J.Basrah Researches (Sciences) Vol.31. Part.2. 1-7 (2005)

Calculating the Annihilation Parameters for the Interaction of Positrons-Noble systems

A.A.Khalf

Physics Department, College of science, University of Basrah, Basrah, Iraq

Received 12/9/2004, Accpted 16/1/2005

Abstract

One of the most important events happens when positrons interact with atoms is the annihilation process of the positronium (e^-+e^+) atom, which is a probable structure, forming during the interaction. We have extended our previous work on the partial wave approximation, to the treatment of annihilation process for positron-atom system in the elastic scattering region. We have use a formula of annihilation parameter (Z_{eff}) proposed by Gribakin (Phys.Rev.A,61,22720(200)) depending in it's general formula on Phase shift, which in turn had calculated using the Polarized Orbital method, whereas our method in calculating that factor was the Partial Wave method. Good agreement is obtained between our results and those of Gribakin concerning (Z_{eff}), also we calculate the annihilation rate (λ_a), and the annihilation cross section (σ_a), where both depends on (Z_{eff}) in explicit mathematical formulas.

Keywords: scattering-annihilation-cross section-positron-inert gases.

Introduction

In this work we apply partial-wave method to calculate the annihilation parameter (Z_{eff}) for low-energy positron scattering from Noble atoms, also we calculate the annihilation rate & cross section in low-density atomic gases. The interaction of the positron with the atom is described by means of a non-local energy dependent correlation potential[1].The definition of the annihilation parameter (Z_{eff}) is the effective number of target electrons contributing to the annihilation process [2]. This parameter is independent of the density of positrons, it characterizes the annihilation of positron on a single atom. One could expect that (Z_{eff}) is comparable to the number of electron (Z) in an atom. Moreover, low-energy positron does not penetrate deep into the atom, and most probable annihilate with the valance electrons only [3].

One of the future work that we had propose is the calculating of annihilation parameters ($Z_{eff}, \lambda_a, \sigma_a$) [4]. The interaction of positron with noble gas and the annihilation rates of positrons in these systems is interesting for a number of reasons, for example (i) the stability of these systems (ii) the large value of it's inelastic channels (energies) like (excitation, ionization, and positronium formation). Although the electronic structure of noble gases is rather simple, the phenomena that have been observed (annihilation) demonstrate that the description of a positron-atom system is quite complicated concerning the experimental field because of the densities of gas required using current experimental technique [5]. An important and interesting feature of low energy positron collision with atoms is the possibility of annihilation of the positron with one of the electrons in the target. This has been the subject of extensive experimental [6-8] and theoretical [9-12] studies.

Low-energy positron scattering and annihilation from atomic targets such as the noble gases is very difficult to describe using theoretical methods such as variational technique [13] or close coupling approach [14]. The difficulty lies in accurately describing both the polarization of the atom by the incident positron and virtual positronium (Ps) formation when the target has more valance electrons. This has led to the application of more approximate methods such as the polarization orbital method [15], which uses an adiabatic treatment of the positron and neglect virtual posironium formation. There are two mechanisms of positron-

atom annihilation. The first mechanism is call the *direct annihilation* of the incoming positron with one of the atom electrons. The contribution of this mechanism to the annihilation rate is proportional to the number of valence electrons available for annihilation. The second mechanism is call the *resonant annihilation*, this mechanism dominant for large molecules capable of forming bound states with the positron [3,4].

A recent formula has been formulated of (Z_{eff}) by Gribakin [3]; it is very successful giving results consistent with other researches [15-18], for the same approximation method used in his calculations which is the polarized orbital in calculating the phase shift, where the formula of (Z_{eff}) depend on that effective factor. We had used the same formula of (Z_{eff}) proposed by Gribakin but with using of partial wave method in calculating the phase shift. Either the annihilation rate (λ_a) and annihilation cross section (σ_a) correlate with (Z_{eff}) in a mathematical relations, and as result of that we can calculate these parameters of annihilation.

Mathematical Description

The scattering of positrons by atoms differs considerably from the case of electron scattering. This is due to the possibility of positronium formation and annihilation. For atoms whose ionization potential (I) are lower than the positronium binding energy $/E_{1s}/ \approx 6.8$eV it is open at all positron energies. For atoms with ($I \rangle 6.8eV$), e.g., noble gases, positronium formation is often the first inelastic scattering channel to open with threshold $\varepsilon_{th} = I - / E_{1s} /$ [2].

The positron annihilation rate (λ_a) in a gas of density (n) is usually expressed in terms of the effective number of electrons (Z_{eff}) as [3]:

$$\lambda_a = \pi r_o^2 c Z_{eff} n \qquad (1)$$

Where, $r_o = e^2 / mc^2$ is the classical electron radius, (c) the speed of light, and (n) is the gas density, its unit is the (g/cm^3) or (Amagat); (1 Amagat=2.69*10^{19}g/cm^3) [1], since we depend in all calculations the atomic unit ($\hbar = m = / e / = 1$), then we'll consider the value of (n=1) for all systems.

