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Monte Carlo calculation of the distributions of interatomic separation and relative velocity resulting from the dissociation of fast molecular ions by thin foils

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A Monte Carlo program to calculate the distributions of separation and relative velocity resulting from the dissociation of fast molecular ions traversing thin foils, including effects of Coulomb explosion, multiple scattering, and differential energy loss, has been developed. Here it is used to explore the effect of the single-scattering cross section employed on the distributions which result. It is demonstrated that different single-scattering distributions—based upon different assumptions concerning atomic screening—give rise to differing separation distributions even though they result in essentially identical multiple-scattering distributions. Such effects must be taken into account in models of subsequent molecular or atomic recombination of the exiting particles.

We have recently studied the alignment of the $n=3$ levels of neutral hydrogen produced by the traversal of fast H_2^+ molecular ions through thin foils.[1] As part of this study, it is important to know the distributions of interatomic spacing and relative velocity which are obtained as the dissociated H_2^+ molecules exit the foil. For example, Cue *et al.*[2] have obtained remarkable agreement between the observed transmission of H_2^+ molecules through thin C foils and a simple model of the recombination process which utilizes such distributions. Consequently, we have developed a Monte Carlo computer program to obtain conveniently the desired separation and velocity distributions. This calculation accounts for proton-proton repulsion due to a Coulomb potential screened by target electrons, for multiple scattering of the protons by target atoms, and for energy loss of the protons as they traverse the foil. Distributions of initial separations of the sort encountered by Kanter *et al.*[3] are employed. Details of the program and a tabulation of results obtained through its use are planned to be presented elsewhere. It is the purpose of this paper to point out that these calculations may also be used to explore two physically interesting questions: (1) do the distributions so obtained depend upon the detailed form of the single-scattering cross section assumed, and (2) to what extent can the Coulomb explosion and multiple scattering be treated incoherently, as has been done in previous discussions?[2,4]

For the purposes of this calculation, the foil is divided into a large number N_s of thin parallel slabs such that the probability of a proton with velocity equal to that of the incident ion undergoing one scattering by a carbon nucleus within that slab is approximately 0.1. N_s depends upon foil thickness, incident ion energy, and the single-scattering parameters assumed; it varies from a few hundred to several thousand for the cases of interest here. The incident H_2^+ molecule is assumed to dissociate upon contact with the foil. The resulting two protons Coulomb explode for one slab thickness; at that point each proton may or may not undergo one or more scatterings by the screened carbon nuclei; finally, their speeds are adjusted in a probabilistic fashion for possible energy loss due to electronic scattering in the slab. The process is then repeated N_s times until the protons exit the foil. Standard Monte Carlo techniques[5] are employed. At that point the separations and relative velocities are recorded. A large number of ions are followed through the foil in this fashion and distributions of interatomic separation and energy of relative motion in the form of histograms are obtained.

Much work—both theoretical and experimental—has been done in studying the scattering of charged particles traversing solids.[6-17] Among the most significant differences of the theoretical treatments are the methods used to treat the electron screening of the nuclear scattering center and the assumptions made about the number of scatterings which occur. Snyder and Scott[9] treat the single scattering using the Born-approximation cross section for an exponentially screened nucleus, which for scattering at a small angle θ is proportional to $\theta/(\theta^2+\theta_c^2)^2$ with θ_c determined by the screening parameter. Goudsmit and Saunderson[7] use this Born-approximation calculation as well as that for the more realistic Thomas-Fermi screening. Lindhart *et al.*[12] use a classical approximation to calculate scattering by a Thomas-Fermi atom and Meyer[13] has extended these results to derive multiple-scattering distributions. The single-scattering cross sections described above must of course agree for "large" θ (where they approach the Rutherford $1/\theta^3$ cross section) but differ at intermediate and small θ; for very

small θ, both the Snyder-Scott and Meyer cross sections become unphysical, the former predicting too few very-small-angle scatterings and the latter predicting too many (actually an infinite total cross section, a difficulty overcome by Meyer through the introduction of a cutoff). Bethe[10] has emphasized that measurements of multiple-scattering angular distributions cannot alone determine the single-scattering cross section (and, hence, the screening function); rather, the experiments simply determine a single parameter—the characteristic screening angle χ_a, which in turn determines the observed multiple-scattering distribution. Several experimenters[16,17] have suggested that the screening parameters experimentally obtained are inconsistent with those obtained in other ways, thus indirectly questioning the screening model employed. Bednyakov[11] has suggested that for carbon targets, the Thomas-Fermi approximation is expected to be inadequate and that more exact Hartree-Fock wave functions must be considered.

