Angular Distributions of Electrons Ejected from Helium by Proton Impact*

D. H. Madison

Department of Physics and Astronomy, University of North Carolina, Chapel Hill, North Carolina 27514

(Received 22 June 1973)

Angular distributions of electrons ejected from helium by proton impact are calculated in the plane-wave Born approximation using bound and continuum electron wave functions obtained from a Hartree–Fock potential. The results of this calculation are compared with experimental data and good agreement is found when the relative electron-proton velocity is larger than the proton velocity. The good agreement observed for large angles of the ejected electron is to be contrasted with previous calculations, which fell lower than the large-angle-scattering experimental data.

I. INTRODUCTION

Comparison of theoretical and experimental angular-distribution results can yield valuable information about various theoretical approximations. Over the last several years, a wealth of information has been compiled comparing experimental total cross sections (integrated over ejected electron energy and angles and projectile angles) with various theoretical predictions. By studying angular distributions, it becomes possible to gain insight into the strengths and weaknesses of these predictions.

In this paper, we shall examine the problem of angular distributions of electrons ejected in ionizing collisions between 0.1–2-MeV protons and helium atoms. Doubly differential cross sections for ionization of helium have been experimentally measured by Stolterfoht,[1] Rudd *et al.*[2] and Toburen.[3] These experimental measurements have been compared with various theoretical predictions of the plane-wave Born approximation (PWBA)[2,4-6] and the binary-encounter approximation (BEA)[3,7,8]. The procedures used in obtaining the various PWBA angular distributions for helium varied from scaling the results for hydrogen[2] to representation of the ground state of helium by a 12-term correlated wave function.[6] In the case of the BEA calculation of Bonsen and Vriens,[7] five different wave functions were used in obtaining the necessary velocity distribution. Comparison of the various theoretical predictions with experimental results exhibited a common feature: The theoretical values agreed fairly well with the absolute measurements for ejected electron angles near the conservation of momentum-energy peak, but large discrepancies often occurred for angles away from this peak. The most pronounced disagreements were seen at large angles, where the BEA calculations, for example, underestimated the data sometimes by orders of magnitude.

For small angles of the ejected electron, theoretical predictions were generally lower than the experimental data, with the largest discrepancy occurring when the velocity of the outgoing electron and proton was comparable. This observation led Oldham[5] to suggest that the disagreement between theory and experiment at small angles might originate from a final-state interaction between the outgoing electron and proton. As a result, Salin,[9] Macek,[10] and Bonsen and Banks[11] reformulated the problem including an asymptotic three-body interaction. Salin generalized the theory of Rudge and Seaton[12] for incident electrons to incident heavy particles, Macek used the first term of the Neumann expansion of Faddeev's equations, and Bonsen and Banks used a classical three-body approach. These treatments gave improved agreement with the experimental small-angle data. They did not, however, improve the disagreement noted for large ejected electron angles.

At large angles, the theoretical predictions consistently underestimated the experimental data. Since fairly accurate bound-state wave functions had been used in these calculations, it was assumed that the disagreement arose from a deficiency in the theories. Consequently, Oldham and Miller[6] attributed part of the problem to neglect of contributions from events which leave the atom in an excited state. Salin[13] examined the amplitude for ejection of the spectator electron due to correlations between atomic electrons. Bonsen and Vriens[8] investigated the effect of atomic distortion caused by the incident proton in their calculation. The poor agreement at large angles obtained in the BEA calculations of Bonsen and Vriens[7,8] led them to conclude that large-angle ejection must be a quantum-mechanical phenomena.

In this paper, it will be demonstrated that the PWBA will give good agreement with experimental measurements if good wave functions are used, not only for the initial state but also for the final state. In previous PWBA calculations, continuum wave functions have been assumed to be hydro-

genic. In one calculation, Oldham[5] replaced the $l=1$ part of the hydrogenlike continuum by a Hartree-Fock continuum. This alone was sufficient to improve agreement between theory and experiment at large angles. We shall show here that calculation of angular distributions of ejected electrons in the PWBA using bound and continuum wave functions calculated as eigenfunctions of a Hartree-Fock potential will yield good agreement with experimental data at all angles for which the relative electron-proton velocity is larger than the proton velocity. In Sec. II we discuss the theory and Sec. III contains the results and conclusions.

