ELASTIC SCATTERING OF SLOW POSITRONS ON ATOMS

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The results of calculations of the elastic scattering cross section of positrons on noble gas and alkali atoms are presented. The calculations are performed within the one-electron Hartree–Fock approximation with multi-electron correlations in the so-called random phase approximation with exchange taken into account. Virtual positronium formation is taken into account and proved to be very important. Arguments are presented that the positron polarization potential is repulsive for alkali atoms. The results obtained are in a reasonable agreement with experiment and with some previously reported calculations.

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1. INTRODUCTION

The studies of positron–atom and positron–molecule scattering, in spite of their development during already several decades, is still quite an active area of research (see [1–3] and references therein). The interest in positron slowing and annihilation in gases and other media motivates the investigation of these processes. The photons emitted in the course of annihilation carry extremely valuable information on the electron structure of different objects, from isolated atoms in gases to solid bodies. But the process of positron collisions on atoms and molecules is also of interest by itself and in comparison to electron collisions on the same objects. The projectile-target interaction mechanisms are most transparent in the collision process at low energies, and we therefore concentrate on this energy region in what follows.

For both the electron and positron scattering, the cross section is determined by the electrostatic and polarization potentials by which the target acts on the projectile. For incoming electrons, however, the exchange with the target electrons is important. It does not exist for positrons at all. At a first glance, the positron scattering process therefore appears to be simpler than that for electrons. Moreover, the positron–atom static potential, being repulsive in general, forces the positron to move into the areas of the target where the potential is the smallest, thus diminishing its overall action. This is opposite to the case of electron–atom (molecule) collision. The contrast looks even stronger if we take into account that as it seems, the polarization potential is attractive for both electrons and positrons. The total potential for electrons must therefore be stronger than for positrons. It thus seems at the first glance that any simple approach that is good for electrons should work least not worse for positrons. For instance, the second-order approximation to the polarization potential is good for electron–atom scattering [4] and can be expected to be at least equally good in describing positron–atom scattering. But this view has proved to be incorrect.

Indeed, the positron that is «pushed» out of the target can interact strongly with a temporarily, or virtually, excited electron that is outside the target. They form a kind of a bound state that can be called the «virtual positronium». We show that this is a very important mechanism that dramatically affects the scattering cross section.

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Our aim in this paper is to calculate the slow positron–atom elastic scattering cross sections and to demonstrate the efficiency of a very simple method first proposed in [5] and then developed in [6, 7] that allows taking the virtual positronium formation into account in this process. The latter effect has proved to be extremely important. The suggested method allows us to considerably improve the agreement with experiment and to give a simple qualitative explanation of a large difference between cross sections for noble gases and their neighbors, alkali atoms. Since the introduction of this approach in [5], a number of other calculations were performed (e.g., [6–10]) based on the idea of the virtual positronium formation but using much more complicated methods (see [8–10]).

2. DETAILS OF CALCULATIONS

The elastic scattering cross section $\sigma(E)$ of a positron with the energy E is determined by the partial scattering phases $\delta_\ell(E)$, where ℓ is the positron angular momentum, as [11][1)]

$$\sigma(E) = \frac{2\pi}{E} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell(E). \qquad (1)$$

In the calculations, we limit ourselves by the first four phase shifts $\ell = 0, 1, 2, 3$, which is sufficient for relatively low positron energies up to 30–40 eV.

The first step of our approach is the Hartree–Fock (HF) calculations, which means the HF approximation for the target atom and the frozen core approximation for the incoming positron, naturally without exchange of the positron and the core electrons. To calculate the

HF positron phase shifts $\delta_\ell^{HF}(E)$, we therefore solve the equation

$$\left[-\frac{\triangle}{2} + \frac{Z}{r} - \int \frac{d\mathbf{r}\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \right] \varphi_{e^+}(\mathbf{r}) = E\varphi_{e^+}(\mathbf{r}) \qquad (2)$$

for the positron wave function $\varphi_{e^+}(\mathbf{r})$; here, Z is the nuclear charge and $\rho(r)$ is the atomic electron density. The asymptotic form of the radial part $P_{E\ell}^{e^+}(r)$ of $\varphi_{e^+}(\mathbf{r})$ for large r determines the phase shift,

$$P_{E\ell}^{e^+}(r) = \frac{1}{\sqrt{\pi r}} \sin\left[pr - \frac{\pi\ell}{2} + \delta_\ell^{HF}(E) \right], \quad r \to \infty. \quad (3)$$

Here, $p = \sqrt{2E}$. The density is obtained by solving the HF equations for the target atom.

