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Classical calculation of high-energy electron capture in 5-MeV proton-hydrogen collisions

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The existence of the classical Thomas peak in the angular distribution of projectiles undergoing capture in collisions of 5-MeV protons with atomic hydrogen is explored using the three-body, three-dimensional classical-trajectory Monte Carlo technique. A method that selects only that portion of the initial phase space which yields capture at this energy was developed to make the calculation tractable due to the extremely small cross section. The spectrum obtained displays only a small shoulder near the angle predicted by Thomas on the basis of successive classical binary collisions and the total (integral) cross section is overestimated by a factor of 26 compared to recent experimental measurements. The overestimation originates from too large a contribution from velocity matching direct capture; the energy regime in which it is significant is discussed. In addition, the double-scattering events in this model which contribute significantly to the cross sections are found to differ substantially from the Thomas picture.

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Almost 70 years ago, Thomas [1] suggested that at high velocity the dominant mechanism for charge transfer in ion-atom collisions would be double scattering, since capture in a single binary event is classically, and quantum mechanically, forbidden by conservation of energy and momentum. In such a Thomas collision, the projectile first interacts with the target electron, scattering it towards the nucleus, which then deflects it in such a way that its final velocity vector matches that of the projectile, resulting in capture. The analysis of Thomas was based entirely on classical mechanics, and energy and momentum conservation for this geometry yields the result that for proton impact, the projectile should be scattered to an angle of about 0.5 mrad, the so-called Thomas angle. As this mechanism becomes dominant, the capture cross section differential in the scattering angle of the projectile should display a peak centered at about this angle, since the background cross section decreases very rapidly from a maximum at an angle of zero. A considerable amount of theoretical work since the suggestion of Thomas has been devoted to exploring the quantum-mechanical consequences of this picture and towards developing theories of high-energy capture (see, for example, the reviews by Shakeshaft and Spruch [2] and by Belkić, Gayet, and Salin [3]).

Experimentally, the Thomas peak has recently ("recently" when placed in context with the date of the Thomas prediction) been directly observed by Horsdal-Pedersen, Cocke, and Stockli [4] and by Vogt *et al.* [5] for proton impact of helium and atomic hydrogen, respectively, both in the collision energy range of several MeV. Quantum-mechanically, this double scattering must be represented as a second-order term in a perturbative expansion such as the Born series and its variants (see, in addition to the reviews, Macek and Taulbjerg [6], Miraglia *et al.* [7], Macek and Alston [8], McGuire, Eichler, and Simony [9], Taulbjerg and Briggs [10], Macek and Dong [11], Alston [12], and Crothers and Dunseath [13]). Models based on quantum-mechanical perturbation theory have found reasonably good agreement with the experimental measurements. However, much conjecture has existed as to whether the Thomas peak could actually be obtained using a purely classical theory or whether it actually arises due to an inherently quantum-mechanical interference of first- and second-order terms.

Since no exact analytical solution exists for the classical Coulomb many-body problem, exploration of this possibility must proceed by numerical simulation. In addition, to obtain cross sections which relate to the quantities which are observed experimentally, the electronic structure of the target atom must be modeled. A procedure to do this was developed for ion-atom collisions by Abrines and Percival [14] based in part on classical models of atom-molecule scattering [15,16]. In this method, an ensemble of projectile-target configurations is prepared in which the electron's initial position and momentum are chosen at random from a distribution whose average properties mimic the quantum-mechanical values. Following Abrines and Percival [14], we have utilized the microcanonical distribution, which, for atomic hydrogen, reproduces exactly the quantum-mechanical momentum distribution and approximately the quantum-mechanical position distribution. The subsequent motion of all the particles is then determined by iterative solution of the classical equations of motion. After the particle trajectories have been integrated into the asymptotic regime, it may be determined what reaction, if any, has occurred, as well as the energies and scattering angles of each of the particles. This method has come to be known as the classical-trajectory Monte Carlo (CTMC) technique, and its utility for describing particularly ionization and charge transfer in ion-atom collisions has been demonstrated by a large body of investigations [17–28]. Thus, if classical scattering alone were to give rise to the Thomas peak, this method should definitively find its signature.

