PHYSICAL REVIEW LETTERS

VOLUME 16 | 21 MARCH 1966 | NUMBER 12

# IMPORTANCE OF RELATIVISTIC EFFECTS IN THE SCATTERING OF SLOW ELECTRONS*

H. N. Browne and E. Bauer

Michelson Laboratory, China Lake, California

(Received 31 January 1966)

In the past it has been generally assumed that the total and differential scattering cross section for slow electrons could be calculated using nonrelativistic quantum mechanics. It is the purpose of this Letter to demonstrate that this assumption is erroneous and that relativistic effects play a very important role at low electron energies, at least in the scattering by heavy atoms.

In order to simplify the theoretical treatment, we prove our statement in the static central field approximation, i.e., we neglect spin-spin correlation (exchange) and charge-charge correlation (polarization) between the free and the atomic electrons. In this approximation the $l$th partial wave $F_l(r)$ in the partial-wave expansion of the scattered wave is obtained from the following equations (in Hartree atomic units):

$$F_l'' + \left[k^2 + 2V(r) - \frac{l(l+1)}{r^2}\right]F_l = 0 \qquad (1)$$

in the nonrelativistic treatment, and

$$F_\lambda'' + \left[\frac{1+\gamma}{2}k^2 + 2\gamma V(r) - \frac{l(l+1)}{r^2} + \alpha^2\left(V^2(r) + \frac{\lambda+1}{r}\frac{V'(r)}{\gamma+1+\alpha^2V(r)} + \frac{1}{2}\frac{V''(r)}{\gamma+1+\alpha^2V(r)} - \frac{3}{4}\frac{\alpha^2V'^2(r)}{[\gamma+1+\alpha^2V(r)]^2}\right)\right]F_\lambda = 0 \qquad (2)$$

in the relativistic treatment,[1,2] with the usual initial condition that $F_l$ (respectively, $F_\lambda$) be zero at $r=0$.

Here $k^2$ is the kinetic energy measured in units of 13.6 eV, $V(r)=Z(r)/r$ is the potential energy of the electron in the field of the atom with $Z(r)$ being the effective nuclear charge, $\gamma=(1-\beta^2)^{-1/2}$ with $\beta=v/c$; $\alpha=1/137.037$ is the Sommerfeld fine-structure constant; and $\lambda$ assumes two values depending on the relative direction of spin $\frac{1}{2}$ and angular momentum $l$:

$$\lambda^+ = +l \text{ if } j = l+\tfrac{1}{2},$$

$$\lambda^- = -(l+1) \text{ if } j = l-\tfrac{1}{2}.$$

For $l=0$ there is only one equation and $\lambda=0$.

The differential scattering cross section is obtained from the phase shifts $\eta_l$, $\eta_\lambda{}^+$, $\eta_\lambda{}^-$ of the asymptotic form of the partial waves $F_l$, $F_{\lambda+}$, $F_{\lambda-}$ with respect to the solutions of Eqs. (1) and (2) with vanishing $V(r)$:

$$I(\theta) = f(\theta)f^*(\theta) \text{ with}$$

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)[\exp(2i\eta_l)-1]P_l(\cos\theta) \qquad (3)$$

in the nonrelativistic case, and

$$I(\theta) = f(\theta)f^*(\theta) + g(\theta)g^*(\theta) \text{ with}$$

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}\{(l+1)[\exp(2i\eta_\lambda{}^+)-1] + l[\exp(2i\eta_\lambda{}^-)-1]\}P_l(\cos\theta),$$

$$g(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}[\exp(2i\eta_\lambda{}^-)-\exp(2i\eta_\lambda{}^+)]P_l^1(\cos\theta) \qquad (4)$$

in the relativistic case.

The total scattering cross section $Q$ is given by

$$Q = 2\pi \int_0^{\pi} I(\theta) \sin\theta d\theta$$

or by the optical theorem: $Q = (4\pi/k)\,\mathrm{Im} f(0)$. Equation (2) differs from (1) in two aspects: (a) in the first two terms, and (b) in the $\alpha^2$ term. Aspect (a) represents the relativistic effect proper since these two terms increase with increasing energy. Regarding aspect (b), the terms in the parenthesis are either independent of energy or their moduli decrease with energy. However, their contributions are in general small because they are of order $\alpha^2$ or higher order in $\alpha^2$. Only near $r = 0$, where $V(r) = Z(r)/r$ has a first-order pole, can the terms become significant. This is probably the reason for the general belief that relativistic effects have no influence on $I(\theta)$ and $Q$ at low electron energies as slow electrons do not penetrate very deeply into the atom so that their $I(\theta)$ and $Q$ are largely determined by the outer part of the atom. Although this is true—as indicated by the small amplitude of the partial waves near the nucleus—the potential near the nucleus has nevertheless considerable influence on the phase and amplitude of the partial waves (Fig. 1). For low electron energies ($\gamma \approx 1$) and small $r$ [$Z(r) \approx Z_0$] Eq. (2) simplifies to

