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ELASTIC SCATTERING OF LOW-ENERGY POSITRON BY ATOM

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Abstract. *In this paper, we present our calculation for the elastic scattering of the slow positron from atoms. The calculation is performed for He, Ne, Xe and Kr. In the calculations we used Random phase approximation. By slowing Dyson equation we take into account the correlation effects. Our results are consistent with experimental and other theoretical results.*

Key words: *positron-atom elastic scattering, random phase approximation*

1. INTRODUCTION

The scattering of positrons by atoms is very different from the corresponding electron-atom scattering. Apparently it may be seen that only a charge of sign in the interaction potential is involved. In the presence of a projectile, the atomic cloud is distorted. It is interesting to note that the effect of distortion of the atom is attractive in nature for both cases. The importance of the polarization potential in low energy electron-atom scattering processes is well known. For electrons, the potential due to polarization tends to add to the static potential which, being attractive, tends to cancel the static interaction which is repulsive. These differences provide useful information in assessing the relative importance of the polarization potential. At low incident positron energies the effect of polarization is found to be large enough to cause the positron to be, on the whole, attracted to the atom.

The interaction of a low-energy positron with a many-electron atom is characterized by strong correlation effects. Apart from the dynamic polarization of the electron cloud by the field of the positron, the positron can also form positronium (Ps), by picking up one of the atomic electrons. When the positron energy is below the Ps-formation threshold, $\varepsilon_{Ps} = I + E_{1s}(Ps) = I - 6.8\text{eV}$ where I is the atomic ionization potential, positronium formation is a virtual process. Another fundamental difference between positron and electron scattering is that the positron, unlike the electron, is distinguishable from the target

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electrons. In the case of electron scattering, the nature of the total wave function is fully guided by Pauli's principle, whereas in the positron scattering case, our knowledge of the total wave function is incomplete for small separations.

In common with electron-atom collisions, many processes can occur during the interaction of positrons with atoms. At low energies, elastic scattering is usually the only open channel apart from annihilation which has a relatively negligible effect compared with any other processes. As the incident positron energy increases, various inelastic channels become accessible, including positronium formation, target excitation and ionization. For positron-helium collisions, for example, the elastic scattering remains the only open channel for energies below the Ps formation threshold of 17.8 eV [1].

During the last 20 years positron-atom collision problems have been studied extensively. The development of new experimental techniques to obtain low energy monoenergetic beam has stimulated this surge of activity [2]. A comprehensive review of progress in the positron—atom (--molecule) scattering has been given by many researchers [3]. In spite of the important advances in recent years, both theoretically and experimentally, our knowledge of positron-atom scattering is still incomplete.

The change of the sign of the charge in e^+-atom scattering as opposed to the e^--atom scattering has several important consequences. The exchange effects between the projectile and the target electrons are absent. In contrast to the electron, the positron is attracted by the target electrons and repelled by the nuclei. This attraction must be taken into account adequately if accurate results are to be obtained. In the case of positron scattering by atoms the static potential energy is positive, whereas the lowest order term in the polarization potential is negative. Thus two major components in the e^+-target interaction tend to cancel each other.

The slow positron scattering has the specificity that the incident e^+ combines with one of the electrons in the target to produce a bound positron-electron system (positronium). That is to say, a new inelastic threshold appears where positronium formation is energetically allowed. This inelastic threshold always lies below the first inelastic threshold of excitation.

The theoretical analysis of positron scattering from atomic systems represents a very difficult task of scattering theory, requiring that a double perturbative expansion, with respect to both e^+ - e^- and e^- - e^- Coulomb interactions, respectively, be carried out. In the case of e^+- He scattering, accurate results have been obtained by the variational methods [4,5,6], and the optical potential method [6,7,8,9].

In this paper, we have improved a method, which recently was suggested in ref [7,8]. This method is based on the many-body theory, namely, the random phase approximation (RPA) [9], and a simple "energy shift" technique was suggested whereby the influence of the virtual positronium formation (VPF) channel (i.e. the spatial correlation between the projectile and target electrons during the scattering) could be taken into account. All notations used in the paper follow those in ref. [7].

