Positron scattering from krypton and xenon

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The elastic scattering of positrons from the heaviest noble gases has been formulated by using a parameter-free semiclassical model for the polarization forces in the short- and intermediate-range distances. The exact Coulomb repulsive interaction has been obtained from self-consistent-field wave functions of near-Hartree-Fock quality and the scattering equations have been solved over a broad range of collision energies. The elastic integral cross sections agree well with experiments in spite of the great simplicity of the employed computational model. Angular distributions also compare favorably with available experiments and the relative importance of various second-order corrections is discussed in relation to their bearing on the final results.

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I. INTRODUCTION

The low-energy scattering of positrons from atomic targets in the gas phase still constitutes a very sensitive test for atomic interactions and for studying the effects of a positive probe on the dynamic response functions of many-electron target systems. In particular, the behavior of the simpler elastic cross sections, integral and differential, below the thresholds of the formation of additional bound particles, i.e., of either positronium (ps) or of positron-atom bound states, is also an ideal ground for testing possible descriptions of the interaction forces within nonrelativistic quantum dynamics.

It is well known in fact that the behavior of low-energy electrons in collisions with atoms and molecules is controlled by three kinds of interactions: electrostatic, exchange, and polarization [1–3]. Outside the region where the target charge density is localized, a region usually referred to as the "target core," the latter interaction can be understood as an induced effect arising from distortions of the molecular electronic wave function by the charged projectile, be it negatively or positively charged [4]. Rigorously speaking, this effect arises in quantum collision theory as virtual excitations of closed electronic states, including in principle those in the continuum [5]. In practice, however, the infinity of such states precludes treating polarization rigorously. Considerable effort has therefore been expended in the past three decades trying to include it as accurately as possible, albeit not rigorously.

In the case of the positron projectile, on the other hand, the absence of some nonlocal effects such as the exchange interaction should make the treatment of its low-energy scattering from many-electron atoms less difficult in principle and computationally less demanding in practice. The electrostatic interaction can in fact be treated exactly and therefore the way one handles the polarization effects plays an essential role in deciding on the quality of the employed theoretical model.

As in the case of an impinging electron, what makes this so difficult is not the representation of the distortion of the target electronic density as function of a charge fixed some distance away from the origin of all charges but rather the additional effects which come into play near and within the target core mentioned before. At large distances from the core in fact the velocity of the slow positron can be considered low enough that the bound molecular electrons respond adiabatically to the impinging projectile without specific dependence on its local velocity [6]. As the projectile nears the target, however, the repulsive Coulomb core further slows it down while the attraction from the bound electrons increases and strongly modifies its asymptotic motion via correlation processes similar to multiple-scattering effects [7]. The polarization potential at short range is therefore not only energy dependent but also nonlocal. In the case of the scattering of electrons a further complication comes from when the projectile's wave function strongly overlaps the target core: in that instance the scattering electron loses its identity, the independent-particle model breaks down, and many-body effects predominate.

In conclusion, in the cases of both electron and positron scattering one distinguishes a long-range region of interaction where perturbative polarization effects are dominant. The ensuing interaction acquires a local form which is adiabatic on the projectile's velocity and independent of the sign of its charge [8]. In addition the intermediate- and short-range regions of interaction are where nonadiabatic nonlocal effects play an important role and where differences appear between the behaviors of electrons and positrons as projectiles [9].

In order to devise simpler ways of handling the polarization forces over the whole range of relative distances various approaches have been tried in recent years, either

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by designing an effective optical-potential form [10–13] or by developing model potentials that strive to treat the single-particle aspects of this phenomenon as accurately as possible while approximating short-range many-body core-polarization effects [14–16]. Ideally, such model correlation-polarization potentials should be free of parameters which need adjustment to experimental cross sections, and it is in this sense that they are often described as *ab initio* potentials.

In the present work we discuss a model potential to treat both polarization forces in the long-range region and correlation-polarization forces in the intermediate- and short-range regions of interaction for the scattering of slow positrons from complex, rare-gas atoms in their ground electronic states. We will show that such a potential requires very little computational effort for its implementation and can provide very good results for the heaviest rare gases for which *ab initio* results are seldom available, due to the complexity of treating correlation via CI expansions, and for which rather complicated model potentials have been previously suggested.

The following section discusses the general outline of our model and its specific derivation. Section III presents our computational results for krypton and xenon. Our final conclusions are collected in Sec. IV.

II. THE SEMICLASSICAL MODEL

The chief interest of our present treatment of correlation-polarization forces is to find a description, in simple terms, of the field experienced by the impinging positron as it penetrates the atomic electrons of the target. The asymptotic form of such a field is simply given by the well-known second-order perturbation expansion formula [4]

$$V_{\rm pol}^{(2)}(r_p)\approx -\sum_{l=1}^{\infty}\frac{\alpha_l q^2}{2r_p^{2l+2}} \quad \text{for } r_p\to\infty \tag{1}$$

for a spherical potential, where r_p represents the coordinate of the positron, q is the charge of the projectile, and the α_1 are the multipolar static polarizabilities of the target atom. In most treatments [1] only the lowest-order term is kept in expansion (1), thereby viewing the target-electron distortion as resulting from the formation of an induced dipole that leads to the familiar r_p^{-4} asymptotic form of the potential with the scalar, atomic dipole polarizability $\alpha_{l=1}=\alpha_D$ as its only coefficient. It is also one of the aims of the present study, as we shall see below, to analyze the effects of the higher-order terms which can be included in Eq. (1) on the computed positron-atom cross sections below the threshold of Ps formation.