This was investigated quite recently by Toshima [29],

who found evidence of Thomas double-scattering events in a two-dimensional (2D) simulation of 5-MeV proton-hydrogen collisions based on the CTMC method. Due to the extremely small total cross section for charge transfer in this reaction (3×10^{-26} cm^2 measured by Schwab *et al.* [30]), a full three-dimensional simulation must have seemed intractable. In a three-dimensional CTMC model, this cross section corresponds to on the order of one capture event out of every 10^7 projectile-target configurations. To obtain enough capture events to produce an angular differential cross section with sufficiently small statistical errors to resolve unambiguously the Thomas peak would require at least 500 times this many counts, so that 5×10^9 trajectories would be needed (Toshima estimated that 10^{12} trajectories would be needed). Using the current vectorized versions of the CTMC codes on a CRAY-2 machine, this would require on the order of 2000 CPU hours (=83.3 CPU days) by our estimate. This is at least two orders of magnitude greater than the largest CTMC studies conducted thus far, and almost three orders of magnitude greater than typical production run times. Thus, to reduce this requirement to a feasible level and still demonstrate the existence of Thomas scattering, Toshima resorted to a two-dimensional model. Even so, that simulation used about 1.1×10^8 2D trajectories requiring 300 hours of CPU time on a FACOM 780 to glean only 82 capture events.

The present authors have also investigated the possibility of calculating the differential cross section for the same case, namely that measured by Vogt *et al.* [5] [p(5 MeV)+H] using the full three-dimensional CTMC method. In this attempt, it was noticed that all capture events recorded resulted from a very narrow range of initial orbital eccentricites. The initial distribution is produced so that the square of the eccentricity is uniformly sampled between zero and 1, but only extremely large values near 1 produced charge transfer. That is, to have an appreciable chance to be captured by the projectile traveling at a velocity of 14.15 a.u. in this case, the orbits had to be highly eccentric to allow electron speeds to be comparable. These high electron velocities are attained when the nearly straight-line orbits approach the nucleus quite closely, near the perigee. These orbits are typical of the high-momentum portion of the distribution. We note that capture from these orbits is more consistent with the capture expected in the Oppenheimer-Brinkman-Kramers (OBK) theory in which a velocity matching occurs than with the idealized Thomas scattering where the electron's initial momentum is assumed to be zero. Nevertheless, double-scattering events have also clearly been recorded in this calculation. Also, since to be captured the electron had to come close to the projectile while it is traveling at these speeds, the impact-parameter dependence of the cross section indicated that beyond 0.065 a.u. the capture probability is negligible. Therefore, because all the projectiles in the ensemble are started at the same distance from the target center of mass, in order for the projectile to meet the electron near the nucleus, all electrons had to start within some small shell of orbits. In other words, the projectile travels in what may be regarded as essentially a straight line, and, since it always begins at some fixed distance away from the target, it always takes roughly the same amount of time to reach the point at which an electron must meet it to have a good chance of capture. In summary, the initial conditions which led to capture in the present model were characterized by having highly eccentric orbits which, for a fixed projectile starting distance, originated from a small range of initial orbital distances.

These observations provided a simple method of tremendously reducing the number of trajectories which actually had to be integrated after the initial conditions were chosen. After a few preliminary runs were completed, a plot of initial orbital eccentricity versus initial orbital distance for each event that had led to capture was made in order to determine the range of these variables. Then a much larger run was made in which initial conditions outside the range were rejected. It was necessary to keep track of how many sets of initial conditions were generated to normalize the final result. This method of restricting the initial phase space led to the result that 7.8×10^8 sets of initial conditions were generated, about 2.3×10^6 were accepted, and 1702 led to capture, just enough to produce a reasonable differential cross section out to about 1 mrad. The eccentricity was limited to $\epsilon>0.94$ and the initial orbital radius to $0.68<r_0<0.78$ a.u. for an initial projectile distance of 5 a.u. This required about 30 CPU hours on a CRAY-2. To illustrate this selection of a portion of the initial phase-space distribution, in Fig. 1 are displayed the values of eccentricity and initial orbital radius which led to capture, plotted over the whole range that they would ordinarily take. Clearly, this method of restricting, or filtering, the initial conditions which are accepted should be applicable to other processes which similarly come from a particular region of phase space. A simple yet important application of this idea is the selection of a maximum impact parameter $b_{\max}$ chosen so that beyond $b_{\max}$ there is only a negligible probability of reaction.

