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ELASTIC POSITRON SCATTERING FROM ZINC AND CADMIUM IN THE RELATIVISTIC POLARIZED ORBITAL APPROXIMATION

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Results of relativistic calculations on the elastic positron scattering from zinc and cadmium atoms are presented in the low-energy region. The *ab initio* calculated polarization potentials applied in these calculations were obtained by solving the coupled Dirac–Hartree–Fock equations. It is shown that the indirect relativistic effects play an important role in the description of the scattering process. Particularly, relativity has a great influence on values of scattering lengths.

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The relativistic polarized orbital theory of the elastic electron and positron scattering from closed-shell atoms has been formulated some time ago [1] and applied to the low-energy positron scattering from mercury [2] and alkaline-earth atoms [3]. In the present work we extend our previous calculations to positron scattering from zinc and cadmium atoms.

So far, positron scattering from cadmium atoms has been investigated only theoretically. Pangantiwar and Srivastava [4] used an optical real model potential in the Schrödinger equation to obtain cross-sections for elastic scattering in the impact energy range 40–150 eV while Nahar [5] performed model relativistic calculations by solving the Dirac equation for both the elastic and total scattering for energies varying from 6.4 to 300 eV. As far as e^+–Zn scattering is concerned, no other investigations, theoretical or experimental, are available for comparison.

In present calculations the motion of the projectile positron in atomic field is described using the Dirac radial equation

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

where E is the total energy of the positron (including the rest energy mc^2) and $V(r)$ is the central potential which consists of two parts

$$V(r) = V_S(r) + V_P(r). \tag{2}$$

The static potential V_S can be calculated in a standard way [1] using the radial atomic orbitals generated by the MCDF code of Grant et al. [6]. The *ab initio* calculation of the polarization potential V_P is much more difficult and requires solving the coupled Dirac–Hartree–Fock equations [1, 2]. This work was done with the aid of a program POLAR [7]. For the reasons explained in the previous papers [2, 3] we decided to retain only the dipole term in the polarization potential V_P. Once the scattering potential V is known, scattering phase shifts δ_κ can be extracted and for this purpose, instead of solving Eq. (1), the relativistic version of the variable phase method [2] was used. Then the total elastic cross-section was calculated using a formula

$$Q_T = \frac{4\pi}{K^2} \sum_{\kappa=-\infty}^{+\infty} |\kappa| \sin^2 \delta_\kappa, \tag{3}$$

where

$$K^2 = (E - mc^2)(E + mc^2)/(c\hbar)^2. \tag{4}$$

The relativistic formulation of the polarized orbital method gives an opportunity to study the role of direct and indirect relativistic effects in the description of the scattering process. It is well known [8, 9] that in the case of low-energy positron scattering the direct effects are negligible. This is caused by the fact that the Coulomb repulsion between a nucleus and a projectile prevents the latter to penetrate the region near origin where the interaction potential is large. This results in a very small spin–orbit coupling which means that the positron could be described nonrelativistically. Our test calculations confirm this conclusion. Therefore, the only important relativistic effects could be relativistic effects in the target structure.

To study this problem more precisely we performed our calculations using relativistically and nonrelativistically obtained static and polarization potentials (Figs. 1 and 2). The calculations of the polarization potentials yield as a by-product the electric dipole polarizabilities of the targets. This is useful, because to some extent differences between the relativistic (α_R) and nonrelativistic (α_N) polarizabilities can serve as a measure of the importance of the relativistic effects in Zn and Cd atoms. The calculated values of dipole polarizabilities are given in Table I. It is found that the relative differences $\eta = 1 - \alpha_R/\alpha_N$ are 6% and 16% for Zn and Cd, respectively and, as could be expected, the corresponding value is greater for cadmium.

