Calculation of Cross Sections for Electron Ionization of Atoms Using Classical Mechanics*

A. E. KINGSTON
Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado
(Received 27 April 1964)

In order to determine the range of validity of Gryzinski's classical theory for inelastic electron-atom scattering, we evaluate exactly the classical cross section for the electron ionization of atomic hydrogen. At large electron-impact energies the exact classical cross section disagrees with the experimental cross section. This is due to the inability of the classical theory to describe an electron-atom collision if the energy of the incident electron is large. For low-impact energies the classical description of a collision becomes valid. The electron energy at which the classical theory becomes applicable is in good agreement with the energy predicted by the uncertainty principle.

INTRODUCTION

USING a theory formulated by Chandrasekhar[1] for stellar encounters, Gryzinski[2] has derived an exact classical theory for the inelastic scattering of electrons by atoms in which we only take account of the Coulomb interaction between the incident and bound electrons. By making certain approximations Gryzinski was able to obtain simple analytical formulas for the cross sections for electron excitation and ionization of atoms. Comparison[2–5] of his cross-section formulas with experimental data shows that the classical theory reproduces the experimental cross sections with considerable success.

To obtain some insight into the range of validity of the classical method we consider the effect of the approximations made in Gryzinski's calculations.

EXACT CLASSICAL CALCULATIONS

In order to calculate cross sections for electron-atom scattering processes, Gryzinski[2] assumes that the only force which contributes to the scattering is the Coulomb interaction between the bound and incident electrons. Hence to obtain classical cross sections he considers the classical motion of two electrons which have a repulsive Coulombic force acting between them. Distinguishing the electrons by subscripts 1 and 2, denoting the initial velocities and energies[6] of the electrons by $\mathbf{v}_1$, $\mathbf{v}_2$ and E_1 and E_2, respectively, and letting θ be the angle between the vectors $\mathbf{v}_1$ and $\mathbf{v}_2$, Gryzinski shows that the cross section for a collision between two electrons in which electron 2 undergoes a change in energy ΔE is given by

$$\sigma(\Delta E)=2\pi\frac{1}{\Delta E^2}\int_{\theta_{\min}}^{\theta_{\max}}\frac{f(\theta)}{V^4}\times\left(v_1^2v_2^2\frac{\sin^2\theta}{2\Delta E}-E_2+E_1\right)d\theta\cdots, \quad (1)$$

where V = the initial relative velocity of the two electrons,

$$=(v_1^2+v_2^2-2v_1v_2\cos\theta)^{1/2};$$

$f(\theta)$ = the relative angular distribution function between vectors $\mathbf{v}_1$ and $\mathbf{v}_2$,

$=(\sin\theta)V/v_2$, if electron 2 moves through a collection of electrons 1 which have an isotropic distribution of velocities;

$$\cos\theta_{\max,\min}=\pm x \quad \text{if} \quad |x|\leqslant 1,$$
$$=\pm 1 \quad \text{if} \quad |x|\geqslant 1,$$

and where

$$x=[(1-\Delta E/E_1)(1+\Delta E/E_2)]^{1/2}.$$

The cross section for a collision in which electron 2 loses energy greater than U is

$$Q(U)=\int_U^{E_2}\sigma(\Delta E)d(\Delta E)\cdots. \quad (2)$$

We now identify electron 1 with a bound atomic electron and electron 2 with an incident free electron. Hence, denoting the velocity distribution of the electrons in the jth electronic shell of an atom by $N_j(v_1)$ and the ionization potential by U_j, we find that the electron ionization cross section for an atom is

$$Q_{\text{ion.}}=\sum_j\int_0^\infty N_j(v_1)Q(U_j)dv_1\cdots. \quad (3)$$

Gryzinski has shown that we can simplify the calculations greatly if we replace the relative velocity V in Eq. (1) by $(v_1^2+v_2^2)^{1/2}$ and also replace the exact electron velocity distribution $N_j(v_1)$ in Eq. (3) by $N_j\delta[v_1-(2U_j)^{1/2}]$, where N_j is the number of electrons in the jth electronic shell and δ is the Kronecker δ-function. Using these two approximations, we find that the

* This research was supported in part by the Advanced Research Projects Agency (Project DEFENDER), and was monitored by the U. S. Army Research Office-Durham, under Contract DA-31-124-ARO-D-139.

[1] S. Chandrasekhar, Astrophys. J. 93, 285 (1941).
[2] M. Gryzinski, Phys. Rev. 115, 374 (1959).
[3] S. S. Prasad and K. Prasad, Proc. Phys. Soc. (London) 82, 655 (1963).
[4] V. I. Ochkur and A. M. Petrun'kin, Opt. i Spectroskopiya 14, 457 (1963) [English transl.: Opt. Spectry. (USSR) 14, 245 (1963)].
[5] A. E. Kingston, Phys. Rev. 135, A1529 (1964), preceding paper.
[6] We use atomic units throughout the discussion.