Even though this method allowed a tremendous reduction in the amount of CPU time required to produce enough events, there was still a serious shortcoming in that the total cross section for charge transfer (CT) was overestimated. This cross section is given by

$$\sigma_{\mathrm{CT}}=\pi b_{\max}^2(N_{\mathrm{CT}}/N_{\mathrm{MC}}) , \tag{1}$$

where N_{CT} is the number of capture events and N_{MC} is the total number of Monte Carlo initial conditions generated. It was found to be [for p(5 MeV)+H]

$$\sigma_{\mathrm{CT}}^{\mathrm{CTMC}}=8.12\times10^{-25}\ \mathrm{cm}^2 , \tag{2}$$

whereas the recent experimental measurements of Schwab *et al.* [30] had found

$$\sigma_{\mathrm{CT}}^{\mathrm{expt}}=3.10\times10^{-26}\ \mathrm{cm}^2 , \tag{3}$$

indicating an overestimation by approximately a factor of 26. Thus, not as many trajectories were required as were predicted to obtain the desired statistical uncertainty because of this large overestimation. The degree of overestimation is put in context with the results at other impact

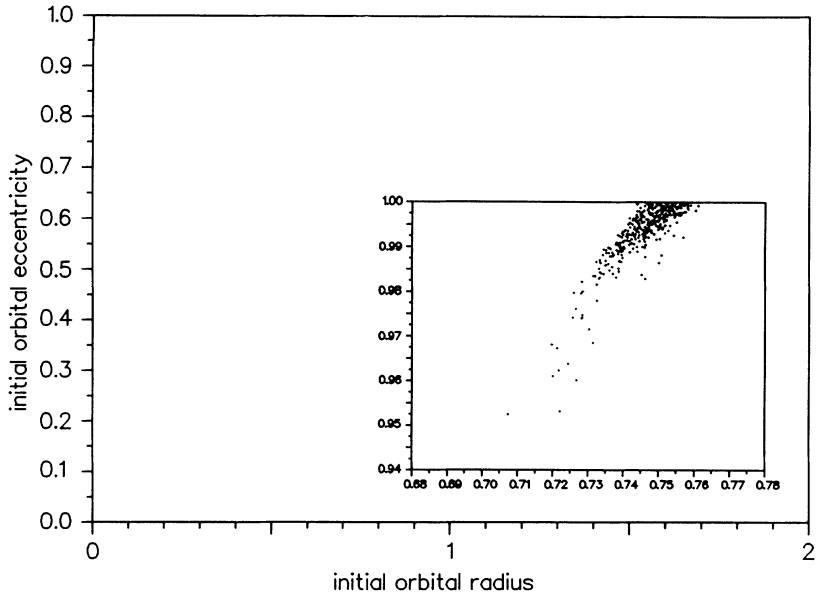

FIG. 1. Scatter plot of the Monte Carlo generated initial conditions which led to capture in the collision of 5-MeV protons with atomic hydrogen. The plot illustrates the full range of initial orbital distance separating the electron and target nucleus ("orbital radius") and eccentricity possible in a projection of the initial phase space onto these variables. The inset is an enlargement of the region which contributed to capture and indicates the range over which these variables were selected by the filtering method.

energies in Fig. 2, which displays the CTMC total cross section compared with experiment. At very low energies, the CTMC method underestimates the cross section for $p+H$ since it lacks the quantum-mechanical resonance present in this symmetric collision. At intermediate energies, the regime in which the method is expected to be most applicable, the agreement is very good, as has been shown previously in a number of works [36]. At high energies, however, there is a systematically increasing overestimation, which has been noted previously by a number of authors as well [37,38]. This problem arises simply due to the fact that there is no classical minimum binding energy that may be accessed in the capture process. That is, an electron may be captured to an arbitrarily deeply bound level in a momentum-matching collision. Thus the calculated cross section fails to drop off with energy as rapidly as it should. It should be noted that for impact by multiply charged ions, this overestimation does not occur until much higher energies, since in this case capture proceeds predominantly to excited states.

