RELATIVISTIC EFFECTS IN HIGH-ENERGY INELASTIC ELECTRON-ATOM COLLISIONS

ALBERT C. YATES
Department of Chemistry, Indiana University, Bloomington, Indiana 47401, USA

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In the approximation that electron–electron interactions at high incident electron energies (≈40 keV) may be taken as coulombic, an expression for the integral inelastic cross section for all inelastic collisions is given for the hydrogen atom and is easily generalizable to more complex atoms. Results are presented which indicate that relativistic effects in the above energy range can amount to upwards of 15% of the nonrelativistic results. For the differential cross sections, it is found that such corrections are most important for small-angle scattering.

1. INTRODUCTION

In a recent letter by Bonham and Ng [1], the importance of determining high-energy total inelastic cross sections for electron–atom collisions has been discussed, and calculations of these quantities, using non-relativistic equations, have been presented for a select group of atoms. The present preliminary investigation shows that in the energy range under consideration (≈ 40 keV), contributions to the cross sections resulting from relativistic effects can be appreciable, and complement earlier work concerning elastic scattering [2]. Such effects might be expected, however, if one notes that for such collisions, $v/c \approx 0.4$, where v is the velocity of the incident electron and c is the velocity of light.

It appears that the scattering of very fast electrons by atomic systems was first treated by Møller [3], who, for his considerations, found it necessary to include magnetic and retardation effects in the formulation. An application of Møller's work, pertinent to the present study, has been made by Rose and Bethe [4], who were interested in the effect of inelastic scattering on the depolarization of electron beams. They were able to show that for incident electron energies below 100 keV, retardation effects and magnetic interactions may be essentially neglected. Thus, in the following, the electron–electron interactions are treated as coulombic.

2. THEORY

Expressions for the cross sections may be derived in a manner which parallels that given by Newton [5] for double scattering of electrons by nuclear magnetic moments. For simplicity, the two-electron system is treated; however, the extension to many-electron atoms should appear obvious. Symbolically, we write the Dirac equations for the total system of electron plus atom as

$$(E - H - V)\Psi = 0\,, \tag{1}$$

where E is the total energy available to the system, $H = H_0 + H_A$, with H_0 and H_A as the Dirac operators [6], respectively, of the incident electron and atom in the absence of any mutual interaction, V. Consider

$$(E - H)\Psi^{(0)} = 0\,, \tag{2}$$

then clearly,

$$\Psi = \psi^{(0)} + G_0[1 - VG_0]^{-1} V\Psi^{(0)} = \psi^{(0)} + G_0 H' \psi^{(0)}, \tag{3}$$

with $G_0 \equiv (E - H)^{-1}$. In the coordinate representation, (3) becomes (for two particles)

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \psi^{(0)}(\boldsymbol{r}_1, \boldsymbol{r}_2) + \int d\boldsymbol{r}_1' \ldots \int d\boldsymbol{r}_2'' \langle \boldsymbol{r}_1, \boldsymbol{r}_2 | G_0 | \boldsymbol{r}_1', \boldsymbol{r}_2' \rangle \langle \boldsymbol{r}_1', \boldsymbol{r}_2' | H' | \boldsymbol{r}_1'', \boldsymbol{r}_2'' \rangle \psi^{(0)}(\boldsymbol{r}_1'', \boldsymbol{r}_2''), \tag{4}$$

where G_0 satisfies *

$$[E - H(\boldsymbol{r}_1, \boldsymbol{r}_2)] G_0(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}_1', \boldsymbol{r}_2') = \delta(\boldsymbol{r}_1 - \boldsymbol{r}_1')\, \delta(\boldsymbol{r}_2 - \boldsymbol{r}_2'). \tag{5}$$

From (5), it follows, with little effort, that

$$G_0(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}_1', \boldsymbol{r}_2') = -\frac{1}{4\pi c^2} \sum_\lambda [E_{k_\lambda} + H_0(\boldsymbol{r}_1)] \frac{\exp[ik_\lambda |\boldsymbol{r}_1 - \boldsymbol{r}_1'|]}{|\boldsymbol{r}_1 - \boldsymbol{r}_1'|} \psi_\lambda(\boldsymbol{r}_2) \psi_\lambda^+(\boldsymbol{r}_2'), \tag{6}$$

with $E_{k_\lambda}^2 \equiv (E - E_\lambda)^2 = c^2 k_\lambda^2 + c^4$, and ψ_λ, in this case, is a Dirac eigenfunction for the hydrogen atom with E_λ, as the corresponding eigenvalue. The fact that solutions of the Dirac equation form a complete set [7] has also been used. Note also that Hartree atomic units have been assumed, i.e., $\hbar = m_0 = e = 1$ and $c = 137$. Using (6) in (4) and taking the limit as $r_1 \to \infty$ gives