In our previous studies on the use of this model for electron-atom scattering processes [17,18], we analyzed higher-order perturbation terms and examined the effects of third- and fourth-order contributions [19] on the computed elastic cross sections, integral and differential, for He, Ne, and Ar targets. In the case of positrons as projectile, however, one should keep in mind that the strong Coulomb repulsion from the nuclei of complex atoms, such as those examined here, plays a rather important role in keeping the slow positron away from the inner core of the bound electronic density. As a consequence, it is the outer region of such a density that is mostly sampled by the impinging projectile at low energies, hence the likely dominance of the contributions to polarization forces which come from the lower orders of the perturbation expansion and which go to zero in the asymptotic region at the slowest rates. We therefore feel that the second-order contributions implied by expansion (1) will be the most important to analyze for low-energy positron scattering processes. As we shall see, they are also the ones which have been most often considered in previous studies via model potentials [15].

The main drawback of Eq. (1), however, is that it fails to correctly represent the true short-range behavior of polarization forces since it diverges at the origin. The present approach provides instead a smooth modification of the divergent series in Eq. (1) without having to invoke any adjustable parameters for its implementation. Our present method originates from a semiclassical model recently applied to the H_2^+ molecule [20], where an analogous problem occurs in connection with the Heitler-London perturbation calculations of the chemical-bond total energy. More recently, we have demonstrated that the previous approach could be successfully applied to the cases of both electron and positron scattering from the two-electron He atom [17] and we have further extended successfully the use of such a global model to the scattering of electrons from many-electron atoms [18].

The essential point of our treatment simply consists in noting that, as the relative target-to-projectile distance is reduced, the interposed electronic charge density goes to zero and consequently the corresponding long-range polarization potential will tend to vanish [8]. In the case of an impinging positron, this amounts to saying that the short-range correlation of its motion with that of the bound electrons will effectively reduce the overall attractive potential given by the long-range terms of Eq. (1). A practical ansatz for the total correlation-polarization potential $V_{cp}^{(2)}$ over the full range of relative distances could thus be given by the expression

$$V_{cp}^{(2)}(r_p)\approx -\sum_{(2l+2)}^{\infty} f_{2l+2}^{(2)}(r_p)V_{\rm pol}^{l}(r_p)\ , \tag{2}$$

where

$$V_{\rm pol}^{l}(r_p)=\frac{\alpha_l}{r_p^{2l+2}} \tag{3a}$$

and

$$f_{2l+2}^{(2)}(r_p)\approx \begin{cases} 0 \ \text{ as } r_p^{2l+2+l'} \ \text{ with } l'\geq 1 \ \text{ when } r_p\to 0 \\ 1 \ \text{ when } r_p\to\infty . \end{cases} \tag{3b}$$

Thus the correcting functions which we are searching for are required to go to zero at short distances and to approach unity at large distances from the origin.

The second-order perturbation energy due to the Coulomb interaction between a continuum electron and the bound electron of the H atom target has been given long ago by Dalgarno and Lewis [21] in a simpler form

which uses the closure approximation

$$J_2=\langle\phi_1|V|\phi_0\rangle=-\frac{1}{\varepsilon}\{\langle\phi_0|V^2|\phi_0\rangle-|\langle\phi_0|V|\phi_0\rangle|^2\}\ , \tag{4}$$

where ϕ_1 is the first-order target wave function and ϕ_0 is the unperturbed wave function. According to those authors [21], Eq. (4) is exact at any given r_p for some value of ε such that $\frac{8}{9}<\varepsilon<2$ [20]. Within the familiar random-phase approximation [4] the quantity ε describes the average excitation energy. The perturbation potential for the one-electron target atom can be written in our case as

$$V=+\frac{1}{r_p}-\frac{1}{r_i}\ , \tag{5}$$

where r_p is the distance of the scattering positron from the nucleus and r_i its distance from the bound electron. If we denote by r_b the coordinate of the bound electron with respect to the nucleus, then the interaction of Eq. (5) can be rewritten as a multipolar expansion

$$V=\sum_{l=0}^{\infty}V_l(r_b,r_p,\cos\vartheta)=\begin{cases}-\dfrac{1}{r_p}\displaystyle\sum_{l=1}\left[\dfrac{r_b}{r_p}\right]^l P_l(\cos\vartheta), & r_p>r_b \qquad (6)\\[2ex] +\dfrac{1}{r_p}-\dfrac{1}{r_b}\displaystyle\sum_{l=0}\left[\dfrac{r_p}{r_b}\right]^l P_l(\cos\vartheta), & r_b>r_p, \qquad (7)\end{cases}$$

where ϑ describes the angle between r_b and r_p. We can now make use of the familiar polarized orbital approximation [22,23], whereby the dominant part of the perturbation interaction is assumed to come from that spatial region where $r_b\le r_p$ and the bound charge distribution to be considered is only the one contained within the sphere of radius r_p. One can therefore write the interaction in an approximate form by keeping only the contribution from Eq. (6),

$$J_2=V_{\rm pol}^{(2)}(r_p)=-\frac{1}{\varepsilon}\left\langle\phi_0\left|\left\{\frac{1}{r_p}\sum_{l=1}\left[\frac{r_b}{r_p}\right]^l P_l(\cos\vartheta)\right\}^2\right|\phi_0\right\rangle\ . \tag{8}$$

To consider the positron as a pointlike projectile fixed in space and not affecting the potential calculation with change overlap effects or with the further interaction from Eq. (7) amounts to using some classical picture in our model, hence its being called a semiclassical model, as discussed in [20].

