Semiempirical potentials for positron scattering by atoms

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We report calculations of differential and integral cross sections for positron scattering by noble gas and alkaline-earth atoms within the same methodology. The scattering potentials are constructed by scaling adiabatic potentials so that their minima coincide with the covalent radii of the target atoms. Elastic differential and integral cross sections are calculated for Ne, Ar, Be, and Mg, and the results are very close to experimental and best theoretical data. Particularly, elastic differential cross sections for Be and Mg at low energies are reported.

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I. INTRODUCTION

Positron scattering by atoms has been subject to intensive experimental and theoretical research in recent years. Despite these efforts, theory in this field still fails in giving a proper account to low-energy elastic cross section measurements [1]. Remarkably, diverging results have been presented even for the simplest problems, such as the total elastic cross section (TECS) from helium target.

The detailed interaction of a positron with electrons and nuclei is quite complicated, so it becomes extremely attractive to search for methodologies in which the scattering dynamics can be described through a preferably *ab initio* positron-target local potential (depending only on the positron coordinates). This fact gives theorists in the field a double challenge: to produce potentials simple enough to be useful but, at the same time, able to describe an involving interaction. To the best of our knowledge, two such approaches appeared in the literature: One is the model potentials for rare gas targets from Gianturco *et al*. [2] in which the repulsive part is obtained exactly at the Hartree-Fock level and the attractive polarization and correlation parts come from approximate density functional theory. The other is from Bromley *et al*. [3], applied to Be and Mg targets, in which free parameters of the potentials are adjusted to reproduce calculated positron binding energies for e^+Be and e^+Mg, as in Fig. 1 complexes. Despite the important progress reported by both approaches, they are clearly limited to particular targets or to cases in which positron binding is predicted.

We have already reported on the generation of adiabatic potentials in which the positron is treated on a common footing with the nuclei, which were applied to different processes involving a positron, such as binding energies, annihilation rates, and molecular properties relaxation [4–6]. They are expected to display the correct repulsive behavior as well as the polarization effects and they generate TECSs that show a proper qualitative dependence with incident energy. Nevertheless, the total TECSs appear too large, probably due to the lack of positron-electron correlation on a nonadiabatic level. In this paper we develop these potentials further by introducing an empirical nonadiabatic scaling that accounts for further positron-electron correlation. Applications are made to Ne, Ar, Be, and Mg targets.

A few theoretical applications are found for Be and Mg among which we can mention the distorted-wave polarized orbital method from Szmytskovisk [7], the already cited calculations from Bromley *et al*. [3], the low-energy many-body perturbation theory application by Gribakin *et al*. [8], and the orbital polarized method by Drachman *et al*. [9] and by Campeanu *et al*. [10], only for Mg. Measurements have been made by Stein *et al*. [11] with incident energies above 2 eV. As for noble gases we detected the measurements by Stein *et al*. (for Ne) [12], Charlton *et al*. [13], Coleman *et al*. [14], Kauppila *et al*. [15]; Kauppila *et al*. [16] (for Ar) (showing the Ramsauer minimum), Coleman *et al*. [17] and Kauppila *et al*. [18]. Theoretical works were from McEachran *et al*. (for Ne) [19], McEachran *et al*. (Ar) [20], based on the polarized orbital approximation; McEachran and Stauffer (Ar) based on an optical potential including absorption [21]; Nakanishi and Schrader (Ne and Ar) [22,23] with polarized orbital approximation plus an effective radius for the target; the already cited work by Gianturco *et al*. [2] and theeikonal Born series method by Byron *et al*. (Ne) [24]. Finally, a recent experimental and theoretical paper has been published by Jones *et al*. on Ne and Ar [25].

II. CONSTRUCTION OF ADIABATIC POTENTIALS AND THE SCATTERING DYNAMICS

The first step in the construction of potentials for positron interaction with an n electron atom is to consider the positron