The annihilation cross section (σ_a) appears in two formulas; (i) the Para-Positronium (in this case the spin of the positron and electron be in opposite direction) which predominantly decay into 2γ-rays (each of energy ≈ 0.511 MeV), (ii) the Ortho-Positronium (in this case the positron and electron spin be in the same direction) which predominantly decay into 3γ-rays. The two formulas can be expressed as [11]:

$$\sigma_{2\gamma} = \pi r_o^2 (c / \upsilon) Z_{eff} \qquad (2)$$

$$\sigma_{3\gamma} = [4(\pi^2 - 9) / 3] \alpha r_o^2 (c / \upsilon) Z_{eff} \qquad (3)$$

Where (α) is a constant, ($\alpha = e^2 / \hbar c \approx 1/137$), ($\upsilon$) is the incident positron velocity. In what follows we use atomic units ($\hbar = m = / e / = 1$), so that, e.g., $\upsilon = k$, where (k) is the incident positron momentum.

The general expression of the effective number of electrons (Z_{eff}) can be expressed by the formula [3]:

$$Z_{eff} = \int \sum_{i=1}^{Z} \delta(r - r_i) \left| \Psi_k(r_1, ..., r_Z, r) \right|^2 dr_1 ... dr_Z dr \qquad (4)$$

Where (Z) is the number of the target electrons, r_i and r are the coordinate of the electrons and positron, respectively, and $\Psi_k(r_1,...,r_Z,r)$ is the total wave function of the system, and ($\delta(r-r_i)$) is the Kronecker delta which obey the conditions:

1) $\delta(r-r_i)=0$ if $r \neq r_i$

2) $\int \delta(r-r_i)dr = 1$ if $r = r_i$

3) $\int_{\Delta\tau} \delta(r-r_i)d\tau = \begin{Bmatrix} 1 & if & r=r_i \\ 0 & if & r\neq r_i \end{Bmatrix}$

Equation (4) describes the scattering of the positron with initial momentum (*k*) from atomic target in the ground state (Φ_0), and is normalized as:

$$\Psi_k(r_1,...,r_Z,r) \approx \Phi_0(r_1,...,r_Z)e^{ik\cdot r} \qquad (r\rangle\rangle R_a) \qquad (5)$$

Where (R_a) is the radius of the target, and not the cut-off radius (r_o).

The scattering wave function is determined by the positron interaction with the charge distribution of the ground-state target and electron-positron correlation interaction [4]. Let us denote the corresponding wave function as (Ψ_k^0).

The *direct annihilation* can be expressed as [3]:

$$Z_{eff}^{(dir)} = \langle \Psi_k^{(0)} \left| \sum_{i=1}^{Z} \delta(r-r_i) \right| \Psi_k^{(0)} \rangle \qquad (6)$$

is a smooth function of the positron energy. Let us estimate its magnitude and find its energy dependence at small (low) positron energies (0.01-0.85) eV. When the positron is outside the atomic system, ($r\rangle R_a$), the wave function ($\Psi_k^{(0)}$) contains contributions of the incoming and scattered positron waves,

$$\Psi_k^{(0)}(r_1,...,r_Z,r) = \Phi_0(r_1,...,r_Z)\left[e^{ik\cdot r} + f(\Omega)\frac{e^{ikr}}{r} \right] \qquad (7)$$

Where $f(\Omega)$ is the scattering amplitude.

Because of the repulsion from the atomic nuclei the low-energy positron does not penetrate deeply inside the atomic system. Accordingly, the positron annihilates mostly with the outer valence electrons, where the electron and positron densities overlap [3].

After substitution of expression (7) into Eq. (6), one obtains

$$Z_{eff}^{(dir)} = \int \rho(r)\left[e^{ik\cdot r} + f(\Omega)\frac{e^{ikr}}{r} \right] \times \left[e^{-ik\cdot r} + f^*(\Omega)\frac{e^{-ikr}}{r} \right] r^2 dr d\Omega \qquad (8)$$

Where

$$\rho(r) \equiv \langle \Phi_0 \left| \sum_{i=1}^{Z} \delta(r-r_i) \right| \Phi_0 \rangle \qquad (9)$$

is the electron density in the ground state of the system.

Then Eq. (8) will become

$$Z_{eff}^{(dir)} = \int \rho(r)\left[1 + f^*(\Omega)e^{ik\cdot r}\frac{e^{-ikr}}{r} + f(\Omega)e^{-ik\cdot r}\frac{e^{ikr}}{r} + \frac{f(\Omega)f^*(\Omega)}{r^2} \right] r^2 dr d\Omega \qquad (10)$$

$$= \int \rho(r)\left[r^2 + f^*(\Omega)re^{ik\cdot r}e^{-ikr} + f(\Omega)re^{-ik\cdot r}e^{ikr} + f(\Omega)f^*(\Omega) \right] dr d\Omega \qquad (11)$$