Because of the orthogonality of the P_l's, all the cross terms in l of Eq. (8) will vanish and the sign of the potential will not depend anymore, in the second-order term, on the sign of the impinging projectile [17]. One can now rewrite Eq. (8) as given by, for a one-electron target [20],

$$V_{\rm pol}^{(2)}(r_p)=\sum_{l=1}^{\infty}\frac{k_l}{2r_p^{2l+2}}\int_0^{\infty}\rho_0(r_b)r_b^{2l+2}dr_b\ , \tag{9}$$

where the k_l factor contains all the necessary normalization factors [20]. If we now compare the above result with Eq. (3a), then we obtain

$$\alpha_l=k_l\int_0^{\infty}\rho_0(r_b)r_b^{2l+2}dr_b\ , \tag{10}$$

where the integration runs over the whole range of the radial variable for the bound electron for which the target has nonvanishing charge density $\rho_0(r_b)$. One can also define an r_p-dependent polarizability coefficient by writing an approximate expression for it [20]

$$\alpha_l(r_p)=k_l\int_0^{r_p}\rho_0(r_b)r_b^{2l+2}dr_b\ , \tag{11}$$

which then allows us, by using Eqs. (2) and (9)–(11), to obtain an explicit expression for the damping function of Eq. (2)

$$\alpha_l(r_p)=f_{2l+2}^{(2)}(r_p)\alpha_l \tag{12}$$

with

$$f_{2l+2}^{(2)}(r_p)=\frac{\int_0^{r_p}\rho_0(r_b)r_b^{2l+2}dr_b}{\int_0^{\infty}\rho_0(r_b)r_b^{2l+2}dr_b}\ , \tag{13}$$

which now behaves asymptotically as required by conditions (3b). We therefore see that the present model simply employs the electronic density of the target atom to scale the asymptotic polarization potential coefficient into the short-range and intermediate-range regions where Eq. (1) is no longer valid. The basic assumption is therefore classical in nature, in the sense that the only target charge distribution being considered for the scaling is the one up to the local position of the impinging positron, now treated as a fixed pointlike particle.

The final correlation-polarization potential of Eq. (2) can also be written explicitly as the sum of the contributions from the first three leading terms of the second-order expansion (1), in the case one wishes to include more contributions from that expansion

$$V_{cp}^{(2)}(r_p)=-f_4^{(2)}(r_p)\frac{\alpha_D}{2r_p^4}-f_6^{(2)}(r_p)\frac{\alpha_Q}{2r_p^6}-f_8^{(2)}(r_p)\frac{\alpha_0}{2r_p^8}+\cdots\ , \tag{14}$$

where the further two coefficients correspond to the quadrupole and octupole static polarizabilities α_Q and α_0, respectively [19], and the individual scaling functions can be obtained from numerical integrations of Eq. (13).

Higher-order terms can also be obtained and have been discussed by us for electron scattering processes [17,18], but, as we shall see below, they are not expected to improve on the present model unless many more terms are included in the treatment. Therefore we will not explicitly include them in the present work.

We should point out that various approximations have been either used or implied in deriving Eqs. (4), (8), (11), and (14), which describe our present model, and the scope of our comparison with experiments is essentially to see how realistically it will be able to describe integral and differential elastic cross sections given the various simplifications that were needed for its derivation. That it will turn out to yield a rather reasonable picture for complex systems is an indication of the basic validity of the approximations made.

One further aspect of our derivation from the treatment for chemical bonds [20] requires the extension of our formulas to the many-electron atomic targets which are our main concern in the present work. So far, in fact, the interaction has been obtained via a semiclassical model discussed earlier [17,20] for one-electron target atoms. The simplest generalization therefore is obtained, as discussed in Ref. [18], for targets with an arbitrary number N_e of bound electrons by assuming that (i) the ensuing effective potential can still be considered as spherical and (ii) it is given by the polarized-orbital approximation. It therefore follows that the scaling of our previous potential to the actual N_e-electron density within the sphere of radius r_p provides the expression

$$V_{N_e}(r_p)=f_2^{N_e}(r_p)V_1(r_p)\ , \tag{15}$$

where $V_1(r_p)$ is given by Eq. (6) and the scaling factor is obtained as

$$f_2^{N_e}(r_p)=\frac{\int_0^{r_p}\rho_{N_e}(r_b)r_b^2dr_b}{\int_0^{\infty}\rho_{N_e}(r_b)r_b^2dr_b}\ , \tag{16}$$

where $\rho_{N_e}(r_b)$ is now the ground-state charge density of the target atom with N_e bound electrons. By inserting this result in Eq. (8), the final correlation-polarization potential contributions of Eq. (14) become further modified accordingly and can now be written down as follows for the case in which the first three coefficients of the second-order adiabatic, asymptotic potential are included:

$$V_{cp}^{(2)}(r_p,N_e)=-(f_2^{N_e})^2f_4^{(2)}(r_p)\frac{\alpha_D}{2r_p^4}-(f_2^{N_e})^2f_6^{(2)}(r_p)\frac{\alpha_Q}{2r_p^6}$$
$$-(f_2^{N_e})^2f_8^{(2)}(r_p)\frac{\alpha_0}{2r_p^8}+\cdots\ . \tag{17}$$

This correlation-polarization potential now behaves correctly over the whole range of r_p values and holds for N_e-electron targets. In the following section we will show the application of the present effective potential to positron scattering from Kr and Xe targets.