One could naively think that differences between relativistic and nonrelativistic cross-sections should be of the same order as differences between corresponding polarizabilities. In fact, the situation is different in the very low-energy region. To illustrate this let us compare in Table II the relativistically and nonrelativistically calculated scattering lengths a_R and a_N. In the last column we give also the ratio a_R^2/a_N^2. In view of the well known relation between the zero-energy cross-section $Q_T(0)$ and the scattering length a [10]:

$$Q_T(0) = 4\pi a^2, \tag{5}$$

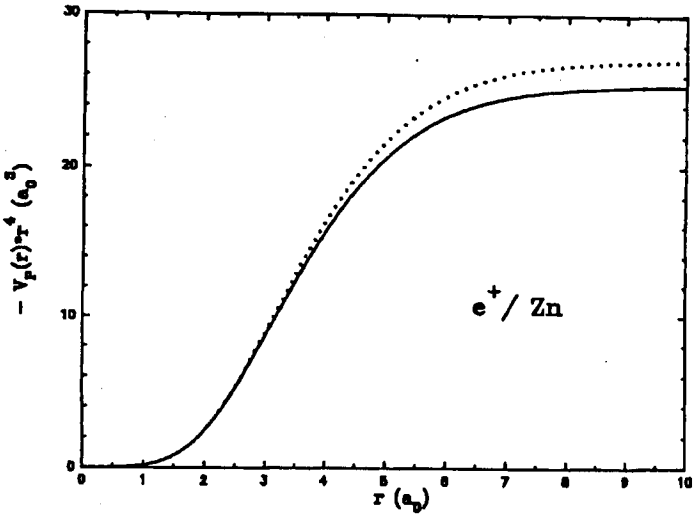

Fig. 1. Dipole polarization potential for zinc: —— relativistic, · · · · · nonrelativistic.

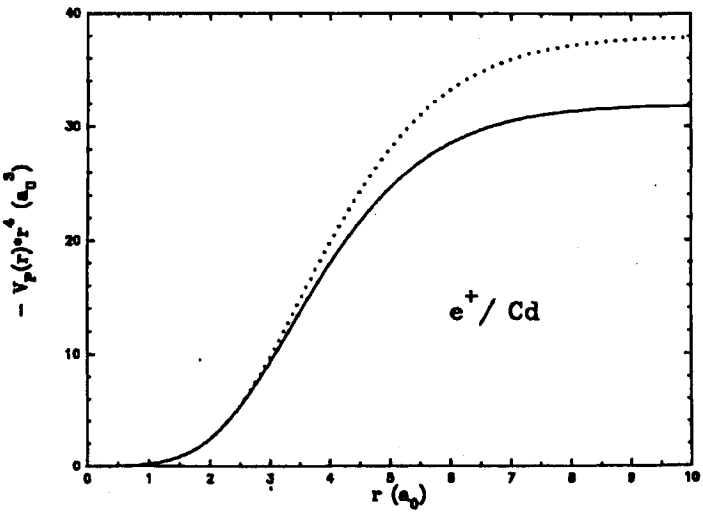

Fig. 2. Dipole polarization potential for cadmium: —— relativistic, · · · · · nonrelativistic.

this ratio is equal to

$$(a_R/a_N)^2 = Q_T^R(0)/Q_T^N(0). \tag{6}$$

As is seen from Table II, there is a large enhancement of the zero-energy scattering in the relativistic case and, at first sight paradoxically, this enhancement is much greater for zinc than for cadmium. This apparent paradox can be resolved if we

TABLE I

Relativistic (α_R) and nonrelativistic (α_N) dipole polarizabilities for zinc and cadmium atoms (in atomic units). Relativistic values agree almost exactly with results obtained in the same approximation by Kolb et al. [11] while nonrelativistic results almost coincide with values calculated by McEachran and Stauffer [12].

Atom	α_R	α_N
Zn	50.81	54.06
Cd	63.68	76.02

TABLE II

Relativistic (a_R) and nonrelativistic (a_N) positron scattering lengths for zinc and cadmium atoms (in atomic units).

Atom	a_R	a_N	$(a_R/a_N)^2$
Zn	1144.3	163.6	48.8
Cd	94.05	42.58	4.9

consider the relativistic changes in terms of positron binding energies. It is well known [10] that the large positive value of the scattering length indicates that the scattering potential supports a weakly bound state of energy

$$E_b \approx \frac{\hbar^2}{2ma^2} = \frac{13.6\,\mathrm{eV}}{(a/a_0)^2}, \tag{7}$$

where a_0 is the Bohr radius. Substituting to the above formula values of the scattering lengths presented in Table II we obtain that relativistically and nonrelativistically calculated positron binding energies are

$$E_b^R \approx 1 \times 10^{-5}\,\mathrm{eV} \quad \text{and} \quad E_b^N \approx 5 \times 10^{-4}\,\mathrm{eV} \quad \text{for zinc,}$$

$$E_b^R \approx 1.5 \times 10^{-3}\,\mathrm{eV} \quad \text{and} \quad E_b^N \approx 7.5 \times 10^{-3}\,\mathrm{eV} \quad \text{for cadmium.}$$

It is evident that an *absolute* change of the binding energy is, as could be expected, greater for heavier cadmium than for zinc but in view of the functional relation between E_b and a the smaller absolute values of E_b for zinc result in much greater change of the scattering length for this atom than for cadmium.