THEORY

A conventional treatment of positron scattering from an N-electron target would start from the Schrödinger equation for the total wave function for the N+1 particles. In many body theory we start instead from Dyson equation [10]

$$(H_0 + \Sigma_\varepsilon)\psi_\varepsilon = \varepsilon\psi_\varepsilon \tag{1}$$

where ψ_ε is the single-particle (quasiparticle) wave function of the positron, ε is its energy, and H_0 is a central-field Hamiltonian of the zero approximation, which describes the motion of the positron in the static field of the target. The many-body dynamics in Eq. (1) is represented by Σ_ε, a non-local energy-dependent correlation potential. This quantity, also known as the optical potential, is equal to the self-energy part of the single-particle Green's function of the positron in the presence of the atom [11]. Due to its non-local nature, Σ_ε operates on the quasiparticle wave function as an integral operator

$$\Sigma_\varepsilon\psi_\varepsilon = \int \Sigma_\varepsilon(r,r')\psi_\varepsilon(r')dr'. \tag{2}$$

For systems containing more than one electron the Hartree-Fock (HF) Hamiltonian (without exchange, for the positron) is the best choice. The correlation potential Σ_ε is given by an infinite perturbation series in powers of the residual electron-electron and electron-positron interaction. Inclusion of the electrostatic interaction in H_0 and the use of the HF approximation for the target electrons means that the perturbation theory expansion for Σ_ε starts with the second-order diagrams, and that the diagram does not contain elements which describe the electrostatic potential (for electrons this also means the absence of the contributions of the target exchange potential).

Owing to the spherical symmetry of the problem, Eq. (1) can be solved separately for each positron partial wave. So, in particle one deals with radial quasiparticle wave functions, $\widetilde{P}_{\varepsilon\ell}(r)$, related to ψ_ε by $\psi_\varepsilon(r) = r^{-1}\widetilde{P}_{\varepsilon\ell}(r)\,Y_{\ell m}(\Omega)$, where $Y_{\ell m}(\Omega)$ is the spherical harmonic for the orbital angular momentum ℓ. Accordingly, the self-energy operator is also found for each partial wave separately as

$$\Sigma_\varepsilon(r,r') = \frac{1}{rr'}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{m=\ell} Y_{\ell m}(\Omega)\Sigma_\varepsilon^{\ell}(r,r')Y_{\ell m}^{*}(\Omega') \tag{3}$$

Rather than solving the Dyson equation for the quasiparticle wave function in the coordinate approximation it is easier to work with the self-energy matrix,

$$\langle\varepsilon'|\,\Sigma_\varepsilon\,|\,\varepsilon\rangle = \int \varphi_{\varepsilon'}^{*}(r)\Sigma_\varepsilon(r,r')\varphi_\varepsilon dr dr' \tag{4}$$

where φ_ε are the positron eigen function of the HF Hamiltonian

$$H_0\varphi_\varepsilon = \varepsilon\varphi_e \tag{5}$$

with a given angular momentum ℓ, $\varphi_\varepsilon(r) = r^{-1}P_{\varepsilon\ell}(r)Y_{\ell m}(\Omega)$.Since the static potential of the atom is repulsive, all positron states φ_ε lie in the continuum ($\varepsilon > 0$). The radial wave function is normalized to a δ-function of energy, $\delta(k^2 - k'^2)$, where k is the positron momentum. This corresponds to the asymptotic behavior

$$P_{\varepsilon\ell}(r) \sim (\pi k)^{-1/2}\sin(kr - \frac{\ell\pi}{2} + \delta_\ell^{(0)}) \tag{6}$$

where $\delta_\ell^{(0)}$ is the scattering phase shift in the static potential.