III. THE SCATTERING CALCULATIONS

As mentioned in our previous papers [17,18], the knowledge of the ground-state electronic densities for the target atoms was taken from linear combination of atomic orbitals wave functions published earlier [24], where they were given by near-Hartree-Fock nonrelativistic calculations for the bound electrons. In the case of scattering of electrons, it has often been suggested that if one wishes to include relativistic effects, then it is best to go directly to a Dirac formulation for both the structure and the scattering parts of the problem [25,26]. In the case of positron scattering, on the other hand, the static potential is repulsive and no exchange terms appear in the interaction. Both these effects mean that the impinging positron, especially at low collision energies below Ps formation, does not penetrate deeply enough into the atom to significantly "feel" the inner orbitals, which would be most affected by relativistic corrections [27]. We therefore carried out the scattering calculations within a nonrelativistic treatment, as recently done by other calculations on the same systems [28].

The numerical methods employed in calculating elastic cross sections, integral and differential, have been discussed before in connection with the study of electron-atom scattering processes [29] and will not be repeated here in detail. The coupled differential equations were solved numerically for each partial wave and for all the examined collision energies. The radial solutions were propagated using a Numerov's algorithm with an energy-dependent radial mesh, with step size ranging from $10^{-3}a_0$ up to $10^{-2}a_0$. The positions of the outer matching radii were tested against the stability of the calculated phase shifts and were typically at around $200a_0$, leading to a numerical error of less than 0.1%. Individual phase shifts were directly computed up to $l\approx 15$, while an effective-range formula [30] was employed for higher l values. For computing differential cross sections (DCSs) the number of partial waves included was extended up to $l\approx 500$. While convergence at most angles was achieved with $l_{\max}\approx 100$, the higher angular momenta were necessary to obtain stable results in the small-angle scattering.

In order to assess the reliability of the present model, we show in Fig. 1 the computed DCSs for scattering of positrons from N_e at 13.6 eV, i.e., below the threshold of Ps formation. The calculations were carried out at the simplest level of the $V_{cp}^{(2)}$ potential presented in our work, i.e., by including only the dipole polarizability term in Eq. (14). One clearly sees that they agree remarkably well with the most recent experimental data on this system [31], as well as the more complicated polarized-orbital calculations done earlier on by McEachran, Rayman, and Stauffer [32].

A similar set of comparisons is shown in Fig. 2, where the DCSs for the argon atom are presented at two different collision energies: at 5 eV (top) and at 8.7 eV (bottom). The experimental points are from Ref. [33]. When we consider the lower-energy data (top part of the

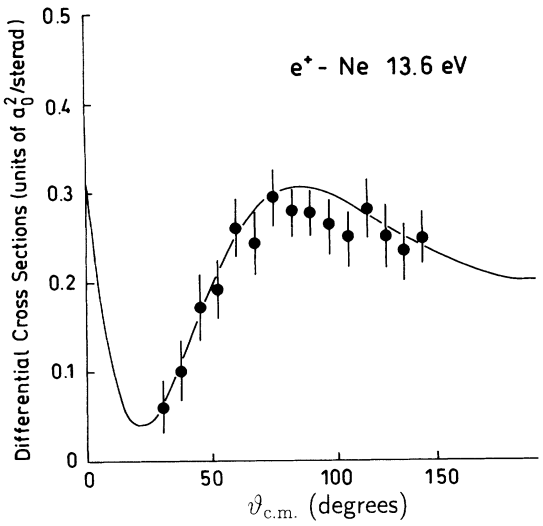

FIG. 1. Computed and measured differential cross sections for positron scattering from neon at 13.6 eV of collision energy. The solid line gives our present calculations with α_D only in Eq. (14), while the experimental points are from Ref. [33].

figure) we see that the $V_{cp}^{(2)}$ potential of Eq. (14) needs to be used with its quadrupole and octupole contributions. The solid line shows in fact our calculations with α_D only, while the long-dashed line reports calculations with both α_D and α_Q coefficients. Finally the short-dashed line results include the α_0 coefficient in Eq. (14). The agreement with the position of the experimental minimum at $\sim 57°$ and with the low-angle sharp increase of the DCS is rather good when only the quadrupole term is added to the $V_{cp}^{(2)}$ potential and is not changed very much by the further addition of the octupole polarizability coefficient in Eq. (14).

