

## Elastic scattering of electrons by strontium and barium atoms

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Differential, total, and momentum transfer cross sections for the elastic scattering of low- and intermediate-energy (0.2–100 eV) electrons by strontium and barium atoms were calculated in the relativistic polarized-orbital approximation. A static part of the projectile-target interaction potential was generated by solving the Dirac-Hartree-Fock (DHF) equations for the isolated target. A polarization potential was obtained by solving the coupled DHF equations for the target perturbed by an electric field produced by the projectile. Only the dipole term in the polarization potential was included in scattering calculations. For low angular momenta ( $0 \leq l \leq 5$ ) relativistic phase shifts were extracted by solving a continuum state DHF equation in an inner region, where exchange between the projectile and the target electrons was important, and then a relativistic variable phase (RVP) equation in an outer region, where exchange was negligible. For intermediate angular momenta ( $6 \leq l \leq 17$ ) exchange was neglected and the phase shifts were calculated by solving the RVP equation in the whole configuration space. Higher ( $l \geq 18$ ) phase shifts were obtained using the Born approximation and their contributions to scattering amplitudes and cross sections were evaluated analytically. At low energies (0.2–10 eV) our total cross sections for both strontium and barium atoms differ seriously from experimental data of Romanyuk, Shpenik, and Zapesochnyi (Pis'ma Zh. Eksp. Teor. Fiz. **32**, 472 (1980) [JETP Lett. **32**, 452 (1980)]). At energies up to 60 eV our differential cross section for barium differs both in magnitude and shape from experimental data of Jensen, Register, and Trajmar [J. Phys. B **11**, 2367 (1978)] but quite satisfactorily reproduces shapes of curves measured recently by Wang, Trajmar, and Zetner [J. Phys. B (to be published)]. At energies above 80 eV the agreement between the present results and the data of Jensen, Register, and Trajmar is much more satisfactory.

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### I. INTRODUCTION

Recently, we formulated the relativistic polarized-orbital approximation [1] and applied it to the elastic positron [2–5] and electron [6,7] scattering from a majority of heavy closed-shell atoms. In this paper we complete our investigations considering electron collisions with strontium and barium atoms.

To the best of our knowledge the only experiment concerning the elastic scattering of electrons by strontium atoms was performed by Romanyuk *et al.* [8], who reported total cross sections in the energy region 0.1–10 eV. For energies below the first ( $^3P$ ) excitation threshold their results provide the total elastic cross section. On the theoretical side, the elastic  $e^- + \text{Sr}$  collisions were investigated by Fabrikant in the static [9], polarized-orbital [10], and three-channel close-coupling [11] approximations, by Yuan *et al.* [12–14] and Kumar *et al.* [15] in the “static-exchange plus parameter-free correlation-polarization potential” calculations, and by Gribakin *et al.* [16,17] using Dyson’s approach to the many-body theory.

With regard to the elastic  $e^- + \text{Ba}$  scattering, the experimental results were reported by Romanyuk *et al.* [8] for the total cross sections and by Trajmar *et al.* [18–21] for the differential, total, and momentum transfer cross sections. This process was investigated theoretically by Fabrikant [9–11,22,23], Yuan and Zhang [13,24,14], Kumar *et al.* [15], and Gribakin *et al.* [16,17] in the same

approximations as for Sr. In addition, Gregory and Fink [25] reported differential cross sections in the high- (100–1500 eV) energy region while Dzuba *et al.* [26] performed model studies on collisionally induced spin polarization of very slow electrons.

As previously mentioned, the polarized-orbital calculations concerning electron collisions with strontium and barium atoms were already carried out by Fabrikant [10] and it might seem that the present calculations are needless. However, there are two serious differences between the present work and the work of Fabrikant. First, he kept the core of the target atom frozen and assumed that only the outermost atomic orbital was influenced by the electric field produced by the projectile. In contrast, in the present calculations all atomic orbitals were allowed to be distorted. Second, the importance of the relativistic effects in strontium and barium atoms has been recognized a long time ago. In spite of that Fabrikant’s approach was completely nonrelativistic. The present work is free of that shortcoming as in our calculations both the target and the projectile were described relativistically. Therefore our results are expected to be much more reliable than those reported by Fabrikant in Ref. [10].

