PHYSICAL REVIEW A VOLUME 9, NUMBER 3 MARCH 1974

# Binary-encounter stopping cross sections. I. Basic theory and calculations for helium in hydrogen*

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(Received 1 August 1973)

A model to describe the slowing down of fast-moving heavy particles in matter owing to inelastic collisions is devised using the binary-encounter approximation, and stopping cross sections are calculated specifically for helium in hydrogen. In performing the calculations, each incident-beam charge-state component is treated separately, and the results are combined using the best available experimental information on the equilibrium charge-state fractions. The results, both for the partial stopping cross sections of the individual charge-state components and the total stopping cross section of the equilibrium mixture, are compared as a function of incident energy with the results of various experiments and with other theories. The calculated total stopping cross section is in reasonable agreement with experiment over a rather wide energy range and is superior at energies below 1 MeV to the results of the Bethe theory, but discrepancies exist between calculated and experimentally determined partial stopping cross sections. These discrepancies are discussed and possible explanations for them are suggested.

## I. INTRODUCTION

Phenomena associated with the slowing down of heavy charged particles in matter are of considerable interest in several fields, including nuclear, atmospheric, and radiation physics. A basic quantity associated with these phenomena is the electronic stopping cross section, which is a measure of the average rate at which the particles of a beam passing through matter lose energy to electronic excitation or ionization as the result of inelastic collisions with the target atoms.

Although electronic stopping cross sections have been studied for many years, no completely satisfactory method for calculating them over a broad energy range exists. For large incident speeds the standard method makes use of a well-known formula which Bethe[1] derived in 1930 using approximations similar to but more restrictive than the Born approximation. The Bethe formula contains a parameter $I$ called the mean excitation energy which in principle can be calculated from a knowledge of the target-atom wave functions, but since these calculations are very difficult except for simple target atoms $I$ is usually determined empirically by fitting the formula to high-energy stopping cross-section data.[2] Even considered semiempirically, the Bethe formula is good only for incident particle speeds much greater than any of the target-atom electron speeds. However, the average speed of an electron in a bound state of principal quantum number $n$ is approximately given by $Z\alpha c/n$. Thus the uncorrected Bethe formula is severely restricted in its range of usefulness. Shell corrections which extend the Bethe formula to lower energies have been applied, but unfortunately such treatments require excessive labor.[3,4]

We have developed a model of the stopping process which permits relatively simple calculations of stopping cross sections and which can be applied for any target atom even at intermediate incident speeds. To describe the collision process, we have employed a modification of Gryzinski's binary-encounter approximation.[5] Like the Born approximation, the binary-encounter approximation is strictly a first-order theory and assumes static undistorted atomic wave functions that are inappropriate at low incident energies. However, in contrast to the Bethe formula, the binary-encounter approximation has been developed within a theoretical framework that does not exclude low-incident particle velocities. Thus we might expect it to be superior in those energy regions in which the uncorrected Bethe formula is invalid. To precisely test the validity of our model, we consider it necessary to treat separately the interactions of each individual charge-state species which comprise the energy-dependent distribution of the incident beam.

In principle, our model is applicable to any incident species, but the required calculations rapidly become complicated for heavier atoms because of the large number of possible charge states which must be considered. For this reason, and because much recent stopping cross-section data exists for this system, we will discuss only incident helium. In Paper I of this series we will present the model, develop formulas, and make stopping cross-section calculations specifically for hydrogen targets. We will also compare our results for total stopping cross sections and for the stopping cross sections of the individual charge states with experimental values and the results of other theories. In Paper II we will generalize our formulas and calculations to more complicated targets and, in particular, discuss the variation of our calculated results with target-atom atomic number as well as the corresponding variations in experimental stopping cross-section values.

## II. THEORY

### A. General

An atomic beam passing through matter will in general contain ions in all possible charge states. Regardless of the composition of the beam upon entering the target, the mean relative populations of these various charge-state components will quickly reach equilibrium values which change slowly as a function of velocity as the beam particles slow down. In solids, for instance, equilibrium may be reached after penetration of only a few atomic layers. The target-dependent total electronic stopping cross section $S_e$ for the incident beam will be a weighted average of the stopping cross section for the individual components given by

$$S_e = \sum_i F_{i\infty} S_{ei} , \tag{1}$$

where $F_{i\infty}$ is the equilibrium fraction of the $i$th charge-state component and the corresponding partial stopping cross section $S_{ei}$ includes contributions from all excitation processes including charge transfer. For incident helium $i$ goes from 0 to 2.

From Eq. (1) it can be seen that the solution of the stopping problem conveniently separates into two parts: the determination of the equilibrium charge-state fractions and the calculation of the corresponding partial stopping cross sections. The calculation of the partial stopping cross sections in turn requires the evaluation of the equation

$$S_{ei} = \sum_n E_n Q_{ni} \tag{2}$$

for each incident charge species. Here $Q_{ni}$ represents the total excitation cross section of the $n$th target state by an incident particle of the $i$th charge species, and $E_n$ is the corresponding excitation energy. The summation includes an integration over the continuum of ionized states as well as a summation over all accessible discrete states.

To solve Eq. (2) we exclude processes such as charge transfer or projectile excitation. Generally speaking, charge-transfer contributions to the energy loss will be small for multiply charged incident-beam components and for the singly charged component at large energies. At low energies charge transfer will also be small unless an accidental or symmetric resonant process can occur. Such processes are relatively infrequent, however. The amount of projectile excitation depends on the number and binding energies of the projectile electrons. It will generally be small for the charged incident-beam components, and therefore for large incident speeds, but it may be important for neutral projectiles. In the case of helium, however, the large excitation energies will inhibit projectile excitation even for the neutral species.

### B. Binary-encounter partial stopping cross sections

The binary-encounter approximation is used to determine the inelastic-scattering cross sections $Q_{ni}$ needed for the evaluation of Eq. (2). In this approximation inelastic processes are considered to result from binary collisions between the incident system and the individual electrons of the target atom. These collisions, although elastic in a coordinate system moving with the center of mass of the binary-collision partners, result in energy transfers to the target electrons in a coordinate system at rest with respect to the target nuclei. The influence of the target nuclei during the collision is ignored except insofar as it determines the electron speed distribution.