A prominent difference between the HF and experimental results at low positron energies in positron–atom elastic scattering exists for almost all atoms considered, for example, He. The next step must therefore be made by taking the polarization interaction into account. This interaction appears in the second order in the positron–electron interaction, in the same way as for the electron–atom scattering (see [4, 12] for details). Assuming that the polarization interaction Σ is weak, we can express the correction $\Delta\delta_\ell(E)$ to the HF partial positron scattering phase due to the action of Σ as

$$\Delta\delta_\ell(E) = -\pi \langle E\ell \, \| \Sigma_\ell(E) \| \, E\ell \rangle, \qquad (4)$$

where $\Sigma_\ell(E)$ is the ℓth component of Σ and $E\ell$ denotes the radial part of the positron wave function $P_{E\ell}^{e^+}(r)$.

In the second order in the Coulomb interaction $V = 1/|\mathbf{r} - \mathbf{r}'|$ between the incoming positron and atomic electrons, the reduced matrix element in the right hand side of (4) is given by

$$\langle E\ell \, \| \Sigma_\ell(E) \| \, E\ell \rangle = \sum_{L \geq 0} \frac{1}{2L+1} \times$$
$$\times \sum_{i \leq F; \varepsilon_2\ell_2 > F} \int_0^\infty \frac{\langle E\ell, \varepsilon_i\ell_i \, \| V_L \| \, E_1\ell_1, \varepsilon_2\ell_2 \rangle \langle E_1\ell_1, \varepsilon_2\ell_2 \, \| V_L \| \, E\ell, \varepsilon_i\ell_i \rangle}{(2\ell+1)(E - E_1 - \varepsilon_2 + \varepsilon_i + i\delta)} dE_1 \, d\varepsilon_2, \quad (5)$$

where $E_1\ell_1$ denotes the intermediate positron state, which is determined by solving Eq. (3), and $\varepsilon_2\ell_2$ and $E_i\ell_i$ stand for the energies and angular momenta of atomic electrons in the virtually excited and ground states, respectively (with their wave functions found in the HF approximation [12]). The reduced Coulomb matrix elements V_L are defined in [12]. The conditions $i \leq F$ and $\varepsilon\ell > F$ indicate occupied and vacant electron states, respectively. Equation (5) corresponds

to the lowest order correlation correction in the frame of the Random Phase Approximation with Exchange (RPAE). It differs from the expression for the second-order polarization interaction for electron–atom scattering described in [4, 12] because it does not include the exchange between the incoming particle and target electrons. The scattering cross section with the polarization interaction taken into account is determined by Eq. (1) where $\delta_\ell^{HF}(E)$ is replaced by the phases

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[1)] Atomic units are used in this paper, with m and e being the electron mass and charge.

$$\delta_\ell(E) = \delta_\ell^{HF}(E) + \Delta\delta_\ell(E) \qquad (5a)$$

for $E < I$ with I being the target atom ionization potential. For higher positron energies, the scattering phases given by (4) and (5a) are complex, and the imaginary part $\operatorname{Im}\Delta\delta_\ell(E) \equiv \Delta\delta_\ell'(E)$ determines the inelastic scattering cross section of the positron by an atom.

The elastic scattering cross section for $E > I$ is given by [4, 12]

$$\sigma(E) = \frac{\pi}{E} \sum_\ell (2\ell+1)\left[\operatorname{ch}(2\Delta\delta_\ell'(E)) - \cos(2\delta_\ell(E))\right] \times$$
$$\times \exp\left[-2\Delta\delta_\ell'(E)\right], \quad (6)$$

where $\delta_\ell(E)$ is the real part of the positron ℓ-wave scattering phase shift.

Similarly to Eq. (5), the method described in [4, 12] in some aspects apply well beyond the simple second-order perturbation theory in the inter-electron interaction. Important higher-order corrections are taken into account by calculating the HF wave function of the electron $\varepsilon_2\ell_2$ in the atomic field with the vacancy i. With this improvement, even the lowest order in the polarization interaction gives good results for the elastic scattering of electrons on noble gases. This interaction depends on the projectile energy, is nonlocal, and does not contain free adjustable parameters. Far from the atom, it can be approximated as the polarization potential

$$V_{pol} = -\frac{\alpha(\varepsilon)}{2r^4}, \qquad (7)$$

where $\alpha(\varepsilon)$ is the atom dipole polarizability, ε is the mean excitation energy of the incoming electron in the intermediate state, and r is the distance between the projectile and the center of the target. In phenomenological calculations or estimations for low incoming positron energy E, it is usually assumed that $\varepsilon = 0$. For $0 \le \varepsilon < I_1$, where I_1 is the energy of the first atom excitation level, the dipole polarizability is positive and the polarization potential is therefore attractive. It should be kept in mind, however, that $\alpha(\varepsilon)$ as a function of ε can become negative, at least for alkali and alkali earthes, at $\varepsilon > I$, where I is the atomic

ionization potential. As a result, the polarization potential in (7) can become repulsive. It is essential to note that $\alpha(\varepsilon)$ is complex at $\varepsilon > I$, its imaginary part being proportional to the atom photoionization cross section. The polarization potential can therefore also be complex in principle.