II. THEORY

In the PWBA, the triply differential cross section (differential in energy and angle of the ejected electron and angle of the projectile) for ionization of an atom initially in state i and finally in state f is given in atomic units by[14,15]

$$d\sigma_{fi} = (2Z_p^2/V^2)\,|F_{fi}(q, \phi_p, E_e, \Omega_e)|^2 \times q^{-2}\, d(\ln q^2)\, d\phi_p\, dE_e\, d\Omega_e \ , \tag{1}$$

where Z_p is the charge of the incident projectile, V is the initial relative velocity of the projectile-target system, q is the magnitude of the momentum change of the projectile, ϕ_p is the azimuthal scattering angle of the projectile, E_e is the ejected electron energy, and Ω_e is the solid angle of observation for the ejected electron. The cross section is expressed in a coordinate system attached to the target atom. The form factor is given by

$$F_{fi} = \langle \Psi_f^{(-)}(1\ldots N)\,|\sum_{j=1}^{N} e^{i\vec{q}\cdot\vec{r}_j}\,|\,\Psi_i(1\ldots N)\rangle \ . \tag{2}$$

Here N is the number of electrons initially in the atom, Ψ_i is the properly antisymmetrized initial atomic wave function, and $\Psi_f^{(-)}$ is the properly antisymmetrized wave function for the combined atom-outgoing-electron system. The minus superscript indicates that the continuum component of the wave function must satisfy the usual incoming wave boundary conditions. If Ψ_i and Ψ_f can be expressed in terms of products of orthogonal single-particle wave functions, it can be seen that (2) reduces to

$$F_{fi} = \langle U_f^{(-)}(\vec{k}, \vec{r})\,|\,e^{i\vec{q}\cdot\vec{r}}\,|\,U_i(\vec{r})\rangle \ , \tag{3}$$

where $U_f^{(-)}$ is the final continuum wave function for the ejected electron of wave number $\vec{k}$, and U_i is the initial bound-state wave function. In obtaining (3), it was also assumed that wave functions of the nonparticipating core electrons were unchanged by the ionizing collision. The initial-state wave function is given by

$$U_i(\vec{r}) = r^{-1} u_{nl_0}(r)\, i^{l_0} Y_{l_0 m_0}(\Omega) \ , \tag{4}$$

where u_{nl_0} is the radial wave function for the initially bound electron and $Y_{l_0 m_0}$ is a spherical harmonic. Making the usual distorted-wave expansion[16] for the continuum electron, we have

$$U_f^{(+)}(\vec{k}, \vec{r}) = (k\pi)^{-1/2} r^{-1} \times \sum_{lm} i^l \chi_l(k, r)\, Y_{lm}(\Omega_e) Y_{lm}^*(\Omega) \ , \tag{5}$$

where

$$\chi_l(k, r) \underset{r\to\infty}{=} e^{i(\sigma_l + \delta_l)} \times \sin[kr - k^{-1}\ln 2kr - \tfrac{1}{2}(l\pi) + \sigma_l + \delta_l] \tag{6}$$

and

$$U^{(-)*}(\vec{k}, \vec{r}) = U^{(+)}(-\vec{k}, \vec{r}) \ . \tag{7}$$

Here σ_l is the Coulomb phase shift[17] and δ_l is the phase shift originating from the non-Columbic portion of the potential used in the calculation of the continuum wave function. The wave function in (5) is normalized to $\delta(E_e' - E_e)$.

If (4)–(7) are inserted into (3) and the absolute square of the resulting expression is summed over final magnetic states, averaged over initial magnetic states, and integrated over ϕ_p, it can be shown after some angular-momentum algebra that

$$\int d\phi_p \frac{1}{2l_0+1}\sum_{m_0} |F_{fi}|^2 = \frac{1}{2\pi k}\sum_{l\lambda} i^{l-\lambda}(2\lambda+1)(2l+1)^{1/2}\, C(l_0\lambda l;000) f_{l\lambda l_0}^{kq} \times \sum_{l'\lambda'} i^{l'-\lambda'}(2\lambda'+1)(2l'+1)^{1/2} C(l_0\lambda' l';000) f_{l'\lambda' l_0}^{kq*} \times \sum_{l_3} C(ll'l_3;000)\, C(\lambda'\lambda l_3;000)\, W(\lambda l_0 l_3 l';l\lambda')\, P_{l_3}(\beta) P_{l_3}(\theta) \ . \tag{8}$$