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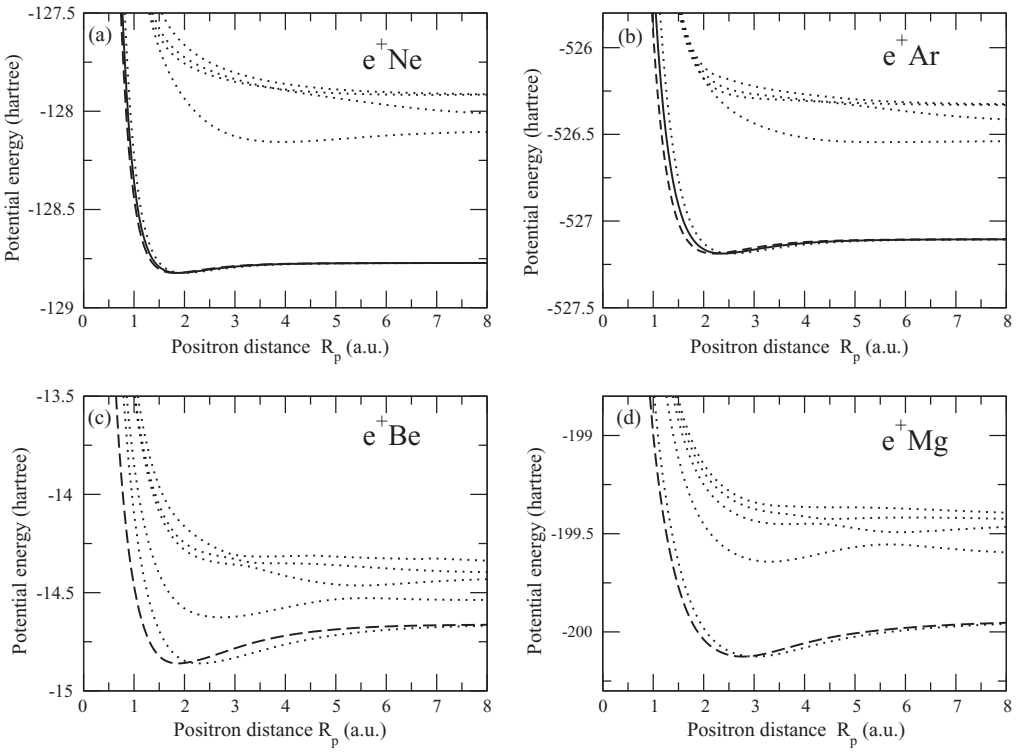

FIG. 1. Potential energy curves for all systems: $\cdots$ nonscaled PEC ($\lambda = 1.0$) for ground state and low-lying excited PECs; scaled ground state PEC for (a) $- - --$, $\lambda = 1.10$ and —— $\lambda = 1.06$, (b) $- - --$, $\lambda = 1.16$ and —— $\lambda = 1.08$, (c) $- - --$, $\lambda = 1.23$, and (d) $- - --$, $\lambda = 1.08$.

on the same footing of the nucleus (both represented generically by A) and to take advance of a previously introduced electronic Hamiltonian (in atomic units, a.u.) [26] given by

$$H_{\rm el} = \sum_{A}^{2}\left(-\sum_{i}^{n} P_A \frac{\nabla_i^2}{2M_A} P_A\right) - \sum_{i}^{n}\frac{\nabla_i^2}{2} + V. \qquad (1)$$

Here M_A represents the mass of the standard and the exotic nucleus (e^+), $P_A = |\phi_A\rangle\langle\phi_A|$ projects a generic electronic wave function on the space of the atomic-like wave functions ϕ_A, centered on A, and V stands for the Coulombic attraction and repulsion terms. The last two terms in Eq. (1) correspond the common Born-Oppenheimer Hamiltonian. The first term stands for adiabatic corrections of atomic character, since the projections impose its crossing atomic ($B \neq A$) matrix elements to vanish. This correction is equivalent of changing the masses of all electrons [27] in order to keep the center-of-mass of the whole system at rest. Particularly when $A = e^+$, the correction energy term becomes $-\langle\phi^i_{e^+}\sum_i^n \frac{\nabla_i^2}{2M_{e^+}}\phi^i_{e^+}\rangle$, that is, the i electron occupying an orbital $\phi^i_{e^+}$ centered on e^+ is given the appropriate reduced mass, a huge correction since M_{e^+} is the same as the electron mass.

TABLE I. Scaling data for each system [all defined in text, see particularly Eq. (6)]. Distances are in a.u.

	Ne	Ar	Be	Mg
R_m	2.00	2.55	2.30	3.03
$R_{\rm cov}$	1.81[a]	2.19[b]	1.87[b]	2.79[b]
$\lambda_{\rm cov}$	1.10	1.16	1.23	1.08
$\lambda_{\rm opt}$	1.06	1.08	–	–
$R_{\rm opt}$	1.90	2.35	–	–

[a]Reference [34].
[b]Reference [35].