The comparison of our calculated cross sections with further experiments at a higher collision energy is shown in the bottom part of Fig. 2. Here again the use of $V_{cp}^{(2)}$ with quadrupole and octupole contributions exhibits reasonable accord with the measured data, especially beyond the minimum at $\vartheta_{c.m.} \sim 48°$. Both the minimum and the maximum in the cross sections are, however, closely reproduced by our model. Considering the general simplicity of our treatment of correlation effects and the computational ease with which our results are obtained, it is certainly very reassuring that we get so close to experiments and perform, in the comparison, as well as the more sophisticated calculations of Ref. [25]. Furthermore, the marked existence of such features has been related, in the experiments, to possible absorption effects from inelastic channels on the elastic DCS as the energy increase [33]. Since our elastic calculations do not include such effects, the fact that they show deeper minima than the experiments at 8.7 eV is in keeping with earlier calculations [25] and somehow confirms that the present correlation-polarization potential can realistically describe short-range effects on the elastic cross section part of the measured DCS. Our results also indicate that when the complexity of the target atom increases, more terms in Eq. (1) should be included. This is certainly a well-known result and the inclusion of nonadiabatic contributions for coefficients beyond the dipole polarizability has important consequences on the final results for electrons. One should therefore suspect that our simple model for the short-range correction produces here some cancellations when using only adiabatic terms beyond the leading dipole coefficient.

A. Integral cross sections

Having established in the previous analysis of our results for Ne and Ar the general good quality of the present semiclassical model, we can now go on to examine its performance for the calculations of integral cross sections of the heaviest rare gases Kr and Xe as ground-

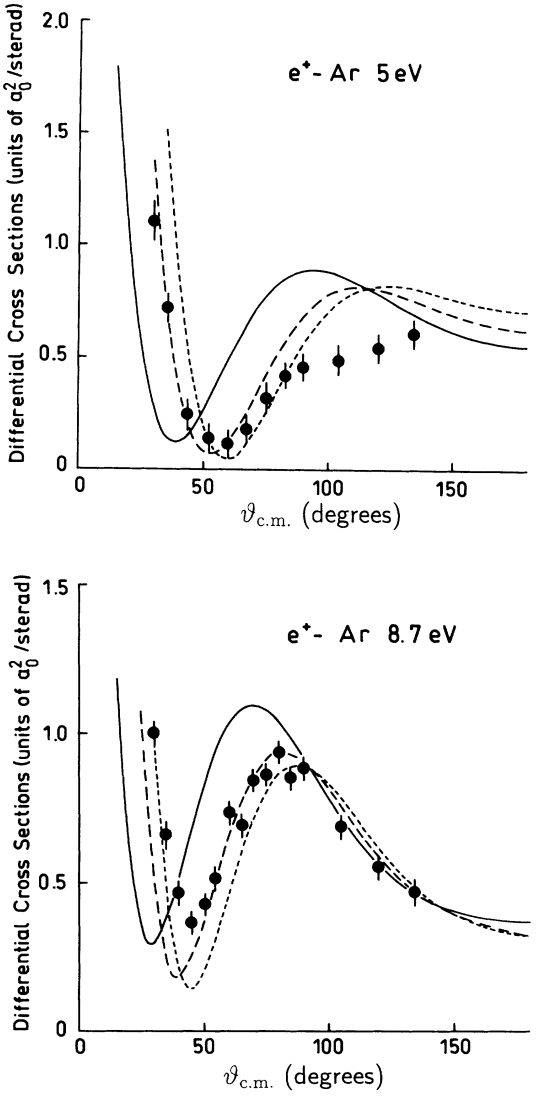

FIG. 2. Computed and measured differential cross sections for positron scattering from argon atoms (top) at a collision energy of 5 eV and (bottom) at a collision energy of 8.7 eV. Solid line, present calculations with α_D coefficient only in Eq. (14); long-dashed line, calculations with α_D and α_Q coefficients; short-dashed line, calculations with α_D, α_Q, and α_0 coefficients. The experimental points are from Ref. [33].

state atomic targets. The range of energies examined will be below the respective threshold of Ps formation ($\sim$7 eV for Kr and $\sim$5 eV for Xe, respectively), where several experimental data have been available over the years.

The results of our calculations for krypton are shown in Fig. 3 together with the experimental data [34–36]. It is interesting to note at the outset the rather wide range of uncertainty existing between experiments: the squares are the data from Ref. [35] and the circles are those from Ref. [37]. Both sets of experiments, however, indicate the existence of a rather marked increase of the cross sections below 2 eV of energy.

The calculations reported include, successively, the contributions of the first three multipolar coefficients of Eq. (14) for the $V_{cp}^{(2)}$ potential of the present work. Thus the solid line shows results with only the dipole polarizability coefficient, the long-dashed line the results obtained with α_D and α_Q coefficients, and the short-dashed line the calculations with all three coefficients included. As expected, the computed cross sections get larger at very low energy as an increasingly more attractive potential is employed to treat the long-range part of the polarization interaction. On the other hand, the first two leading terms of the second-order contribution to the perturbative treatment of polarization (long-dashed line) provide very good quantitative agreement with experiments. The addition of the r_p^{-8} coefficient with the octupole static polarizability appears to improve agreement with experiments above 4 eV, but yields cross sections which are too large below that energy. In other words, the inclusion of higher multipoles in the polarization potential is not sufficient if one uses adiabatic contributions only, and before convergence can be reached, one should include the higher-order terms of the perturbation expansion from both adiabatic and non-adiabatic effects [28]. These higher-order coefficients in fact appear with different signs for the different contributions [18] and therefore are possibly needed to very high-order before such cancellation effects are all correctly included [9].

