Vol. 86 (1994) *ACTA PHYSICA POLONICA A* No. 3

ELASTIC POSITRON SCATTERING FROM KRYPTON AND XENON IN THE RELATIVISTIC POLARIZED ORBITAL APPROXIMATION

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(Received December 27, 1993)

We present results of *ab initio* relativistic calculations on the elastic positron scattering from Kr and Xe atoms in the energy region below 10 eV. The approach employed was the relativistic polarized orbital approximation in which we tried to keep correctly orders of various contributions to positron–atom interaction potentials. In view of the serious disagreement between the present results and experimental data we conclude that the polarized orbital approximation, even in its relativistic version, is not able to provide reliable values of positron scattering cross-sections.

PACS numbers: 34.80.Bm, 34.90.+q

1. Introduction

The relativistic polarized orbital theory of the elastic electron and positron scattering from closed-shell atoms has been recently formulated [1] and applied to the low-energy positron scattering from mercury [2], zinc and cadmium [3] and alkaline-earth-metals [4]. In the present paper we extend our previous calculations to positron scattering from krypton and xenon which enables us to verify our theoretical predictions by comparing them with experimental data.

There has been a lot of interest in positron scattering from krypton atoms. Experimentally, total cross-section measurements were made by Canter et al. [5, 6], Dababneh et al. [7, 8] and Sinapius et al. [9] while Charlton et al. [10] and Diana et al. [11] carried out measurements of the total positronium formation cross-section. Recently, measurements of the elastic differential cross-section were made by Dou et al. [12]. Theoretically, Massey et al. [13], Schrader [14], McEachran et al. [15], Sin Fai Lam [16] and Basu et al. [17] investigated the low-energy total elastic cross-section. Wadehra et al. [18] predicted existence of a critical minimum in the low-energy differential cross-section. Moreover, Schultz et al. [19] and McAlinden and Walters [20] carried out calculations of the positronium formation cross-section while Baluja and Jain [21] reported the total (elastic plus inelastic) cross-sections at intermediate and high energies.

For the case of positron scattering from xenon, the total collision cross-sections for energies of up to 1000 eV were measured by Canter et al. [6], Coleman et al. [22], Dababneh et al. [7, 8] and Sinapius et al. [9] while the total positronium formation cross-sections were measured by Charlton et al. [10] and Diana et al. [23]. On the theoretical side, calculations of the total elastic scattering include those of Schrader [14], McEachran et al. [15] and Sin Fai Lam [16]. The differential cross-sections for elastic scattering at intermediate energies were reported by Hasenburg et al. [24]. Wadehra et al. [18] predicted existence of a critical point in the angular distribution of elastically scattered slow positrons. Moreover, Baluja and Jain [21] presented results of their calculations of the total (elastic plus inelastic) cross-sections in the energy range 20–1000 eV and McAlinden and Walters [20] reported cross-sections for positronium formation.

So far, the non-relativistic polarized orbital calculations of McEachran et al. [15] seemed to be the most sophisticated attempt to describe the elastic positron scattering from both targets. One might suppose that inclusion of the relativistic effects in the description of the considered processes should improve the quite satisfactory agreement between theoretical results of this group and some of the experimental data. However, below we question an internal consistency of the approach used by McEachran et al. and show that the non-relativistic polarized orbital approximation, if correctly used, gives results disagreeing with experimental data and that inclusion of the relativity does not improve a quality of theoretical results.

2. Results and discussion

A detailed treatment of the theoretical and numerical methods used is given in our previous papers [1, 2] and will not be presented here. Calculations of the polarization potentials were performed in the fully coupled approach, i.e. all atomic subshells were allowed to be polarized. In scattering calculations only the dipole terms in the polarization potentials were used with the corresponding relativistic (α_R) and non-relativistic (α_N) polarizabilities $\alpha_R = 16.47a_0^3$ and $\alpha_N = 16.48a_0^3$ for krypton and $\alpha_R = 26.97a_0^3$ and $\alpha_N = 27.10a_0^3$ for xenon.

In Fig. 1a and 1b we compare our relativistic differential cross-sections for elastic e^+–Kr scattering with results of very recent measurements of Dou et al. [12] and theoretical values obtained by this group using non-relativistic phase shifts of McEachran et al. [15]. It is seen that although present results generally agree with experimental data with respect to the shapes, the results based on the phase shifts of McEachran et al. better predict locations of cross-sections minima.