In the adiabatic approximation, we consider that the relative nucleus-positron motion can be separated from the electronic motion. The full Hamiltonian is taken as having the form $H = T_A + H_{\rm el}$, where the first term stands for the kinetic energy of the nucleus and the positron. The total wave function is then

$$\Psi(R,\vec{r}) = \chi_A(R)\phi_{\rm el}(\vec{r};\overline{R}), \qquad (2)$$

in which R represents the nuclei-positron distance, χ_A is the unknown scattering (or eventually bound state) wave function, and $\overline{R}$ means parametric dependence on R. The electronic function $\phi_{el}(\vec{r};\overline{R})$, in which $\vec{r}$ represents all electrons is obtained by the minimization of the functional

$$E_{\rm el}(R) = \frac{\langle\phi_{\rm el}|H_{\rm el}|\phi_{\rm el}\rangle}{\langle\phi_{\rm el}|\phi_{\rm el}\rangle}. \qquad (3)$$

Finally, the potential energy curve (PEC) is obtained as

$$U(R) \equiv E_{\rm el}(R) + V_A, \qquad (4)$$

in which V_A represents the nucleus-positron repulsion.

Standard approximations involve the construction of the positron-target potential by partitioning it in a static part, containing all Coulombic interactions, and a correlation-polarization potential, describing electron-positron correlations, that is, $V(R) = V_{\rm est}(R) + V_{\rm corr,pol}(R)$. The static

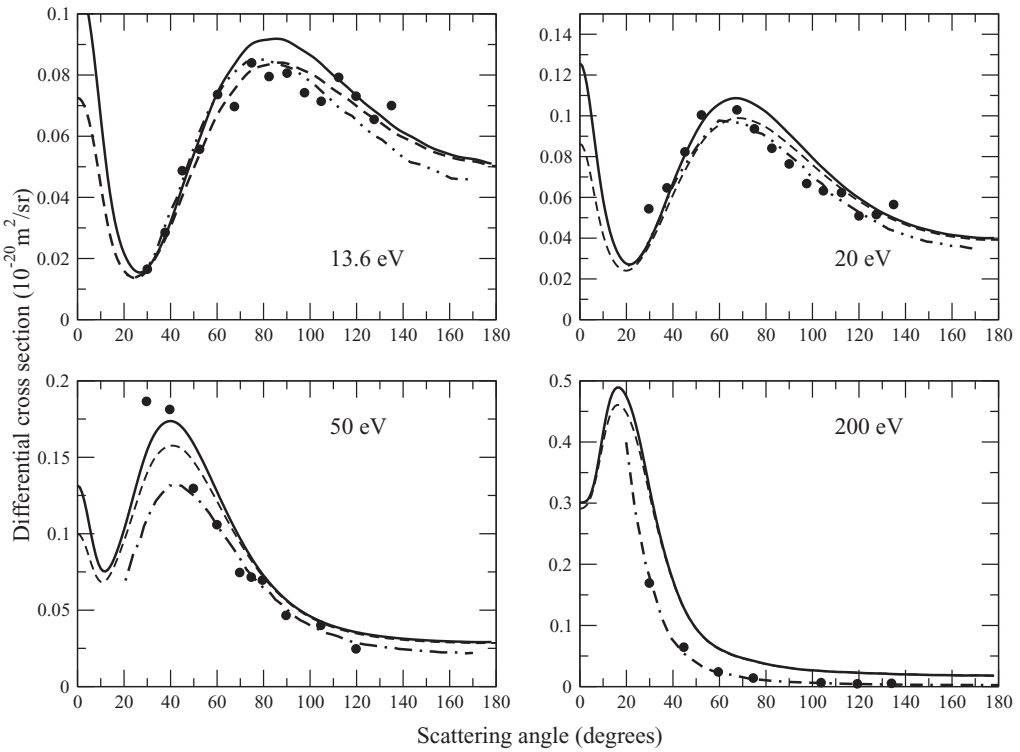

FIG. 2. Differential cross section for positron scattering from neon at some energies. Theoretical curves: present work – – –– ($\lambda = 1.10$) and —— ($\lambda = 1.06$); – · · – · · – from [19]; – · – · – from [22]; and – – · – – · –– from [24]. Experimental data: • • • from [15]. All data taken from [15].

potential is constructed by bracketing the Coulombic terms with the electronic ground state target wave function. For the correlation-polarization potential two main approaches have been tried, namely the multichannel methods, involving excited target wave functions [21], and the use of empirical potentials $V_{\rm corr,pol}(R)$ [2,3]. In the present approach the basis wave functions refer to the whole system, so that an *ab initio* adiabatic potential $U(R)$ is straightforwardly yielded as explained above. On the other hand, to take advantage of standard computational codes based on the cited partition, in which $V_{\rm est}(R)$ is generated automatically by the codes, we just define our effective correlation-polarization potential as $V_{\rm corr,pol}(R) = U(R) - V_{\rm est}(R)$ and add it *a posteriori* to $V_{\rm est}(R)$.