### II. SCATTERING CALCULATIONS

The reader is referred to our previous papers for details concerning mathematical formulation of the rela-

tivistic polarized-orbital approximation [1] and numerical methods used in calculations of polarization potentials [2]. Our scattering equation is the radial continuum Dirac-Hartree-Fock equation [see Ref. [1], Eq. (43)]

$$\begin{pmatrix} mc^2 - E + V(x) & -c\hbar \left( \frac{d}{dx} - \frac{\kappa}{x} \right) \\ c\hbar \left( \frac{d}{dx} + \frac{\kappa}{x} \right) & -mc^2 - E + V(x) \end{pmatrix} \begin{pmatrix} F_\kappa(x) \\ G_\kappa(x) \end{pmatrix} = \begin{pmatrix} X_{F_\kappa}(x) \\ X_{G_\kappa}(x) \end{pmatrix} \quad (1)$$

with an initial condition  $F_\kappa(0) = G_\kappa(0) = 0$ . Here  $E$  is the total energy of the scattered electron (including its rest energy  $mc^2$ ),  $\kappa = \pm(j + \frac{1}{2})$  for  $l = j \pm \frac{1}{2}$ , and  $V(x)$  is a spherically symmetric scattering potential which consists of static and polarization parts.  $X_{F_\kappa}(x)$  and  $X_{G_\kappa}(x)$  are the exchange terms and have been explicitly given in our previous work [1]. The static potential used in the present work has been calculated using the Dirac-Hartree-Fock code of Desclaux [27] while the polarization potential has been obtained by solving the coupled Dirac-Hartree-Fock equations [1,2].

Solving Eq. (1) we make two simplifications. First, because of limitations of our computational facilities we are not able to include exchange-polarization terms in our calculations and we omit them. Thus in present calculations  $X_{F_\kappa}(x)$  and  $X_{G_\kappa}(x)$  are the static-exchange terms. Second, we retain only the dipole term in the polarization potential. We justify it as follows. The polarization potential is defined as a second-order perturbation correction to the interaction energy [28]. It is well known [29] that the second order of the perturbation theory gives correct values of only first two terms in an asymptotic expansion of the interaction energy in powers of  $x^{-1}$  (i.e., terms proportional to  $x^{-4}$  and  $x^{-6}$ ; here  $x$  denotes a distance between the projectile and the nucleus). The third term, which is proportional to  $x^{-8}$ , is dominated by a leading term in the third-order perturbation theory correction falling off asymptotically as  $x^{-7}$  (neglected in the calculations). In view of this neglect it is methodologically incorrect to retain terms in the polarization potential other than monopole, dipole, and quadrupole ones. Moreover, since the polarized-orbital method is based on the adiabatic approximation, it does not take into account dynamic effects in the interaction potential while it is known [30,31] that such effects are not negligible. Particularly, monopole and dipole terms in a multipole expansion of the nonadiabatic (i.e., dynamic) correction to the polarization potential are comparable in magnitude but of opposite sign to monopole and quadrupole terms in the polarization potential. Therefore we conclude that by neglecting the dynamic distortion effects (as it has been done in the formulation of the polarized-orbital theory) one is forced to drop other than dipole contributions to the polarization potential.

Evaluating phase shifts for  $0 \leq l \leq 5$  we divide the configuration space into two regions which are separated by a sphere of radius  $R$ . In the inner region ( $x < R$ ), where exchange is important, we perform direct outward integration of the Dirac equation (1) using a modified version of Desclaux's program [27,32]. We stop this integration

at the surface of the sphere and extract "short-range" phase shifts  $\delta_\kappa^s$  from the equation

$$\frac{G_\kappa(R)}{F_\kappa(R)} = \pm \lambda \left( \frac{\hat{j}_{l\mp 1}(kR) - \hat{n}_{l\mp 1}(kR) \tan \delta_\kappa^s}{\hat{j}_l(kR) - \hat{n}_l(kR) \tan \delta_\kappa^s} \right), \quad (2)$$

where

$$\lambda = \left( \frac{E - mc^2}{E + mc^2} \right)^{1/2}, \quad k^2 = \frac{(E - mc^2)(E + mc^2)}{(c\hbar)^2} \quad (3)$$

while  $\hat{j}_l(kR)$  and  $\hat{n}_l(kR)$  are the Riccati-Bessel functions. In Eq. (2) the upper sign should be taken for  $\kappa > 0$  and the lower one for  $\kappa < 0$ . In the outer region ( $x > R$ ), where the exchange terms on the right-hand side of Eq. (1) may be neglected, we use the relativistic version of the variable phase method [2] solving the equation