Except for the work of Gryzinski,[5] application of the binary-encounter theory to the calculation of stopping cross sections has been somewhat neglected, although many cross-section calculations for individual processes, particularly ionization, have been made. Most of the results, as well as recent theoretical developments, are summarized in review articles by Bates and Kingston[6] and Vriens.[7] Among other things, it has been shown that the binary-encounter approximation correctly describes contributions to excitation and ionization from close collisions insofar as distortion effects can be disregarded, but that it completely neglects resonant excitation and ionization due to distant encounters. For incident bare charges at large velocities, close and distant collisions have been found to contribute about equally to the energy loss of the projectile,[7] and consequently stopping cross sections calculated using the binary-encounter approximation should underestimate those calculated using the Born approximation by a factor of about 2 at large velocities. On the other hand, for neutral incident species or for any incident species at low speeds, resonant processes will be relatively unimportant and the binary-encounter and Born approximations should yield approximately equal results.

Most previous applications of the binary-encounter approximation have been limited to Coulomb interactions; however, as has been suggested by Gerjuoy[8] and Bates and McDonough,[9] the theory can be extended to quite general binary interactions, provided the appropriate center-of-mass (c.m.) scattering cross sections can be determined. Flannery[10] has recently presented formulas for this generalization and made calculations of ionization and excitation cross sections of hydrogen and helium atoms and singly charged lithium ions for incident neutral hydrogen. In this paper we will generalize the formulation of Gerjuoy[8] to determine the inelastic cross section for the incident $He^+$ and $He^0$ components.

When the binary-encounter approximation is applied to the calculation of cross sections for the excitation of discrete electronic states, a difficulty arises because the approximation treats all excitations as continuous. The customary method of dealing with this problem has been to equate the excitation cross section $Q_{ni}$ to the integral of the binary-encounter "differential" cross section $Q_i(\Delta E)$ for energy transfers within a small interval around $\Delta E$ between the limits $E_n$, the excitation energy of the $n$th excited state, and $E_{n+1}$, the next-highest excitation energy. As has been mentioned by Flannery,[11] this procedure yields excitation cross sections which do not satisfy detailed balancing; nevertheless, it has the advantage of simplicity. We will define the contribution to the stopping cross section from excitation of the $n$th state by a similar integral between $E_n$ and $E_{n+1}$, in which the "differential" cross section $Q_i(\Delta E)$ is weighted by $\Delta E$. Using this definition we can write Eq. (2) as

$$S_{ei} = \int_{\Delta E_1}^{\infty} \Delta E Q_i(\Delta E)\, d\Delta E \ , \qquad (3)$$

where $\Delta E_1$ is the lowest allowed excitation energy of the target electron. For hydrogen $\Delta E_1$ is the excitation energy of the $n=2$ states and equals three quarters of the binding energy.

In the following discussion, when referring to quantities describing the binary-collision partners, we will adopt the subscript convention in which 1 refers to the incident particle and 2 refers to the target electron. A prime will be used to distinguish quantities before and after a collision.

The binary-encounter "differential" cross section $Q_i(\Delta E)$ is derived starting from the c.m. electron-scattering cross section $\sigma_i$ for the potential appropriate to the $i$th charge state. As has been shown by Gerjuoy,[8] this electron-scattering cross section can be related to a "differential" cross section $\sigma_{i\Delta E}$ for energy transfer $\Delta E$ in the laboratory coordinate system at rest with respect to the target nucleus. In particular $\sigma_{i\Delta E}$, which is considered to be a function of the incident- and target-particle velocities $\vec{v}_1$ and $\vec{v}_2$, as well as the energy transfer $\Delta E$, can be expressed in terms of $\sigma_i$, which is a function of the relative velocity $\vec{v}$ and c.m. scattering angle $\chi$. The appropriate formula given by Gerjuoy is

$$\sigma_{i\Delta E}(\vec{v}_1, \vec{v}_2) = \frac{1}{mvV} \int_0^{2\pi} d\phi\, \sigma_i(v, \chi) \ , \qquad (4)$$

in which $m = m_1 m_2/(m_1 + m_2)$ is the reduced mass, $\phi$ is the collisional change in the azimuthal angle of the relative velocity in a coordinate system with its $z$ axis along the c.m. velocity vector $\vec{V}$, and $\chi = \chi(\phi, \Delta E)$. The energy transfer $\Delta E$ can be expressed in terms of the polar angles $\theta$, $\theta'$ of the relative velocity vectors before and after the collision by

$$\Delta E = mvV(\cos\theta - \cos\theta'). \qquad (5)$$

The geometrical requirement that $\cos\theta$ and $\cos\theta'$ be between $+1$ and $-1$ imposes limits on $\Delta E$ which are easily obtained from this equation. If $\Delta E$ lies outside of these limits, $\sigma_{i\Delta E}$ vanishes. For a typical target in which the atoms (molecules) are randomly oriented, we may assume that the electron velocity distribution is isotropic. Following Gerjuoy,[8] we may replace $\sigma_{i\Delta E}$ by an effective cross section, $\sigma_{i\Delta E}^{\rm eff}(v_1, v_2)$, which is characteristic of the $i$th charge state and represents an average over the relative orientations of $\vec{v}_1$ and $\vec{v}_2$ for an isotropic distribution of $\vec{v}_2$.[12] The cross section $Q_i(\Delta E)$ can then be found directly by averaging $\sigma_{i\Delta E}^{\rm eff}$ over the target-electron speed distribution $f(v_2)$, with the result that

$$Q_i(\Delta E) = \int_0^{\infty} f(v_2)\sigma_{i\Delta E}^{\rm eff}(v_1, v_2)\, dv_2 \ . \qquad (6)$$

Finally, by substituting Eq. (6) for $Q_i(\Delta E)$ into Eq. (3), the partial stopping cross section can be written as

$$S_{ei} = \int_{\Delta E_1}^{\infty} \Delta E \int_0^{\infty} f(v_2)\sigma_{i\Delta E}^{\rm eff}(v_1, v_2)\, dv_2\, d\Delta E \ . \qquad (7)$$

