3} rad.

In Figs. 1 and 2, the differential cross sections calculated by the formula (6) are compared with experiments[8] for $p+\mathrm{H}\rightarrow\mathrm{H}+p$ at 60- and 125-KeV proton energies, respectively. For the two-body potential $V(R)$ that is indispensable for the relation between scattering angles and impact parameters, we have used the static potential

$$V(R) = \frac{Z_A(Z_B+Z_C)}{R} + (Z_AZ_B + Z_A/R)\exp(-2Z_BR)\ , \tag{7}$$

which is obtained by averaging the potential $Z_AZ_B/R + Z_AZ_C/|\mathbf{r}-\mathbf{R}|$ over the quantum-mechanical $1s$ orbital of the target atom. Also shown in these figures are quantal calculations, namely, the Oppenheimer-Brinkmann-Kramers approximation[9] (OBK), the eikonal

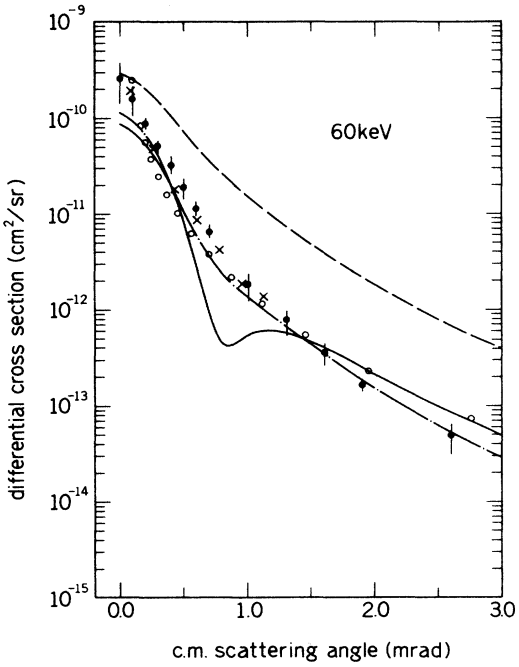

FIG. 1. Differential cross sections for $p+\mathrm{H}(1s)\rightarrow\mathrm{H}+p$ in center-of-mass coordinates and a proton energy of 60 keV. CTMC cross sections: ○, present results; ×, "exact" CTMC (Ref. 4). Quantal cross sections: ———, OBK; —·—·—, eikonal; ——, B1B. CTMC cross sections are the sum over all final bound states and quantal cross sections are the sum up to $n=3$. Quantal cross sections are calculated by the present authors and they are consistent with previous calculations (Refs. 10 and 12). Experimental cross sections are denoted by circles with error bars (Ref. 8).

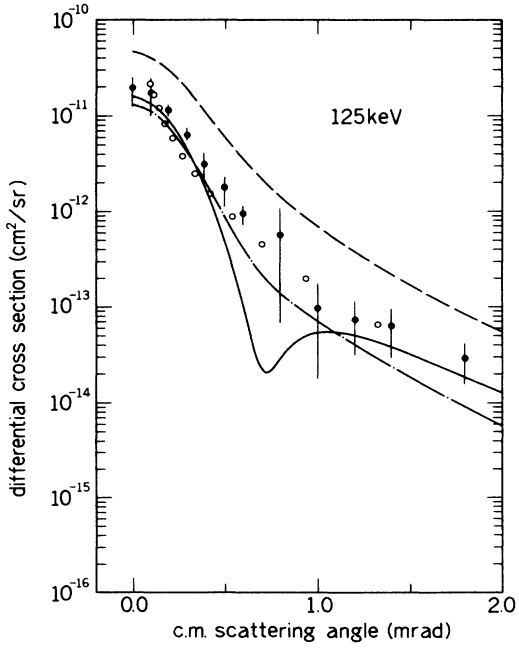

FIG. 2. Same as Fig. 1 but for 125 keV. The "exact" CTMC cross sections are not available.

approximation,[10] and the boundary-corrected first-order Born approximation[11,12] (B1B). The present results are in excellent agreement with experiments. It is as good as the best of the quantal calculations. We have also compared our results with the "exact" CTMC cross sections[4] reported by Olson at 60 keV. They agree well within the accuracy of statistical errors which are not shown in these figures. The behavior of our cross sections near the forward direction seems to be a little different from the experimental data. The static potential $V(R)$ becomes zero rapidly outside the region of the bound-electron distribution of the target, and this makes the scattering angles too small at large impact parameters. As a result, $|d\chi/db|$ becomes small and hence increases differential cross sections at forward direction. Better agreement may be obtained by using a more realistic internuclear potential $V(R)$.

SUMMARY

We have shown that the impact-parameter treatment of CTMC calculations serves to reduce computing time without significant loss of accuracy. In the present calculations the elastic deflection function uniquely determined the relation between the scattering angle and the impact parameter. This is in contrast to the usual CTMC method in which the scattering angle cannot be predicted before solving equations of motion for a three-body system. The transition probability $P(b)$ is insensitive to the trajectory assumed. Satisfactory agreement of our results with the "exact" CTMC calculations and with experiments implies that the physics that determines the angular distribution of projectiles may be much simpler than usually anticipated.

[1]R. Abrines and I. C. Percival, Proc. Phys. Soc. London **88**, 861 (1966); **88**, 873 (1966).

[2]R. E. Olson and A. Salop, Phys. Rev. A **16**, 531 (1977); M. L. McKenzie and R. E. Olson, *ibid.* **35**, 2863 (1987); J. S. Cohen, *ibid.* **26**, 3008 (1982).

[3]A. Ohsaki, T. Watanabe, N. Nakanishi, and K. Iguchi, Phys. Rev. A **32**, 2640 (1985); J. S. Cohen, *ibid.* **35**, 1419 (1987).

[4]R. E. Olson, Phys. Rev. A **27**, 1871 (1983).

[5]G. Schiwietz and W. Fritsch, J. Phys. B **20**, 5463 (1987).

[6]M. R. C. McDowell and J. P. Colman, *Introduction to the Theory of Ion-Atom Collisions* (North-Holland, Amsterdam, 1970).

[7]L. D. Landau and E. M. Lifshitz, *Mechanics* (Pergamon, Oxford, England, 1960).

[8]P. J. Martin, D. M. Blankenship, T. J. Kvale, E. Redd, J. L. Peacher, and J. T. Park, Phys. Rev. A **23**, 3357 (1981).

[9]J. R. Oppenheimer, Phys. Rev. **31**, 349 (1928); H. C. Brinkmann and H. A. Kramers, Proc. Acad. Sci. Amsterdam **33**, 973 (1930).

[10]K. Kobayashi and T. Ishihara, Phys. Rev. A **34**, 626 (1986).

[11]D. P. Dewangan and J. Eichler, J. Phys. B **19**, 2939 (1986); Comments At. Mol. Phys. **21**, 1 (1987).

[12]Dž. Belkić, S. Saini, and H. S. Taylor, Z. Phys. D **3**, 59 (1986).