The scattering wave function $\chi(R)$ is then expanded in partial waves $u_l(R)$, as usual, to get the radial equation (a.u.)

$$\left[\frac{d^2}{dR^2} + k^2 - 2V(R) - \frac{l(l+1)}{R^2}\right] u_l(R) = 0 \qquad (5)$$

($k = \sqrt{2E}$, E being the energy of the incident positron).

Since the problem has already spherical symmetry, the identification $\chi_A(R) \equiv u_l(R)$ for each value of the angular momentum quantum number l holds. To obtain the differential elastic cross sections (DECSs) and TECSs, we consider just the ground state PEC and Eq. (5) is solved by the R-matrix method [28] within the pseudostate algorithm of Walters *et al.* [29,30]. The partial waves are obtained for l up to 25.

A. Scaling the potentials

The crude adiabatic potentials described above account for the scattering physics, namely, the TECS has a qualitative correct dependence on the incident energy, but at too high values. The apparently obvious reason for this misbehavior is the lack of nonadiabatic positron-electron correlation in the adiabatic PEC. This hypothesis is supported by the fact that this wrong raising of the TECS is observed as being somehow proportional to the number of electrons of the target. The *ab initio* inclusion of nonadiabatic effects should involve excited PECs or a previously obtained effective mass for the projectile [31], formidable tasks capable of compromising the simple model of positron scattering in a single potential. Instead, we resort here to an empirical scaling of $V(R)$ that improve nonadiabatic positron-electron correlation, namely,

$$V_{\rm esc}(R) \equiv V(\lambda R), \qquad \lambda_{\rm cov} = \frac{R_m}{R_{\rm cov}}. \qquad (6)$$

Here R_m corresponds to the minimum distance in the PEC and $R_{\rm cov}$ is the so called covalent radius, roughly half of the bond distance of the molecule formed by two target atoms.

The major effects of such scaling are moving R_m to effective lower values ($\lambda > 1$), and improving the attractive part of the PECs (see Fig. 1).

The introduction of an effective reduced radius for the target can be traced back to the works of Nakanishi *et al.* [22,23], based on a model polarization potential, aimed at reproducing established reference values for scattering lengths and binding energies for both positron and electron projectiles.