Here $C(j_1 j_2 j_3;000)$ is a Clebsch-Gordan[18] coefficient, $W(j_1 j_2 j_3 j_4;j_5 j_6)$ is a Racah[18] coefficient, P_l is a Legendre polynomial, β is the angle between $\vec{q}$ and the direction of the incident projectile, θ is the angle between $\vec{k}$ and the direction of the incident projectile, and

$$f^{kq}_{l\lambda l_0} = \langle r^{-1}\chi_l(kr) | j_\lambda(qr) | r^{-1}u_{nl_0}(r)\rangle , \qquad (9)$$

where $j_\lambda(qr)$ is a spherical Bessel function. To obtain the doubly differential cross section (differential in ejected electron angle and energy), it is necessary to integrate over q as indicated in (1). This integration must be performed numerically. The resulting cross section expresses the probability of ejecting one of the electrons in a shell. The total cross section is obtained by multiplying by the number of electrons in the shell.

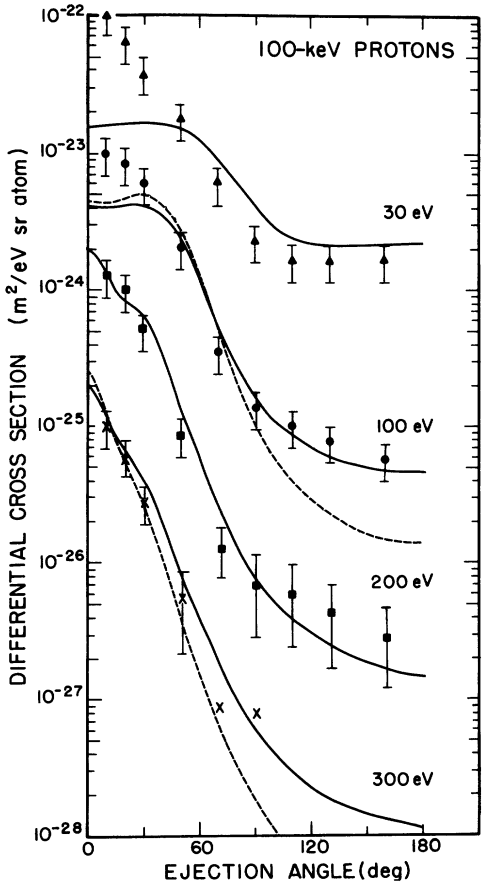

FIG. 1. Angular distributions of electrons ejected from helium by 100-keV protons. Full curves: present calculation; broken curves: scaled-Born cross sections; triangles, circles, squares, and crosses: experiment of Rudd *et al.* Experimental points at 300 eV without error bars have an uncertainity of 100%. The numbers associated with the various curves indicate the energy of the ejected electron.

III. APPLICATION TO IONIZATION OF HELIUM BY PROTONS

A. Numerical Procedure

The formulation given in Sec. II is expressed in terms of a coordinate system attached to the target atom. However, it is necessary to know the cross section in the laboratory-reference frame for comparison with experimental data. Noting that the protons are basically undeflected in these collisions, a simple kinematics argument shows that the ratio of the recoil velocity of the target to the velocity of the electron is of the order of 10^{-4} for energies of interest in this paper. Therefore, the two reference frames are assumed to be the same.

The following procedure was used in obtaining the bound and continuum wave functions used in the evaluation of the form factor (9). The $1s$ core wave function was obtained from a Hartree-Fock calculation for the ground state of He using the numerical program described by Froese-Fischer.[19] This wave function was used to cal-

