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Short Communication

Theoretical study of low-energy positron scattering on alkaline-earth atoms in the relativistic polarized orbital approximation

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Abstract. — The elastic low-energy positron scattering on Be, Mg, Ca, Sr, Ba and Ra atoms has been investigated at energies below 100 eV. The *ab initio* calculated polarization potentials applied in these calculations were obtained by solving the coupled Dirac-Hartree-Fock equations. Comparison between present results and those of previous model calculations shows serious discrepancies. Particularly, we do not predict existence of the Ramsauer-Townsend minima in total elastic cross sections.

The low-energy elastic scattering of electrons from light (Be, Mg and Ca) and heavy (Sr, Ba and Ra) alkaline-earth metals has attracted considerable interest in the past few years [1-8]. However, only a few investigations have been made for the scattering of slow positrons on these targets. Kurtz and Jordan [9] carried out model calculations on elastic e^+-Be, Mg and Ca scattering for positron energies varying from 0 to 5 eV. In turn Khare and co-workers employed the optical model potential approach in their studies on e^+-Mg [10] and e^+-Ca [11] scattering in the impact energy ranges 10-500 eV and 10-75 eV, respectively. For heavy targets the only calculation was performed by Jaskólski [12] who obtained s and p-wave phase shifts for e^+-Ra scattering in the static field approximation. So far, no experimental data on e^+-alkaline-earth atom collisions have been reported. In this paper, we present results of the first *ab initio* study of elastic positron scattering from Be, Mg, Ca, Sr, Ba and Ra atoms in the energy region below 100 eV. The approach employed has been the relativistic polarized orbital theory formulated some time ago [13] and applied to the elastic scattering of slow positrons from Hg [14] and Zn and Cd [15] atoms.

In the relativistic polarized orbital approximation the positron scattered elastically on a closed-shell atom is treated as the Dirac particle moving in a central field and a system of two radial differential equations describing the projectile has a form

$$
\begin{aligned}
c\hbar\,\frac{\mathrm{d}P(r)}{\mathrm{d}r}+c\hbar\frac{\kappa}{r}P(r)+\left(-mc^2-E+V(r)\right)\;Q(r)=0,\\
c\hbar\,\frac{\mathrm{d}Q(r)}{\mathrm{d}r}+c\hbar\frac{\kappa}{r}Q(r)+\left(-mc^2+E-V(r)\right)\;P(r)=0,
\end{aligned}
\qquad (1)
$$

where E is the total energy of the positron (including its rest energy mc^2) and $\kappa=(2j+1)\cdot(L-j)$, while j and L have their usual meanings [16]. The spherically symmetric potential V consists of static (V_{S}) and polarization (V_{P}) parts

$$
V(r)=V_{\mathrm{S}}(r)+V_{\mathrm{P}}(r). \qquad (2)
$$

In our calculations the static potential V_{S} has been obtained in a standard way [13] using the radial atomic orbitals generated in a single-configuration approximation by the MCDF code of Grant *et al.* [17]. The feature which distinguishes the relativistic polarized orbital method from many other approaches is the fact that in this approximation the polarization potential V_{P} is calculated in a fully *ab initio* manner by solving the coupled Dirac-Hartree-Fock equations [13, 14]. This very laborious work has been done with the aid of a program POLAR [18].

Only the dipole term in the polarization potential has been used in present calculations. The dropping of the other multipole terms is justified by the fact that in the relativistic polarized orbital approximation the non-adiabatic dynamic distortion effects are not taken into account. Far from the atom the scattering potential should be of the form

$$
V(r)=-\frac{\alpha_1 e^2}{2r^4}-\sum_{k=2}^{\infty}\frac{(\alpha_k-6\beta_{k-1})\,e^2}{2r^{2k+2}}, \qquad (3)
$$

where the coefficients α_k and $6\beta_{k-1}$ are both positive and comparable in magnitude. Therefore, neglecting the dynamic distortion effects (i.e. putting $\beta_{k-1}=0$) we were forced to drop out other than dipole contributions to the polarization potential.