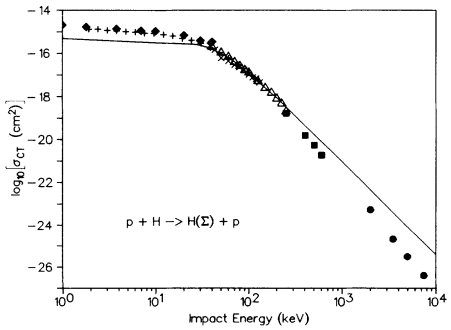

FIG. 2. The total cross section for charge transfer in proton–atomic-hydrogen collisions as a function of impact energy. The CTMC result is indicated by the solid curve and is compared to the experimental measurements of Fite *et al.* [31] (diamonds), McClure [32] (plus signs), Gilbody and Ryding [33] (crosses), Wittkower, Ryding, and Gilbody [34] (triangles), Hvelplund and Andersen [35] (squares), and Schwab *et al.* [30] (circles).

The differential cross section obtained is displayed in Fig. 3 along with the experimental measurements of Vogt *et al.* [5]. Clearly only a shoulder is shown by the calculation near the experimental peak. The statistical errors in the calculation around the Thomas peak are about 12% at the one-standard-deviation level. The lack of a peak is simply due to the overestimation of the velocity-matching, OBK-like captures, which swamp the cross section in this model. In addition, the double-scattering events found with the CTMC model show large departures from the prototypical Thomas scattering in that they involved electrons initially with high momentum and which followed trajectories differing from the successive 60° scatterings expected in the idealized model [1,2]. This observation was also made by Toshima in the two-dimensional model, who also implicitly showed that events with low-momenta electrons and nearly 60° intermediate scattering angles occurred at much larger impact parameters. These more idealized Thomas double scatterings, by being confined to large impact parameters,

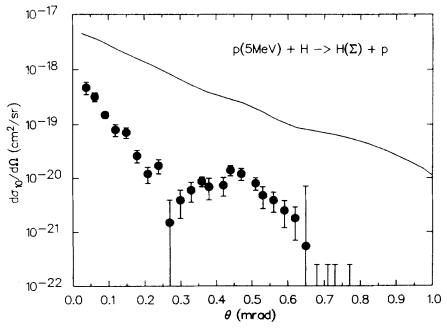

FIG. 3. The cross section for charge transfer in 5-MeV proton–atomic-hydrogen collisions differential in the scattering angle of the projectile illustrating the Thomas peak. The experimental measurements of Vogt *et al.* [5] are plotted along with the result of the present CTMC calculation.

contribute negligibly to the CTMC differential cross section due to their negligible probability of occurrence.

We note that the role of nonidealized Thomas double scatterings has been explored in the quantum-mechanical treatments of Briggs, Greenland, and Kochbach [39] and Nagy, Macek, and Miraglia [40], which utilized Coulomb rather than plane-wave functions in the propagation of the intermediate state between the two successive collisions. Briggs, Greenland, and Kochbach [39] point out that this results in the fact that the scatterings are not binary collisions, and a variety of geometries result in scattering to the Thomas angle. Further work with a more elaborate classical model may find a connection with these results if the unphysical velocity matching collisions can be avoided.

We would like to emphasize that the conclusion we reach is not dependent on the use of the method of filtering the initial conditions which we have adopted. That is, if larger impact parameters and smaller eccentricities were also selected, as would be expected in the idealized Thomas picture, no Thomas peak would be observed, since the conventional CTMC model cannot discriminate against the unphysical single-scattering events which completely dominate the capture process. By allowing such large impact parameters and small eccentricities, Thomas-scattering events can be observed, but they occur very infrequently compared to the OBK-like events. The unphysically deeply bound captured electrons could simply be discarded, but this in no way corrects the model. Also, since the bound levels form a continuum, and capture at this impact energy proceeds to very tightly bound orbits, there is no way to do this without being quite arbitrary.