In actual calculations we have interchanged the order of integration in Eq. (7) and adopted the notation

$$G_i(\Delta E_1, v_1, v_2) = \int_{\Delta E_1}^{\infty} \Delta E \sigma_{i\Delta E}^{\text{eff}}(v_1, v_2)\, d\Delta E \ . \tag{8}$$

The resulting equation for $S_{ei}$ is given by

$$S_{ei} = \int_0^{\infty} f(v_2) G_i(\Delta E_1, v_1, v_2)\, dv_2 \ . \tag{9}$$

### C. Incident He$^{++}$ component

For the Coulomb potential of He$^{++}$ appropriate formulas for $\sigma_{2\Delta E}^{\text{eff}}$ have been developed by Gerjuoy.[8] To simplify comparison with the other charge-state components, we will present his results in terms of the nondimensional variables $\omega_{1,2} = v_{1,2}/v_\lambda$ and $\delta = \Delta E/E_\lambda$, where $v_\lambda$ and $E_\lambda = \frac{1}{2} m v_\lambda^2$ characterize the particular interaction and can be chosen arbitrarily for a Coulomb interaction without changing the form of the resulting equations. Specifically,

$$\sigma_{2\Delta E}^{\text{eff}} = (\pi/\omega_1^2\omega_2)(e^4/E_\lambda^3)(1/\delta^3)[(\omega_1^2 - \omega_2^2)(\omega_2'^2 - \omega_1'^2)(\omega_l^{-1} - \omega_u^{-1}) + (\omega_1^2 + \omega_2^2 + \omega_1'^2 + \omega_2'^2)(\omega_u - \omega_l) - \tfrac{1}{3}(\omega_u^3 - \omega_l^3)] \ , \tag{10}$$

where

$$\omega_1' = [\omega_1^2 - (m/m_1)\delta]^{1/2} \ ,$$
$$\omega_2' = [\omega_2^2 - (m/m_2)\delta]^{1/2} \ . \tag{11}$$

The quantities $\omega_l$ and $\omega_u$ are limiting values of the relative velocity for a given $\delta$ and are related to the geometrical requirement mentioned earlier that $\cos\theta$ and $\cos\theta'$ lie between $+1$ and $-1$. In the event that $m_1 \gg m_2$, as will be the case for heavy particles incident on electrons, and for $\delta > 0$, the following three cases depending on the value of $\delta$ are important.

Case (i): $\delta < \delta_1$,

$$\omega_l = \omega_1 - \omega_2, \quad \omega_u = \omega_1 + \omega_2; \tag{12}$$

case (ii): $\delta_1 \leqslant \delta < \delta_2$ ,

$$\omega_l = \omega_2' - \omega_1', \quad \omega_u = \omega_1 + \omega_2; \tag{13}$$

case (iii): $\delta \geqslant \delta_2$, $\sigma_{\Delta E}^{\text{eff}} = 0$ , (14)

where

$$\sigma_1 = [4/(m_1 + m_2)](\omega_1 - \omega_2)(m_1\omega_1 + m_2\omega_2) \ ,$$
$$\sigma_2 = [4/(m_1 + m_2)](\omega_1 + \omega_2)(m_1\omega_1 - m_2\omega_2) \ . \tag{15}$$

Using Eq. (10) for $\sigma_{2\Delta E}^{\text{eff}}$, $G_2$ given by Eq. (8) can be evaluated analytically with the aid of the following expressions for the indefinite integral:

$$\int^E \sigma_{2\Delta E}^{\text{eff}} \Delta E\, d\Delta E = E_\lambda^2 \int^\delta \sigma_{2\Delta E}^{\text{eff}}\, \delta\, d\delta = \frac{4\pi e^4}{3\omega_1^2 E_\lambda}\left(\frac{3m_1}{m_1 + m_2}\ln\delta - \frac{4\omega_2^2}{\delta}\right) \quad \text{for} \quad \delta < \delta_1 \ ,$$
$$= \frac{4\pi e^4 m}{3\omega_1^2\omega_2 E_\lambda}\left[2\left(\frac{\omega_2^2/m_2}{\omega_2' + \omega_2} - \frac{\omega_1^2/m_1}{\omega_1 - \omega_1'}\right) + 3\left(\frac{\omega_2}{m_2}\ln(\omega_2' + \omega_2) - \frac{\omega_1}{m_1}\ln(\omega_1 - \omega_1')\right) - \left(\frac{\omega_2'}{m_2} + \frac{\omega_1'}{m_1}\right)\right] \quad \text{for} \quad \delta_1 \leqslant \delta < \delta_2 \ . \tag{16}$$

Then, choosing $f(v_2)$ to be the ground-state electron speed distribution of atomic hydrogen given by

$$f(v_2) = 32 v_2^2 v_0^5 / \pi(v_2^2 + v_0^2)^4 \ , \tag{17}$$

where $v_0$ is the electron speed in the ground-state Bohr orbit, we can integrate Eq. (9) for $S_{e2}$ numerically.

### D. Incident He$^0$ component

To determine $\sigma_{\Delta E}^{\text{eff}}$ for He$^0$ a number of additional assumptions are made. First, the incident atom electrons are represented by 1$s$ hydrogenic wave functions of the form

$$\psi_{1s}(r) = (\lambda^3/8\pi)^{1/2} e^{-\lambda r/2} \ , \tag{18}$$

with $\lambda = 2Z_{\text{eff}}/a_0$ where $a_0$ is the classical radius of the ground-state Bohr orbit of a hydrogen atom, and according to Slater's rules $Z_{\text{eff}} = 1.7$ for helium.[13] From Coulomb's law the interaction potential created by such atoms is

$$V(r) = -2e^2(r^{-1} + \tfrac{1}{2}\lambda)e^{-\lambda r} \ . \tag{19}$$

We also assume that electron scattering is ade-

TABLE I. Coefficients $A_{ij}$ to be used in the evaluation of the cross sections for energy transfer to an electron by an incident atomic hydrogen or atomic helium beam.