Once the scattering potential V is known, the scattering phase shifts δ_κ can be calculated and the relativistic version of the variable phase method has been used for this purpose. In this method one introduces a so-called phase function $\delta_\kappa(r)$ which satisfies a first-order nonlinear differential equation

$$
\begin{aligned}
\frac{\mathrm{d}\delta_\kappa(r)}{\mathrm{d}r}=-\lambda^{-1}\;\frac{V(r)}{c\hbar}\cdot\left[\hat{\jmath}_L(Kr)\cdot\cos\,\delta_\kappa(r)-\hat{n}_L(Kr)\cdot\sin\,\delta_\kappa(r)\right]^2-\\
-\lambda\cdot\frac{V(r)}{c\hbar}\cdot\left[\hat{\jmath}_{L\mp1}(Kr)\cdot\cos\,\delta_\kappa(r)-\hat{n}_{L\mp1}(Kr)\cdot\sin\,\delta_\kappa(r)\right]^2
\end{aligned}
\qquad (4)
$$

with an initial condition

$$
\delta_\kappa(0)=0. \qquad (5)
$$

Here

$$
\lambda=\left(\frac{E-mc^2}{E+mc^2}\right)^{1/2} \qquad (6)
$$

and

$$
K^2=\left(E-mc^2\right)\cdot\left(E+mc^2\right)/(c\hbar)^2, \qquad (7)
$$

while $\hat{\jmath}_L(Kr)$ and $\hat{n}_L(Kr)$ are the Riccati-Bessel functions. In the equation (4) the upper sign ($-$) should be taken for $\kappa>0$ and the lower one ($+$) for $\kappa<0$. Then the phase shift δ_κ can be obtained from the relation

$$
\delta_\kappa=\lim_{r\to\infty}\;\delta_\kappa(r). \qquad (8)
$$

and the total elastic cross section Q_T can be calculated *via* expression

$$Q_T = \frac{4\pi}{K^2} \cdot \sum_{\kappa=-\infty}^{+\infty} |\kappa| \cdot \sin^2\delta_\kappa \tag{9}$$

The variable phase approach offers also a method of calculation of a scattering length a which is defined as

$$a = -\lim_{K\to 0} \frac{\tan \delta_{-1}}{K} \tag{10}$$

In this method the scattering length is calculated by solving the equation [14]

$$\frac{db(r)}{dr} = \frac{2mV(r)}{a_0\hbar^2} \cdot [r \cdot \cos b(r) - a_0 \cdot \sin b(r)]^2 + \frac{V(r)}{2a_0mc^2} \cdot \left[\frac{a_0}{r} \cdot \sin b(r)\right]^2 \tag{11}$$

with an initial condition

$$b(0) = 0 \tag{12}$$

and then using a formula

$$a = a_0 \cdot \tan b(\infty), \tag{13}$$

where a_0 denotes the Bohr radius.

The calculations of the polarization potentials yield as a by-product the electric polarizabilities of the targets. In table I we present the dipole polarizabilities obtained both in the relativistic and nonrelativistic cases. As could be expected, the relativistic effects in target structures are almost negligible for the three lighter atoms while it is evident that they play a significant role for heavier targets. In table I we also list relativistic results obtained in the same approximation by Kolb *et al.* [19]. An excellent agreement between the two sets of relativistic data confirms correctness and accuracy of the program POLAR.

Table I. — *Relativistic and nonrelativistic dipole polarizabilities for alkaline-earth atoms (in a_0^3).*

	nonrelativistic	relativistic	
Atom	present	present	Kolb *et al* [19]
Be	45.62	45.59	45.6
Mg	81.59	81.16	81.2
Ca	185.5	182.8	182.8
Sr	246.0	232.6	232.6
Ba	368.2	324.0	324.0
Ra	441.5	296.2	—

In table II we present calculated values of the positron scattering lengths. Their large positive values signify that scattering potentials can support weakly bound states with binding energies E_b

$$E_b \simeq \frac{\hbar^2}{2ma^2}. \tag{14}$$

Table II. — *Positron scattering lengths a (in a_0) and binding energies E_b (in eV) for alkaline-earth atoms.*

Atom	Present		Kurtz and Jordan [9]	
	a	E_b	a	E_b
Be	67.6	0.003	26.1	0.02
Mg	30.1	0.02	58.3	0.004
Ca	14.3	0.07	82.5	0.002
Sr	12.7	0.08	—	—
Ba	8.6	0.2	—	—
Ra	10.8	0.1	—	—