$$\begin{aligned} \frac{d\delta_\kappa(x)}{dx} = & -\lambda^{-1} \frac{V(x)}{c\hbar} [\hat{j}_l(kx) \cos \delta_\kappa(x) \\ & - \hat{n}_l(kx) \sin \delta_\kappa(x)]^2 \\ & - \lambda \frac{V(x)}{c\hbar} [\hat{j}_{l\mp 1}(kx) \cos \delta_\kappa(x) \\ & - \hat{n}_{l\mp 1}(kx) \sin \delta_\kappa(x)]^2 \end{aligned} \quad (4)$$

subject to an initial condition

$$\delta_\kappa(R) = \delta_\kappa^s \quad (5)$$

and then obtaining the phase shift from the formula

$$\delta_\kappa = \lim_{x \rightarrow \infty} \delta_\kappa(x). \quad (6)$$

A choice of the sign in Eq. (4) is the same as in Eq. (2).

For  $6 \leq l \leq l_0 = 17$  we neglect the exchange between the atomic electrons and the projectile and evaluate the phase shifts solving Eq. (4) in the whole configuration space subject to an initial condition  $\delta_\kappa(0) = 0$ . For higher partial waves ( $l > l_0$ ) we estimate values of the phase shifts using the nonrelativistic Born approximation [33]

$$\delta_{-l-1} \simeq \delta_l \simeq \delta_l^B = \pi \left( \frac{me^2\alpha}{\hbar^2} \right) \frac{k^2}{(2l-1)(2l+1)(2l+3)}, \quad (7)$$

where  $\alpha$  is a dipole polarizability of the target atom extracted from a long-range part of the polarization potential. This leads to the following expressions for the direct  $f(\theta)$  and spin-flip  $g(\theta)$  scattering amplitudes:

$$\begin{aligned} f(\theta) \simeq & \frac{1}{2ik} \sum_{l=0}^{l_0} [(l+1) (e^{2i\delta_{-l-1}} - 1) \\ & + l (e^{2i\delta_l} - 1)] P_l(\cos \theta) \\ & - \pi \left( \frac{me^2\alpha}{\hbar^2} \right) k \sum_{l=0}^{l_0} \frac{P_l(\cos \theta)}{(2l-1)(2l+3)} \\ & - \frac{\pi}{2} \left( \frac{me^2\alpha}{\hbar^2} \right) k \sin \frac{\theta}{2}, \end{aligned} \quad (8)$$

$$g(\theta) \simeq \frac{1}{2ik} \sum_{l=1}^{l_0} (e^{2i\delta_{-l-1}} - e^{2i\delta_l}) P_l^1(\cos \theta). \quad (9)$$

Given the scattering amplitudes, we calculate the differential  $I(\theta)$ , total  $Q_T$ , and momentum transfer  $Q_M$  cross sections using formulas

$$I(\theta) = |f(\theta)|^2 + |g(\theta)|^2, \quad (10)$$

$$Q_T = 2\pi \int_0^\pi d\theta \sin \theta I(\theta) \\ \simeq \frac{4\pi}{k^2} \sum_{l=0}^{l_0} [(l+1) \sin^2 \delta_{-l-1} + l \sin^2 \delta_l] - \frac{4\pi}{k^2} \sum_{l=0}^{l_0} (2l+1) (\delta_l^B)^2 + \frac{\pi^3}{2} \left( \frac{me^2\alpha}{\hbar^2} \right)^2 k^2, \quad (11)$$

$$Q_M = 2\pi \int_0^\pi d\theta \sin \theta (1 - \cos \theta) I(\theta) \\ \simeq \frac{4\pi}{k^2} \sum_{l=0}^{l_0-1} \left( \frac{(l+1)(l+2)}{(2l+3)} \sin^2 (\delta_{-l-1} - \delta_{-l-2}) + \frac{l(l+1)}{(2l+1)} \sin^2 (\delta_l - \delta_{l+1}) \right. \\ \left. + \frac{(l+1)}{(2l+1)(2l+3)} \sin^2 (\delta_{-l-1} - \delta_{l+1}) \right) + \frac{4\pi}{k^2} \frac{(l_0+1)}{(2l_0+1)} [(l_0+1) \sin^2 (\delta_{-l_0-1} - \delta_{l_0+1}^B) + l_0 \sin^2 (\delta_{l_0} - \delta_{l_0+1}^B)] \\ - \frac{4\pi}{k^2} \sum_{l=0}^{l_0} (l+1) (\delta_l^B - \delta_{l+1}^B)^2 + \frac{2\pi^3}{3} \left( \frac{me^2\alpha}{\hbar^2} \right)^2 k^2. \quad (12)$$

Notice that all the summations in Eqs. (8)–(12) have finite limits.

