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OPTICAL POTENTIAL APPROACH TO THE SLOW POSITRON SCATTERING FROM HELIUM ATOM

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A. R. Tančić[1], M. R. Nikolić[2]

[1]Institute for Nuclear Science Vinča, lab 020, Belgrade, Yugoslavia
[2]University of Niš, Faculty of Science and Mathematics, Department of Physics

Abstract. *We have extended our previous calculations to include the contribution of the random-phase approximation (RPA) (improved) optical potential to the low energy elastic scattering in the electron+He system. Our improved RPA calculations are shown to be in better agreement with the experimental values than other theoretical results.*

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

INTRODUCTION

The existence of positron was predicted theoretically by Dirac [1], and [2] and Oppenheimer [3], and confirmed experimentally by Anderson [4] Blackett and Occhialini [5]. Positron has been extensively used as probes in different areas of physics: in the high energy physics, where the interaction of positrons with electrons gives very interesting information; in the condensed matter physics the beams of positrons are used to obtain unique information about crystal defects, their formation and configuration, and, to determinate the Fermi (F) surface, too. The study of atomic collision phenomena has great importance in the theory of thermonuclear research, chemical reactions, gaseous electronics and lasers. The electron-atom approximate theories may be used as a sensitive self-test by applying them in the case of positron-atom scattering.

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 [6]. A comprehensive review of progress in the positron–atom (molecule) scattering has been given by many researchers [7]. In spite of 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

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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 [12,13,14], and the optical potential method [14,15,16,17].

In this paper we have improved a method, which recently was suggested in ref [15,16]. This method is based on the many-body theory, namely, the random phase approximation (RPA) [19], 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. [15].

THEORY

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 [7]:

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

where H_ℓ^{HF} is the radial part of the single-particle HF Hamiltonian ($P_{E\ell}^{N+1}$ are its eigenfunctions) 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). $P_{E\ell}^{\Sigma}$ have the asymptotic form

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

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, $\delta_\ell(E) = \delta_\ell^{HF}(E) + \Delta\delta_\ell(E)$.

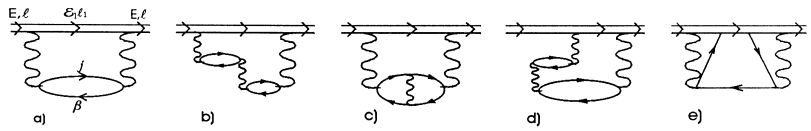

Fig. 1. Some of the RPA diagrams coreesponding to (3)

The RPA contribution to the scattering process was determined by using the relationship [7]

$$\Delta\delta^{RPA}(E) \cong -\pi\langle P_{E\ell}^{N+1} \| \Sigma_{\ell}^{RPA}(E) \| P_{E\ell}^{N+1}\rangle \tag{3}$$

$\Delta\delta_{\ell}^{RPA}(E)$ gives the 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" [19]. The effect of the Hartree distorting field (the first potential) is fully taken into account, in terms of the P^{N+1} functions.

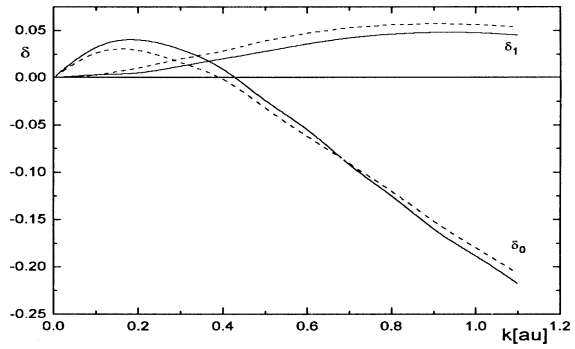

Fig. 2. Phase shift for s (δ_0) and p (δ_1) waves,---- our RPA results, - - - our HF results

For the process which will be considered the momentum-space T-matrix elements can be expressed in terms of the following Lippmann-Schwinger relationship [15]:

$$\langle k_i\ell \,|\, T_{\ell}(\varepsilon_i) \,|\, k_i\ell\rangle = \langle k_i\ell \,|\, \Sigma_{\ell}(\varepsilon_i) \,|\, k_i\ell\rangle + \frac{2}{\pi}\int_0^{\infty} dk_1 \frac{\langle k_i\ell \,|\, \Sigma_{\ell}(\varepsilon_i) \,|\, k_1\ell\rangle\langle k_1\ell \,|\, T_{\ell}(\varepsilon_i) \,|\, k_i\ell\rangle}{k_i^2 - k_1^2 + i\delta} \tag{4}$$