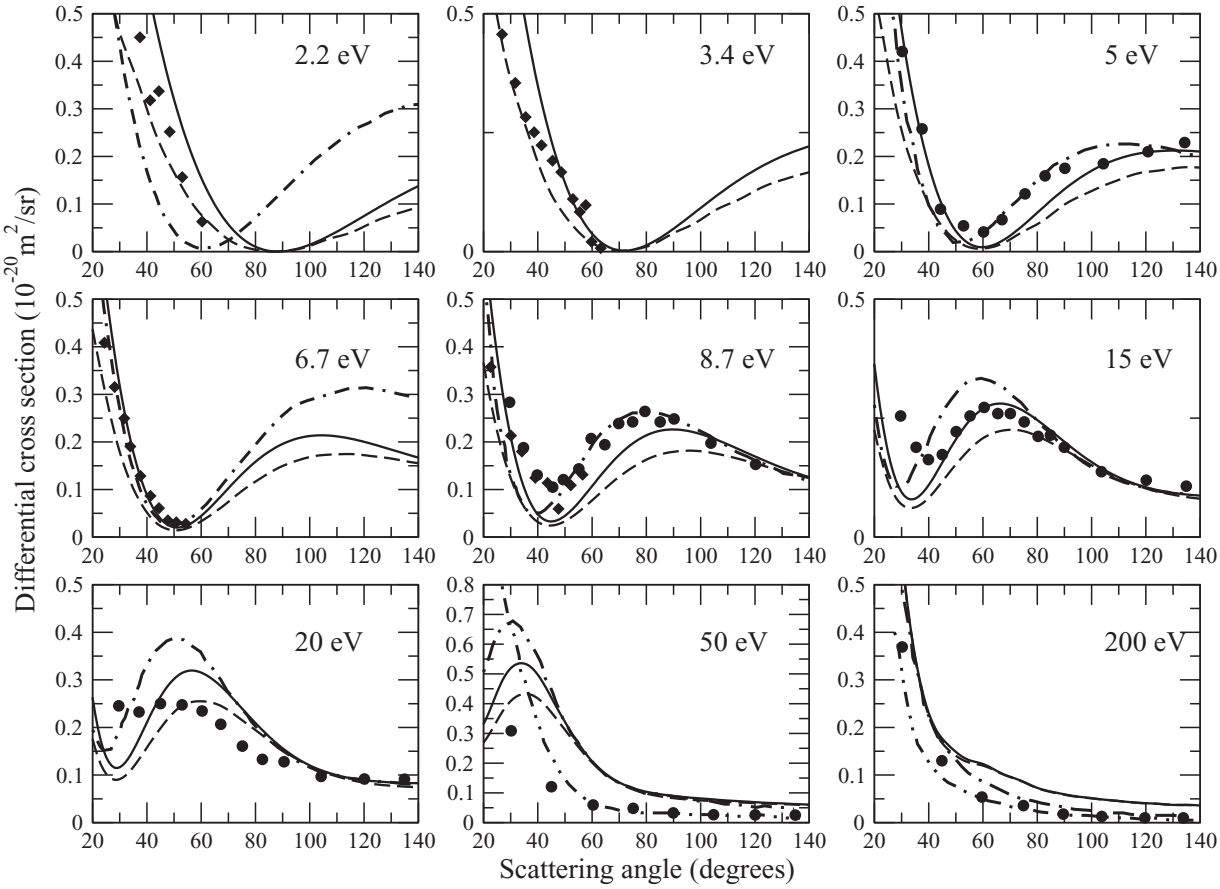

FIG. 3. Differential cross section for positron scattering from argon at some energies. Theoretical curves: present work – – –– ($\lambda = 1.16$) and —— ($\lambda = 1.08$); – · – · – (without absorption) and – · · – · · – (with absorption) from [21];– – · – – · –– from [2]. Experimental data: ● ● ● from [18]; ♦♦♦ from [17].

In the present application the positron, a light nucleus, is able to modify the size of the target by attracting its electronic cloud [5,32,33] while extruding the positive nuclei, so the main region of interaction needs to be larger than the usual atomic radius (in agreement with [22,23]). Without scaling ($\lambda = 1$), the minimum of the PEC is outlying to the target atomic radius,

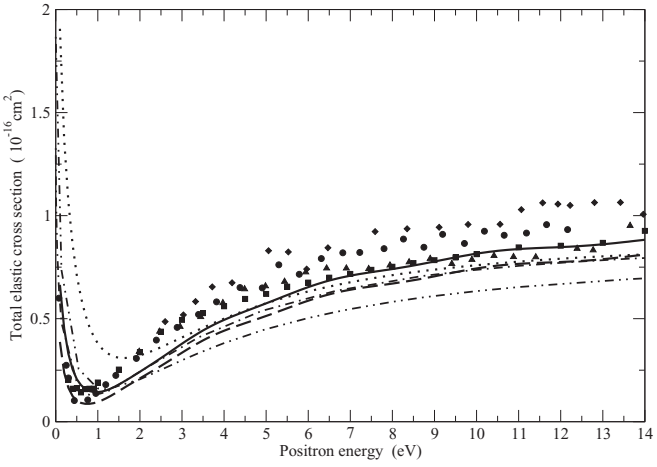

FIG. 4. Total elastic cross section for positron scattering from neon. Theoretical curves: present work · · · · ($\lambda = 1.00$), – – –– ($\lambda = 1.10$) and —— ($\lambda_{opt} = 1.06$); – · · – · · – from [19]; – · – · – from [23]. Experimental data: ● ● ● from [12]; ♦♦♦ from [13]; ▲▲▲ from [14]; ■■■ from [25].

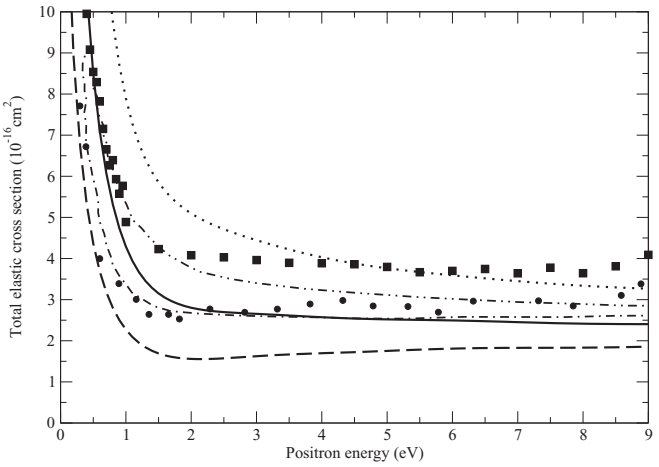

FIG. 5. Total elastic cross section for positron scattering from argon. Theoretical curves: present work · · · · ($\lambda = 1.00$), – – –– ($\lambda = 1.16$) and —— ($\lambda_{opt} = 1.08$); – · · – · · – from [20]; – · – · – from [23]. Experimental data: ● ● ● from [12]; ■■■ from [25].