### III. RESULTS

As a test of correctness of our polarization potential calculations we compared our values of electric dipole polarizabilities for strontium ( $\alpha = 232.6a_0^3$ ) and barium ( $\alpha = 324.0a_0^3$ ) atoms with those obtained in the same approximation by Kolb *et al.* [34]. Both sets of results agree exactly.

It may be interesting to answer a question regarding the necessity of using the relativistic approach. In order to study this problem we performed both relativistic and nonrelativistic calculations of  $e^- + \text{Sr}$  and  $e^- + \text{Ba}$  total elastic cross sections. (In the nonrelativistic case *both* a projectile and a target were treated nonrelativistically—the speed of light  $c$ , appearing in *all* our equations as a parameter, was multiplied by  $10^6$ .) Our results for electron impact energies varying from 0.2 to 10 eV are shown in Fig. 1. It is seen that for strontium relativistic effects (direct plus indirect) do not exceed 7%, but for barium they are as high as 25% at an energy of 1.8 eV

and 30% at an energy of 10 eV. Thus in our opinion the relativistic approach seems to be justified.

In Fig. 1 we compare our results for the total elastic cross section with experimental data of Romanyuk *et al.* [8] and theoretical results of Fabrikant [11,22]. Serious disagreement between the present data and the experiment below the first inelastic thresholds is somewhat surprising and it is difficult to point at its origin. Discrepancies may be partly attributed to some shortcomings of the present approach (see below), but in view of the fact that the close-coupling results of Fabrikant [11,22] also differ seriously from data of Romanyuk *et al.* [8], we suspect that at least in the very-low-energy region the experimental results may be in error. It should be mentioned that Yuan *et al.* [12,13] came to the same conclusion using a different approach. Independent measurements resolving this discrepancy would be highly desirable. Results obtained by Fabrikant [10] in the nonrelativistic valence-only polarized-orbital calculations (not shown in figures) are approximately one order of magnitude higher than other data and thus seem to be completely unreliable. This confirms the necessity of using the relativistic approach and allowance for distortion of all atomic orbitals.

Obviously, the present approach, as a single-channel

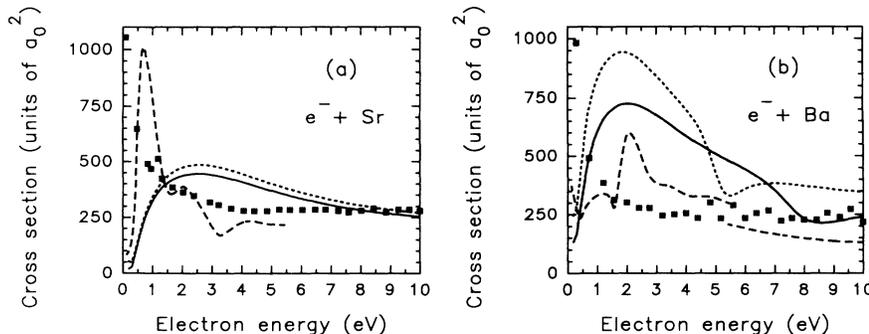


FIG. 1. Total cross sections for electron scattering from (a) strontium and (b) barium atoms. Theory (total elastic): - - -, present nonrelativistic; —, present relativistic; — —, Fabrikant (from Ref. [11] below 5.442 eV and Ref. [22] above 5.442 eV). Experiment (total): ■, Romanyuk *et al.* [8].

one, cannot predict near-threshold resonance structures in cross sections. However, it can predict eventual shape resonances and we found that broad structures with maxima located at energies of 2.5 eV for Sr and 2.0 eV for Ba are due to the appearance of such resonances in  $d$  partial waves.