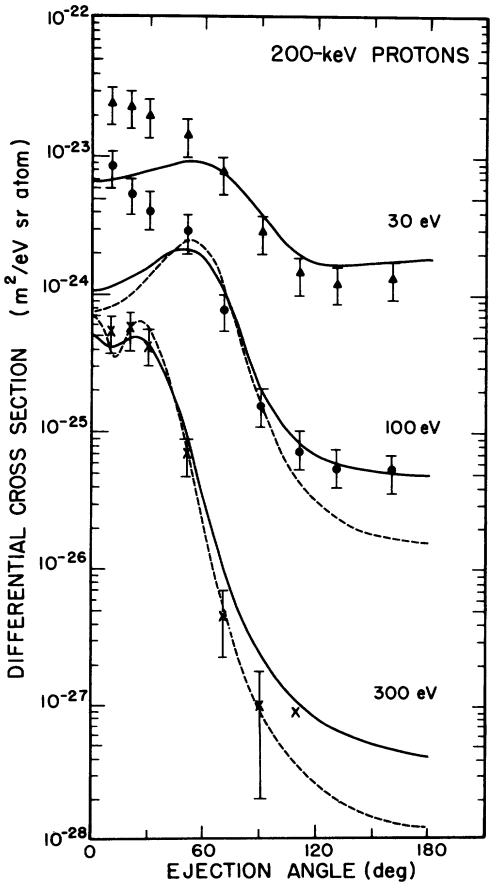

FIG. 2. Same as Fig. 1, except here the proton energy is 200 keV.

culate the effective potential seen by the initial bound and final outgoing electron. The initial and final wave functions are then calculated as eigenfunctions of this effective potential. The orthogonality requirement discussed in Sec. II precludes the use of the exact Hartree-Fock 1s wave function.

The calculation was performed on the IBM 370 model No. 165 computer at Triangle Universities Computation Center (TUCC). The maximum number of partial waves used in the expansion of the continuum wave function was 15. The largest contributions to errors in the calculation resulted from using an insufficient number of partial waves. Comparing numerical and analytic calculations for ionization of hydrogen revealed that the average error ranged from 2 to 5%. The numerical errors are largest for large angles of the ejected electron where the cross sections are smallest.

B. Results and Conclusions

The results of the present calculation using a Hartree-Fock potential for obtaining the bound and continuum wave functions are shown in Figs. 1–4. Also shown in the figures are PWBA calculations obtained by scaling from hydrogen[2] and the experimental data of Rudd, Sautter, and Bailey[2] and Toburen.[3] It is seen that the angular distributions obtained from the Hartree-Fock potential gave good agreement with the experimental data at large angles for all the electron and proton energies displayed here. This is to be contrasted with all previous calculations which fell lower than the experimental data at large angles as previously discussed.

It can be seen from the figures that the agreement between the present calculation and experiment at small angles varies with different electron and proton energies. The largest small-angle disagreement occurs when the relative velocity between the outgoing electron and proton is small. As has been noted,[9,10] it is necessary to include a final-state interaction between the outgoing electron and proton when these relative velocities are small. It then becomes desirable to be able to predict the relative velocities at which these final-state distortions may be ignored. This knowledge would give the angular range in which the present theory would be expected to be valid, since the relative velocity depends on the

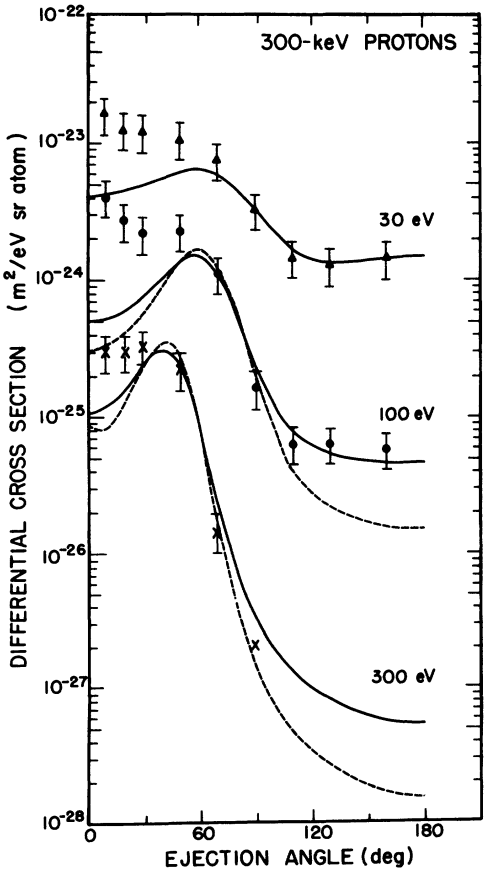

FIG. 3. Same as Fig. 1, except here the proton energy is 300 keV.