$$\Psi_{k_0\gamma}(\boldsymbol{r}_1, \boldsymbol{r}_2) \xrightarrow[r_1 \to \infty]{} u_\gamma(\boldsymbol{k}_0) \exp[i\boldsymbol{k}_0 \cdot \boldsymbol{r}_1] \psi_0(\boldsymbol{r}_2) + \sum_\lambda \frac{\exp[ik_\lambda r_1]}{r_1} \psi_\lambda(\boldsymbol{r}_2) \Big\{ -\frac{1}{4\pi c^2} (E_{k_\lambda} - c\boldsymbol{\alpha}_1 \cdot \boldsymbol{k}_\lambda - \beta_1 c^2)$$

$$\times \int d\boldsymbol{r}_1' \ldots \int d\boldsymbol{r}_2'' \exp[-i\boldsymbol{k}_\lambda \cdot \boldsymbol{r}_1'] \psi_\lambda^+(\boldsymbol{r}_2') \langle \boldsymbol{r}_1', \boldsymbol{r}_2' | H' | \boldsymbol{r}_1'', \boldsymbol{r}_2'' \rangle \exp[i\boldsymbol{k}_0 \cdot \boldsymbol{r}_1''] \psi_0(\boldsymbol{r}_2'') \Big\} u_\gamma(\boldsymbol{k}_0), \tag{7}$$

where $u_\gamma(\boldsymbol{k}_0)$ is a normalized Dirac spinor and γ denotes the direction of spin; α_x, α_y, α_z and β are the Dirac matrices. Hence, the amplitude for scattering into the direction determined by $\hat{k}_\lambda$, while exciting the λth state of the target atom is,

$$A_\gamma(\boldsymbol{k}_0, \boldsymbol{k}_\lambda) = -\frac{1}{4\pi c^2} (E_{k_\lambda} - c\boldsymbol{\alpha}_1 \cdot \boldsymbol{k}_\lambda - \beta_1 c^2) H'(\boldsymbol{k}_0, \boldsymbol{k}_\lambda) u_\gamma(\boldsymbol{k}_0). \tag{8}$$

The definition of the 4×4 matrix $H'(\boldsymbol{k}_0, \boldsymbol{k}_\lambda)$ is obvious on comparing with (7).

The differential cross section for exciting the γth state is obtained from its definition as the ratio of the outgoing to incident flux, and is

$$\sigma_{\gamma(0\to\lambda)}(\boldsymbol{k}_0, \boldsymbol{k}_\gamma) = \frac{v_\lambda}{v_0} |A_\gamma(\boldsymbol{k}_0, \boldsymbol{k}_\lambda)|^2, \tag{9}$$

where v_0 and v_λ are the velocities of the incident and scattered electrons, respectively, e.g. $v_\lambda = c^2 k_\lambda / E_{k_\lambda}$. Eq. (9) may be verified by writing the current vector as $\boldsymbol{J} = -c\Psi^+ \boldsymbol{\alpha} \Psi$, and using (7). The cross section of interest here is that for an unpolarized incident electron beam and detection of the outgoing electrons without regard to spin state. Thus, σ must be averaged over initial and summed over final spin states, i.e. form the average,

$$\sigma_{0\to\lambda}(\boldsymbol{k}_0, \boldsymbol{k}_\lambda) = \tfrac{1}{2} \sum_{\gamma=1}^{2} \sigma_{\gamma(0\to\lambda)}(\boldsymbol{k}_0, \boldsymbol{k}_\lambda). \tag{10}$$

Such sums are routinely evaluated [8] by constructing the projector onto the electron states, $\Lambda_+ = \frac{1}{2}[1 - (c\boldsymbol{\alpha} \cdot \boldsymbol{k}_0 + \beta c^2)/E_{k_0}]$, and extending the sum to include positron states. On doing this, it is found that

$$\sigma_{0\to\lambda}(\boldsymbol{k}_0, \boldsymbol{k}_\lambda) = \frac{1}{32\pi^2 c^4} \frac{v_\lambda}{v_0} \mathrm{Tr}\, H'^+(\boldsymbol{k}_0, \boldsymbol{k}_\lambda) (E_{k_\lambda} - c\boldsymbol{\alpha} \cdot \boldsymbol{k}_\lambda - \beta c^2)^+ (E_{k_\lambda} - c\boldsymbol{\alpha} \cdot \boldsymbol{k}_\lambda - \beta c^2) H'(\boldsymbol{k}_0, \boldsymbol{k}_\lambda) \Lambda_+, \tag{11}$$

where Tr denotes the trace. One should observe that the sum over final states is implicit in the above approach.