Our relativistic results for differential cross section are shown in Fig. 2 along with experimental data of Trajmar and co-workers [18,20,21] and theoretical close-coupling results of Fabrikant [22,23]. First of all, we notice that the results of Fabrikant, when available, are in much better qualitative agreement with the results of the present cal-

culations than in a case of low-energy total cross section. A qualitative agreement between the present results and the recent experimental data of Wang *et al.* [21] at 15 and 20 eV is also satisfactory. Quantitative deviations may be partly attributed to experimental errors (estimated to be less than 25%) and partly to shortcomings of the present theory (see below). Analysis of all results available at an energy of 20 eV suggests that results of measurements performed by Trajmar and co-workers in the 1970s [18–20] suffer probably from large experimental errors. It explains why at energies up to 60 eV the present results do not agree even qualitatively with these

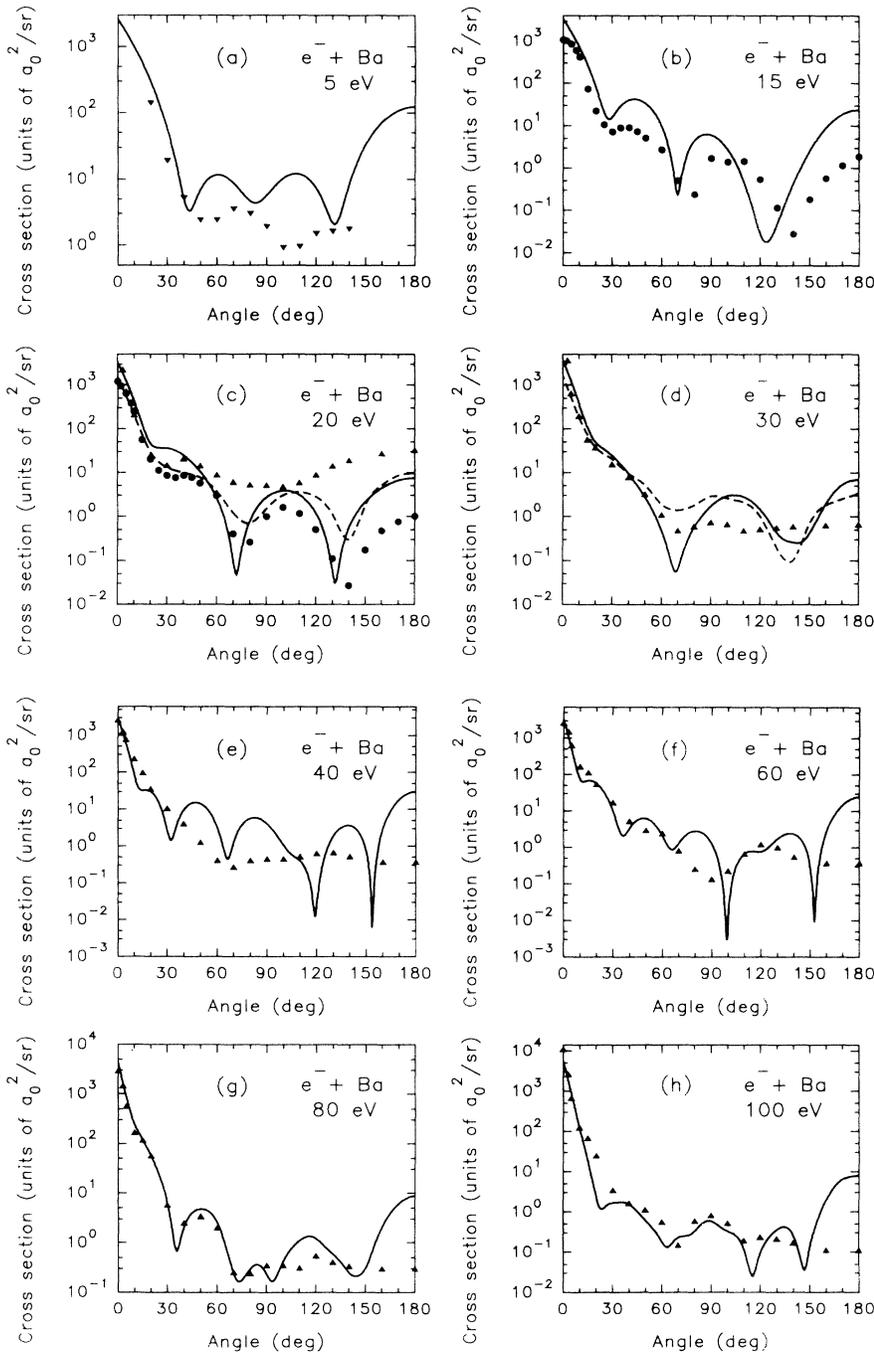


FIG. 2. Differential cross section for elastic electron scattering from barium atoms. Theory: —, present relativistic; — —, Fabrikant [22] and [23]. Experiment:  $\blacktriangledown$ , Trajmar and Williams [18];  $\blacktriangle$ , Jensen *et al.* [20];  $\bullet$ , Wang *et al.* [21].

TABLE I. Total ( $Q_T$ ) and momentum transfer ( $Q_M$ ) cross sections for electrons elastically scattered by barium atoms.

Energy (eV)	Experiment				Theory			
	Jensen <i>et al.</i> [20]		Wang <i>et al.</i> [21]		Fabrikant [22,23]		Present work	
	$Q_T (a_0^2)$	$Q_M (a_0^2)$	$Q_T (a_0^2)$	$Q_M (a_0^2)$	$Q_T (a_0^2)$	$Q_M (a_0^2)$	$Q_T (a_0^2)$	$Q_M (a_0^2)$
15			123.6	14.6			311.5	58.8
20	216.3	145.7	95.4	13.1	113.7		206.9	36.6
30	129.8	11.6			108.1		175.1	23.6
40	99.2	8.84					105.1	38.5
60	112.0	12.4					95.3	26.7
80	98.1	8.11					127.9	15.5
100	90.6	5.50					82.1	7.84

data. At energies of 80 and 100 eV deviations become small apart from angles larger than  $130^\circ$  where the experimental data were obtained by, probably incorrect, extrapolation. Such a satisfactory agreement suggests that at least for energies greater than 80 eV the present results are reliable both in magnitude and shape.

Finally, for the sake of completeness, in Table I we compare our values of total and momentum transfer cross sections at selected intermediate and higher energies with available experimental and theoretical data.