The next step beyond the HF approximation in our analysis of positron–atom scattering consists in taking the polarization interaction into account in the first order, in the same manner as this is done for the electron–atom scattering in [4]. The results obtained improve the correspondence with experimental data, but they are still far from being satisfactory. As an illustration, we can use the respective results for any atom, for instance He (see below).

3. METHOD OF CALCULATIONS

The lack of a decisive success after the second-order polarization correction (5) has been taken into account means that something qualitatively important is missing. We believe that as suggested in [5], this is the positronium formation in the intermediate state, that is, the possibility of a temporary binding of the incoming positron and the excited electron (the one located far from the atomic core). We assume that being almost unaffected by the core action, these electron and positron can form a bound state that is almost identical to the free positronium Ps. This alters the energy of the intermediate state, shifting it by the positronium binding energy I_{Ps} and modifies the wave function of the intermediate state, which is no longer the product of HF-wave functions of the positron, the excited electron, and the vacancy created after the virtual excitation of the atomic electron. Instead, the motion of the positron relative to the electron is strongly modified by the binding.

To take the energy shift into account, we must subtract I_{Ps} from the sum of the positron and electron energies $E_1 + \varepsilon_2$ in the denominator of the second-order polarization interaction (5). The modified matrix element is then given by

$$\left\langle E\ell \left\| \widetilde{\Sigma}_l(E) \right\| E\ell \right\rangle = \sum_{L \ge 0} \frac{1}{2L+1} \sum_{i \le F, \varepsilon_2\ell_2 > F} \int_0^\infty \frac{\langle E\ell, \varepsilon_i\ell_i \left\| V_L \right\| E_1\ell_1, \varepsilon_2\ell_2 \rangle \langle E_1\ell_1, \varepsilon_2\ell_2 \left\| V_L \right\| E\ell, \varepsilon_i\ell_i \rangle}{(2\ell+1)(E - E_1 - \varepsilon_2 + I_{\mathrm{Ps}} + \varepsilon_i + i\delta)} dE_1 d\varepsilon_2. \qquad (8)$$
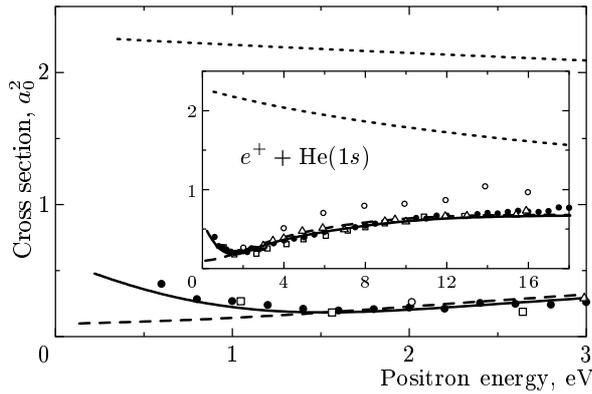
Fig. 1. Cross sections of the elastic positron scattering on He. The dotted line is the HF approximation, the dashed line is the RPAE without positronium formation taken into account; the solid line is the RPAE with the positronium formation taken into account. Experimental data: triangles — [15]; open circles — [16], open squares — [17], solid circles — [18]; a_0 is the Bohr radius

The additional phase shifts $\Delta\delta_\ell(E)$ are determined by Eq. (4) with $\widetilde{\Sigma}_\ell(E)$ instead of $\Sigma_\ell(E)$.

We note that far from the target atom, Eq. (8) leads to a rather simple expression for the polarization potential,

$$V_{pol} = -\frac{\alpha(\varepsilon + I_{\mathrm{Ps}})}{2r^4}. \tag{9}$$

According to the discussion at the end of the previous section, it is essential to have in mind that if $I_{\mathrm{Ps}} > I$, then $\alpha(I_{\mathrm{Ps}})$ is a complex quantity, usually with a considerable imaginary part and $\alpha(I_{\mathrm{Ps}})$ can be not only positive but also negative.

It would be much simpler to use (9) (or (7)) instead of (8) (or (5)), but the asymptotic expressions are valid at so large distances from the atom that their contribution to the total phase shift is small. This is why we used Eq. (8) in our calculations. The advantage of our approach is obvious: to describe the positron–atom scattering, we can use almost the same system of computing codes that was used in studying the electron–atom scattering [12].