* In the following equations the explicit appearance of the 4×4 unit matrix has been suppressed.

In order to put eq. (11) into a calculable form, it is necessary to simplify $H'(k_0, k_\lambda)$. This may be accomplished by expanding the operator H' and retaining only the first term (the first Born approximation). Thus, for the simple electron–electron interaction, we have

$$H'(k_0, k_\lambda) = \int \mathrm{d}r_1' \int \mathrm{d}r_2' \exp[\mathrm{i}(k_0 - k_\lambda)\cdot r_1']\psi_\lambda^\dagger(r_2') V(r_1, r_2')\psi_0(r_2') . \tag{12}$$

The cross section may be further simplified by using Darwin's approximation [9] to the Dirac eigenfunctions since $E_\lambda \ll c^2$. This consists essentially of writing $\psi_{\nu s} = O_s\omega_\nu$, where the dependence on the spin quantum number has been made explicit, and ω_ν ($\nu \equiv nlm$) is a solution of the Schrödinger equation. O is a four component spinor operator, whose two small components may be set to zero since magnetic interactions are being neglected*. Making this approximation in (12) and subsequently averaging the cross section over initial target spin states and summing over final states, gives finally

$$\sigma_{0\to\lambda}(k_0, k_\lambda) = \frac{1}{32\pi^2c^4}\frac{v_\lambda}{v_0}|H'(k_0, k_\lambda)|^2 \operatorname{Tr}(E_{k_\lambda} - c\alpha\cdot k_\lambda - \beta c^2)^+ (E_{k_\lambda} - c\alpha\cdot k_\lambda - \beta c^2)\Lambda_+$$

$$= \frac{1}{8\pi^2c^4}\frac{k_\lambda}{k_0}(E_{k_0}E_{k_\lambda} + c^4 + c^2 k_0\cdot k_\lambda)\,|H'(k_0, k_\lambda)|^2 . \tag{13}$$

$H'(k_0, k_\lambda)$ is given by (12) with ψ_λ replaced by ω_{nlm}. Note that this result approaches the correct limit [10, ch. 16, p. 475] as $c \to \infty$, where $E_k \sim c^2$. The integral cross section for exciting the λth state is obtained on integrating (13) over all angles. This equation may be viewed as a generalization of the potential scattering result of Parzen [11]**.

The angular distribution of all inelastically scattered electrons is obtained by summing (13) over all discrete levels and integrating over the continuous levels, i.e.,

$$\sum_{\lambda\neq 0}\sigma_{0\to\lambda}(k_0, k_\lambda) = \frac{2}{k_0c^4}\sum_{\lambda\neq 0}\frac{k_\lambda}{K_{0\lambda}^4}(E_{k_0}E_{k_\lambda} + c^4 + c^2k_0\cdot k_\lambda)\,|\langle\omega_\lambda|\exp[\mathrm{i}K_{0\lambda}\cdot r]|\omega_0\rangle|^2 , \tag{14}$$

which follows from (13) with $V(r_1, r_2) = |r_1 - r_2|^{-1}$, and $K_{0\lambda} = k_0 - k_\lambda$. An estimate of this cross section is easily obtained if the energy transferred in the collision is small compared to the energy of the incident electron. In this case $|k_\lambda| \approx |k_0|$, and $K_{0\lambda} \approx K_{00} \equiv K$; therefore, following the procedure outlined in ch. 16, p. 493 of ref. [10], one gets

$$\sigma_{\mathrm{inel}}(K)\,\mathrm{d}K = \sum_{\lambda\neq 0}\sigma_{0\to\lambda}(K)\,\mathrm{d}K \approx \frac{4\pi}{c^4k_0^2}\frac{\mathrm{d}K}{K^3}(2E_{k_0}^2 - \tfrac{1}{2}c^2K^2)[1 - |\langle\omega_0|\exp[\mathrm{i}K\cdot r]|\omega_0\rangle|^2] . \tag{15}$$

The integral cross section for all inelastically scattered electrons is the integral over K, and is the quantity discussed by Bonham and Ng [1].