$$F_\lambda'' + \left[k^2 + 2\frac{Z_0}{r} - \frac{l(l+1)}{r^2} + \alpha^2 \frac{Z_0^2}{r^2} - \frac{\lambda y + \frac{3}{4}y^2}{r^2}\right] F_\lambda = 0, \quad (5)$$

with

$$y = \frac{\alpha^2 Z_0/r}{2 + \alpha^2 Z_0/r} \quad (0 \leq y < 1).$$

This equation shows that the influence of the last two terms which distinguish the relativistic from the nonrelativistic case increase with (1) increasing $Z_0$ and (2) increasing contributions of the partial waves with small $l$ to the scattering cross section, i.e., with decreasing electron energy.

To determine the magnitude of the influence of the extra terms in the relativistic equations, numerical calculations are necessary. Such calculations have been performed for He, Kr, Cs, and Hg for 2-, 20-, and 200-eV electrons in order to obtain quantitative information on the energy and $Z_0$ dependence of the difference between nonrelativistic and relativistic scattering cross sections. The total scattering cross sections are shown in Table I, typical differential scattering cross sections in Fig. 2. Most of the calculations were performed with a program written by Hückel and modified by Holzwarth and Meister[2] which uses a simplified Numerov integration method. The accuracy was checked by varying the integration step size and by comparison with data obtained with another extensively checked program using a Runge-Kutta procedure.[3,4] The atomic potentials used are taken or derived from data given in the references listed in the tables together with the scattering cross sections. In most cases the numerical integration was terminated at $r_{max} \approx 5$, but for Hg at 2 eV the influence of $r_{max}$ on the data was examined and found to be qualitatively insignificant (Table II). For Kr the energy dependence of the contributions of the different partial waves was studied more carefully (Fig. 3).

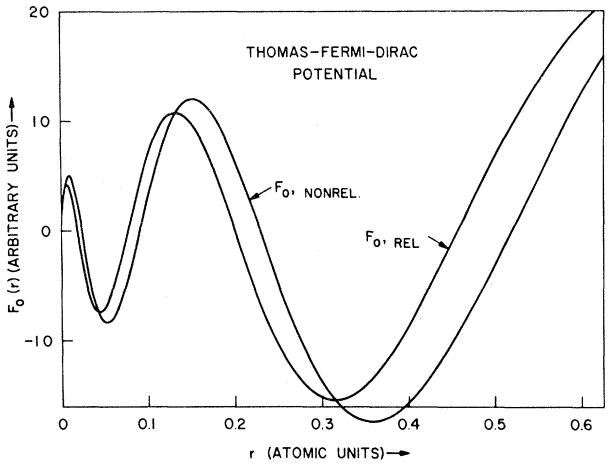


FIG. 1. $s$ wave for the scattering of 2-eV electrons by Hg. The relativistic and nonrelativistic wave functions as obtained by solving Eqs. (2) and (1), respectively, for $l = 0$ are shown only for small $r$ values. At $r_{max} = 8.2$ we obtain $F_{0,\,nonrel} = 76.6$ and $F_{0,\,rel} = 42.9$.

The results in Table I clearly indicate that the relativistic effects have the following behavior: (1) They increase with the nuclear charge $Z_0$. In He they are hardly noticeable, in Hg they are very large. (2) They decrease with increasing electron energy. At 200 eV they amount only to a few percent in the total scattering cross section $Q$ while at 2 eV they can change $Q$ by an order of magnitude. (3) They exist independently of the type of potential used. The strong variation of the scattering cross sections at low energies with potential which

Table I. Total scattering cross sections of He, Kr, Cs, and Hg for 2-, 20-, and 200-eV electrons.