It is of particular interest, therefore, to ascertain if the separation distributions and relative energy distributions which result from the traversal of H_2^+ ions through carbon foils contain any sensitivity to the form of the single-scattering cross section assumed, even though the multiple-scattering distributions do not. We have used our Monte Carlo program to investigate this question quantitatively. Figure 1(a) shows the distribution of interparticle separations which results from following five hundred 200-keV/amu H_2^+ molecules through a C foil of thickness 15 $\mu g/cm^2$, using the single-scattering cross section of Lindhart[12] with the cutoff used by Meyer[13]; Fig. 1(b) shows the result of a similar calculation with the exponential screening Born-approximation result $\sigma(\theta) \sim \theta/(\theta^2+\theta_c^2)^2$ and θ_c chosen to give the same χ_a. In order to allow quantitative comparison of resulting distributions as well as to allow convenient use of these results in further calculation, an empirical analytic approximation to these distributions was obtained. A satisfactory fit was obtained with the function

$$F(s)=\begin{cases}\left[A\exp\left(-\dfrac{(s-s_0)^2}{2\sigma^2}\right)\right], & s\leq s_0\\ \dfrac{A}{1+\left(\dfrac{s-s_0}{\Gamma/2}\right)^2}, & s\geq s_0.\end{cases} \tag{1}$$

The fits obtained by a nonlinear-least-squares fit to Eq. (1) are displayed as dashed curves in Fig. 1. The rms separations obtained and the appropriate fit parameters of Eq. (1) are displayed in Table I, columns 1 and 2. It is clear that, even though the two single-scattering functions give rise to essentially identical multiple-scattering angular distributions (this was directly verified by using the same Monte Carol program with the initial internucleon separation fixed at zero and with Coulomb explosion disabled), the *separation* distributions are significantly different. Most important is the fact that use of the Lindhart single-scattering cross sections shifts the most likely separation to values which are more than 3 Å larger than for exponential screening. Clearly, the additional small-angle scatterings of this model have more influence on the internucleon separation than upon the net scattering angle. This result is of particular significance when recombination into a given state is being consid-

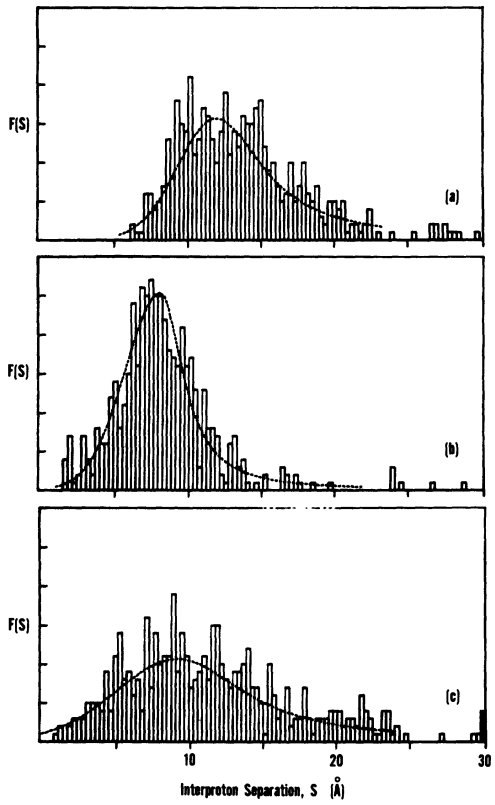

FIG. 1. Interproton separations resulting from the passage of 200-keV/amu H_2^+ molecules through 15-$\mu g/cm^2$ carbon foils. (a) Single-scattering cross section of Lindhart (Meyer)—full Monte Carlo calculation. (b) Exponential screening Born approximation single-scattering cross section—full Monte Carlo calculation. (c) Coulomb explosion and multiple scattering (Meyer theory) treated incoherently. Dashed curves: Least-squares fit to the empirical equation (1) of the text.

ered since the distributions of Figs. 1(a) and 1(b) can give rise to very different probabilities of finding protons emerging from the foil with a given separation. For example, the predicted number of protons emerging with separations between 5 and 10 Å differ from each other by a factor of 3. This unexpectedly large sensitivity to the choice of a single-scattering model assumed gives extra impetus to the evaluation of the effect of using a more realistic single-scattering model derived from Hartree-Fock wave functions, and such a calculation is now in progress. This sensitivity of the separation distribution to the single-scattering cross section also suggests its use as a method for obtaining additional experimental information concerning atomic screening. For example, we have examined our Monte Carlo generated results and find that if the overall angular distribution of outgoing protons from H_2^+ dissociation is measured, the results predicted by the two differing models employed here are—as might have been expected—indistinguishable. If, however, a coincidence measurement were to be carried out, and the angular distribution obtained for protons in coincidence with a second proton scattered through a "large" angle were to be determined, the effects seen in Fig. 1 persist: The angular distribution predicted by Meyer-Lindhard scattering is shifted to larger angles than that predicted by the exponential screening model. Thus, χ_a may be obtained by measuring the angular distribution for incident protons and further information about the actual screening may be obtained by molecular dissociation studies.