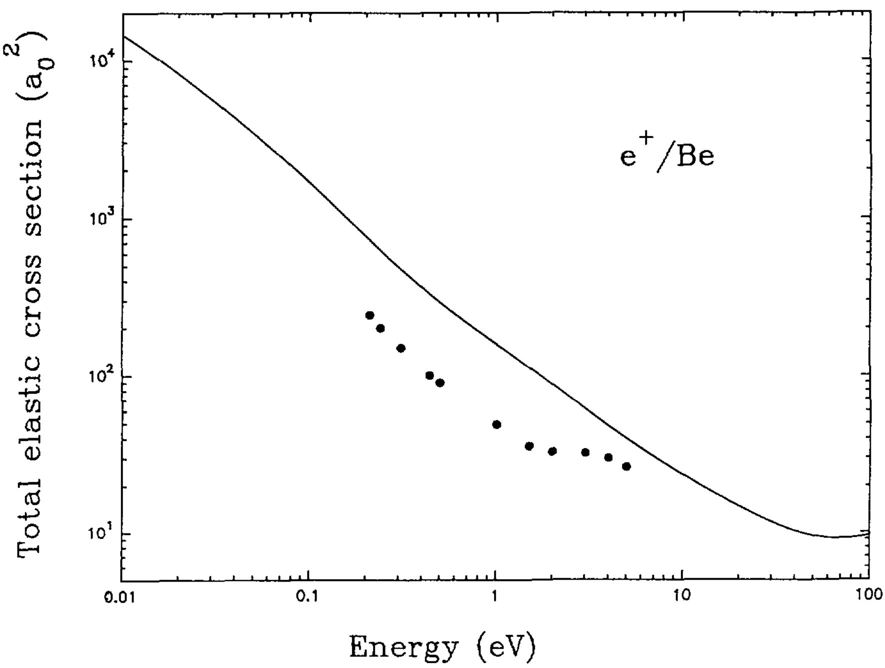

Fig. 1. — Total cross sections for elastic scattering of positrons on beryllium: (—), present; (•), Kurtz and Jordan [9].

The predicted values of E_b are also given in table II where for Be, Mg and Ca they are compared with those obtained by Kurtz and Jordan [9].

The results of calculations of total elastic cross sections for Be, Mg and Ca are presented in figures 1-3, where they are also compared with the theoretical results of Kurtz and Jordan [9] and Khare *et al.* [10, 11]. The results of Kurtz and Jordan are available only at energies varying from 0-5 eV and, as is seen, they are substantially lower than the present results. Moreover,

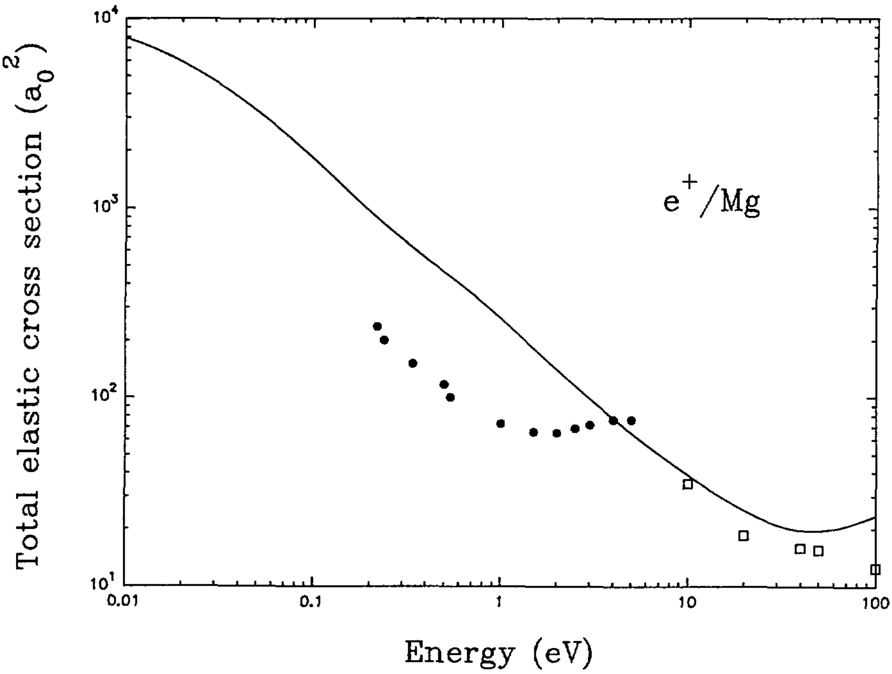

Fig. 2. — Total cross section for elastic scattering of positrons on magnesium: (—), present; (•), Kurtz and Jordan [9]; (□), Khare *et al.* [10].