Before we proceed to conclusions, a few comments on the shortcomings of the approximation used should be given. Recent calculations of other authors (e.g., Kim and Greene [35] and Froese Fischer [36]) show that the configuration mixing was very important for a description of  $e^- + \text{Sr}$  and  $e^- + \text{Ba}$  bound complexes and thus it is expected to play a significant role in low-energy electron scattering from these atoms. In spite of this, in describing the unperturbed target we used a single Dirac-Hartree-Fock determinant. That led to some inaccuracies in calculated static and polarization potentials. For instance, the present calculations overestimated values of atomic polarizabilities ( $\alpha = 232.6a_0^3$  for Sr and  $\alpha = 324.0a_0^3$  for Ba) when compared with values recommended by Miller [37] ( $\alpha = 186.3a_0^3$  for Sr and  $\alpha = 267.9a_0^3$  for Ba). That in turn could give rise to an overestimation of small-angle scattering contributions to cross sections. Neglect of higher-order multipole terms in the polarization potential seems to be *methodologically* justified (see the discussion in Sec. II). However, in practice it might happen that retaining some of these terms we would obtain better agreement with experimental data. This ambiguity is certainly a weak side of the polarized orbital approximation. Finally, we neglected polarization contributions to the exchange terms in the scattering equation. It might influence the quality of low-energy ( $E \leq 10$  eV) cross sections, but should not affect the reliability of our results at higher energies ( $E > 10$  eV) as model calculations of

one of the present authors (see Ref. [38]) have shown that with increasing impact energy the effect of exchange in the polarization potential very quickly becomes negligible. However, one should keep in mind that at higher energies the dynamical polarization terms in the scattering potential (neglected in the present theory) become more important.

#### IV. CONCLUSIONS

We performed relativistic calculations on the elastic scattering of low- and intermediate-energy electrons from strontium and barium atoms. The approach employed was the relativistic polarized-orbital approximation. The most important result is qualitative confirmation of reliability of the very recent differential cross section measurements carried out for barium by Wang *et al.* [21]. However, quantitative agreement with other available experimental data is generally poor at low energies and moderate at intermediate energies. Thus alternative theoretical methods based on the nonperturbative relativistic treatment of polarization and electron correlation in targets, such as the relativistic  $R$  matrix [39–41], should be favored in future.

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