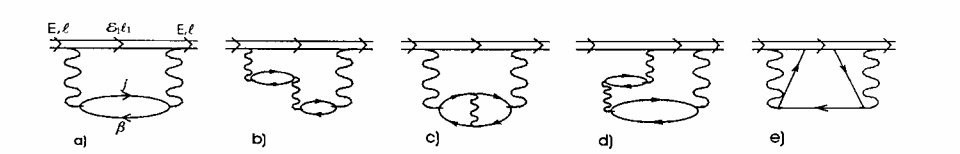

Fig. 1. Some of the RPA diagrams corresponding to (10)

The matrix (4) can be used to obtain the phase shifts directly [12]. A "reducible" self-energy matrix $\langle\varepsilon'|\,\widetilde{\Sigma}_\varepsilon\,|\varepsilon\rangle$ is found via the integral equation

$$\langle\varepsilon'|\,\widetilde{\Sigma}_\varepsilon\,|\varepsilon\rangle = \langle\varepsilon'|\,\Sigma_E\,|\varepsilon\rangle + P\int \frac{\langle\varepsilon'|\,\widetilde{\Sigma}_E\,|\varepsilon''\rangle\langle\varepsilon''|\,\Sigma_E\,|\varepsilon\rangle}{E-\varepsilon''}d\varepsilon'' \tag{7}$$

As an initial approximation for the positron, the wave functions $P_{E\ell}^{N+1}$ (radial part) are used, which were obtained from the "frozen" Hartree-Fock (HF) atomic state. The excited continuum state radial functions are normalized to the δ-functions of the energy. The scattered positron wave function can be written as a solution of the following equation [3]:

$$P_{E\ell}^{\Sigma} = P_{E\ell}^{N+1} - \frac{1}{H_\ell^{HF}-E}\int \Sigma_\ell(r,r';E)P_{E\ell}^{\Sigma}(r')dr' \tag{8}$$

where H_ℓ^{HF} is the radial part of the single-particle HF Hamiltonian $P_{E\ell}^{N+1}$ are its eigen-functions) and $\Sigma_\ell(r,r';E)$ is the optical potential (i.e. the irreducible part of the single-particle Green function in the coordinate representation). $P_{E\ell}^{\Sigma}$ has the asymptotic form

$$P_{E,\ell}^{\Sigma} \approx \frac{1}{\sqrt{\pi k}}\{\sin[kr-\frac{1}{2}\ell\pi+\delta_\ell^{HF}(E)]+\tan\Delta\delta_\ell\cos[kr-\frac{1}{2}\ell\pi+\delta_\ell^{HF}(E)]\} \tag{9}$$

where $k=\sqrt{E}$ is the positron momentum, and $\Delta\delta_\ell$ is the correlation correction to the frozen-core HF value (δ_ℓ^{HF}) of the phase shift, $\delta_\ell(E) = \delta_\ell^{HF}(E) + \Delta\delta_\ell(E)$.
The RPA contribution to the scattering process was determined by using the relationship [3]

$$\Delta\delta^{RPA}(E) \simeq -\pi\langle P_{E,\ell}^{N+1}\,\|\,\Sigma_\ell^{RPA}(E)\,\|\,P_{E,\ell}^{N+1}\rangle. \tag{10}$$

$\Delta\delta_\ell^{RPA}(E)$ makes contribution to the phase shift, due to the RPA optical potential and double vertical line represents reduced matrix elements. The expression (3) corresponds to a first Born approximation to a "two-potential formula" [9]. The effect of the Hartree distorting field (the first potential) is fully taken into account, in terms of the P^{N+1} functions.

For the process which will be considered, the momentum-space T-matrix elements can be expressed in terms of the following Lippmann-Schwinger relationship [7]:

$$\langle k_i\ell\,|\,T_\ell(\varepsilon_i)\,|\,k_i\ell\rangle = \langle k_i\ell\,|\,\Sigma_\ell(\varepsilon_i)\,|\,k_i\ell\rangle + \frac{2}{\pi}\int_0^\infty dk_1\,\frac{\langle k_i\ell\,|\,\Sigma_\ell(\varepsilon_i)\,|\,k_1\ell\rangle\langle k_i\ell\,|\,T_\ell(\varepsilon_i)\,|\,k_i\ell\rangle}{k_i^2-k_1^2+i\delta} \tag{11}$$

where the ℓ-th radial component of the optical potential have been evaluated at the $\varepsilon = k_i^2$ scattering energy. The optical potential Σ is given by Hartree term augmented by the RPA contribution: $\Sigma(\varepsilon_i) = \Sigma^H + \Sigma^{RPA}(\varepsilon_i)$. Their matrix elements can be conveniently given according to Fig. 1a (the positron is depicted by double line, the electron and hole by a single line and the Coulomb interaction by a **wavy** line):