An interesting deduction from the present calculation, however, seems to be that the lowest-order terms of the second-order perturbative treatment included in our model are sufficient to provide good accord with experiments, thus allowing us to keep the present model to a rather simple level by having it include only the lower-order multipoles appearing in Eq. (1). In other words, the present semiclassical model provides an effective local potential in the inner region of interaction which realistically describes short-range correlation effects on the full polarization potential by a global scaling function, which acts only on the second-order lower coefficients included in Eq. (1). That the global damping of the lowest static multipoles of that equation is sufficient to provide a reliable V_{cp} potential seems to be indicated by the calculations we have shown here and appears to suggest that, in spite of its approximate nature, our simple prescription catches the main physics involved in the positron scattering even from complex targets.

A similar set of calculations was also carried out for Xe targets and is reported in Fig. 4 together with the experimental data. Here again the existing measurements appear to span a very large range of uncertainty, especially in the very-low-energy regime.

The calculations shown involve the $V_{cp}^{(2)}$ potential of Eq. (14) and include the $(\alpha_D+\alpha_Q)$ coefficients in the results given by the long-dashed curve and all three multipolar coefficients in the results given by the short-dashed curve. Both calculations follow very closely the experimental findings. The computations with the α_D

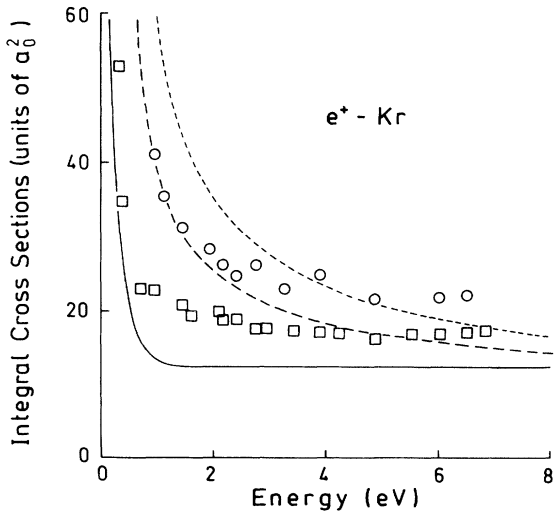

FIG. 3. Computed and measured elastic integral cross sections for positron scattering from krypton. The experimental values are from Refs. [35] (squares) and [37] (circles). The present calculations employ the $V_{cp}^{(2)}$ potential of Eq. (14): α_D coefficient only (solid line); α_D and α_Q coefficients (long-dashed line); all three coefficients in Eq. (14) (short-dashed line).

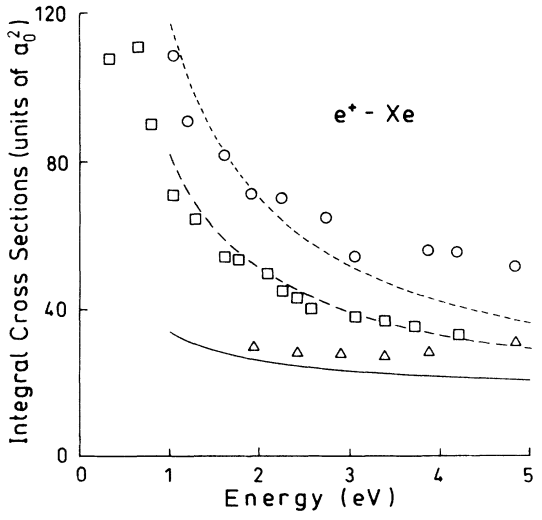

FIG. 4. Computed and measured elastic integral cross sections for positron scattering from xenon atoms. The experimental data are from Refs. [35] (triangles), [37] (squares), and [37] (circles). The present calculations include the α_D coefficient only (solid line), the $(\alpha_D+\alpha_Q)$ coefficients in Eq. (14) (long-dashed line), and all three coefficients in Eq. (14) (short-dashed line).

coefficient only are reported in Fig. 4 by the solid curve and follow very closely the lowest set of experiments from Ref. [35]. Here again the comparison with measured data clearly shows the good quality of our global scaling model potential, which is applied to the second-order perturbative coefficients and only to the lower polarizabilities of Eq. (1).

It is also interesting to note that both the calculations given by the short-dashed line for Kr and Xe are very close to the earlier theoretical calculations which employed a frozen-core version of the polarized-orbital approximation [28] and which require a more substantial computational effort than that needed by our present semiclassical approximation.

B. Differential cross sections

One of the reasons of interest in measuring and computing positron-atom scattering cross sections is connected with the possibility of observing positron scattering resonances [38] and absorption effects [33]. Both effects have been related to the likely modifications of structured differential cross sections around specific collision energy values, either below or above the threshold of Ps formation [39]. Thus it is very important to be able to unquestioningly assign to elastic channel only the oscillations observed below Ps formation and to a coupling with inelastic channels its damping as the energy is increased [40].