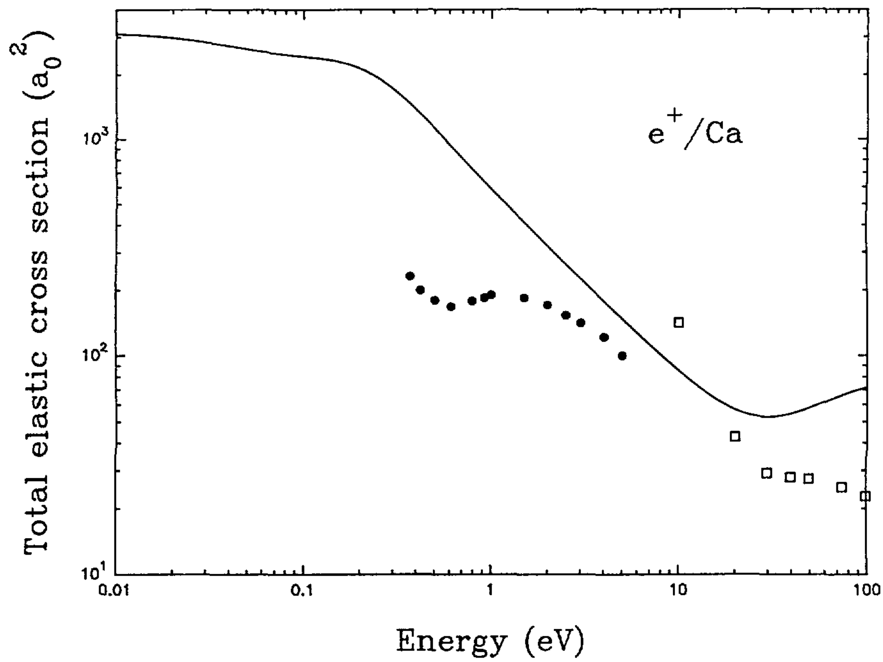

Fig. 3. — Total cross section for elastic scattering of positrons on calcium: (—), present; (•), Kurtz and Jordan [9]; (□), Khare *et al.* [11].

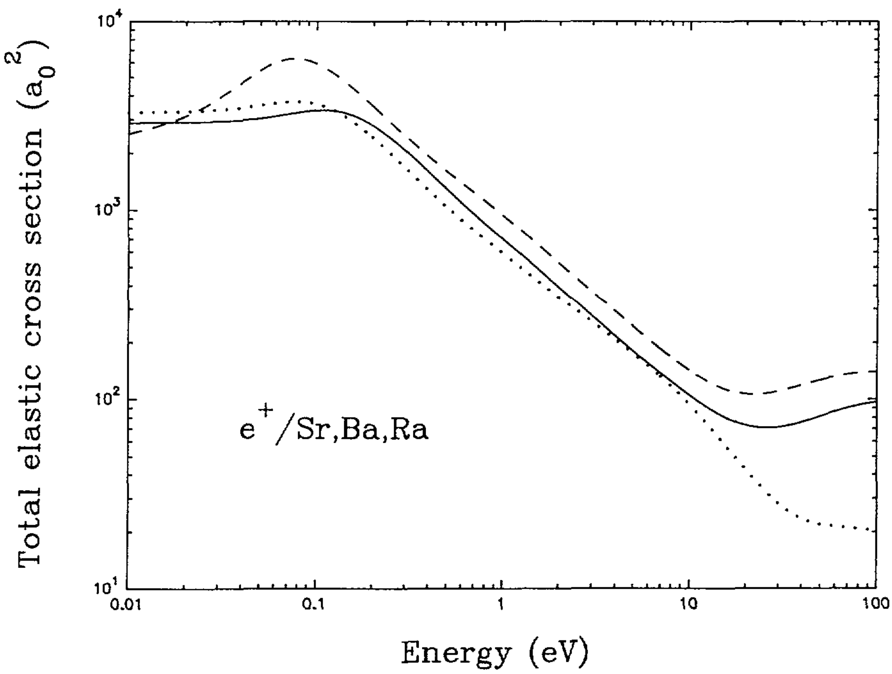

Fig. 4. — Total cross section for elastic scattering of positrons on strontium, barium and radium: (—), Sr, present; (- - - -), Ba, present; (...), Ra, present.

calculations of Kurtz and Jordan predict the existence of the very shallow Ramsauer-type minima for Mg and Ca at energies 0.6 and 1.5 eV, respectively, while our curves decrease monotonically in this energy region. At higher energies differences between present results and those of Khare *et al.* are not so large but still significant. Our results for Sr, the Ba and Ra are plotted in figure 4. For radium the results obtained using the phase shifts of Jaskólski [12] are not shown because of the unreliability of the approximation used in his calculations. No other investigations are available for comparison for these three targets.

We also carried out a number of calculations of differential elastic cross sections at various energies but in view of the lack of relevant experimental data we do not present results here. The numerical values of the phase shifts, differential, total elastic and elastic momentum transfer cross sections are available from the author upon request.

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