| $i \backslash j$ | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| 0 | 25 | | | |
| 1 | $19a_1$ | $-19a_2-47\delta^2$ | | |
| 2 | $15a_1^2$ | $-6a_1(5a_2+7\delta^2)$ | $3(a_2+\delta^2)(5a_2+9\delta^2)$ | |
| 3 | $5a_1^3$ | $-15a_1^2(a_2+\delta^2)$ | $15a_1(a_2+\delta^2)^2$ | $-5(a_2+\delta^2)^3$ |

quately described by the Born approximation, which neglects electron exchange and distortion of the helium-atom wave functions during the collision. This approximation is consistent with the binary-encounter approximation which neglects target-atom distortion and precludes the possibility of electron exchange by considering the projectile to be a structureless particle. The appropriate Born cross section for the interaction of Eq. (19) is

$$\sigma_0(k) = 4\left(\frac{2me^2}{\hbar^2}\frac{2\lambda^2+k^2}{(\lambda^2+k^2)^2}\right)^2 , \tag{20}$$

where $k^2=(2m^2v^2/\hbar^2)(1-\cos\chi)$.[14]

Determination of $\sigma_{0\Delta E}^{\text{eff}}$ corresponding to the c.m. scattering cross section given by Eq. (20) follows the procedure used by Gerjuoy for the Coulomb interaction. In this case, however, considerable simplification results if we let $v_\lambda=\hbar\lambda/m$. Details of the straightforward but somewhat tedious analysis are given in the unpublished dissertation of one of the authors.[15] Only the results will be presented here. The cross section $\sigma_{0\Delta E}^{\text{eff}}$ can be represented by the formula

$$\sigma_{0\Delta E}^{\text{eff}} = \frac{\pi}{16}\frac{1}{\omega_1^2\omega_2}\frac{e^4}{E_\lambda^3}\sum_{\substack{i=0\\ j\le i}}^{3} A_{ij}f_{ij}(x)\Bigg|_{x_l}^{x_u} , \tag{21}$$

where $x=\omega^2$ and expressions for $A_{ij}$ and $f_{ij}(x)$ are obtained from Tables I and II, respectively. The constants $a_1$ and $a_2$ in Table I are given by

$$a_1=(m_1\omega_1^2+m_2\omega_2^2)/(m_1+m_2) , \quad a_2=m/(m_1+m_2) . \tag{22}$$

The variable $y$ in Table II satisfies the equation

$$y^2=y_0+y_1x-x^2 , \tag{23}$$

and the coefficients of $x$ in this equation can be written in one of the alternate forms

$$y_0=\omega_1^2\Delta_1^+-\omega_2^2\Delta_2^- -(\omega_1^2-\omega_2^2)^2 , \quad y_1=2(\omega_1^2+\omega_2^2)+\Delta_1^+\Delta_2^- , \tag{24}$$

or

$$y_0=\omega_2'^2\Delta_2^+-\omega_1'^2\Delta_1^- -(\omega_2'^2-\omega_1'^2)^2 , \quad y_1=2(\omega_1'^2+\omega_2'^2)+\Delta_1^-\Delta_2^+ , \tag{25}$$

where

$$\Delta_i^{+,-}=\delta\pm m_i/(m_1+m_2) . \tag{26}$$

The auxiliary functions $t$ and $q$ in Table II are given by

$$t=2x-y_1 , \quad q=y_1^2+4y_0 . \tag{27}$$

When evaluated at $\omega_u$ and $\omega_l$, expressions for $x$, $y$, and $t$ can be written in comparatively simple form, depending on the value of $\delta$, according to Eqs. (12)–(14). In all cases for $\omega=\omega_u$,

$$x_u=(\omega_1+\omega_2)^2 , \quad y_u=\omega_1\Delta_1^+ +\omega_2\Delta_2^- , \quad t_u=4\omega_1\omega_2-\Delta_1^+\Delta_2^- . \tag{28}$$

For $\omega=\omega_l$, on the other hand, we have

case (i): $\delta<\delta_1$ ,

$$x_l=(\omega_1-\omega_2)^2 , \quad y_l=|\omega_1\Delta_1^+ -\omega_2\Delta_2^-| , \quad t_l=-4\omega_1\omega_2-\Delta_1^+\Delta_2^- ; \tag{29}$$

TABLE II. Functions $f_{ij}(x)$ needed in the evaluation of the cross sections for energy transfer to an electron by the neutral or singly charged species in an incident helium beam.

| $i \backslash j$ | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| 0 | $\sin^{-1}\left(\frac{t}{q^{1/2}}\right)$ | | | |
| 1 | $\frac{2t}{qy}$ | $\frac{1}{y}+\frac{y_1f_{10}}{2}$ | | |
| 2 | $\frac{2}{3q}\left(\frac{t}{y^3}+4f_{10}\right)$ | $\frac{1}{3y^3}+\frac{y_1f_{20}}{2}$ | $\frac{1}{2}\left(\frac{x}{y^3}+\frac{y_1}{2}f_{21}-y_0f_{20}\right)$ | |
| 3 | $\frac{2}{5q}\left(\frac{t}{y^5}+8f_{20}\right)$ | $\frac{1}{5y^5}+\frac{y_1f_{30}}{2}$ | $\frac{1}{4}\left(\frac{x}{y^5}+\frac{3}{2}y_1f_{31}-y_0f_{30}\right)$ | $\frac{1}{3}\left(\frac{x^2}{y^5}+\frac{y_1}{2}f_{32}-y_0f_{31}\right)$ |

case (ii): $\delta_1 \leqslant \delta < \delta_2$ ,

$$x_l = (\omega_2' - \omega_1')^2 ,$$

$$y_l = |\omega_2' \Delta_2^+ - \omega_1' \Delta_1^-| ,$$

$$t_l = -4\omega_1'\omega_2' - \Delta_1^- \Delta_2^+;$$

case (iii), given by Eq. (14), also applies for incident neutral systems.

The final evaluation of $G_0(\Delta E, v_1, v_2)$ from Eq. (8) and $S_{e0}$ from Eq. (9) using $f(v_2)$ given by Eq. (17) is done numerically.