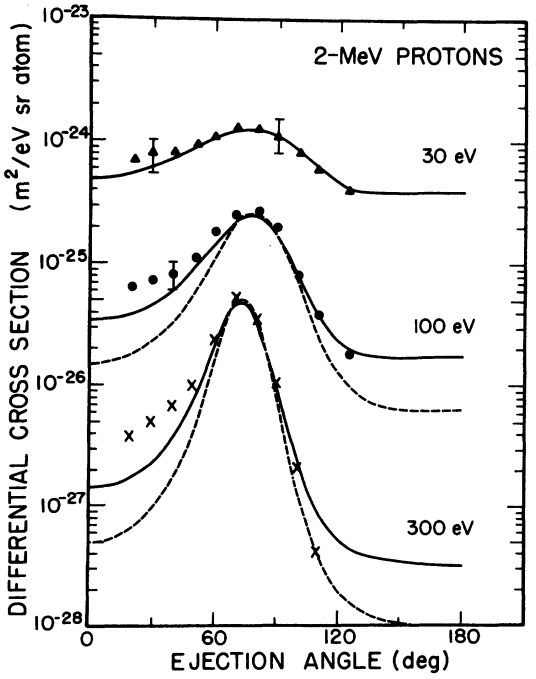

FIG. 4. Angular distributions of electrons ejected from helium by 2 MeV protons. Full curves: present calculation; broken curves: scaled-Born cross sections; triangles, circles, and crosses: experiment of Toburen. The numbers associated with the various curves indicate the energy of the ejected electron.

angular separation of the particles. A straightforward calculation of the relative velocities corresponding to the angles where experiment and the present theory came into agreement revealed that the agreement was achieved for relative electron-proton velocities greater than 0.8–0.9 of the proton velocity. This factor was moderately stable considering the range of electron and proton velocities and the uncertainty in the angle where agreement is achieved. This observation explains how good agreement can be observed over the whole angular range for 100 KeV protons and 200 eV electrons but not over the whole angular range for 2 MeV protons and 300 eV electrons, where intuitively one might expect better agreement (the ratio of the relative velocity to the proton velocity at 0° is 0.9 for the former and 0.5 for the latter: This ratio becomes 0.8 around 50° in the case of the latter.)

Salin[13] has treated the asymptotic three-body problem quantum mechanically. He concludes that the PWBA cross sections should be multiplied by a normalization factor that depends upon the relative electron-proton velocities. The effect of multiplying the present PWBA calculation by this normalization factor is shown in Figs. 5 and 6. It is seen that this normalization factor does improve agreement between theory and experiment at small angles. Unfortunately, however, the agreement at large angles becomes less satisfactory.

One may think that it is somewhat unusual that the present calculation should give such good agreement with experiment for the case in which the electron is leaving the collision much faster than the proton. In this situation, the electron should asymptotically see a charge of two, instead of one, as assumed here. This paradox may be understood from the following explanation. The present cross sections are obtained from the form factor [Eq. (9)] which is completely determined by the radial range in which the bound-state wave function is finite. Therefore, the contribution to the scattering cross section from the continuum wave function is determined by its behavior in this radial range. The behavior of the continuum wave function in this range is determined by the actual potential through which the electron moves. In this calculation, we have replaced this actual potential by a Hartree-Fock atomic potential, and have treated the interaction of the electron with the projectile as a small perturbation. For this approximation to be valid, the projectile must not be near the nucleus when the electron is ejected. The results of the present paper imply that this is the case when the relative electron-proton velocity is large. Further, it may be

