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Absence of the Thomas peak in the classical-trajectory Monte Carlo calculations for proton-hydrogen collisions in the MeV region

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Large-scale classical-trajectory Monte Carlo calculations are executed in three-dimensional space for proton-hydrogen collisions at 2.8 and 5 MeV. The Thomas peak that has been confirmed in the experimental data and in the quantal calculations is invisible in the classical calculations. This unexpected result is due to the peculiar character of classical bound states that have no minimum binding energy. The Oppenheimer-Brinkmann-Kramers-type capture by means of the velocity-matching mechanism dominates even in the MeV region owing to the classical peculiarity, and the Thomas double-scattering contribution is embedded in this background.

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The mechanism of the Thomas double-scattering process [1] has been one of the long-standing subjects in the physics of ion-atom collisions. Following the pioneering study of Drisko [2], many theoretical methods based on perturbation theory have been proposed and applied to the analysis of this process. Though the exact calculation of the second-order terms has become feasible owing to the progress of high-speed computers [3], the perturbative approaches have the shortcoming that the contribution of higher-order terms are not taken into account. A variety of higher-order theories that contain a part of interactions to all orders have been developed [4] but they are obliged to employ further approximations for evaluating the transition matrix elements. The accuracy of these secondary approximations is difficult to assess quantitatively. The success of the measurements of the Thomas peak for proton-helium [5] and for proton-hydrogen [6] collisions has made more elaborate theoretical investigations desirable.

Nonperturbative theoretical studies of the Thomas process have been carried out recently using the coupled-channel method [7] and the classical-trajectory Monte Carlo (CTMC) method [8]. The coupled-channel method is a quantum-mechanical approach in which all the electronic wave functions including very-high-lying continuum states are expanded in Gaussian orbitals. Significant knowledge of the Thomas process beyond the second order was obtained and good agreement with the experimental cross sections was achieved. On the other hand, the CTMC method is a purely classical approach. Though quantum-mechanical studies continue successfully, it is of great interest to see how the Thomas double-scattering process is described in classical mechanics since it was originally predicted in the framework of purely classical formalism [1]. The CTMC study has shown that classical captures can be classified into three types, in analogy with quantum-mechanical theory: knock-on captures, the Oppenheimer-Brinkmann-Kramers (OBK) type, and Thomas double scatterings. Knock-on capture takes place through a head-on collision of the projectile and the target nucleus resulting in a replacement of the two nuclei. This can occur only at extremely small impact parameters of the order 10^{-3} a.u. The OBK-type capture is the process in which the electron is transferred through the mechanism of momentum matching as in the quantal OBK approximation [9]. The OBK-type capture also occurs at small impact parameters $b \leq 0.05$ a.u. Only the Thomas double scattering can occur even at large impact parameters. While this CTMC calculation is useful for studying how the trajectories are deformed from the idealized picture of the Thomas process in close encounters, the treatment was based on a two-dimensional collision model for simplicity and hence it does not give complete information for quantities such as differential cross sections.

In the present study we execute three-dimensional CTMC calculations for the process

$$p + \mathrm{H} \rightarrow \mathrm{H} + p \tag{1}$$

at 2.8 and 5 MeV. The details of the CTMC method are described in many papers [10] and we give only a brief remark here. The classical equations of motion for three-particles interacting through Coulomb potentials are solved directly by numerical integration under initial conditions that simulate the quantum-mechanical distribution of the bound state. For the initial Kepler orbits, we adopt the microcanonical distribution [10], in which the square of the eccentricity is uniformly distributed and the momentum distribution coincides exactly with the quantal prediction. Since the correct description of the momentum distribution is the most important factor for the determination of high-energy capture cross sections, the microcanonical distribution is more suitable for the present study than other distributions [11]. The impact parameter b is generated randomly in linear scale between 0 and 1.0 a.u. at 2.8 MeV and between 0 and 0.5 a.u. at 5 MeV. We solve the equations of motion from the moment at which the projectile is located 5 a.u. from the closest-approach point before the collision to the moment at which the projectile is separated from the closest point 5 a.u. after the collision. We have checked the invariance of the results by shifting the starting and ending points between 5 and 10 a.u. We need an enormous number of trajectories since the probability of the Thomas process is extremely small. Special consideration for the generating code of the random numbers is required. We have used a shuffling technique in order to make the period 5×10^8 of a standard generating code larger than 10^{12}: the order of generated random numbers is rearranged using another set of random numbers generated independently. The differential cross sections are calculated by the formula [12]