3. RESULTS AND DISCUSSION

The differential cross section, $\sigma_{0\to\lambda}$, has been evaluated over the range of energies 1 to 50 keV for the 1s – 2s and 1s – 2p transitions of hydrogen, where it has been found that at 50 keV relativistic corrections to the cross section can amount to upwards of 15% of the nonrelativistic result, with no significant differences being found below about 10 keV. By inspection of eq. (13), it is seen that these differences are determined by the importance of the term proportional to $k_0\cdot k_\lambda$. Hence, such effects will tend to increase the cross section for scattering angles less than 90°, and will be most important for small-angle scattering, decreasing with increasing angles. A comparison of the relativistic and nonrelativistic total cross sections for exciting the 2s and 2p states is given in table 1 for various incident electron energies. Needless to say, the only value of such numbers is to exemplify differences in the two treatments. A few values of the total inelastic differential cross section are presented in table 2 for small-angle scattering at 40 keV and shows the behavior discussed above. The total inelastic differ-

* That such an approximation is expected to be valid for the present case follows from the results and arguments in refs. [3,4]. See also ref. [10], ch. 9.

** Eq. (13) may be derived by techniques similar to those used by Parzen, but is algebraically more tedious.

Table 1
Integral cross section in units of $10^{-2}\pi a_0^2$ (a_0 = Bohr radius) for exciting the 2s and 2p levels of hydrogen

	Electron energies (keV)					
	1	5	10	20	40	50
σ_{2s} (nonrel.)		0.12	0.060	0.030	0.015	0.012
σ_{2s} (rel.)		0.12	0.062	0.032	0.017	0.014
σ_{2p} (nonrel.)	14.4	3.86	2.14	1.17	0.64	0.52
σ_{2p} (rel.)	14.5	3.91	2.20	1.24	0.71	0.59

Table 3
Integral (all inelastic collisions) cross sections in units of $10^{-2}\pi a_0^2$ for the hydrogen atom

	Electron energies (keV)					
	1	5	10	20	40	50
σ^{-} (nonrel.)	35.7	8.89	4.83	2.60	1.39	1.14
σ^{r} (rel.)	35.8	9.01	4.96	2.74	1.55	1.29

Table 2
Total inelastic differential cross sections for hydrogen at 40 keV

	K							
	0.5	1.0	2.0	3.0	4.0	5.0	6.0	8.0
σ^{nr} (K) inel.	13.78	2.36	0.23	0.048	0.016	0.0064	0.0031	0.00097
σ^{r} (K) inel.	16.03	2.75	0.27	0.067	0.018	0.0074	0.0036	0.0011

r = relativistic. nr = nonrelativistic.

ential cross section in a_0^2/steradian is obtained from $\sigma_{\text{inel}}(K)$ as $\sigma_{\text{inel}}(K)k_0k_\lambda/K$. Absolute measurements of such cross sections have been made by Fink and Kessler [12] for the rare gases. Unfortunately, the uncertainty in these measurements is greater than the expected differences in the relativistic and nonrelativistic treatments.

The quantity of greatest interest, as discussed in ref. [1] is the integral inelastic cross section for excitation originating in the ground state, and is given in table 3 for incident electron energies ranging from 1 to 50 keV. From our previous work [2] on elastic scattering it is expected that differences between relativistic and nonrelativistic treatments will increase with increasing atomic number. Hence we conclude that calculations of these cross sections for incident electrons with energies in the 40 keV range should include relativistic effects in a manner similar to that given here. As a final remark it is to be noted that the often used procedure [13] of replacing the nonrelativistic wave vector by a relativistic one cannot account for the effects which have been reported here.

Calculations extending the above results to larger atoms are currently in progress and will be reported soon.

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REFERENCES

[1] R. A. Bonham and E. W. Ng, Chem. Phys. Letters 4 (1969) 355.
[2] A. C. Yates and T. G. Strand, Phys. Rev. 170 (1968) 184;
A. C. Yates, Phys. Rev. 176 (1968) 173;
A. C. Yates and R. A. Bonham, J. Chem. Phys. 50 (1969) 1056.
[3] C. Møller, Z. Physik 70 (1931) 786; Ann. Physik 14 (1932) 531.
[4] M. E. Rose and H. A. Bethe, Phys. Rev. 55 (1939) 277.
[5] R. G. Newton, Phys. Rev. 103 (1956) 385; 94 (1954) 1773.
[6] M. E. Rose, Relativistic electron theory (Wiley, New York, 1961) chs. III, V.
[7] E. C. Titchmarsh, Proc. Roy. Soc. 262 (1961) 489.

[8] S. S. Schweber, Relativistic quantum field theory (Row, Peterson and Co., Evanston, Illinois, 1961) ch. 3, p. 85.
[9] C. G. Darwin, Proc. Roy. Soc. 118 (1928) 654.
[10] N. F. Mott and H. S. W. Massey, Theory of atomic collisions (Oxford University Press, London, 1965).
[11] G. Parzen, Phys. Rev. 80 (1950) 261.
[12] M. Fink and J. Kessler, Z. Physik 196 (1966) 1.
[13] E. M. A. Peixoto, Phys. Rev. 177 (1968) 204.