TABLE I. Cross section for the ionization of atomic hydrogen by electrons in πa_0^2.

Energy of incident electron in atomic units	Experimental cross section	Classical cross section				Born cross section
		approximate V approximate $N(v_1)$	approximate V exact $N(v_1)$	exact V approximate $N(v_1)$	exact V exact $N(v_1)$	
0.720	0.31	0.401	0.531	0.541	0.692	0.563
0.980	0.53	0.711	0.782	1.280	1.153	0.993
1.280	0.71	0.844	0.861	1.603	1.297	1.166
1.620	0.80	0.866	0.852	1.506	1.270	1.190
2.000	0.82	0.835	0.808	1.333	1.172	1.141
3.125	0.77	0.690	0.651	0.945	0.883	0.930
4.500	0.67	0.548	0.521	0.685	0.659	0.743
8.000	0.45	0.352	0.335	0.400	0.392	0.489
18.000	0.24	0.172	0.168	0.182	0.180	0.247
36.125	0.14	0.089	0.088	0.090	0.091	0.137

cross section for electron ionization from the jth shell of an atom is given by

$$Q_{\text{ion.}}=\begin{cases}\dfrac{N_j}{U_jE_2}\left(\dfrac{E_2}{E_2+U_j}\right)^{3/2}\left(\dfrac{5}{3}-\dfrac{2U_j}{E_2}\right) & \text{if } 2U_j\leq E_2,\\ \dfrac{N_j}{U_jE_2}\dfrac{4\sqrt{2}}{3}\left(\dfrac{E_2-U_j}{E_2+U_j}\right)^{3/2} & \text{if } 2U_j\geq E_2,\end{cases}\quad\cdots\quad(4)$$

where E_2 is the energy of the incident electron.

In order to understand the classical theory, it is necessary to study the effects of these two approximations. For atomic hydrogen the velocity distribution of the atomic electrons may be obtained exactly from the momentum wave function,[7] and it is not difficult to evaluate Eq. (3) exactly.

In Table I we compare the cross section for the electron ionization of atomic hydrogen calculated using various approximations. In the first column we tabulate the experimental cross section,[8] in the second the classical cross section obtained using $(v_1^2+v_2^2)^{1/2}$ for the relative velocity V and $\delta(v_1-(2U_1)^{1/2})$ for the electron velocity distribution, in the third the classical cross section obtained using $(v_1^2+v_2^2)^{1/2}$ for V but the exact electron velocity distribution, in the fourth the classical cross section obtained using the exact V but the approximate $N(v_1)$, in the fifth the classical cross section obtained using the exact relative velocity V and the exact electron velocity distribution $N(v_1)$, and finally in the sixth the quantal cross section obtained using the first Born approximation.[9]

The most interesting feature of this comparison is the disagreement that exists between the quantal calculations and even the exact classical calculations at large impact energies. This is due to the fact that the Born cross section falls off as $\log E_2/E_2$ while the classical cross sections fall off as $1/E_2$ for large values of E_2.

The disagreement between the exact classical and the Born calculations is at first surprising, for in the Born approximation we neglect the distortion of the incident plane wave by the atomic system, the polarization of the atom by the incident electron, exchange effects and only take into account the Coulomb interaction between the bound and the free electron. Similarly in the exact classical approximation we neglect polarization effects, exchange effects and only take into account the Coulomb interaction between the bound and the free electron, but in the classical approximation we do take into account the distortion of the straight line path of the incident electron by the bound electron. However, at high-impact energies this distortion is negligible, and the Born approximation and the exact classical approximation are essentially quantum-mechanical and classical-mechanical descriptions of the same physical phenomena.

To explain the discrepancy between these approximations at high energies we recall that, due to the uncertainty principle, the classical description of a collision is only meaningful if the classical angle of deflection of an incident particle is greater than the uncertainty in the angle of deflection.[10,11] For the Coulomb scattering of one electron by another, it can be shown that for relative energies greater than about 2 atomic units, the classical description is invalid, but for energies less than about 2 atomic units the classical description is valid. This is in quite good agreement with the results in Table I, where we find that for incident electron energies between 2 and 3 atomic units the Born and exact classical approximation are in good accord, but above 3 atomic units they begin to disagree. The disagreement between the Born and classical approximation at electron energies less than 2 atomic units is probably due to the fact that the classical theory does take some account of distortion which tends to increase the cross section.