We compare in Figs. 2 and 3 our results of the total elastic cross-sections for Kr and Xe with the calculations of McEachran et al. [15] and Sin Fai Lam [16]. Theoretical results of Massey et al. [13] and Basu et al. [17], for Kr, and Schrader [14], for Kr and Xe, were obtained using semi-empirical potentials and are not shown. First of all it should be noted that while for krypton present relativistic and

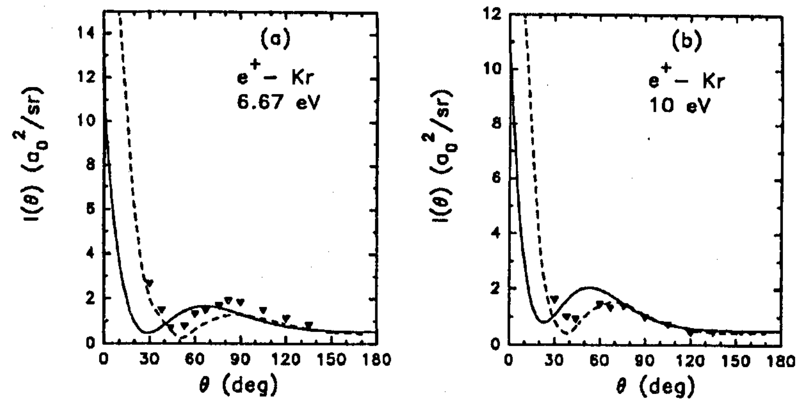

Fig. 1. Differential cross-section for elastic positron scattering from krypton at 6.67 eV (a) and 10 eV (b). Theory: ——, present relativistic; – – – – – –, Dou et al. [12] using non-relativistic phase shifts of McEachran et al. [15]. Experiment: filled ▽, Dou et al. [12].

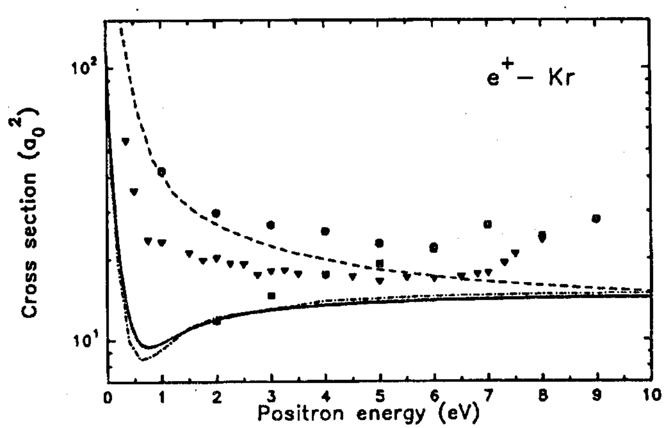

Fig. 2. Cross sections for positron scattering from krypton. Theory (total elastic): ——, present relativistic; · · · · ·, present non-relativistic; – – – – – –, McEachran et al. [15]; – · – · –, Sin Fai Lam [16]. Experiment (total): ■, Canter et al. [5, 6]; filled ▽, Dababneh et al. [7]; •, Sinapius et al. [9].

non-relativistic results almost coincide and both indicate the Ramsauer–Townsend minimum, for xenon both sets of results differ remarkably at energies below 4 eV and only the non-relativistic data exhibit the minimum. As regards comparison with other theoretical data, an overall agreement between present relativistic results and those of Sin Fai Lam [16] should be stressed. That author used in his scattering calculations the Dirac–Hartree–Fock static potentials together with the scaled dipole polarization potentials obtained in the relativistic Pople–Schofield (PS) method [25]. The scaling factors were chosen in such a way that the resulted