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: $\Sigma(\varepsilon_i) = \Sigma^{HF}(\varepsilon_i) + \Sigma^{RPA}(\varepsilon_i)$, 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):

$$\langle k_i\ell \,|\, \Sigma_\ell^{RPA}(\varepsilon_i) \,|\, k\ell\rangle = \sum_{\beta\le F,\, j>F} \sum_{L,\ell_1} [(2\ell+1)(2L+1)]^{-1} \times \int_0^\infty dk_1 \frac{\langle k_i\ell, \beta \,\|\, V_L \,\|\, k_1\ell_1, j\rangle \langle k_1\ell_1, j \,\|\, V_L \,\|\, k\ell, \beta\rangle}{\varepsilon_i - (\varepsilon_j^{RPA} - \varepsilon_\beta^{HF}) - \varepsilon_1 + i\delta} \tag{5}$$

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 contributions was contributions was about 5.3%. Diagram 1e represent the results of the summation of the infinite sequence of diagrams which represents the VPF terms.

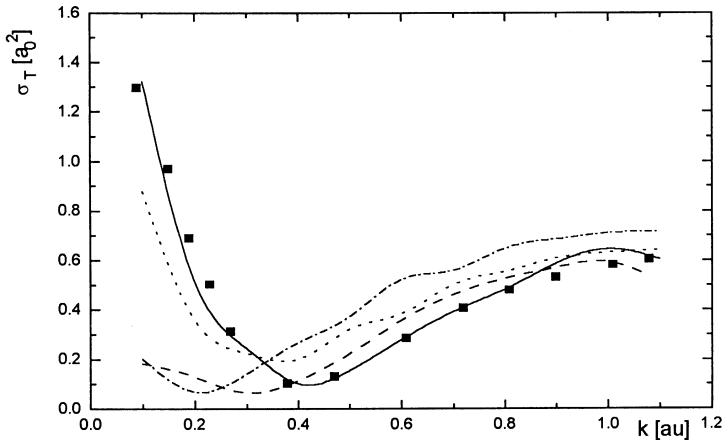

Fig 3. Total cross section: solid line our result, dash [15], dot-dash [16], dots [19], black square [13]

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 [15] 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.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 a suggested in ref. [17] such energy shift is equivalent to lowering the thresholds of the 2^1S and 2^1P inelastic channels by the same amount ($\simeq$6.80eV). 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).

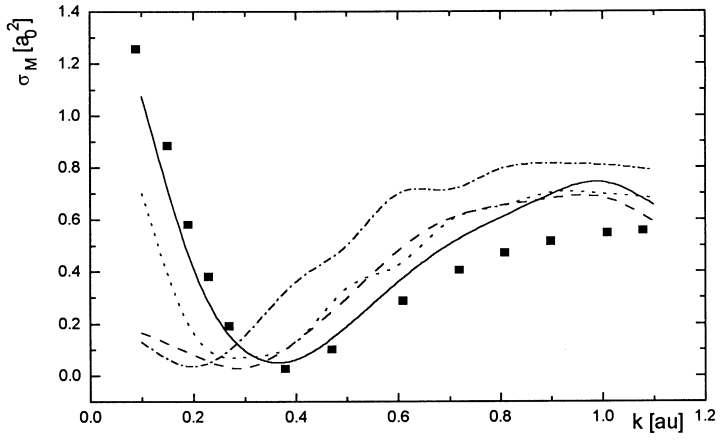

Fig 4. Momentum transfer cross section: : solid line our result, dash [15], dot-dash [16], dots [18], black square [14].

RESULTS AND CONCLUSIONS

The contribution of diagrams with transferred angular momentum $\ell = 0,1,2,3,4$ was calculated, and when $\ell > 4$ the contribution was estimated. The values of the *s* and *p* phases are plotted in figure 2. 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. [16,17]. 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 cross section (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 [13,14] and theoretical results [14,15,16,18,19]. Our previous results (RPA$^{(1)}$) [15] are different from the present results (RPA$^{(imp)}$). On the base 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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RASEJANJE SPORIH POZITRONA NA ATOMU HELIJUMA, TRETMAN PREKO OPTIČKOG POTENCIJALA

A. R. Tančić, M. R. Nikolić

U radu smo proširili naše prethodno izračunavanje uključivanjem doprinosa RPA optičkog potencijala u razmatranju elastičnog rasejanja sporih pozitrona na atomu helijuma. Pokazano je kako se menja faya rasejanje i na osnovu faza izračunati su totalni i momentum transfer efikasni preseci. Dobijeni rezultati su upoređeni sa drugim teorijskim i sa eksperimentalnim rezultatima.