$$\langle k_i\ell \,|\, \Sigma_\ell^{RPA}(\varepsilon_i) \,|\, k\ell\rangle =$$
$$\sum_{\beta\le F, j>F}\sum_{L,\ell_1}[(2\ell+1)(2L+1)]^{-1}\int_0^\infty dk_1 \frac{\langle k_i\ell,\beta \,\|\, V_L \,\|\, k_1\ell_1, j\rangle\langle k_1\ell_1, j \,\|\, V_L \,\|\, k\ell,\beta\rangle}{\varepsilon_i - (\varepsilon_j^{RPA} - \varepsilon_\beta^{HF}) - \varepsilon_1 + i\delta}. \qquad (12)$$

The summation $\beta \le F$ is performed over occupied states, whereas $j > F$ means the summation is carried out over all discrete excited states and integration performed over the continuum. The higher "time-forward" diagrams of the RPA method (Figures 1b. and 1c.) are taken into account by using the wave functions $P_{(\beta)j}^{N(LS)}$ for the states $\varepsilon_2\ell_2$ (i.e. $k_2\ell_2$) (Fig. 1a), calculated in the "frozen" ion core with the hole in the state β. We estimated the contribution of the "time backward" diagrams (for example, Fig. 1d) - their contribution was about 5.3%. Diagram 1e represents the results of the summation of the infinite sequence of diagrams, which represents the VPF terms.

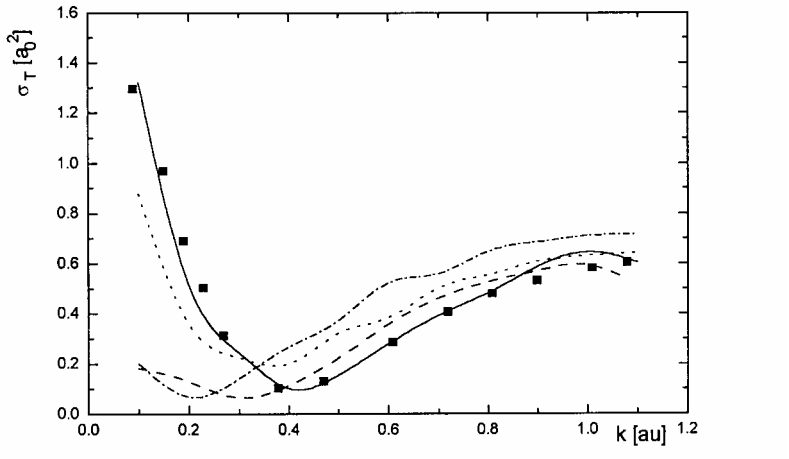

Fig. 2. Total cross section for e^+-He: solid line our result, dash [7], dot-dash [8], dots [9], black square [5]

In order to introduce the effect of virtual positronium formation VPF (the results of the summation of an infinite sequence of the diagrams which represents the VPF terms are presented in Figure 1g) it is suggested [7] the "energy shift" technique by replacing the binding energy hole ε_β in the denominator of Eq. (5) by $\varepsilon_\beta^{HF} - E_p$ (where $E_p = -0.5Ryd$). The bound state of the positron-electron pair is known as positronium.

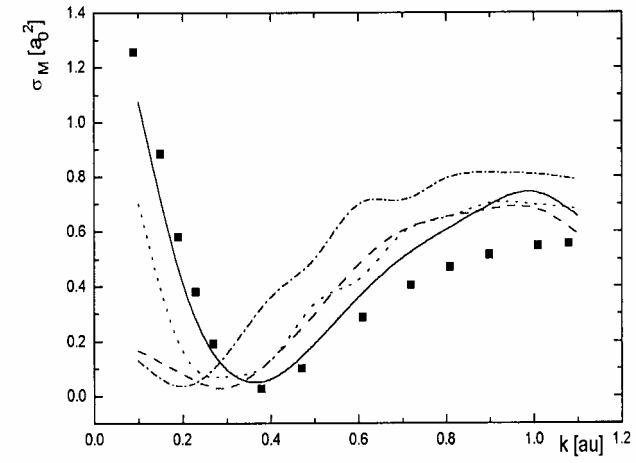

Fig. 3. Momentum transfer cross section for e^+-He : solid line our result, dash [7], dot-dash [8], dots [10], black square [6].