With the development of the filtering technique described here, further study could explore in greater detail the shape of the differential cross section with a larger number of events, but until, and unless, a suitable extension of the model which corrects the overestimation can be made, the present work, along with that of Toshima, should suffice to illustrate the shortcomings of the model for high-energy charge transfer. Such an extension could utilize a constraining potential to prevent capture to bound states below the quantum ground state, thus alleviating the overestimation of the velocity-matching contribution.

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[1] L. H. Thomas, Proc. R. Soc. London, Ser. A **114**, 561 (1927).

[2] R. Shakeshaft and L. Spruch, Rev. Mod. Phys. **51**, 369 (1979).

[3] Dž. Belkić *et al.*, Phys. Rep. **56**, 279 (1979).

[4] E. Horsdal-Pedersen *et al.*, Phys. Rev. Lett. **50**, 1910 (1983).

[5] H. Vogt *et al.*, Phys. Rev. Lett. **57**, 2256 (1986).

[6] J. H. Macek and K. Taulbjerg, Phys. Rev. Lett. **46**, 170 (1981).

[7] J. E. Miraglia *et al.*, J. Phys. B **14**, L197 (1981).

[8] J. H. Macek and S. Alston, Phys. Rev. A **26**, 250 (1982).

[9] J. H. McGuire *et al.*, Phys. Rev. A **28**, 2104 (1983).

[10] K. Taulbjerg and J. S. Briggs, J. Phys. B **16**, 381 (1983).

[11] J. Macek and X. Y. Dong, Phys. Rev. A **38**, 3327 (1988).

[12] S. Alston, Phys. Rev. A **24**, 331 (1990).

[13] D. S. F. Crothers and K. M. Dunseath, J. Phys. B **23**, L365 (1990).

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

[15] F. T. Wall, L. A. Hiller, and J. Mazur, J. Chem. Phys. **29**, 255 (1958); **35**, 1284 (1961).

[16] D. L. Bunker, J. Chem. Phys. **37**, 393 (1962); **40**, 1946 (1964).

[17] I. C. Percival and D. Richards, Adv. At. Mol. Phys. **11**, 1 (1975).

[18] D. Banks *et al.*, J. Phys. B **9**, L141 (1976).

[19] R. E. Olson and A. Salop, Phys. Rev. A **16**, 531 (1977).

[20] E. Teubner *et al.*, J. Phys. B **13**, 523 (1980).

[21] D. Eichenauer, N. Grun, and W. Scheid, J. Phys. B **14**, 3929 (1981); **15**, L17 (1982).

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

[23] R. L. Becker and A. D. MacKellar, J. Phys. B **17**, 3923 (1984).

[24] J. S. Cohen, J. Phys. B **18**, 1759 (1985).

[25] C. O. Reinhold and C. A. Falcón, Phys. Rev. A **33**, 3859 (1986).

[26] R. E. Olson, *Electronic and Atomic Collisions,* edited by H. B. Gilbody, W. R. Newell, F. H. Read, and A. C. H. Smith (Elsevier Science, Amsterdam, 1988), p. 271.

[27] V. J. Montemayor and G. Schiwietz, Phys. Rev. A **40**, 6223 (1989).

[28] D. R. Schultz *et al.*, J. Phys. B **23**, 3389 (1990).

[29] N. Toshima, Phys. Rev. A **42**, 5739 (1990).

[30] W. Schwab *et al.*, J. Phys. B **20**, 2825 (1987).

[31] W. L. Fite *et al.*, Phys. Rev. **119**, 663 (1960).

[32] G. W. McClure, Phys. Rev. **148**, 47 (1966).

[33] H. B. Gilbody and G. Ryding, Proc. R. Soc. London, Ser. A **29**, 438 (1966).

[34] A. B. Wittkower *et al.*, Proc. R. Soc. London **89**, 541 (1966).

[35] P. Hvelplund and A. Andersen, Phys. Scr. **26**, 375 (1982).

[36] D. R. Schultz, Phys. Rev. A **40**, 2330 (1989).

[37] D. R. Schultz *et al.*, Phys. Rev. A **40**, 4947 (1989).

[38] A. Schmidt *et al.*, J. Phys. B **23**, 2327S (1990).

[39] J. S. Briggs *et al.*, J. Phys. B **15**, 3085 (1982).

[40] O. Nagy *et al.*, Phys. Rev. A **43**, 5991 (1991).