To properly include the positron–electron interaction mentioned above, instead of simply adding I_{Ps} to the denominator in (8), we must take the modification of the corresponding wave functions into account. This means that the product of the one-positron Hartree and one-electron Hartree–Fock functions $E_1\ell_1$, $\varepsilon_2\ell_2$ and energies E_1 and ε_2 must be replaced by wave functions and total energies of the interacting or bound positron and electron that move in the atomic field. To
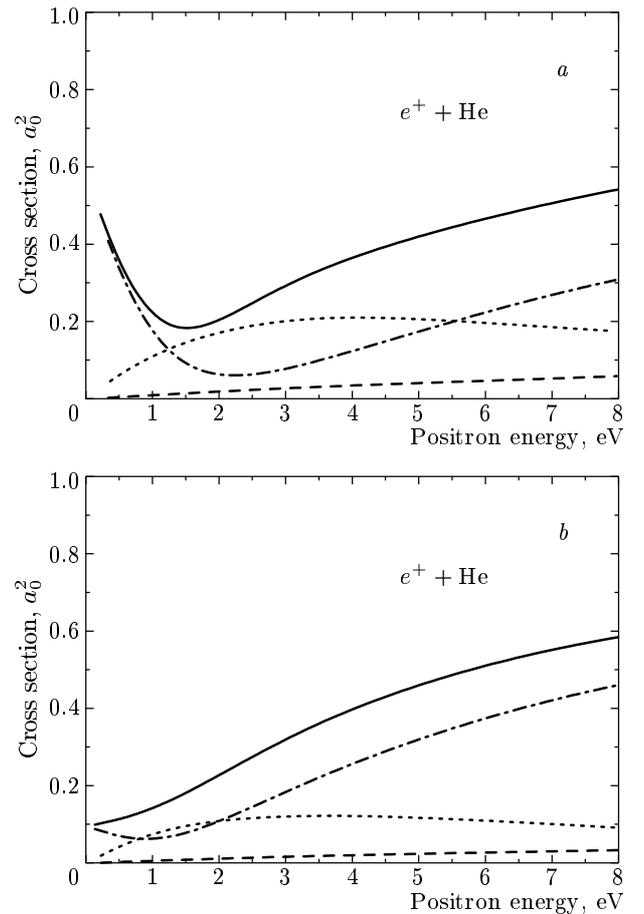

Fig. 2. Partial wave contributions to the cross sections of the elastic positron scattering on He: a — with the inclusion of positronium formation; b — without positronium formation. $I_{\mathrm{Ps}} = 0.5$Ry (a), 0 (b). The dotted-and-dashed line is the s-wave cross section, the dotted line is the p-wave cross section, the dashed line is the d-wave cross section, and the solid line is the sum of s-, p- and d-partial cross sections

find these functions and total energies, the three-body problem must be solved with the interaction between the incoming positron and atomic electron and the vacancy created after the electron virtual excitation taken into account. This is very difficult, and simplifications are inevitable. An attractive option is to describe the relative motion of the positron and the electron by a positronium wave function, while considering their center of mass as moving freely, unaffected by the selfconsistent atomic field and the vacancy field. This approximate approach has been developed in [8–10], but the modification of the energy denominator was entirely neglected there. Here, we present the results of a much simpler approach, where only the energy shift due to

virtual positronium formation is taken into account and the modification of the positron and electron wave functions is completely neglected [5–7].

4. RESULTS OF THE CALCULATIONS

Here, we give the results of our calculations for a number of atoms. We start with He.

The results for elastic scattering of positrons by He obtained using Eq. (8) are demonstrated in Fig. 1. It can be seen that the energy shift due to the positronium formation leads to a prominent decrease of the low-energy cross section. The difference is qualitative at $E \leq 1$ eV. As E grows, the influence of the positronium formation becomes smaller, but the deviation from the HF approximation results is huge in all the
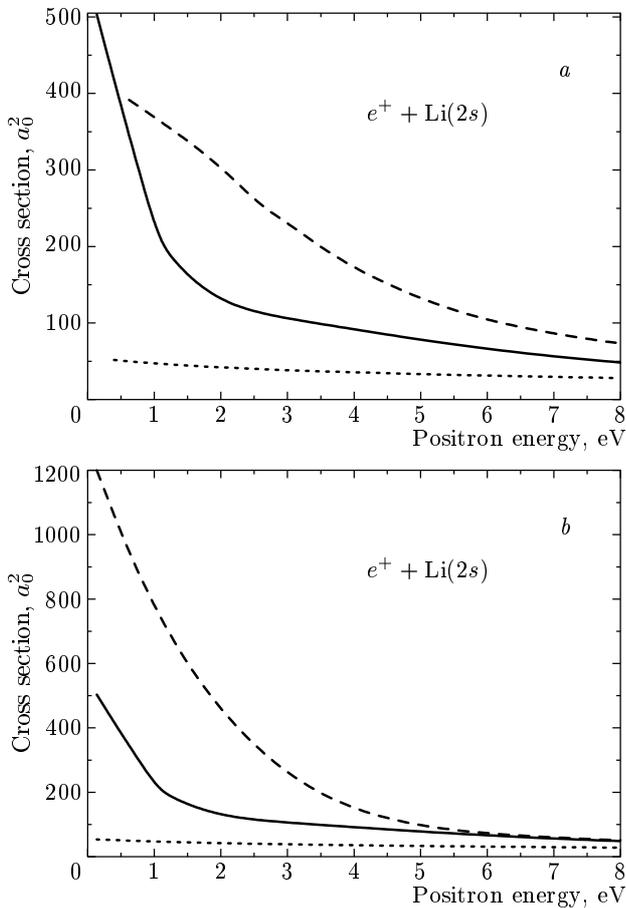
Fig. 3. Cross sections of the elastic positron scattering on Li. The dotted line (a, b) is the HF approximation. The solid line (a, b) is the RPAE with positronium formation taken into account. The dashed line is a — the result of [2], b — the RPAE without positroniun formation