The binding between a positron and an electron is the attractive Coulomb interaction. The energetic of positronium formation is described by the Ore gap model (A.Ore, Naturvidenskap Rekko No.9, Univ. Bergen Arbok. 1973). It states that the probability of positronium formation is maximum when the positron energy during thermalization lies within a gap where no other electronic energy transfer is possible. To capture an electron from an atom or a molecule in a medium with ionization energy E_i, the kinetic energy E_p of the positron must be greater than $E_i - E_{\{ps\}}$, $E_{\{ps\}}$ being the binding energy of the positronium. In vacuum, the binding energy of a positronium atom is 6.8 eV but may be smaller in the medium. If the positron energy E_p is greater than the ionizing energy E_i of the medium, the positronium atom is formed with a kinetic energy greater than its binding energy and it will rapidly break up in further collisions. Furthermore, above the lowest excitation energy $E_{\{ex\}}$, inelastic processes occur. These processes definitely slow down the rate probability of positronium formation. Thus the positronium formation is most probable with the energy in the range $E_i - E_{\{ps\}} < E_p < E_{\{ex\}}$ which is the Ore gap. As suggested in ref. [9] such energy shift is equivalent to lowering the thresholds of the 2^1S and 2^1P inelastic channels by the same amount ($\simeq 6.80$eV). We have solved equation (4) numerically by using the "improper" calculation for contributions of the RPA matrix elements (some of the contributions of estimated RPA third order diagrams).

RESULTS AND CONCLUSIONS

To evaluate the diagrams of the correlation potential Σ, one first needs to generate sets of electron and positron HF basis states. Evaluation of the diagram requires summation over complete sets of electron and positrons intermediate states, including integration over the electron and positron continua.

To perform a numerical calculation, the continuous spectrum can be discretized. The simplest way of doing this is by placing the system in a spherical cavity of radius R. Set-

ting the wave function to zero at the boundary will result in a discrete spectrum of eigenstates with an approximately constant step size in momentum space. The basis states are obtained by expanding the radial wave functions $P_\ell(r)$ in terms of B splines $B_i(r)$

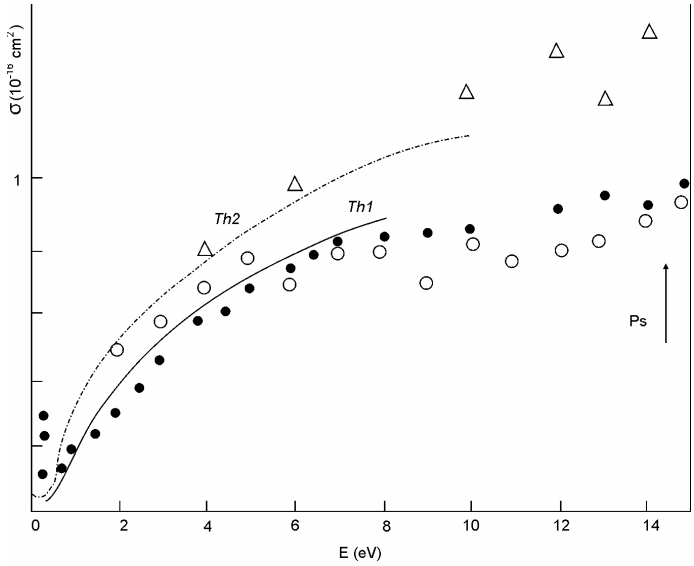

Fig. 4. Total cross section for e^+-Ne: • [15], ○ [16], Δ [17], Th2 [19], Th1 our result.

$$P_\ell(r) = \sum C_i^{(\ell)} B_i(r) \tag{13}$$

where $H_{ij} = \langle B_i \mid H_0^{(\ell)} \mid B_j \rangle$ and $Q_{ij} = \langle B_i \mid B_j \rangle$. Prior to solving Eq. (13) the ground-state atom HF Hamiltonian is generated by a conventional HF routine [14].