| $Z_0$ | Atom | Potential | Case | 2 eV | 20 eV | 200 eV |
|---|---|---|---|---|---|---|
| 2 | He | Hartree-Fock[a] | rel | 76.0 | 8.20 | 0.752 |
| | | | nonrel | 76.1 | 8.20 | 0.753 |
| 36 | Kr | Hartree-Fock[b] | rel | 110 | 31.7 | 13.2 |
| | | | nonrel | 108 | 29.8 | 13.3 |
| 55 | Cs | Hartree-Fock-Slater[c] | rel | 228 | 65.8 | 20.7 |
| | | | nonrel | 286 | 61.2 | 21.0 |
| | | Thomas-Fermi-Dirac[d] | rel | 131 | 17.6 | 15.8 |
| | | | nonrel | 119 | 14.0 | 16.0 |
| 80 | Hg | Hartree-Fock-Slater[c] | rel | 12.8 | 50.9 | 21.1 |
| | | | nonrel | 1.55 | 59.3 | 20.3 |
| | | Relativistic Hartree[e] | rel | 84.1 | 15.1 | 27.2 |
| | | | nonrel | 19.5 | 23.1 | 26.7 |
| | | Thomas-Fermi-Dirac[d] | rel | 99.9 | 9.82 | 28.3 |
| | | | nonrel | 393 | 13.5 | 27.9 |
| | | Thomas-Fermi[f] | rel | 216 | 79.9 | 30.8 |
| | | | nonrel | 328 | 68 | 31.1 |

[a]W. S. Wilson and R. B. Lindsay, Phys. Rev. 47, 681 (1935).
[b]R. E. Watson and A. J. Freeman, Phys. Rev. 124, 1117 (1961).
[c]F. Herman and S. Skillman, Atomic Structure Calculations (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).
[d]A. A. Abrahamson, Phys. Rev. 123, 538 (1961).
[e]P. F. Mayers, Proc. Roy. Soc. (London) A241, 93 (1957).
[f]S. Rozental, Z. Physik 98, 742 (1936).

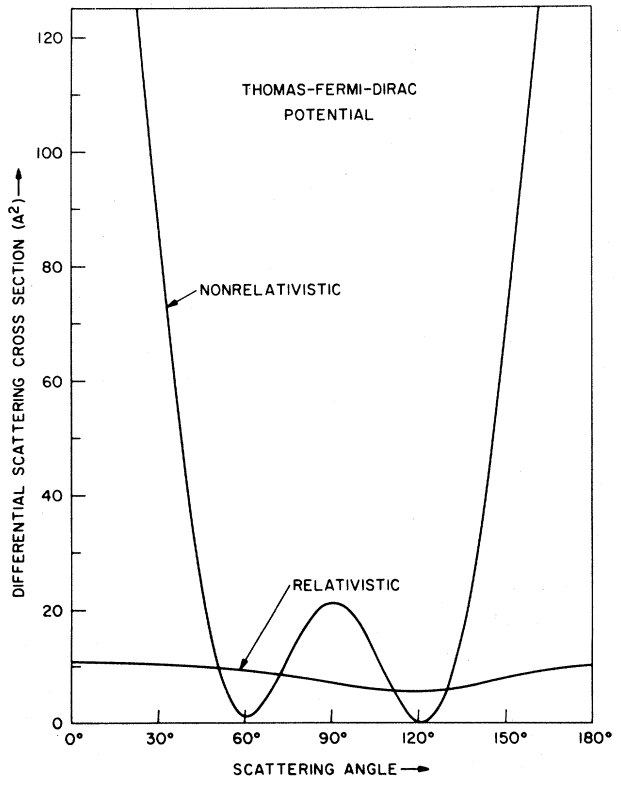


FIG. 2. Differential scattering cross section of Hg for 2-eV electrons.

has been noted earlier (see, e.g., Ref. 3, Fig. 4) clearly demonstrates the need for better wave functions. (4) They may either increase or decrease the total scattering cross section.

A better understanding of the relativistic effects is obtained by studying the partial-wave shifts. The numerical data show that in all cases where the relativistic effects are significant, both $\eta_\lambda{}^+$ and $\eta_\lambda{}^-$ are larger than $\eta_l$ (see, e.g., Fig. 3). This means that the $\lambda$-dependent term which represents spin-orbit coupling and which leads to the Mott polarization of the electrons is smaller than the other terms, so that the relativistic potential is stronger than the nonrelativistic potential. The number of par-

Table II. Influence of $r_{max}$ on the total scattering cross section of Hg for 2-eV electrons.

| Potential | Case | $r_{max}$ 4.7 | 8.2 | 14.0 |
|---|---|---|---|---|
| Hartree-Fock-Slater[a] | rel | 12.8 | 14.1 | 14.1 |
| | nonrel | 1.55 | 1.20 | 1.20 |
| Thomas-Fermi-Dirac[b] | rel | 99.9 | 100 | 100 |
| | nonrel | 393 | 393 | 392 |

[a]P. F. Mayers, Proc. Roy. Soc. (London) A241, 93 (1957).
[b]S. Rozental, Z. Physik 98, 742 (1936).