region considered, up to $E = 18$ eV. To obtain the cross sections, contributions of the positron s-, p-, and d-partial waves were taken into account. We note that the virtual positronium formation leads to prominent variations in all the partial wave contributions. This is illustrated in Fig. 2, where the results with (Fig. 2a) and without (Fig. 2b) the positronium energy shift are presented.

The cross section of the low energy (e^+ +He)-elastic scattering is much smaller than that of (e^- +He). This can be explained qualitatively as follows: while the selfconsistent field V_{sc} acting on the incoming positron is repulsive, the polarization potential V_{pol}, which behaves as $-\alpha_{\text{He}}(I_{\text{Ps}})/2r^4$ far from the atom, is attractive, because $\alpha(I_{\text{Ps}})$ and $\alpha(0)$ for He are positive and of the same order of magnitude as V_{sc}. The contributions of V_{sc} and V_{pol} therefore compensate each other, suppressing the elastic scattering cross section. For the electron scattering, both V_{sc} and V_{pol} are attractive, and instead of compensating, the respective quite big contributions enhance each other.

It is of special interest to compare the (e^+ + He) and (e^+ + Li) scattering because $\alpha_{\text{Li}}(I_{\text{Ps}})$ is negative, complex, and much larger than $\alpha_{He}(I_{\text{Ps}})$ by the absolute value. In accordance with (9), the negative sign of $\alpha_{\text{Li}}(I_{\text{Ps}})$ implies that in this case, the polarization potential is repulsive instead of being always attractive [13] (also see the discussion above). This observation is important for different scattering processes in general. Indeed, if the projectile and the target constituent can form a composite particle in the intermediate state, the polarization interaction can easily change its sign, becoming attractive. This was found to occur, for example, in nuclear physics, namely in π-meson–nuclear scattering, where the (π-meson + nucleon) system forms the so-called Δ_{33}-resonance, leading to a change of the sign in the polarization interaction [14]. The imaginary part, depending on its magnitude, can effectively be of either the repulsive or the attractive nature from the point of view of the elastic scattering. We should therefore expect that because V_{sc} and V_{pol} have the same sign, they contribute constructively and hence lead to an extremely large cross section of the size of, or even bigger than the (e^- + Li) cross section. The results for (e^+ +Li) cross sections are presented in Fig. 3. It follows that the energy shift accounting for the positronium formation in the virtual state affects the low-energy cross section considerably. In Fig. 3a, we show the results obtained in the Hartree–Fock and random phase approximation with exchange with the positronium formation taken into account and the results derived in [2] using a substantially more compli-
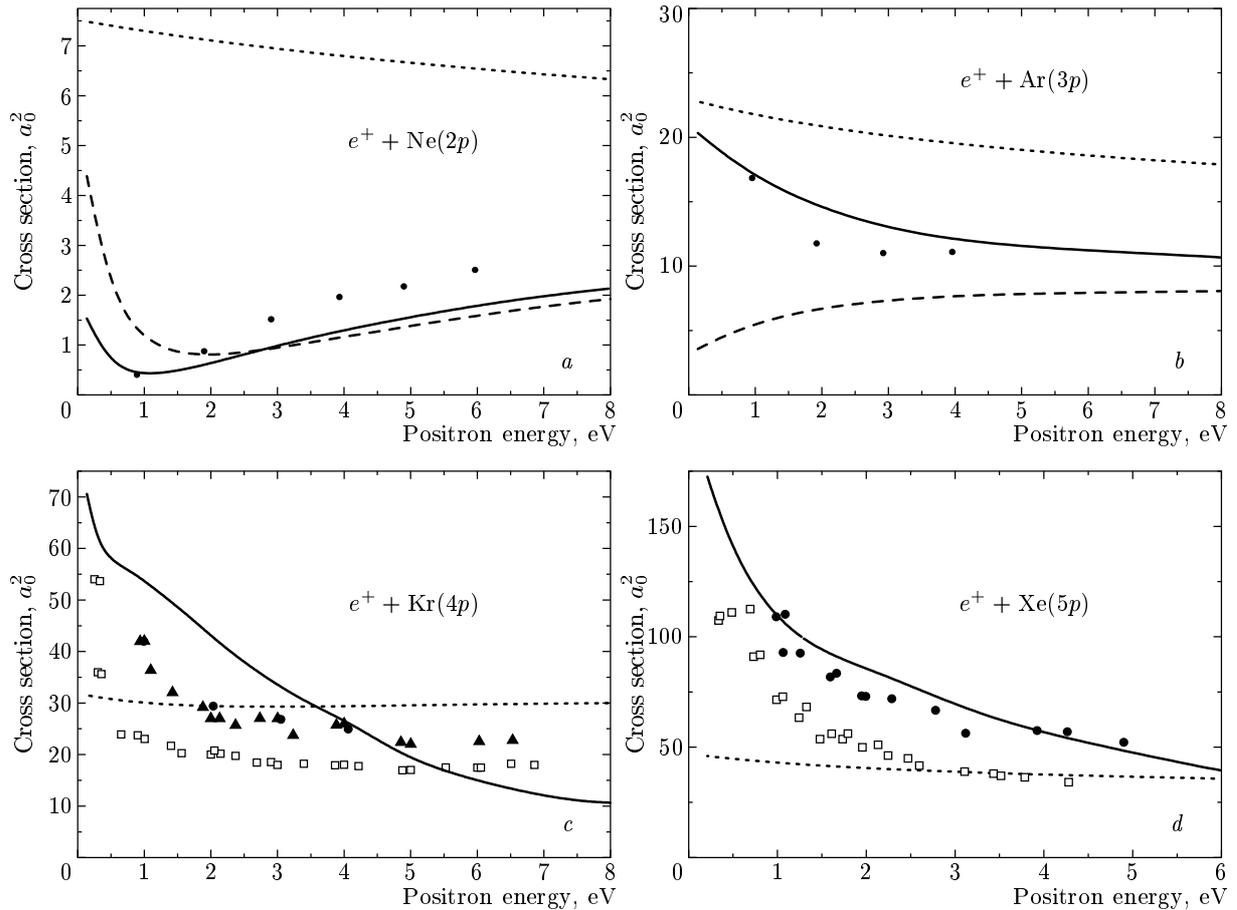
Fig. 4. Calculated cross sections of the elastic positron scattering on noble gases. The dotted line is the HF approximation, the dashed line is the RPAE without taking the positronium formation into account, the solid line is the RPAE with the positronium formation taken into account. a — Ne, experimental points from [19], b — Ar, experimental points from [19], c — Kr, experimental points: solid circles — [19], open squares — [20], solid triangles — [21], d — Xe, experimental points: solid circles — [19], open squares — [17]