### E. Incident $He^+$ component

For $He^+$, as for $He^0$, we assume that the incident systems are in the ground state. However, in this case, their electrons are described exactly by 1$s$ hydrogenic wave functions with $Z_{eff} = 2$. Application of Coulomb's law to the corresponding charge distribution of the incident ion gives

$$V(r) = -e^2[r^{-1} + (r^{-1} + \tfrac{1}{2}\lambda)e^{-\lambda r}] \tag{31}$$

for the interaction potential. The first term of this expression represents the Coulomb potential of the residual ionic charge, and the second term represents the potential of that part of the nuclear charge which is screened by the electron. Except for the value of $\lambda$, the second term has the same form as the potential of a hydrogen atom. Evaluation of the Born approximation to the electron-scattering cross section can be carried out by substituting Eq. (31) into the well-known formula

$$\sigma(k) = \left| \frac{2m}{\hbar^2} \int_0^\infty \frac{\sin(kr)}{kr} V(r) r^2\, dr \right|^2 \tag{32}$$

and performing the integration to obtain

$$\sigma_1(k) = \left(\frac{2me^2}{\hbar^2}\right)^2 \left(\frac{1}{k^4} + \frac{2(2\lambda^2 + k^2)}{k^2(\lambda^2 + k^2)^2} + \frac{(2\lambda^2 + k^2)^2}{(\lambda^2 + k^2)^4}\right) . \tag{33}$$

Most of the work in finding $\sigma_{1\Delta E}^{eff}$ from this equation has already been done, since the first and third terms result in contributions that have the same form as $\sigma_{2\Delta E}^{eff}$ and $\sigma_{0\Delta E}^{eff}$, respectively, except that $v_\lambda$ is now determined with $Z_{eff} = 2$. Consequently, the expression for $\sigma_{1\Delta E}^{eff}$ can be written:

$$\sigma_{1\Delta E}^{eff} = \tfrac{1}{4}\sigma_{2\Delta E}^{eff} + \sigma'^{eff}_{1\Delta E} + \tfrac{1}{4}\sigma_{0\Delta E}^{eff} , \tag{34}$$

in which only the middle term remains to be evaluated. The procedure used for this evaluation, although similar to that for $\sigma_{0\Delta E}^{eff}$, is much simplier and results in the following formula for $\sigma'^{eff}_{1\Delta E}$:

$$\sigma'^{eff}_{1\Delta E} = \frac{\pi}{4\omega_1^2\omega_2} \frac{e^4}{E_\lambda^3} \times \left( \frac{8(\omega_u - \omega_l)}{\delta} - [\, 5f_{00}(x) + a_1 f_{10}(x) - (a_2 + \delta^2) f_{11}(x)]_{x_l}^{x_u} \right) , \tag{35}$$

where the $f_{ij}$ are again obtained from Table II. The second term of Eq. (35) must be integrated numerically over $\Delta E\, d\Delta E$ in Eq. (8) for $G_1$; however, analytic expressions exist for the indefinite integral of the first term. They are

$$\begin{aligned} \int^E \frac{2\pi}{\omega_1^2\omega_2} \frac{e^4}{E_\lambda^3} \left(\frac{\omega_u - \omega_l}{\delta}\right) \Delta E\, d\Delta E &= \frac{2\pi}{\omega_1^2\omega_2} \frac{e^4}{E_\lambda} \int^\delta (\omega_u - \omega_l)\, d\delta , \\ &= (8\pi e^4/\omega_1^2 E_\lambda)\delta \quad \text{for } \delta < \delta_1 , \\ &= (4\pi/\omega_1^2\omega_2)(e^4/E_\lambda)[(\omega_1 + \omega_2)\delta - (2/3m)(m_2\omega_2'^3 + m_1\omega_1'^3)] \\ &\quad \text{for } \delta_1 \leqslant \delta < \delta_2 . \end{aligned} \tag{36}$$

These expressions can be used in the evaluation of $G_1(\Delta E)$ from Eq. (8). Again, the final determination of $S_{e1}$ from Eq. (9) is done numerically.

### F. Equilibrium charge-state fractions

The remainder of the stopping cross-section calculation requires knowledge of the equilibrium charge-state fractions for helium in hydrogen. For the energy range from 0.01 to approximately 1.5 MeV we have used experimental results of Barnett and Stier,[16] Torres *et al.*,[17] and Wittkower *et al.*[18] Above this energy, however, no data exist and we have developed an extrapolation procedure based on an analysis by Armstrong *et al.*[19] of the charge equilibrium process.

Variations in the incident-beam charge-state populations with distance $s$ along the beam path are a direct result of electron capture and loss. It is usually a good assumption that multiple electron-transfer processes can be neglected,[19] in which case the equations governing these variations may be written as

$$\frac{1}{N}\frac{dF_0}{ds} = F_1\sigma_{10} - F_0\sigma_{01} , \tag{37}$$

$$\frac{1}{N}\frac{dF_1}{ds} = F_2\sigma_{21} + F_0\sigma_{01} - F_1(\sigma_{12} + \sigma_{10}) , \tag{38}$$

$$\frac{1}{N}\frac{dF_2}{ds} = F_1\sigma_{12} - F_2\sigma_{21} , \tag{39}$$

where $N$ designates the target-atom number density, $F_i$ designates the $i$th charge-state fraction, and $\sigma_{ij}$ is the cross section for a transition from the $i$th to the $j$th charge state and is a property of the target material as well as the incident species. Equilibrium is reached when the rates of electron capture and loss are balanced. Then the left-hand sides of Eqs. (37)–(39) vanish and we find that

$$F_{0\infty}/F_{1\infty} = \sigma_{01}/\sigma_{10} , \tag{40}$$

$$F_{1\infty}/F_{2\infty} = \sigma_{21}/\sigma_{12} , \tag{41}$$

where $F_{i\infty}$ is the equilibrium fraction of the $i$th charge state.