Recently, Gryzinski[12,13] has been able to obtain almost exact agreement between classical theory and

[7] B. Podolsky and L. Pauling, Phys. Rev. **34**, 109 (1929).
[8] W. L. Fite, in *Atomic and Molecular Processes*, edited by D. R. Bates (Academic Press Inc., New York, 1962).
[9] R. McCarroll, Proc. Phys. Soc. (London) **70**, 460 (1957).
[10] E. J. Williams, Rev. Mod. Phys. **17**, 217 (1945).
[11] C. L. Longmire, *Elementary Plasma Physics* (Interscience Publishers, Inc., New York, 1963), p. 174.
[12] M. Gryzinski, *Proceedings of the Sixth International Conference on Ionization Phenomena in Gases, Paris, 1963* (S.E.R.M.A., Paris, 1963), p. 117.
[13] M. Gryzinski, Institute for Nuclear Research, Warsaw, Poland, Report No. 436/XVIII, 447/XVIII, 448/XVIII (1963).

experiment for the cross section for the electron ionization of atomic hydrogen. To get this agreement it is necessary to use an electron velocity distribution of the form $(v_0/v_1)^3 e^{-v_0/v_1}$; since this distribution is very different from the exact velocity distribution its use cannot be justified theoretically. However, this semiempirical procedure could partially be justified if it gave good results for other atomic systems. Unfortunately, this is not the case. For example, if we compare the cross sections obtained from Gryzinski's semiempirical formula with the Bethe formulas[14] for electron ionization of the states of hydrogen with principal quantum numbers $n=2$, 3, and 4 we find that at high energies the semiempirical classical formula is in error by factors of 2, 3, and 4, respectively.

It is interesting to note in Table I that the two classical cross sections obtained by replacing V by $(v_1^2+v_2^2)^{1/2}$ tend to agree quite closely with the experimental cross section at low energies. Since the result of this approximation is to eliminate collisions with long interaction times it has been suggested[2] that since it has the same effect as the inclusion of the atomic nucleus it is a better approximation than the original classical approximation. By comparing columns one, two, and five of Table I we see that this suggestion is true.

[14] H. Bethe, Ann. Physik 5, 325 (1930).

CONCLUSION

At large impact energies we cannot expect the classical inelastic electron-atom scattering cross sections to agree with experiment, for the classical theory cannot describe an electron-atom collision correctly. However, at incident electron energies of a few atomic units the classical description of a collision is valid and the classical cross sections should be as accurate as the Born-approximation cross sections. If the incident electron energy is close to the ionization or excitation threshold the electron-electron interaction is not the dominant interaction and we cannot expect either the classical or the Born approximations to give accurate cross sections.

ACKNOWLEDGMENT

I wish to thank John Lauer for expert computational assistance.

PHYSICAL REVIEW VOLUME 135, NUMBER 6A 14 SEPTEMBER 1964

Polarization Effects in the Elastic Scattering of Electrons from Helium*†

R. W. LaBahn
U. S. Naval Ordnance Laboratory, Corona, California, and University of California, Riverside, California

AND

Joseph Callaway
Univesrity of California, Riverside, California
(Received 13 April 1964)

The cross section for elastic scattering of electrons from helium atoms has been computed for an energy range from 0 to 50 eV. The formalism used here was obtained from an extension of Hartree-Fock theory wherein the distortion induced in the atom by the scattering electron is approximated by a polarization potential. The method is similar to the "adiabatic-exchange" treatment of electron-hydrogen scattering by Temkin and Lamkin. The computed scattering phase shifts and cross sections are compared with various other calculations and experimental data. A scattering length of 1.13 a_0 is extrapolated from the phase shifts after correcting them for the effects of truncating the polarization interaction as required in the iteration process. The computed total cross sections compare favorably at low energies with the data of Ramsauer and Kollath and at very low energies with the modified effective-range theory of O'Malley, Spruch, and Rosenberg. The differential scattering cross sections follow the effective-range theory in a high backward asymmetry at low energies and the experimental data in a high forward asymmetry at higher energies. The momentum-transfer cross sections agree well with recent microwave drift-velocity measurements, especially those of Pack, Phelps, and Frost.

I. INTRODUCTION

THIS paper is concerned with the elastic scattering of electrons from atomic helium in the energy region from 0 to 50 eV. For this problem, as in all low-energy electron-atom scattering problems, two major effects must be included in the formalism to give adequate description of the scattering. These are the exchange interactions between the scattering electron and the atomic electrons arising from the exclusion principle and the distortion induced in the atomic system by the presence of the scattering electron.

Exchange effects in scattering have been studied by

* A preliminary account of this work was given at the Pasadena meeting of the American Physical Society [Bull. Am. Phys. Soc. 8, 608 (1963)].
† This work was supported in part by the U. S. Bureau of Naval Weapons.