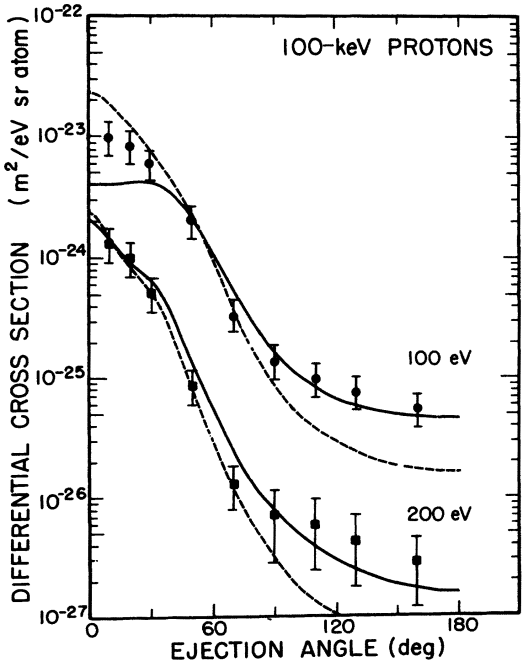

FIG. 5. Angular distributions of electrons ejected from helium by 100 keV protons. Full curves: present calculation; broken curves: present calculation modified by Salin's normalization factor (see Ref. 13); squares and circles: experiment of Rudd *et al.* The numbers associated with the various curves indicate the energy of the ejected electron.

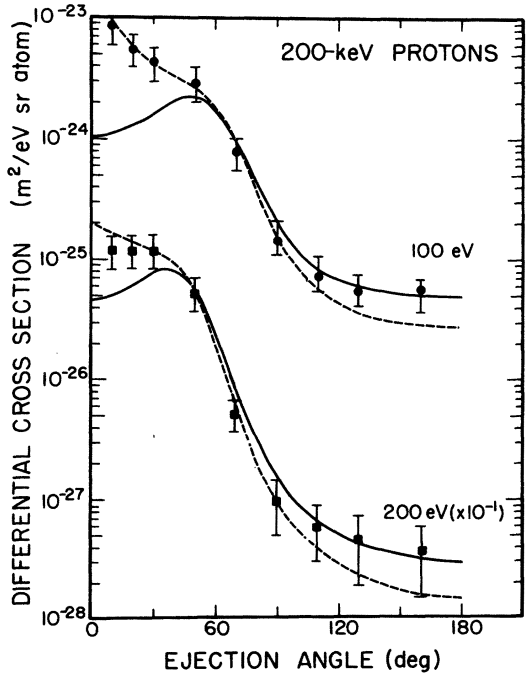

FIG. 6. Same as Fig. 5, except here the proton energy is 200 keV.

surmised that the electron-projectile interaction is not weak when the present calculation fails, i.e., for angles of the ejected electron in a forward cone when relative electron-proton velocities are small. This failure suggests that the proton is also in this cone during these ionizing collisions.

In Table I, PWBA cross sections integrated over angles are presented along with the experimental values. As would be expected, better agreement with experiment is obtained for those energies at which there is good agreement at small angles. In those cases where the relative electron-proton velocity is significantly less than the proton velocity over a large angular range, integrated cross sections obtained from Salin's modification will be superior to the values in Table I. This can be seen from Figs. 5 and 6. The deviations at large angles introduced by Salin's normalization factor do not significantly affect the integrated cross section.

It is interesting to compare the results of the PWBA calculation using hydrogenic wave functions with the results of the PWBA calculation using wave functions obtained from a Hartree-Fock potential. The two PWBA calculations give cross sections integrated over angles that are very similar, and based on the values given in Table I, it would be difficult to say that one calculation was definitely superior to the other. However, Figs. 1–4 show that the calculation using the Hartree-Fock potential is definitely superior. The two angular distributions are similar only over the angular range containing the conservation of momentum-energy peak. The two integrated cross sections are comparable since the largest contribution lies within this peak.

The similarity between quantum and classical results can be understood in a comparable manner. The classical BEA angular distributions[7,8] deviate from experiment at small angles analogous to the hydrogenic PWBA and deviate at large angles by orders of magnitude. However, these BEA angular distributions do contain the conservation of momentum-energy peak. Even though the angular distributions can be very different, integration over angles can yield similar results.

From the results of this calculation, it is seen that angular distributions of electrons ejected from He by 0.1–2-MeV protons given by the PWBA using Hartree-Fock potentials are in good agreement with experiment providing the relative electron-proton velocity is greater than the proton velocity. Agreement with large-angle experimental data was achieved using the quantum-mechanical PWBA only when Hartree-Fock potentials were used to calculate both the initial- and final-state electron wave functions. Sample calculations were also performed using the Hartree-Fock-Slater potential of Herman and Skillman.[20] The results of these calculations were comparable with the results using the Hartree-Fock potential out to about 105°. For angles larger than 105°, the Herman-Skillman potential gave slightly larger cross sections. In spite of the necessity for using Hartree-Fock potentials for predicting the details of angular distributions, cross sections integrated over angles are primarily determined by the conservation of momentum-energy peak.