If the electron-capture and -loss cross sections obey relatively simple power laws for sufficiently large particle velocities, as is suggested by Bohr,[20] for instance, then the equilibirium charge-state fraction ratios will also obey simple power laws. This has been verified by Armstrong *et al.*[19] for carbon, and provides us with an easy method for extrapolating experimental data to high energies. We assume that the ratios have the form

$$f = f_0(E/E_0)^{-\alpha} , \tag{42}$$

$$g = g_0(E/E_0)^{-\beta} , \tag{43}$$

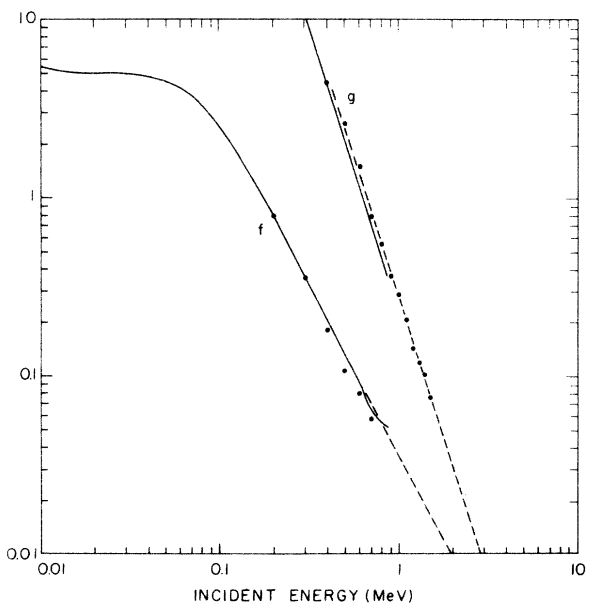


FIG. 1. Equilibrium charge-state fraction ratios for helium in molecular hydrogen gas. Solid lines: smooth curves representing experimental results from Refs. 16 and 17; solid circles: experimental results from Ref. 18; dashed lines: straight-line extrapolations of experimental results to large energies.

where $f \equiv F_{0\infty}/F_{1\infty}$, $g \equiv F_{1\infty}/F_{2\infty}$, and $E_0 = 1$ MeV. Then, noting that $F_{0\infty} - F_{1\infty} + F_{2\infty} = 1$, we develop the following formulas for the equilibrium charge-state fractions:

$$F_{2\infty} = [1 + g(1+f)]^{-1} \tag{44}$$

$$F_{1\infty} = gF_{2\infty} , \tag{45}$$

$$F_{0\infty} = fF_{1\infty} . \tag{46}$$

The constants $f_0$, $g_0$, $\alpha$, and $\beta$ can be found graphically from logarithmic plots of $f$ and $g$ calculated from experimental data versus energy. Then extrapolated values for $f$ and $g$ can be found from Eqs. (42) and (43) and these results may be substituted in Eqs. (44)–(46) to determine values for the equilibrium charge-state fractions. Plots of $f$ and $g$ as functions of energy for helium in hydrogen are shown in Fig. 1. The values of the various constants determined from these graphs are $f_0 = 0.035$, $g_0 = 0.27$, $\alpha = 1.9$, and $\beta = 3.1$. The experimental and extrapolated equilibrium charge-state fractions for helium in hydrogen are given in Table III.

TABLE III. Equilibrium charge-state fractions: Helium on hydrogen.

| $E$ (MeV) | $F_2$ | $F_1$ | $F_0$ |
|---|---|---|---|
| 0.010 | 0.000 | 0.156 | 0.844 |
| 0.013 | 0.000 | 0.164 | 0.836 |
| 0.018 | 0.000 | 0.166 | 0.834 |
| 0.024 | 0.000 | 0.167 | 0.833 |
| 0.032 | 0.000 | 0.170 | 0.830 |
| 0.042 | 0.000 | 0.177 | 0.823 |
| 0.056 | 0.000 | 0.191 | 0.809 |
| 0.075 | 0.000 | 0.224 | 0.776 |
| 0.100 | 0.001 | 0.289 | 0.710 |
| 0.130 | 0.007 | 0.372 | 0.621 |
| 0.180 | 0.012 | 0.503 | 0.485 |
| 0.240 | 0.037 | 0.620 | 0.343 |
| 0.320 | 0.076 | 0.707 | 0.217 |
| 0.420 | 0.173 | 0.703 | 0.124 |
| 0.560 | 0.349 | 0.590 | 0.061 |
| 0.750 | 0.583 | 0.393 | 0.024[a] |
| 1.000 | 0.781 | 0.212[a] | 0.007[a] |
| 1.300 | 0.892 | 0.106[a] | 0.002[a] |
| 1.800 | 0.959[a] | 0.041[a] | 0.000[a] |
| 2.400 | 0.983[a] | 0.017[a] | 0.000[a] |
| 3.200 | 0.993[a] | 0.007[a] | 0.000[a] |
| 4.200 | 0.997[a] | 0.003[a] | 0.000[a] |
| 5.600 | 0.999[a] | 0.001[a] | 0.000[a] |
| 7.500 | 1.000[a] | 0.000[a] | 0.000[a] |
| 10.00 | 1.000[a] | 0.000[a] | 0.000[a] |

[a] Values extrapolated from experimental data.

## III. RESULTS

### A. Total stopping cross sections

Using the procedure described in the previous section, we have calculated both the partial and total stopping cross sections of hydrogen as a function of the incident helium beam energy for the energy range between 0.01 and 10 MeV. Our results for the total stopping cross section are represented in Fig. 2 by the line marked BE. Other theoretical results are also plotted on that figure. Curve L is the prediction of Lindhard's low-energy formula[21] given by

$$S_e = \xi_e 8\pi e^2 a_0 (Z_1 Z_2/Z)(v_1/v_0) , \qquad (47)$$

where

$$Z=(Z_1^{2/3}+Z_1^{2/3})^{3/2}, \quad \xi_e \approx Z_1^{1/6} ;$$

it was developed using qualitative arguments based on the Thomas-Fermi picture of the atom and is expected to give only approximately correct results.