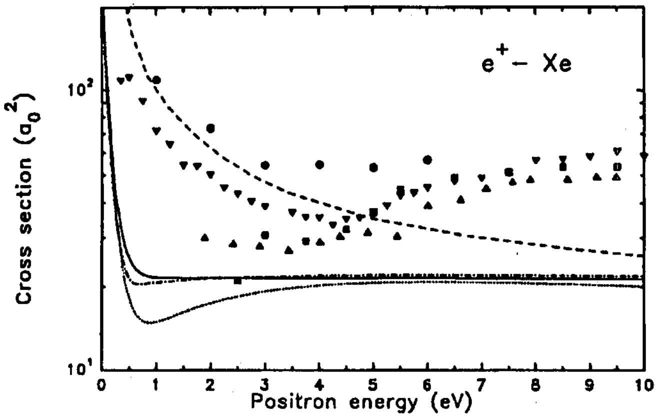

Fig. 3. Cross sections for positron scattering from xenon. Theory (total elastic): ——, present relativistic; · · · · ·, present non-relativistic; – – – – – –, McEachran et al. [15]; – · – · –, Sin Fai Lam [16]. Experiment (total): ■, Canter et al. [6]; filled △, Coleman et al. [22]; filled ▽, Dababneh et al. [7]; •, Sinapius et al. [9].

polarization potentials reproduced the experimental values of polarizabilities. Such good agreement between the two sets of relativistic results can be explained by the conceptual relationship of the relativistic PS method and the relativistic polarized orbital approximation. Some shortcomings of the PS method (which is less sophisticated than the polarized orbital approximation) were overcome by Sin Fai Lam by the scaling procedure which brought the polarization potentials to forms very close to ours.

Turning to comparison with the non-relativistic polarized orbital calculations of McEachran et al. [15] one might be somewhat surprised that their results do not coincide exactly with present non-relativistic data. An explanation is that although in the non-relativistic limit our polarization potential calculations are completely equivalent to the method used by this group, the scattering calculations differ since McEachran et al. retained in their polarization potentials all multipole terms (apart from the monopole ones) while in the present work we have decided to use only the dipole terms. It seems to us, however, that an approach of McEachran et al. is inconsistent with simultaneous neglect of higher order corrections to the projectile–target interaction energy [26]. It is well known [27] 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 other terms than monopole, dipole and quadrupole ones in the polarization potential. 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 [28, 29] that such effects are not negligible. Particularly, monopole and dipole terms in a multipole expansion of the non-adiabatic (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 neglecting the dynamic distortion effects (as it was done in the formulation of the polarized orbital theory) one is forced to drop other than dipole contributions to the polarization potential.

In the same figures we compare the present data with the results of measurements of the total cross-sections performed by Canter et al. [5, 6], Coleman et al. [22], Dababneh et al. [7] and Sinapius et al. [9]. It seems unbelievable that the observed disagreement below positronium formation thresholds (7.20 eV for Kr and 5.33 eV for Xe) could be completely attributed to experimental errors (manifesting themselves in visible scatter between results obtained in different laboratories) and we conclude that it is mainly due to shortcomings of the theory.

In view of the above discussion the quite satisfactory agreement between results of McEachran et al. [15] and experimental data should be attributed to rather fortunate cancellation of dynamic and higher order adiabatic corrections to positron–targets interaction potentials. A failure of our calculations in which we tried to keep correctly orders of various contributions to interaction potentials shows an inapplicability of the polarized orbital theory to provide accurate results on the low-energy positron scattering from atoms.

3. Conclusions

We applied the relativistic version of the polarized orbital approximation to the case of elastic low-energy positron scattering from Kr and Xe atoms. Comparison with available experimental results shows the serious disagreement both for the total elastic and the differential elastic cross-sections. On the theoretical side, our data agree almost excellently with the results obtained by Sin Fai Lam [16] in the relativistic Pople–Schofield approximation but differ seriously from the non-relativistic polarized orbital results of McEachran et al. [15]. We argue that although results of the latter group are in the better agreement with experiment, they were obtained in a methodologically questionable way. We conclude that the polarized orbital approximation does not represent a reliable method for predicting accurate values of *positron* scattering cross-sections.

Despite this fact the relativistic polarized orbital method is interesting in its own right in that it enables one to perform "model" studies on the influence of the relativity on the low-energy positron scattering. Particularly, it was shown that such interesting phenomena as positron attachment to atoms [2] or existence of the Ramsauer–Townsend minima in the total cross-sections might depend on the relativistic effects.

Acknowledgments

This work was supported by the Committee for Scientific Research under grant no PB/0916/P3/92/03. The calculations were performed in the Computer Center at the University of Gdańsk.

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