TABLE I. Differential cross sections for ionization of helium by proton impact in M^2 eV^{-1} $atom^{-1}$.

Proton energy (keV)	Electron energy (eV)	Expt.[a]	Present calculation	Hydrogenic Born[b]
100	30	1.31×10^{-22}	8.97×10^{-23}	9.62×10^{-23}
	100	1.48×10^{-23}	1.18×10^{-23}	1.30×10^{-23}
	200	1.23×10^{-24}	1.40×10^{-24}	1.48×10^{-24}
	300	7.11×10^{-26}	1.08×10^{-25}	7.72×10^{-26}
200	30	8.30×10^{-23}	6.04×10^{-23}	5.95×10^{-23}
	100	1.44×10^{-23}	8.75×10^{-24}	8.84×10^{-24}
	200	2.65×10^{-24}	2.23×10^{-24}	2.35×10^{-24}
	300	7.91×10^{-25}	8.20×10^{-25}	9.04×10^{-25}
300	30	6.62×10^{-23}	4.55×10^{-23}	4.31×10^{-23}
	100	1.06×10^{-23}	6.45×10^{-24}	6.26×10^{-24}
	200	2.45×10^{-24}	1.72×10^{-24}	1.73×10^{-24}
	300	8.86×10^{-25}	7.51×10^{-25}	7.74×10^{-25}

[a]See Ref. 2.
[b]These results were scaled from analytic results for hydrogen as described in Ref. 2.

ACKNOWLEDGMENTS

I am grateful to Dr. M. E. Rudd for providing interpolated values for some of the small-cross-section data and to Dr. B. H. Choi for helpful discussions. The encouragement of Dr. E. Merzbacher during the course of this work is gratefully acknowledged.

---

*Supported by the Materials Research Center, University of North Carolina, Chapel Hill, N. C. under Grant No. GH-33632 from the National Science Foundation.

[1]N. Stolterfoht, Z. Phys. 248, 81 (1971).

[2]M. E. Rudd, C. A. Sautter, and C. L. Bailey, Phys. Rev. 151, 20 (1966); See also M. E. Rudd and T. Jorgensen Jr., Phys. Rev. 131, 666 (1963). Dr. Rudd has supplied interpolated values for some of the small-cross-section data.

[3]L. H. Toburen, in *Proceedings of the Seventh International Conference on the Physics of Electronic and Atomic Collisions*, edited by L. M. Branscomb, H. Ehrhardt, R. Gaballe, F. J. de Heer, N. V. Fedorenko, J. Kistemaker, M. Barat, E. E. Nikitin, and A. C. H. Smith (North-Holland, Amsterdam, 1971), pp. 1120–1122.

[4]W. J. B. Oldham Jr., Phys. Rev. 140, A1477 (1965).

[5]W. J. B. Oldham Jr., Phys. Rev. 161, 1 (1967).

[6]W. J. B. Oldham Jr. and B. P. Miller, Phys. Rev. A 3, 942 (1971).

[7]T. F. M. Bonsen and L. Vriens, Physica (Utrecht) 47, 307 (1970).

[8]T. F. M. Bonsen and L. Vriens, Physica (Utrecht) 54, 318 (1971).

[9]A. Salin, J. Phys. B 2, 631 (1969).

[10]J. Macek, Phys. Rev. A 1, 235 (1970).

[11]T. F. M. Bonsen and D. Banks, J. Phys. B 4, 706 (1971).

[12]M. R. H. Rudge and M. J. Seaton, Proc. R. Soc. A 283, 262 (1964).

[13]A. Salin, J. Phys. B 5, 979 (1972).

[14]E. Merzbacher and H. W. Lewis, in *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, 1958), Vol. 34, p. 166.

[15]M. Inokuti, Rev. Mod. Phys. 43, 297 (1971).

[16]D. H. Madison and W. N. Shelton, Phys. Rev. A 7, 499 (1973).

[17]A. Messiah, *Quantum Mechanics* (Wiley, New York, 1968), Chap. XI.

[18]M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1967).

[19]C. Froese-Fischer, Computer Phys. Commun. 4, 107 (1972).

[20]F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, N. J., 1963).