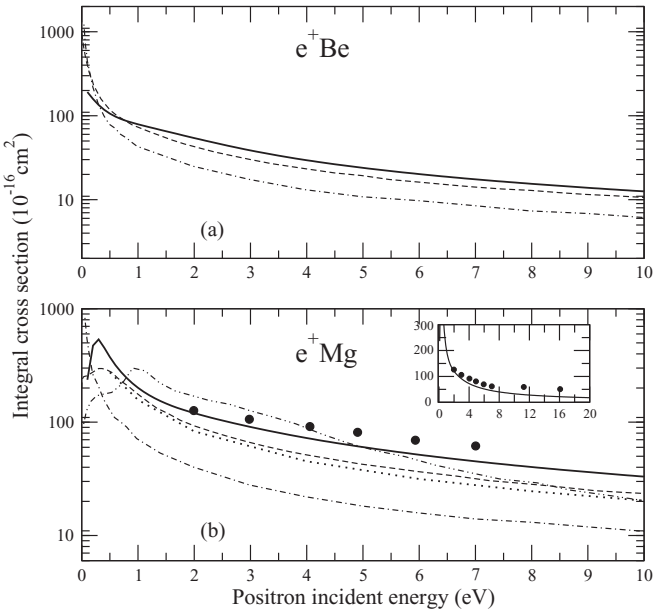

FIG. 6. Total elastic cross section for positron scattering by beryllium: —— present work for scaled PEC ($\lambda = 1.23$); – · – · – from [7]; - - - - from [3] and magnesium: —— present work for scaled PEC ($\lambda = 1.08$); – · – · – from [7]; – · · – · · – from [8]; - - - - from [3]; · · · from [10]; and • • • experimental data from [12]. The inset compares the present results with experimental data [12] in detail.

which results in a repulsive range larger than the actual one and responsible for the increased TECSs. In most cases we found it appropriate to scale the PEC so that its minimum coincides with the covalent radius [34]. With this choice, the short-range nonadiabatic correlation effects are accounted for.

We restrict ourselves to low-energy elastic positron scattering, so only the ground state PECs need to be scaled (as shown in Fig. 1. Table I supplies all data used in the scaling procedure. For all systems considered here, the new minima decrease by about 10% –20%, but the covalent radii keep still larger than the atomic radii: 60% larger for Ne, 38% for Ar, 11% for Be, and 2% for Mg. For comparison, Nakanishi's effective radius for Ne is 45% above the atomic radius.

In the applications we also discuss the possibility of an optimal (though somewhat arbitrary) choice of $\lambda\ (= \lambda_{\rm opt})$ to achieve a fit to some set of experimental results. Table I also shows the corresponding [in the sense of Eq. (6)] values for the optimal distances $R_{\rm opt}$.

III. RESULTS

A. Positron scattering from neon and argon

Figure 2 displays our results for DECSs of a low-energy positron elastically scattered from neon at 13.6, 20, 50, and 200 eV and compares them with previous calculations and measurements. Our results compare well with all data, especially at low incident energy. Particularly for 13.6 eV we were able to reproduce the single minimum around 20°, which might be expected in positron scattering from noble gases [2].

In Fig. 3 we show the DECSs of a low-energy positron scattering by the argon target from 2.2 to 8.7 eV and also at intermediate energies 15, 20, 50, and 300 eV, and compare them with recent theoretical calculations fromRef. [21] and