The experimental results [39] for positron-krypton collisions are shown, at 6.67 eV, in Fig. 5 together with the present calculations. Although the experiments are given on an absolute scale, the authors point out [39] that the uncertainty in their normalization in the energy width of the positron beam and in the angular acceptance of their detector are factors which make the accurate determination of the locations of the maximum and minimum features rather difficult, as well as to correctly establish the height of the maximum. Given the above caveat, therefore, our present calculations are rather close to the measured data: the computations with α_D only are shown by the solid line and those with $(\alpha_D+\alpha_Q)$ and with all three multipolar coefficients are shown by the long-dashed and the short-dashed curves, respectively. If one normalizes the experimental points to the computed minimum value around 50°, then one finds that the calculations given by the dashed curves follow very closely the experiments and reproduce well the strong oscillation in the measured cross sections. This result is also in agreement with the calculations of McEachran, Stauffer, and Campbell using the polarized-orbital approximation [28,39].

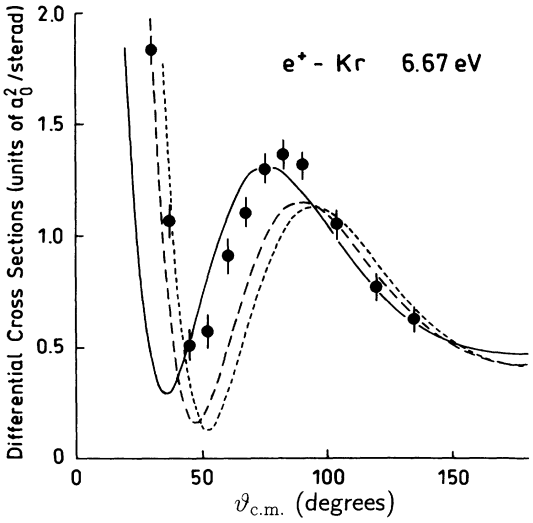

FIG. 5. Computed and measured differential cross sections for positron scattering off krypton at 6.67 eV. The experiments (ϕ) are from Ref. [39]. The calculations follow the notation of the preceding figures: solid line, α_D coefficient only in Eq. (14); long-dashed line $(\alpha_D+\alpha_Q)$ coefficients in Eq. (14); short-dashed line, all three coefficients in Eq. (14).

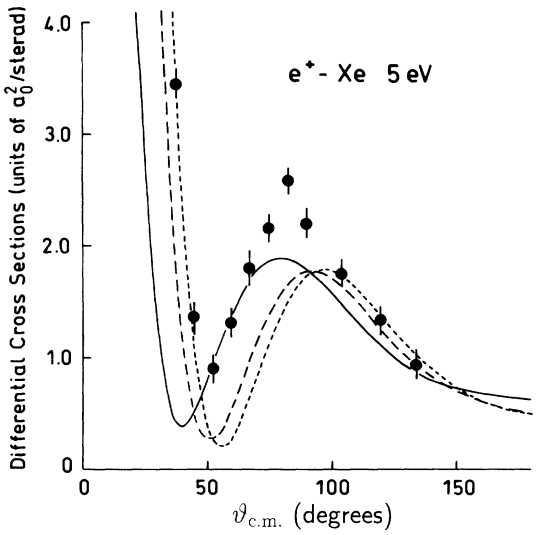

FIG. 6. Computed and measured differential cross sections for positron scattering off xenon atoms. The experiments (ϕ) are from Ref. [41] while the calculations are from the present work and follow the notation of Fig. 5.

Similar calculations for Xe are shown in Fig. 6 for a collision energy of 5 eV. The measurements come from the same experimental group of before [41] and are shown in comparison with our present calculations. Here again no normalization of measured data to experiments is attempted; were this done, for example, at the minimum position, then the calculations including quadrupole and octupole polarizability coefficients would follow closely the experimental findings. Our results are also in accord with the earlier calculations of McEachran, Stauffer, and Campbell [28] as quoted in Ref. [41].

IV. CONCLUSIONS

In the present work we have applied a simple semiclassical model to the treatment of short-range correlation effects in the scattering of positrons from the heaviest rare gases below the threshold of Ps formation. We have

shown that such a model relies on an approximate scaling procedure for treating polarization forces in the overlap region, contains no *ad hoc* empirical parameters, and requires only the knowledge of the target electronic density to compute a global scaling function for the asymptotic polarization potentials. Our model is obviously an approximate effective potential and relies on the accuracy of the polarization potential to describe high-l scattering processes as a starting point of its derivation.

The comparison of calculations with experiments also shows here that the simplest treatment of the polarization forces, i.e., the second-order perturbative term only and the lowest multipolar coefficients that contribute to that term, is sufficient to attain rather good accord with experiments and to avoid the search for the full convergence of the series expansion through the use of many higher-order terms, both adiabatic and energy-independent terms, often unavailable for such systems.

The model suggested is physically rather straightforward to understand and computationally easy to implement, even for complex targets such as those examined in this work. In spite of its approximate nature, it appears to provide a reliable form of a local energy-independent effective potential to treat correlation effects for the scattering of positrons and electrons off ground-state atomic targets. From what has been learned about atoms [17,1], its extension to molecular systems thus appears rather promising and is currently under study in our group.