$$\frac{d\sigma}{d\Omega}=\frac{\Delta\sigma}{2\pi(\sin\theta)\Delta\theta} \quad (2)$$

with

$$\Delta\sigma=\frac{2\pi b_{\max}}{N}\sum_i b_i(\theta-\Delta\theta/2,\theta+\Delta\theta/2)\,, \quad (3)$$

where $\Delta\theta$ is the width of the scattering angle and all the particles scattered into this width is counted as the scattering to the angle θ. In the present calculations, we take $\Delta\theta=0.05$ mrad. $b_{\max}$ is the maximum value of the generated impact parameters, N is the total number of generated trajectories, and b_i is the impact parameter of the ith event among the scatterings into the interval $\Delta\theta$. It is confirmed that the results are independent of the choice of $\Delta\theta$ if it is sufficiently small.

We have generated 8.82×10^9 trajectories for 5-MeV and 1.21×10^9 trajectories for 2.8-MeV collisions. These numbers are too large to calculate all the trajectories directly. We need a device in order to make the calculations feasible. From the two-dimensional CTMC calculations [8] we have learned that charge exchange occurs under restricted conditions when the projectile energy is high:

(a) For small impact parameters $b<0.1$ a.u., only Kepler orbits with high eccentricity ($\epsilon>0.9$) can induce charge exchange, and in this case both the projectile and the electron must come close to the target nucleus simultaneously: the distance of the closest approach is less than 0.1 a.u. This criterion is valid for both OBK-type capture and Thomas double scattering.

(b) For larger impact parameters $b\geq0.1$ a.u., Thomas double scattering selectively occurs. The projectile encounters the electron at a point situated in the interval $-0.8<\tan\alpha<-0.2$, where α is the angle measured from the direction of the impact parameter vector. Note that $\tan\alpha=-1/\sqrt{3}$ corresponds to the typical Thomas double scattering in which the electron is deflected by 60°.

In classical mechanics the Kepler motion is essentially two dimensional. The calculations of Ref. [8] were carried out without imposing any restriction on the equations of motion of the three-particle system on account of this peculiarity of classical mechanics, and information derived from the results is valid for a full three-dimensional treatment. Before solving the equations of motion, we estimate the point of closest encounter of the projectile with the bound electron using the unperturbed Kepler orbit and the straightline projectile trajectory. If neither of the conditions (a) and (b) is satisfied, we judge that this initial condition does not lead to charge exchange.

The number of charge-exchange events is 2075 out of the total 1.21×10^9 trajectories at 2.8 MeV and 4041 out of the total 8.82×10^9 trajectories at 5 MeV. The obtained total capture cross sections are 1.04×10^{-23} cm^2 and 7.98×10^{-25} cm^2 at these energies, respectively. Figures 1 and 2 show the differential cross sections. The statistical errors are kept smaller than 15% at all scattering angles. We easily notice two distinct features of the cross sections: (i) the classical cross sections are larger than the measured cross sections by about a factor of 10 at 2.8

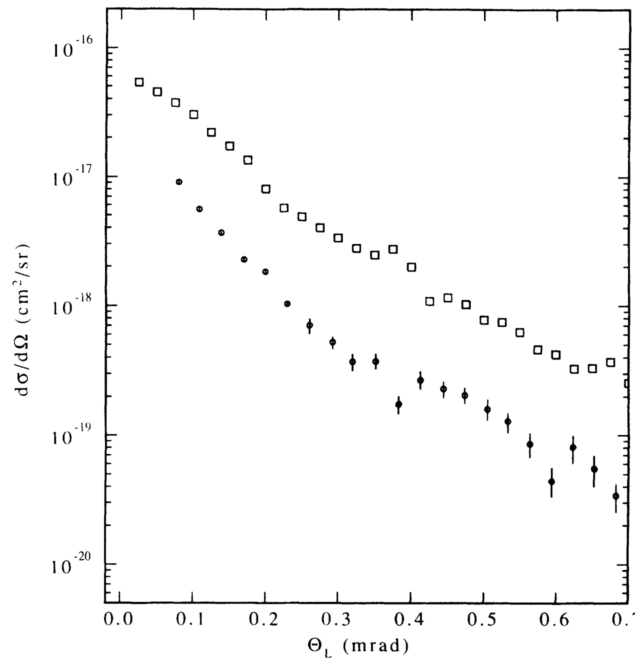

FIG. 1. The CTMC differential cross sections (open squares) in the laboratory frame for $p+H\rightarrow H+p$ at 2.8 MeV. The experimental data is from Ref. [6].