The total cross-sections for elastic e^+–Zn and e^+–Cd scattering are plotted in Figs. 3 and 4. In both cases nonrelativistic cross-sections lie above the corresponding relativistic curves. This is due to more attractive character of the nonrelativistic polarization potentials (see Figs. 1 and 2) resulting in enhanced forward scattering. For cadmium we compare our results with those of Pangantiwar and Srivastava [4] and Nahar [5]. As is seen, the agreement between the

three sets of results is rather poor which is due to differences in employed potentials. It should be pointed that in present calculations we ignored all inelastic and

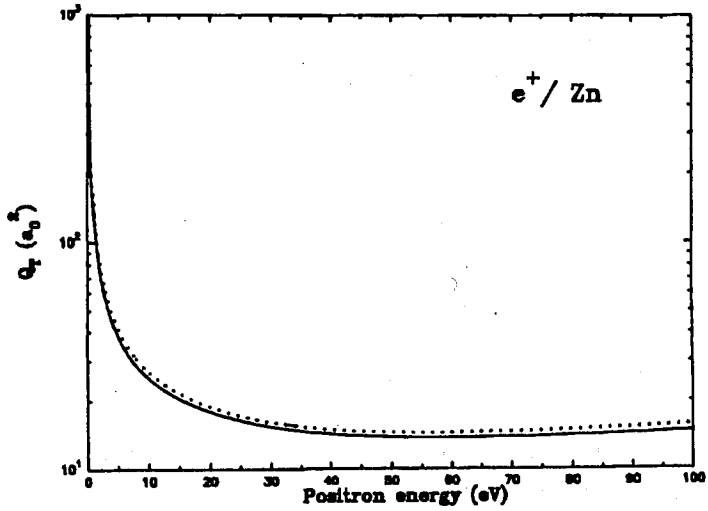

Fig. 3. Total cross-section for elastic positron scattering from zinc: —— present relativistic, · · · · · present nonrelativistic.

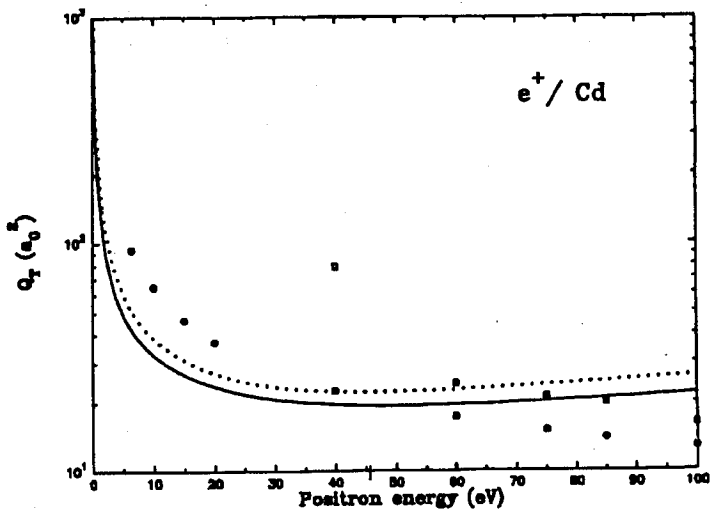

Fig. 4. Total cross-section for elastic positron scattering from cadmium: —— present relativistic, · · · · · present nonrelativistic, □ Pangantiwar and Srivastava [4], • Nahar [5].

rearrangement (Ps formation) open channels [1] and that the same is true for calculations of Pangantiwar and Srivastava. In turn, Nahar took these processes into account representing the positron–atom interaction by a complex potential with a model imaginary part but her approach seems to us to be rather unconvincing. In view of this situation further relativistic *ab initio* calculations including inelastic and Ps formation processes would be highly desirable.

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