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[1] N. F. Lane, Rev. Mod. Phys. **52**, 29 (1980).
[2] F. A. Gianturco and A. Jain, Phys. Rep. **143**, 348 (1986).
[3] M. A. Morrison, Adv. At. Mol. Phys. **24**, 51 (1988).
[4] A. D. Buckingham, Adv. Chem. Phys. **12**, 107 (1967).
[5] L. Castillejo, I. C. Percival, and M. J. Seaton, Proc. R. Soc. London, Ser. A **254**, 259 (1960).
[6] M. Seaton and L. Sternman-Clark, J. Phys. B **10**, 2639 (1977).
[7] M. Puska and R. Nieminen, J. Phys. F **13**, 333 (1963).
[8] T. L. Gibson and M. A. Morrison, Phys. Rev. A **29**, 2497 (1984).
[9] F. A. Gianturco, A. Jain, and J. A. Rodriguez-Ruiz, Phys. Rev. A **48**, 4321 (1993).
[10] H. D. Meyer, Phys. Rev. A **40**, 5605 (1989).
[11] B. I. Schneider and L. A. Collins, J. Phys. B **15**, L335 (1982).
[12] H. D. Meyer, J. Phys. B **25**, 2657 (1992).
[13] M. Berman and U. Kaldor, J. Phys. B **1**, 3993 (1981).
[14] M. A. Morrison and B. C. Saha, Phys. Rev. A **34**, 2786 (1986).
[15] J. K. O'Connell and N. F. Lane, Phys. Rev. A **27**, 1893 (1983).
[16] F. A. Gianturco and J. A. Rodriguez-Ruiz, J. Mol. Struct. **260**, 99 (1992).
[17] F. A. Gianturco, D. De Fazio, J. A. Rodriguez-Ruiz, K. T. Tang, and J. P. Toennies, J. Phys. B **27**, 303 (1994).
[18] F. A. Gianturco, D. De Fazio, J. A. Rodriguez-Ruiz, K. T. Tang, and J. P. Toennies (unpublished).
[19] G. Maroulis and A. J. Thakkar, J. Phys. B **21**, 3819 (1988).
[20] K. T. Tang and J. P. Toennies, J. Phys. Chem. **94**, 7880 (1990).
[21] A. Dalgarno and J. T. Lewis, Proc. Phys. Soc. London Sect. A **69**, 57 (1956).
[22] A. Temkin, Phys. Rev. **107**, 1004 (1957).
[23] A. Temkin and J. C. Lamkin, Phys. Rev. **121**, 788 (1961).
[24] E. Clementi and C. Roetti, At. Data Nucl. Data Tables **14**, 177 (1974).
[25] R. P. McEachran, A. G. Ryman, and A. D. Stauffer, J. Phys. B **12**, 103 (1979).
[26] R. P. McEachran, D. L. Morgan, A. G. Ryman, and A. D. Stauffer, J. Phys. B **10**, 663 (1977).
[27] R. P. McEachran and A. D. Stauffer, in *Positron (Electron) Gas Scattering*, edited by W. E. Kauppila, T. S. Stein, and J. M. Wadehra (World Scientific, Singapore, 1986), p. 122.
[28] R. P. McEachran, A. D. Stauffer, and L. E. M. Campbell, J. Phys. B **13**, 1281 (1980).
[29] F. A. Gianturco and J. A. Rodriguez-Ruiz, Phys. Rev. A **47**, 1075 (1993).
[30] H. P. Saha, Phys. Rev. A **39**, 628 (1989).
[31] S. Smith, W. Kauppila, C. Kwan, and T. Stein, in *Proceedings of the Sixteenth International Conference on the Physics of Electronic and Atomic Collisions, New York, 1989*, AIP Conf. Proc. No. 205, edited by A. Dalgarno, R. S. Freund, M. S. Lubell, and T. B. Lucatorto (AIP, New York, 1990), p. 403.
[32] R. P. McEachran, A. G. Rayman, and A. D. Stauffer, J. Phys. B **11**, 551 (1978).
[33] S. J. Smith, G. M. A. Hyder, W. E. Kauppila, C. K. Kwan, and T. S. Stein, Phys. Rev. Lett. **64**, 1227 (1990); P. G. Coleman and J. D. McNutt, *ibid.* **42**, 1130 (1979).
[34] T. S. Stein, W. E. Kauppila, V. Pol, G. Jesion, and J. H. Smart, in *Abstracts of the Tenth International Conference on the Physics of Electronic and Atomic Collisions, Paris, 1977*, edited by M. Barat and J. Reinhardt (Commissariat à l'Energie Atomique, Paris, 1977), p. 804.
[35] T. S. Stein and W. E. Kauppila, Adv. At. Mol. Phys. **18**, 53 (1982).
[36] H. Nakanishi and D. M. Schrader, Phys. Rev. A **34**, 1823 (1986).
[37] M. Charlton, Rep. Prog. Phys. **48**, 737 (1985).
[38] L. Dou, W. E. Kauppila, C. K. Kwan, and T. S. Stein, Phys. Rev. Lett. **68**, 2913 (1992).
[39] L. Dou, W. E. Kauppila, C. K. Kwan, D. Pryzybyla, S. J. Smith, and T. S. Stein, Phys. Rev. A **46**, 5327 (1992).
[40] K. Higgins and P. G. Burke, J. Phys. B **24**, L343 (1991).
[41] W. E. Kauppila, S. J. Smith, C. K. Kwan, and T. S. Stein, in *Annihilation in Gases and Galaxies*, NASA Conf. Publ. No. 3058, edited by W. E. Kauppila (NASA, Washington, D.C., 1989), p. 113.