cated method. Although the difference between RPAE and [2] is prominent, the deviation of both of them from the HF approximation is qualitative. Figure 3b clearly demonstrates the magnitude of the effect of taking positronium formation into account in the virtual state for $E \leq 4$ eV.

Figures 4a, b, c, and d present our results for noble gas atoms Ne, Ar, Kr, and Xe, respectively. In the case of Ne for $E \leq 2$ eV, the role of positronium formation is significant, while the deviation from the HF approximation is quite dramatic. We can see that the first experimental point at about 1 eV demonstrates the essential role of taking the positronium formation into account in the virtual state. The same effect for even higher E is seen for Ar in Fig. 4b. In Fig. 4c (Kr) and Fig. 4d (Xe), the RPAE results (with the positronium

formation) are qualitatively different from the HF results. The latest experimental points, dark triangles for Kr and dark circles for Xe, are in a reasonable agreement with the RPAE results. More accurate data are desirable, however.

The picture of positron scattering on He and Li described above is also qualitatively valid for the Ne–Na pair. Indeed, the $(e^+ + \text{Ne})$ cross section is small, considerably smaller than the geometrical one, while the $(e^+ + \text{Na})$ elastic scattering cross section (Fig. 5a) is very large. Even larger is the cross section for $(e^+ + \text{Ne})$, as can be seen in Fig. 5b. In Fig. 5, we compare our results with the close-coupling calculations from [22]. Because the calculational approaches are essentially different, the difference is not a big surprise, but experimental data are needed. For noble gases heavier than
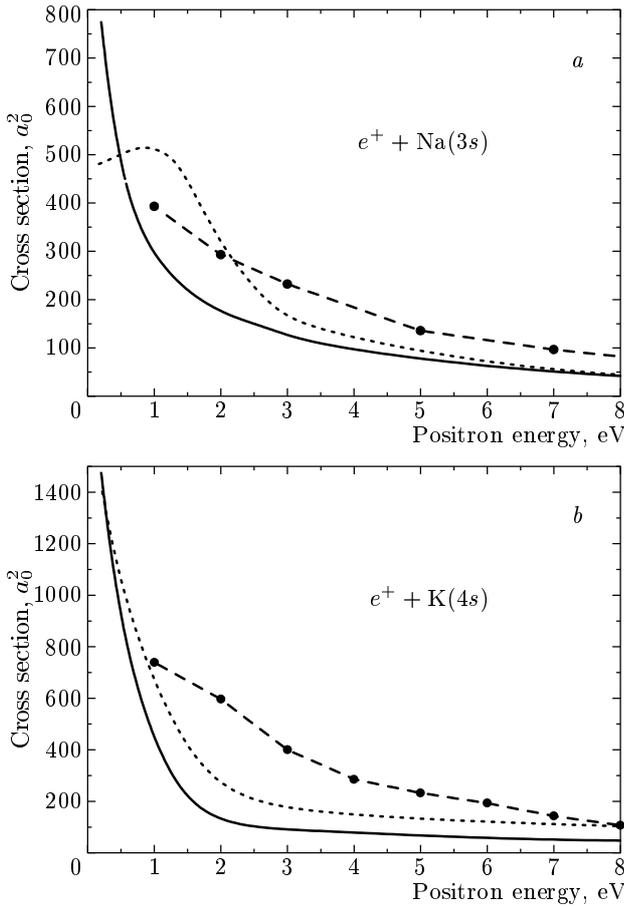