Curve B1 is the well-known Bethe-formula result for incident Coulomb charges[1] given by

$$S_e = (4\pi Z_1^2 Z_2 e^4/mv_1^2)\ln(2mv_1^2/I) , \qquad (48)$$

with the mean excitation energy $I$ set equal to the

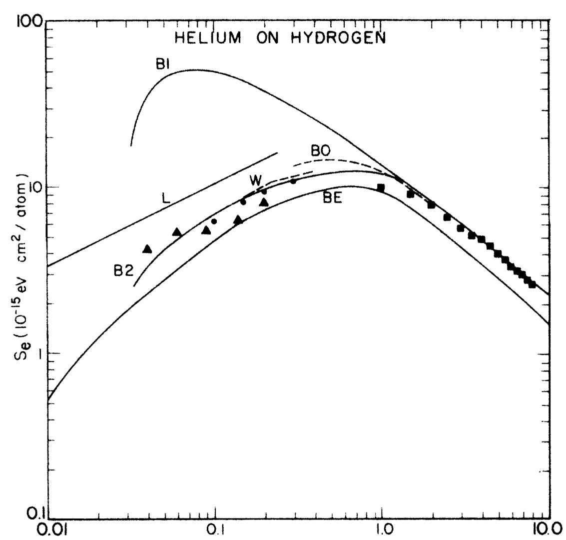


FIG. 2. Total electronic stopping cross section of hydrogen for helium. Curve BE: present binary-encounter calculations; curve B1: Bethe-formula calculation for incident $He^{++}$ from Ref. 22; curve B2: modified Bethe-formula calculation for equilibrium incident beam from Ref. 22; curve L: Lindhard formula calculation. Experimental results: curve BO, Bourland *et al.*, Ref. 23; curve W, Weyl, Ref. 24; circles, Hvelplund, Ref. 25; squares, Palmer, Ref. 26; triangles, Park, Ref. 27.

theoretical value given by Ref. 4, namely $I = 15.0$ eV. Curve B2 is the result of a calculation in which partial stopping cross sections for $He^{++}$, $He^{+}$, and $He^{0}$, determined by Cuevas *et al.*[22] from a modification of the Bethe theory to apply to incident systems other than point charges, are combined using the equilibrium charge-state fractions given in Table III. The various experimental results were obtained from the references cited in the figure. The modified Bethe-formula results are particularly interesting to us because the descriptions of the various helium charge states used to obtain these results are the same as the descriptions used in deriving our binary-encounter results.

From a comparison of curves B1 and B2, it is clear that the effects of the charge-state distribution must be taken into account below about 1.5-MeV incident energy. If this is done, both the binary-encounter approximation (curve BE) and the modified Bethe theory (curve B2) give reasonable results over the entire energy range. As expected, the Bethe theory gives better agreement with experiment at high energies than the binary-encounter theory, owing to the influence of resonance excitations.[7] In addition, the modified Bethe theory appears to give slightly better agreement than the binary-encounter approximation at lower energies, at least for target hydrogen. However, when considering the relative merits of these two approximations, it should be kept in mind that the agreement between either theory and experiment may actually be the result of fortuitous cancellation of errors in the calculated partial stopping cross sections. This possibility will be discussed further in Sec. IV. Both the binary-encounter approximation and the modified Bethe theory appear to give better agreement with experiment than the Lindhard-formula calculations for hydrogen even at low energies, although the significance of this agreement is uncertain since the validity of the binary-encounter approximation and particularly the Bethe theory is questionable at low energies.

### B. Partial stopping cross sections

Very few measurements of partial stopping cross sections have been made owing to the added difficulty of separating the various charge-state components of the incident beam. The measurements of Cuevas *et al.*[22] of the partial stopping cross sections of hydrogen for the charge-state components of helium are notable exceptions. In these experiments a beam of projectiles with an equilibrium distribution of charge states was directed through a stopping gas in the presence of a transverse magnetic field so that particles in different charge states followed different trajectories. A detector was placed in the path of a particular charge-state component to measure its energy decrement, and the value of this quantity was used to deduce the corresponding partial stopping cross section. Since the detector collected only those particles that had not changed their charge state while traversing the stopping gas, the partial stopping cross sections determined from the experiment did not include energy-loss contributions from electron capture and loss by the incident particles. Because our calculations also neglect such capture-and-loss processes, a comparison between them and the experimental results is particularly significant.

Plotted in Fig. 3 are the partial stopping cross sections of hydrogen for the charge-state components of helium obtained from (i) our calculations using the binary-encounter approximation, (ii) the experiment of Cuevas *et al.*, (iii) the calculations of Cuevas *et al.* mentioned above, and (iv) the Born-approximation calculations of Dalgarno and Griffing[28] for protons on hydrogen which have been scaled to apply $He^{++}$ on hydrogen. As can be seen, the agreement between our calculations and experiment is not particularly good at the few energies for which data is available. On the

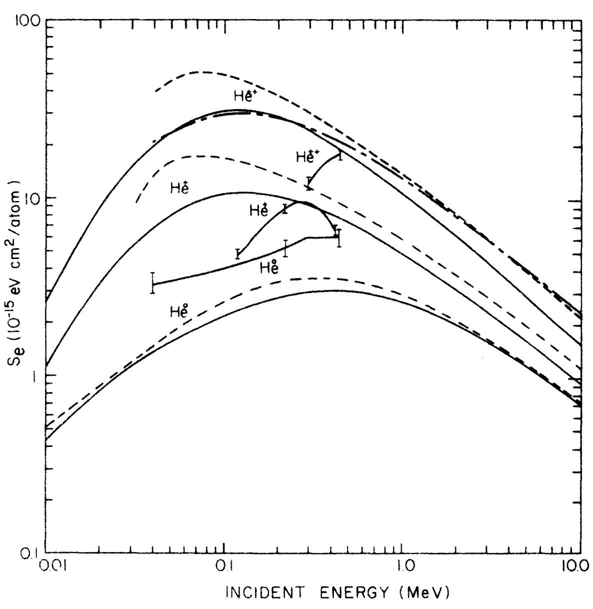


FIG. 3. Partial electronic stopping cross sections of hydrogen for the charge states of helium. (a) Solid lines, binary-encounter calculations; (b) solid lines with error bars, experiments of Cuevas *et al.*, Ref. 22; (c) dashed lines, calculations of Cuevas *et al.*, Ref. 22 using modified Bethe theory; (d) long-dash-short-dashed line, Born approximation calculations of Dalgarno and Griffing, Ref. 28.