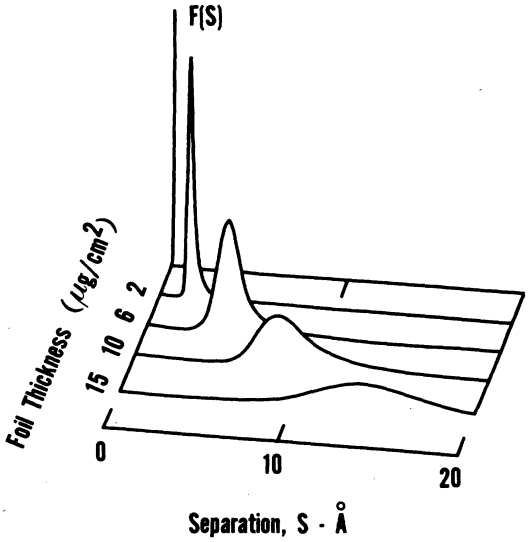

FIG. 2. Interproton separation distributions resulting from the passage of 200-keV/amu H_2^+ molecules through thin C foils as a function of foil thickness.

In earlier work, Escovitz[4] assumed that the changes in the rms separations resulting from Coulomb explosion and from multiple scattering could be added incoherently. Cue *et al.*[2] extended this approach to obtain a quantitative expression for the interparticle separation and relative energy distribution which would result from such an assumption. This calculation is formally equivalent to allowing the Coulomb explosion to develop

TABLE I. Calculated rms separation and empirical fit parameters[a] for Monte Carlo generated separation distributions. 0.2-MeV/amu H_2^+ ions incident upon 15-$\mu g/cm^2$ foils.

Parameters (Å)	(a) Full Monte Carlo treatment Thomas-Fermi screening (Lindhart-Meyer)	(b) Full Monte Carlo treatment exponential screening (Born approximation)	(c) Incoherent treatment of Coulomb explosion and multiple scattering (Lindhart-Meyer)	Coulomb explosion only
rms separation S_{rms}	14.2	9.5	12.8	7
Most probable separation r_0	11.9	8.1	9.2	7
Small-separation distribution width σ	2.6	2.4	4.2	2
Large-separation distribution width Γ	8.0	3.7	11.2	2.5

[a] Fit to empirical relationship

$$F(s)=\begin{cases} A\exp[-(s-s_0)^2/2\sigma^2], & s\leq s_0 \\ A/[1+(s-s_0)^2/(\Gamma^2/4)], & s\geq s_0. \end{cases}$$

through the entire foil and then to follow it with a single scattering chosen from an appropriate *multiple-scattering* distribution. To investigate the validity of this hypothesis, we have used our Monte Carlo routine with the single-scattering cross section which resulted in Fig. 1(a) to generate a multiple-scattering distribution for the parameters specified (protons of the same velocity, no Coulomb explosion). The same Monte Carlo routine was then employed to evaluate the desired numerical integrals by replacing the single-scattering cross section with the multiple-scattering function just derived and treating the entire foil as a single slab, i.e., setting $N_s = 1$. The results of this procedure are shown in Fig. 1(c) and Table I, column 3 and are to be compared with those described earlier, Fig. 1(a) and Table I, column 1. Here the differences are even more pronounced. The incoherent treatment gives a separation distribution shifted to much smaller values and the resultant distribution is much broader. The probability of protons emerging separated by 5–10 Å is 3 times greater than predicted by the more accurate calculation; 1% of all outgoing protons are separated by less than 5 Å in contrast with the almost complete absence of such closely spaced particles in the full Monte Carlo computation.

The comments presented here indicate the importance of carrying out accurate calculations of separation and relative energy distributions for interpretation of molecular-ion dissociation-recombination phenomena. A Monte Carlo computer program for this purpose has been developed and results obtained therewith—a sample of which is displayed in Fig. 2—will be reported elsewhere.

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