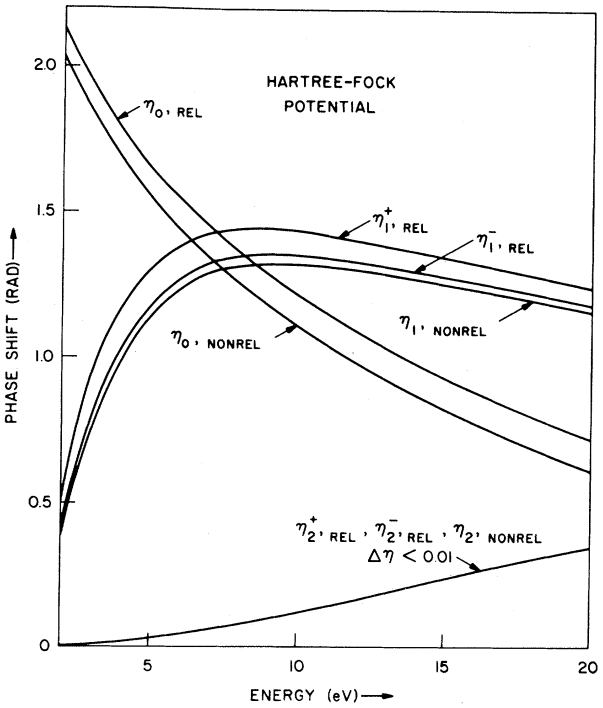


FIG. 3. Partial-wave phase shifts for the scattering of 2- to 20-eV electrons by Kr.

tial waves in which relativistic effects are significant increases with $Z_0$ and $k^2$: In Kr only $\eta_0$ and $\eta_1$ differ considerably at 2 and 20 eV; in Cs $\eta_0$ and $\eta_1$ at 2 eV, $\eta_0$, $\eta_1$, and $\eta_2$ at 20 and 200 eV; in Hg the effects are significant up to $\eta_1$, $\eta_2$, and $\eta_3$ at 2, 20, and 200 eV, respectively.

In the light of these results the agreement between the nonrelativistic theory and experiment which has been obtained previously by other authors for the scattering of slow electrons by heavy atoms has to be considered as fortuitous as the agreement obtained for light atoms neglecting spin and charge correlation.[3] This applies not only to the old work, e.g., on Cd and Hg,[5] but also to recent work on Cs.[6-9] We conclude that in order to obtain reliable scattering cross sections of heavy atoms for slow electrons, not only exchange and polarization but also relativistic effects have to be considered.

We would like to thank Dr. Meister for putting Hückel's IBM program at our disposal.

*This work was supported in part by the National Aeronautics and Space Administration under Grant No. R-05-030-001.

[1]N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Oxford University Press, London, 1949), p. 75.

[2]G. Holzwarth and H. J. Meister, Nucl. Phys. 59, 56 (1964).

[3]E. Bauer and H. N. Browne, in Atomic Collision Processes, edited by M. R. C. McDowell (North-Holland Publishing Company, Amsterdam, 1964), p. 16.

[4]Although the Numerov method is started at the pole ($r=0$) in Ref. 1, we have not seen any breakdown as yet in the calculations.

[5]Ref. 1, p. 213

[6]L. B. Robinson, Phys. Rev. 127, 2076 (1962).

[7]W. R. Garrett and R. A. Mann, Phys. Rev. 130, 658 (1963).

[8]P. M. Stone and J. R. Reitz, Phys. Rev. 131, 2101 (1963).

[9]J. C. Crown and A. Russek, Phys. Rev. 138, A669 (1965).

## SINGLE AND DOUBLE IONIZATION OF He BY ELECTRONS*

Marvin H. Mittleman

Lawrence Radiation Laboratory, University of California, Livermore, California

(Received 21 February 1966)

The double ionization of an atom by a fast electron can come about by two basic processes. In the first, the incident electron hits one of the bound ones and then either of these two hits a third and all three proceed outward. Higher-order processes, i.e., multiple scattering, will also contribute to this result, but for fast electrons these will be small compared to the primary process, the double direct ionization. For high enough energy of the incident electron, both the incident and first recoiling electron will most probably have high energies so the probability of a second interaction will be small. Thus, at high enough energy the double direct process will be improbable. In the second process the first collision takes place suddenly on the time scale of the atomic period and the other electrons are merely spectators. They