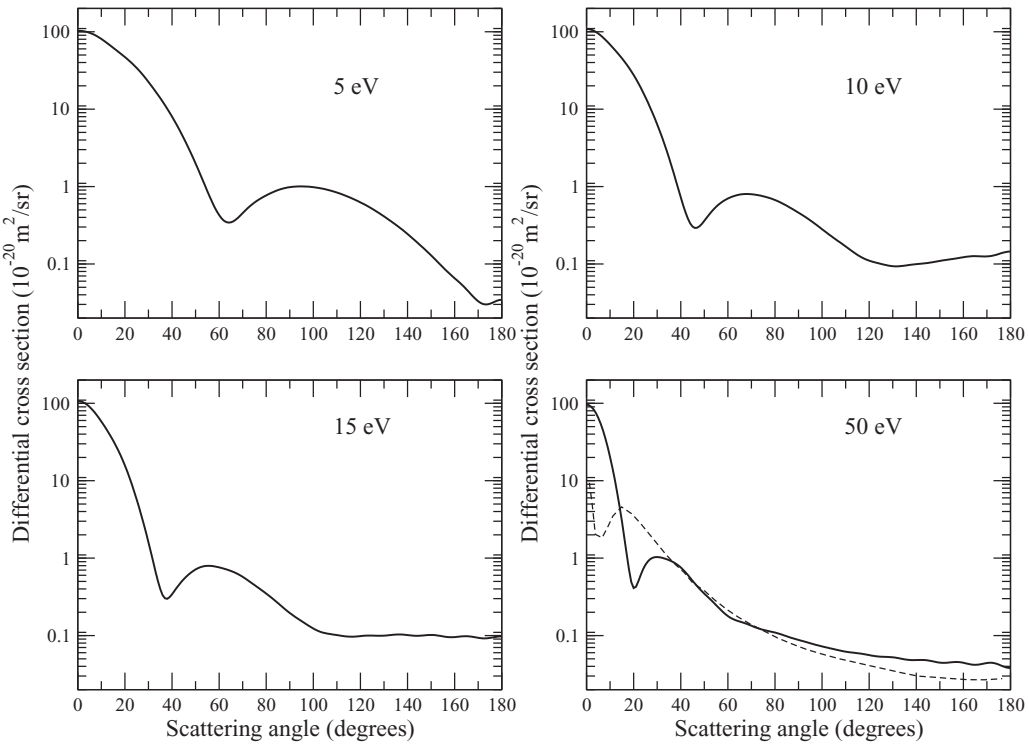

FIG. 7. Differential cross section for positron scattering by Mg at some energies: —— present work for scaled PEC ($\lambda = 1.08$) and - - - - from [37].

experimental data by [18] and [17]. McEachran's results [21] are normalized at 90° to Kauppila's measurements [18] for each energy. As expected, a single minimum is observed around 90° at 2.2 eV, which moves to smaller angles as the positron incident energy increase. This feature is also reported by McEachran *et al.* [21] within their optical model. There are agreement between our results and the experimental and theoretical results for small energies, except for the appearance of minima for 20 and 50 eV, which is likely to be accounted for only with the inclusion of an absorption term in the interaction Hamiltonian [21].

Figures 4 and 5 show the TECSs for positron elastic scattering from Ne and Ar, respectively, up to the positronium (Ps) formation threshold. The unscaled ($\lambda = 1$) result is shown for illustration purpose, while the λ_{opt} result present a slight improvement over the λ_{cov} result. Measurements from Stein *et al.* [12] reported a deep Ramsauer-Townsend minimum of 0.1×10^{-16} cm^2 for the Ne target, around 0.6 eV. McEachran's [19] minimum lies at 0.85 eV while Nakanishi's [23] minimum lies in the vicinity of 1.23 eV. Our minimum lies at 0.8 eV, 25% above the experimental result, and amounts 0.0867×10^{-16} cm^2, only 13% smaller than experiment and 6% better than the best theoretical result so far [19]. From 5 eV up to the Ps formation threshold our results agree almost exactly with McEachran's and are closer to experiments than Nakanishi's.

For the Ar target, our λ_{cov} calculations provide the shallow minimum around 2 eV that is observed in the experimental data from Stein *et al.* [12,16] but is not obtained in any other calculation except that from Gianturco *et al.* [2] which, however, locates it quite apart from that observed. On the other hand, the cross sections for λ_{cov}, though qualitatively good, depart about 33% below from experiment for energies larger than 1 eV. In this case it becomes clear that the covalent radius is not the better choice to fix λ. The λ_{opt} procedure greatly improves the experimental agreement but, unfortunately, makes the minimum vanish. It appears that a more sophisticated scaling procedure should be considered to account for both features.

B. Positron scattering from beryllium and magnesium

Figure 6 shows the TECSs for positron scattering from Be and Mg, compared to previous results. In the Be case, unfortunately, no experimental data for comparison were found, but our results are very close to the previous two calculations from Refs. [3] and [7], diverging significantly from Bromley's just for very small energies. On the other hand, the present results for positron scattering from Mg at energies higher than 2 eV represent nearly full agreement to experimental data [11] so far, as illustrated in the inset. For energies lower than 2 eV we are in agreement with other theoretical approaches, except Szmytkowski's, in obtaining a peak of the TECS. We found this peak around 0.3 eV (below the first inelastic threshold of 0.84 eV). It could be connected to the recent proposal by Mitroy *et al.* [36] of a prominent *p*-wave shape resonance in the TECS at 0.096 eV.

In Fig. 7 we show the DECSs for positron scattering from Mg at low incident energies. To the best of our knowledge, there is no theoretical or experimental data to compare besides the single calculation by Khare *et al.* [37] at 50 eV. For all energies our results present a minimum that moves to smaller angles as the energy increases but, however, differs from Khare's in its position for the 50 eV case. Elsewhere the agreement of the DECSs is considerable.