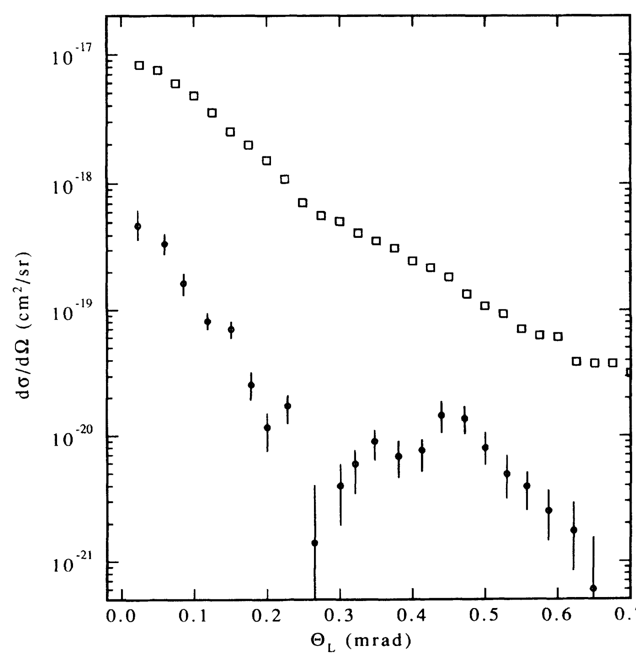

FIG. 2. The CTMC differential cross sections (open squares) in the laboratory frame for $p+H\rightarrow H+p$ at 5 MeV. The experimental data is from Ref. [6].

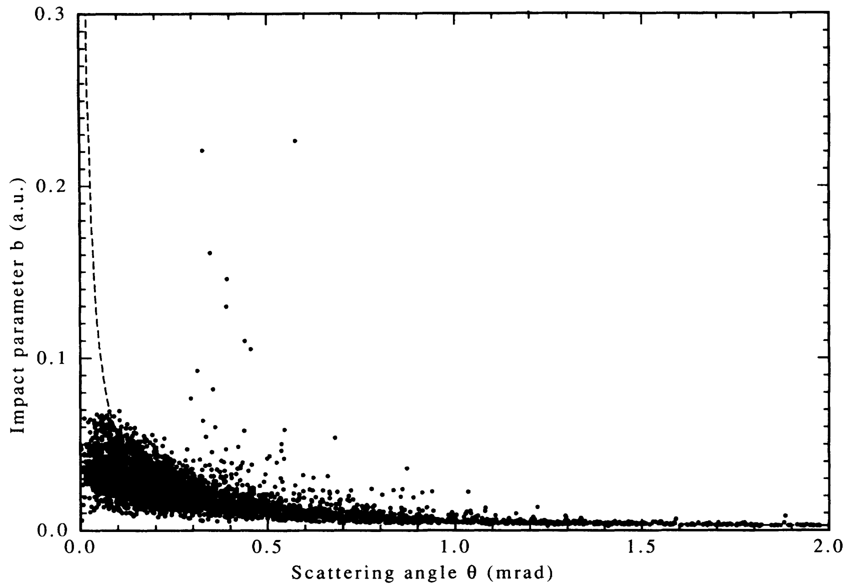

FIG. 3. Plots of the correlation diagram of the impact parameter b and the scattering angle θ in the laboratory frame for proton-hydrogen collisions at 5 MeV. Each dot shows an event that leads to charge exchange. The dashed line is the b vs θ relation of the Rutherford scattering between the projectile and the target nuclei.

MeV and about a factor of 30 at 5 MeV, and (ii) no peak is seen around the critical angle 0.47 mrad. The overestimation of the classical cross sections is attributed to the character of the classical bound states: there exists no minimum binding energy. The OBK-type captures occur thorough momentum matching, and the rapid decrease of the quantal capture probability for high energies is caused by the decline of the large-momentum components of the bound states. On the other hand, there exists in the classical description, for any collision energy, a deep bound state whose average momentum coincides with the required matching momentum. This overestimation of the OBK-type captures is also the cause of the second feature: no Thomas peak is visible in the classical differential cross sections. Because the Thomas process has no preference for large-momentum components, it is not enhanced by the peculiarity of the classical bound states.