Fig. 5. Calculated cross sections of the elastic positron scattering on Na (a) and K (b). The dotted line is the HF approximation, the solid line is the RPAE with positronium formation taken into account, the dashed line with heavy dots is the result of close-coupling calculations [22]
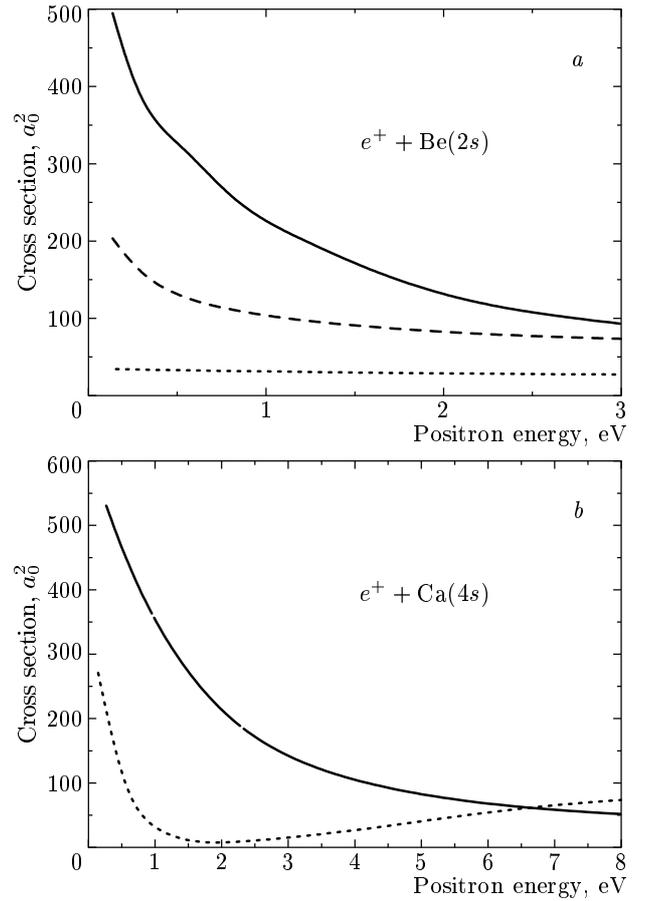
Fig. 6. Calculated cross section of the elastic positron scattering on Be (a) and Ca (b). The dotted line is the HF approximation, the solid line is the RPAE with positronium formation taken into account, the dashed line is the RPAE without positronium formation

Ne, namely Ar, Kr, and Xe, the polarization interaction is much larger and the cross sections increase as the atomic number grows. As in the Li–He case, the cross sections for the alkali neighbors are again much larger. The results for Kr and Xe are in a qualitative agreement with those obtained in [1] using a much more complicated method.

It is interesting to compare the results for a group of three neighbors, a noble gas, alkali, and alkali-earth atom. As a good example, the groups of atoms He, Li, Be (Fig. 6a) and Ar, K, Ca (Fig. 6b) are considered (Figs. 1–6). We checked the role of the positronium formation for Be and found it very important, as previously. For Be, the cross sections proved to be similar in size and shape to those of Li, which is a consequence of the fact that their polarizabilities $\alpha(I_{\mathrm{Ps}})$ are rela-

tively close. The situation is different for Ca, where the cross section is much smaller at very low E, but then decreases much slower than in K. For Ar, K, and Ca, all the three curves are qualitatively similar, but the ($e^+ + $ K) elastic scattering cross section is by an order of magnitude larger than that of ($e^+ + $ Ar).