other hand, the binary-encounter approximation does predict the correct order of magnitude of the partial stopping cross sections and in fact does as well or better than the other calculations. That the binary-encounter approximation overestimates the partial stopping cross sections for $He^{++}$ and $He^{+}$ is consistent with its tendency to overestimate excitation and ionization cross sections especially in the energy range where these cross sections peak.[6] A similar tendency exists for Born-approximation calculations and is illustrated in Fig. 3 by the results of Dalgarno and Griffing. In this regard, it should be mentioned that both the binary-encounter and Born approximations fail to take into account distortion of the target or incident charge clouds due to their mutual interactions during a collision. This distortion usually tends to reduce the probability of scattering and lowers the individual scattering cross sections. It is most prominent when the incident particle is moving more slowly than the target electrons, but, as has been shown by Bates,[29] it remains important even for higher incident speeds. Also, the binary-encounter and Born approximations in their simplest forms incorrectly include as ionization some of the scattered electrons which actually are captured by the incident particles in charge-transfer processes.[6] However, this effect is only important for the ionic components of the incident beam, and even then only for low-incident speeds.

In light of the behavior of calculated partial stopping cross sections for the charged components of an incident helium beam, it is at first surprising that the calculated results for the neutral component rather badly underestimate the experimental values. However, part of this difference in behavior can be accounted for by the fact that distortion effects are not as important for the neutral component as for the charged components because of the short-range forces involved in collisions between neutral atoms. In addition, the partial stopping cross sections for $He^{+}$ and $He^{0}$ determined from experiment include contributions from collisions which excite the incident system without further ionizing them. Our calculations, as well as those of Cuevas *et al.*, have neglected such processes, and while they will probably be insignificant for $He^{+}$ because of the large excitation energies of the ion, they may be important for $He^{0}$. In order to explain the discrepancy between theory and experiment, it would be necessary for the energy losses due to nonionizing excitations of the incident $He^{0}$ to be about as large as energy losses due to both excitation and ionization of the target hydrogen. This seems unlikely, especially since the inelastic-scattering cross sections for helium tend to be smaller than those for hydrogen, owing to the larger energy defects of the excited state of helium. In discussing the results of their calculations, Cuevas *et al.* have come to the same conclusion based on the results of Dalgarno and Griffing,[28] which show that nonionizing excitations of the incident atom account for only about 10% of the partial stopping cross section of hydrogen for neutral hydrogen.

However, excitation of the incident systems will result in an indirect increase in the partial stopping cross sections which could be much larger than the direct increase just discussed. In the binary-encounter calculations we have assumed that the incident neutral atoms are initially in the ground state when they collide with the target-gas atoms. If, in fact, a significant number are initially excited, their nuclear charge will be less effectively screened and the partial stopping cross sections will be correspondingly larger. Based on a target-gas pressure of 35 $\mu$, a total collision cross section of $10^{-16}$ $cm^2$, and incident particle speeds between $10^8$ and $10^9$ cm/sec, we have estimated the mean time between collisions in the Cuevas experiments to be approximately $10^{-7}$ or $10^{-8}$ sec, which corresponds roughly to radiation times for optically allowed transitions. This suggests that a significant number of incident particles may indeed be in excited states. In this regard, it should be noted that target-gas pressures used in stopping cross-section experiments may be greater than in the experiment of Cuevas *et al.* by a factor of 10 or more, especially for larger incident particle energies. In such experiment it seems quite likely that many of the incident atoms are in excited states.

On the other hand, Dalgarno and Griffing have argued that if a significant number of excited projectiles were present in the incident beam, their relative proportion would vary with target-gas pressure and cause a corresponding variation in the measured stopping cross sections. It is not clear that this variation would be easily detectable, however, at least for large target-gas densities, since collision broadening of the radiation lines would tend to cause variations in the mean radiative lifetimes with pressure similar to the variations in the mean times between collisions.[30] Consequently, the relative proportion of atoms in excited states would tend to remain constant.

It should be pointed out that although rather large discrepancies exist between calculated and experimentally determined partial stopping cross sections of hydrogen for helium, cancellation causes the discrepancy between the resulting total cross sections to be reduced when the partial stopping cross sections are combined according to the procedure described in this paper. Consequently, the reasonable agreement between experimentally determined total cross sections and both the binary-encounter and modified Bethe results may be fortuitous. Nevertheless, since the partial stopping cross-section experiments are difficult to perform, and since little data is available, the possibility of experimental error cannot be ruled out either.

## IV. CONCLUSIONS

In this paper we have attempted to develop a realistic model to describe the stopping process over an energy range wider than can be handled by previously existing theories, and although some problems remain, we have been at least partially successful in this regard. Indeed, results of our calculations of the total stopping cross section of helium in hydrogen are in reasonable agreement with experiment for the entire energy range below 10 MeV for which experimental information exists.

On the other hand, certain unresolved discrepancies exist between our calculated values for partial stopping cross sections of helium for hydrogen and measured values. It is significant that the other theories discussed in this paper are also in disagreement with these measurements. Furthermore, the various theories are in fair agreement with one another and the differences between them which do exist are qualitatively understood. Further experimental information, especially for large-incident energies, might be very useful in clearing up the reason for these discrepancies.

Since the binary-encounter approximation does not take into account contributions from resonance excitations, our model is somewhat less accurate than the Bethe theory at large-incident energies. On the other hand, for small energies it has two basic advantages over the Bethe theory. First, in this region the binary-encounter approximation more closely represents the Born approximation than does the Bethe theory, and second, the model takes into account the different charge states present in the incident beam.

Although we have considered only hydrogen targets, the model is also easily generalized to more complicated atoms. In the following paper we will make this generalization and will present results of stopping cross-section calculations for a wide range of target atomic number.

*Work supported by the United States Atomic Energy Commission under Contract No. AT-(40-1)-2911.

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