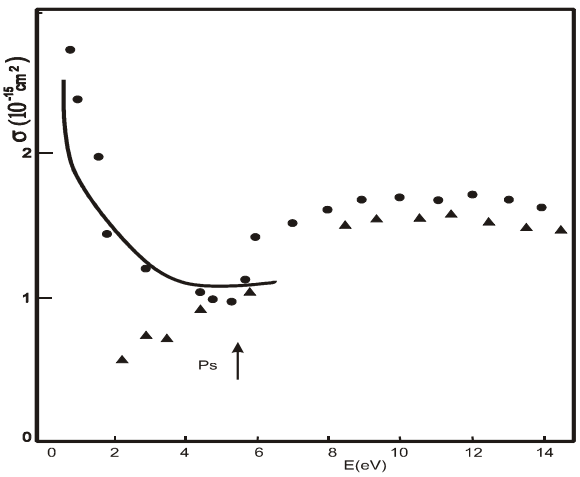

Fig. 5. Total cross section for e^+-Xe: • [15], ▲ [16], solid line our result

The use of a B-spline basis means that fast convergence is achieved with respect to the number of states with a particular orbital angular momentum of the electron and positron intermediate states included in the calculation. It has been known for a while that calculations of positron-atom scattering converge slowly with respect to the number of target angular momentum included in the expansion of the total wave function, notably slower than in the electron-atom case [15]. Physically, the slow convergence rate arises from the need to describe virtual Ps localized outside the atom by an expansion in terms of single-particle orbital centered on the nucleus [16]

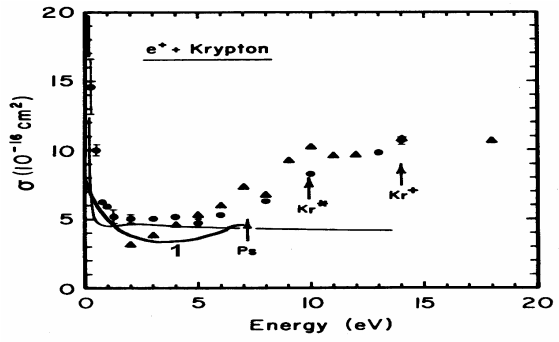

Fig. 6. Total cross section for e^+-Kr: • [15], ▲ [16], – [17], 1 our result

The contribution of diagrams with transferred angular momentum $\ell = 0,1,2,3,4$ was calculated, and when $\ell > 4$ the contribution was estimated. This is a clear indication of the fact that the approximation (3) (while useful for electron atom scattering), breaks down for processes involving positrons, as pointed out in ref. [8,9]. In the lower energy range (below about 4 eV) the contribution of the virtual positronium formation (VPF) channel (missing from RPA calculations) is most important.

The elastic scattering crosssection (both total, $\sigma_T = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$, and momentum transfer, $\sigma_M = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(\ell+1)\sin^2(\delta_\ell - \delta_{\ell-1})$) are plotted in Figures 3 and 4, where they are compared with some experimental [5,6] and theoretical results [6,7,8,9,10]. Our previous results ($RPA^{(1)}$) [7] are different from the present results ($RPA^{(imp)}$). On the basis of the obtained results we conclude that the RPA optical potential, characteristic of many-body formulations, can be expected to lead to reasonable agreement with experimental results for positron-atom scattering processes.

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ELASTIČNO RASEJANNJE SPORIH POZITRONA NA ATOMIMA

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U radu smo prikazali naše proračune elastičnog rasejanja sporih pozitrona na atomima inertnih gasova (He, Ne, Xe, Kr). Za izračunavanje faznih pomeraja koristli smo aproksimaciju slučajnih faza a na osnovu faznih pomeraja računali smo efikasne preseke za rasejanje. Korelacione efekte smo uzimali u obzir rešavanjem Dysonove jednačine. Dobijeni rezultati se dobro slažu sa eksperimentalnim i drugim teorijskim rezultatima.