There is a very important thing which must be taken into account when the probability is extremely small. Under some conditions which are generated randomly, there occurs an exceptional situation that the Thomas double scatterings happen to take place more frequently than the average. This is a particular case allowed by the statistical dispersion. However, even a small number of exceptional events can change the shape of the differential cross section since the probability of total charge exchange itself is very small. Of course, such a "pseudo" peak disappears if we increase the number of samplings.

In order to confirm our assumption that the Thomas double scatterings are hidden in the OBK-type background, we plot the relation between the impact parameters and the scattering angles in Fig. 3 for each trajectory that induces electron capture at 5 MeV. The dense sea of points in the small impact parameter region corresponds to OBK-type captures. Those points are distributed along the line that corresponds to the b vs θ relation of the Rutherford scattering between the projectile and the target nuclei:

$$b = \frac{Z_P Z_T}{mv^2} \cot\theta , \quad (4)$$

where Z_P and Z_T are the charges of the projectile and the target nuclei, respectively, and m and v are the reduced mass and the velocity of the relative motion. A group of

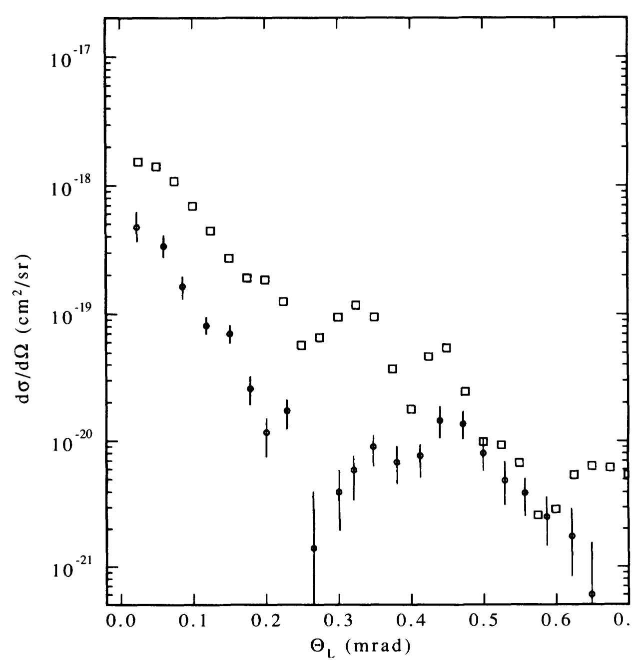

FIG. 4. The reduced differential cross section obtained from the data in which captures to extremely deep bound states are eliminated. The process is the same as Fig. 2.

dispersed points are seen above the dense sea of the OBK-type captures. These dispersed points are the evidence of Thomas double scatterings. They show the typical features of the Thomas process, namely, scattering angles centered at the critical angle 0.47 mrad and large impact parameters. Since the overestimation of the OBK captures is caused by the captures to extremely deep bound states of the projectile, the Thomas peak may be seen in the differential cross-section curve if we remove those components from the events. Figure 4 shows the differential cross sections derived from the reanalyzed data in which captures to bound states below -50 a.u. are eliminated. Oscillatory structures appear in the angular distribution and we see that a local peak exists as the critical angle 0.47 mrad. As seen in Fig. 3, the scattering angles of the Thomas processes are not confined to a small range. The other peaks in Fig. 4 are also produced by the Thomas processes. Because of the broad distribution, the convergence of the statistical dispersion is not good. We need many more samplings of the trajectories, an order of magnitude more at least, in order to judge whether the undulation is an artifact produced by the statistical error. The cutoff energy of -50 a.u. is chosen as the midpoint between the ionization threshold and the energy of the state, the mean orbital velocity of which coincides with the velocity of a 5-MeV proton. It is the high-momentum, high-eccentricity components of weakly bound states which correspond to quantal OBK captures, rather than the high-momentum, low-eccentricity components of strongly bound states. Though the latter components are removed largely by this cutoff procedure, the cross sections are still larger than the experimental data. Choice of a higher cutoff energy is expected to give better agreement but this makes the total number of the capture events still smaller and the statistical uncertainty becomes worse. In any case, we have seen that the Thomas double scatterings are masked by the overestimated OBK captures.

In summary, we have performed large-scale CTMC calculations for proton-hydrogen collisions at 2.8 and 5 MeV. The OBK-type captures are dominant at all the scattering angles in the present application of classical mechanics, in contrast with the quantum-mechanical prediction, and as a result the Thomas peak is hidden by this background. Though the peak is not visible in the differential cross sections, the existence of the Thomas processes is confirmed in the b vs θ plot and in the reduced differential cross-section curve.

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