It is of some interest to study the imaginary parts of the elastic scattering phases. They describe the respective partial wave contributions to the cross section of the inelastic process

$$e^+ + \mathrm{A} \rightarrow \mathrm{Ps} + \mathrm{A}^+. \tag{10}$$

The inelastic positron scattering cross section $\sigma_{in}(E)$ is expressed through the imaginary part of the phase shift $\Delta\,\delta_\ell'(E)$ as

$$\sigma_{in}(E) = \frac{\pi}{E}\sum_{\ell=0}^{2}(2\ell+1)[1-\exp(-4\Delta\,\delta_\ell'(E))]. \tag{11}$$
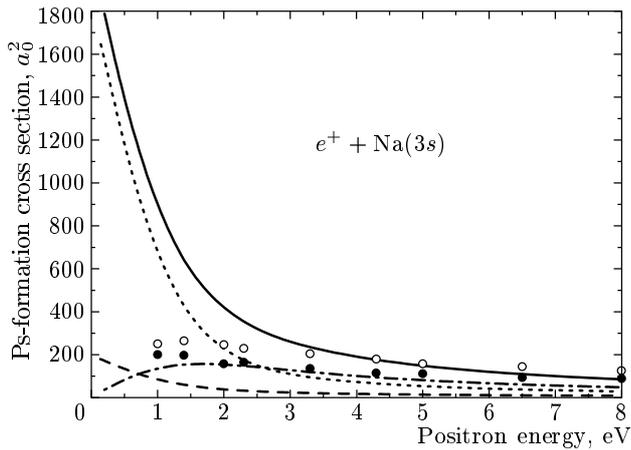
Fig. 7. Ps-formation cross sections for positron–Na scattering in RPAE. The dotted-and-dashed line is the s-wave cross section, the dotted line is the p-wave cross section, the dashed line is the d-wave cross section, the solid line is the sum of s-, p-, and d-partial cross sections. Experimental points are taken from [23], open circles show the upper limit, and solid circles show the lower limit

As in calculations of $\sigma(E)$, we limit ourselves to taking the first three partial waves into account (those with $\ell = 0, 1, 2$). In Fig. 7, we show the results of our calculation of the Ps-formation cross section in positron–Na atom scattering together with the experimental data of [23]. At low energies, there is a strong deviation from the experiment, as in many other calculations [24], but at energies above 3 eV, there is a satisfactory agreement. We note that it is assumed in this calculation that any electron obtained by ionization together with the inelastically scattered positron form a positronium Ps. Obviously, this is an exaggeration: some of the electrons leave the atom without forming a real positronium. This is particularly essential for a small energy E in the cases where the Ps-formation threshold is at $E = 0$ (as in $(e^+ + \mathrm{Na}$ collision).

We note that using Eq. (8), we can also describe the Wigner–Baz' peculiarities in the elastic scattering cross section near the threshold of inelastic channel (10) [11].

5. SUMMARY AND DISCUSSION OF THE RESULTS

We have demonstrated that the relatively simple method with both many-electron correlations and virtual positronium formation taken into account allows obtaining relatively good results for the elastic scattering of positrons on different atoms in the periodic table,

in particular, noble gas and alkali atoms. It also gives an estimate of the Ps-formation cross section. The approach developed in this paper can be applied without any essential difficulty to the study of positron scattering on more complicated targets, such as molecules, clusters, and fullerenes.

It is interesting to know whether the bound states in the $(e^+ + \mathrm{A})$ system can be described within the simple approach developed here. Indeed, given the repulsive nature of V_{sc} and possibly also repulsive nature of V_{pol}, it is far from trivial that the binding can occur at all. We can therefore expect bound states of positrons with those atoms A for which $\alpha_A(I_{\mathrm{Ps}})$ is big (considerably bigger than in noble gases) and positive, $\alpha_A(I_{\mathrm{Ps}}) > 0$, i.e., V_{pol} is sufficiently strong and attractive. An interesting and intriguing possibility is that the $(e^+ + \mathrm{A})$ bound state results from the action of the imaginary part $\mathrm{Im}(V_{pol})$. On the other hand, the binding can originate from the interaction of Ps and A via Van der Waals forces. These are particularly big if A^+ has the electronic structure similar to an atom in the first period of the Mendeleev table, i.e., A is in the second period. To detect the possibility of forming a bound state, one must study the magnitude of the scattering phase shift at zero energy: if it reaches π, a bound state is created in the channel under consideration. It must be checked, however, whether this state is stable against the decay through the $(\mathrm{Ps} + \mathrm{A}^+)$ channel, which requires knowing the bound state energy. Finding it is much more complicated than calculating the phase shifts at zero e^+-energy.

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