The DECSs for positron scattering by the Be target is depicted in Fig. 8, having a similar behavior to the Mg case. No

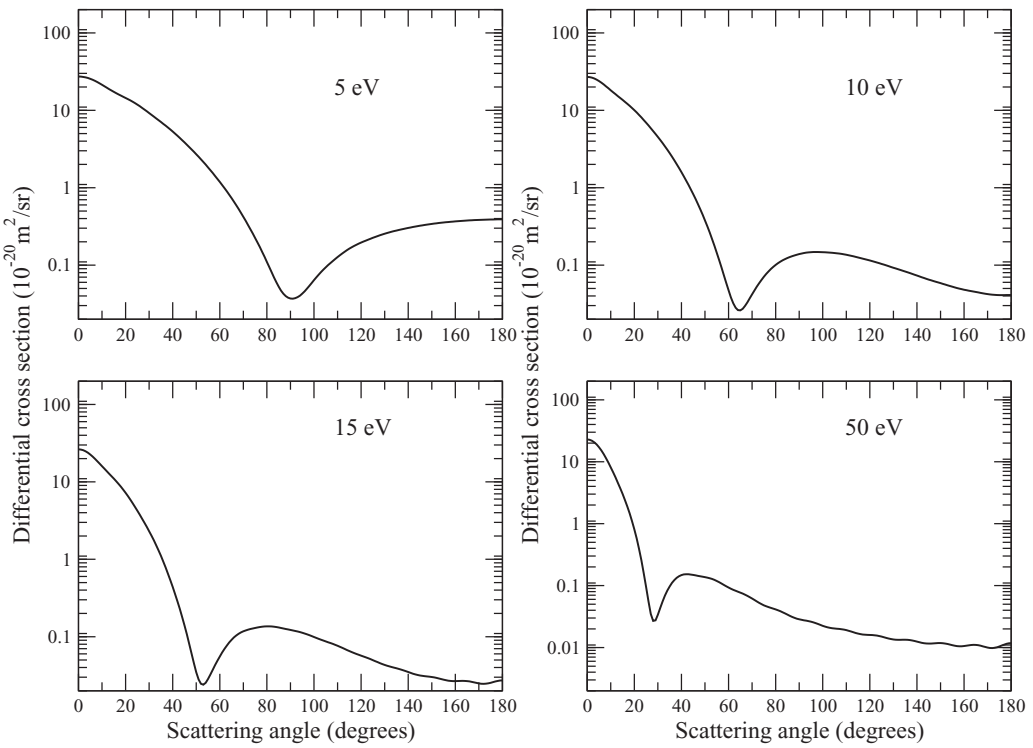

FIG. 8. Differential cross section for positron scattering by Be at some energies for scaled PEC ($\lambda = 1.23$).

other calculations or measurements were found to be compared with our results.

IV. DISCUSSION

Regularly the present potentials seem to behave better than other theoretical approaches for small positron incident energies, where it reproduce details of the DECSs and TECSs not present in most other calculations. Particularly the present calculations of DECSs for the Ar target at 2.2 and 3.4 eV (see Fig. 3) are the only ones at these energies and their agreement with experiments is remarkable. This feature can be connected to an almost exact long- and medium-range behavior of the potentials, where they are able to describe properly the two main components of the wave function, namely the Ps cluster polarized by the ionized atom or the bare positron polarizing the neutral atom. The agreement with the "polarization range" of the PEC is also illustrated by the fact that we do not have to add the empirical α/R^{-4} term (where α is the isotropic atomic polarizability) which is present in almost all other calculations.

It should be noted that, though being a clear correlation effect, virtual Ps formation (that is, a component of the wave function) is contained already in the adiabatic potentials.

As for the scaling procedure, that becomes necessary to adjust DECSs and TECSs as long as the number of electrons becomes larger than a few, we have shown that the scaling factor λ can be fixed by an ad hoc criterion, so to access the predictive capacity of the method, or by fitting it to agree better with experiments, in order to yield useful potentials to further calculations. It is important to observe that noble gases and alkaline-earth-metal atoms are reasonably different elements concerning chemical and physical properties, and the open possibility of treating them within a common methodology might be seen as progress. On the other hand, the direct proportionality of the TECSs with the number of electrons, assumed for the scaling based on atomic or covalent radii, seems to be still a little crude and behind the failure in predicting the Ramsauer minimum of the TECS of Ar. It seems that a more involving model that considers the details of the atomic electronic structure can further improve the present approximation.

ACKNOWLEDGMENTS

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