The electron density drops quickly outside the atom, and the positron density decreases rapidly inside the atom. Therefore the integration in Eq. (11) should be taken over a relatively thin shell of thickness (δR_a) enclosing the atomic system. Let us approximate the integration

domain by a spherical shell of radius ($r = R_a$), where (R_a) is the typical distance between the positron and the target during the annihilation, comparable to the size of the atom. For small positron momentum, ($kR_a \langle 1$), Eq. (11) then yields

$$Z_{eff}^{(dir)} = 4\pi\rho_e \delta R_a (R_a^2 + \frac{\sigma_{el}}{4\pi} + 2R_a \text{ Re } f_\circ) \qquad (12)$$

Where (ρ_e) is the electron density in the annihilation range (which can be to short-range electron-positron correlations), (σ_{el}) is the elastic cross section, $\sigma_{el} = \int |f(\Omega)|^2 d\Omega$, and ($f_\circ$) is the spherical symmetric part of the scattering amplitude, $f_\circ = (4\pi)^{-1} \int f(\Omega) d\Omega$. For positron interaction with an atom, the latter is simply equal to the s-wave scattering amplitude. Its real part is expressed in terms of the s-wave phase shift ($\delta_\circ$) as $\text{Re } f_\circ = \sin 2\delta_\circ / 2k$. The s-wave gives a dominant contribution to the cross section (σ_{el}) at low projectile energies [19], which can be expressed as [3]:

$$\sigma_{el} = \frac{4\pi}{\kappa^2 + k^2} \qquad (13)$$

Where ($\kappa = a^{-1}$), and (a) is the scattering length.

Real atomic targets have nonzero electric dipole polrizabilities (α_d), which give rise to the long-range polarization potential ($V_{pol}(r) = -\alpha_d / 2r^4$) for the positron. The s-wave phase shift formula, which Gribakin [3] has depend it using the polarized orbital method is:

$$\tan\delta_\circ = -ak\left[1 - \frac{\pi\alpha_d k}{3a} - \frac{4\alpha_d k^2}{3}\ln(\frac{C}{4}\sqrt{\alpha_d}k)\right]^{-1} \qquad (14)$$

where (C) is a dimensionless positive constant

Whereas, the partial wave method was our way in calculating ($\delta_\circ$) [4], which have the form:

$$\tan\delta_\ell = -k\int_0^\infty j_\ell(kr) V(r) R_\ell(k,r) r^2 dr \qquad (15)$$

Where $j_\ell(kr)$ is the spherical Bessel function, *V(r)* is the effective potential, and $R_\ell(k,r)$ is the radial wave function, for $\ell = 0$, (ℓ) is the Orbital quantum number.

Results & Discussion

As we notice in Eq. (12) there are many factors effect in the behavior of (Z_{eff}), the three terms in the brackets are due to the incoming positron plan wave, the scattered wave, and the interference term, respectively, whereas the term outside the brackets will be consider as a fitting parameter.

Even if the cross section (σ_{el}), is zero or very small, the annihilation parameter (Z_{eff}) is nonzero. Its magnitude is determine by the effective annihilation radius (R_a), electron density (ρ_e) and (δR_a), also the s-wave phase shift ($\delta_\circ$) is one of the important factors, which effects in that formula. That means (Z_{eff}) depends much more critically on the actual form of the total wave function and hence is likely to be more affected by the approximations made. Table(1), gives us some informations about theses factors for the mentioned systems.

Z_{eff} -the annihilation parameter- is independent of the positron density and characterizes one of the most important events, which happens in the positron-atom system. Our results for this parameter was in a very good agreement with Gribakin data [3], which he use the polarized orbital method in his calculations as shown in figure (1), for the atoms (He, Ne, Ar, Kr, and Xe), the shape of these curves is very similar i.e. quite flat at large energies but rising very steeply as zero energy approached.

In figure (2) & (3) we show the annihilation rate (λ_a) and the annihilation cross section (σ_a) for 2γ or 3γ - rays (for the five mentioned systems) corresponding to (*k*) (the incident positron momentum). Yet, there are no measurements available for these parameters to make a comparison with it, concerning the inert gases. It will be very interesting to study the positronium formation phenomena and their effect on the total cross section in the inelastic region for high-energy incident positrons.

Table(1): Present the polarizability[(1)] (α_d), scattering length[(2)](*a*), fitting parameter[(3)] ($4\pi\rho_e\delta R_a$), the annihilation radius[(3)] (R_a) for noble atoms.

Atom	Z	$\alpha_d (a_o^3)$	*a* (a.u.)	$4\pi\rho_e\delta R_a$ (a.u.)	(R_a)(a.u.)
He	2	1.322	-0.52	0.21	3.9
Ne	10	2.377	-0.61	0.23	5.0
Ar	18	10.76	-5.3	0.42	4.3
Kr	36	16.46	-10.4	0.41	4.2
Xe	54	27.06	-45.3	0.41	4.2

(1)This factor use in calculating the polarization potential, where it is an important part in Schrodinger equation that we depend it in calculating the phase shift [4], and these values has taken from ref. [20].

(2)The values of this factor taken from Ref. [15-18].

(3)These values taken from Ref. [3].

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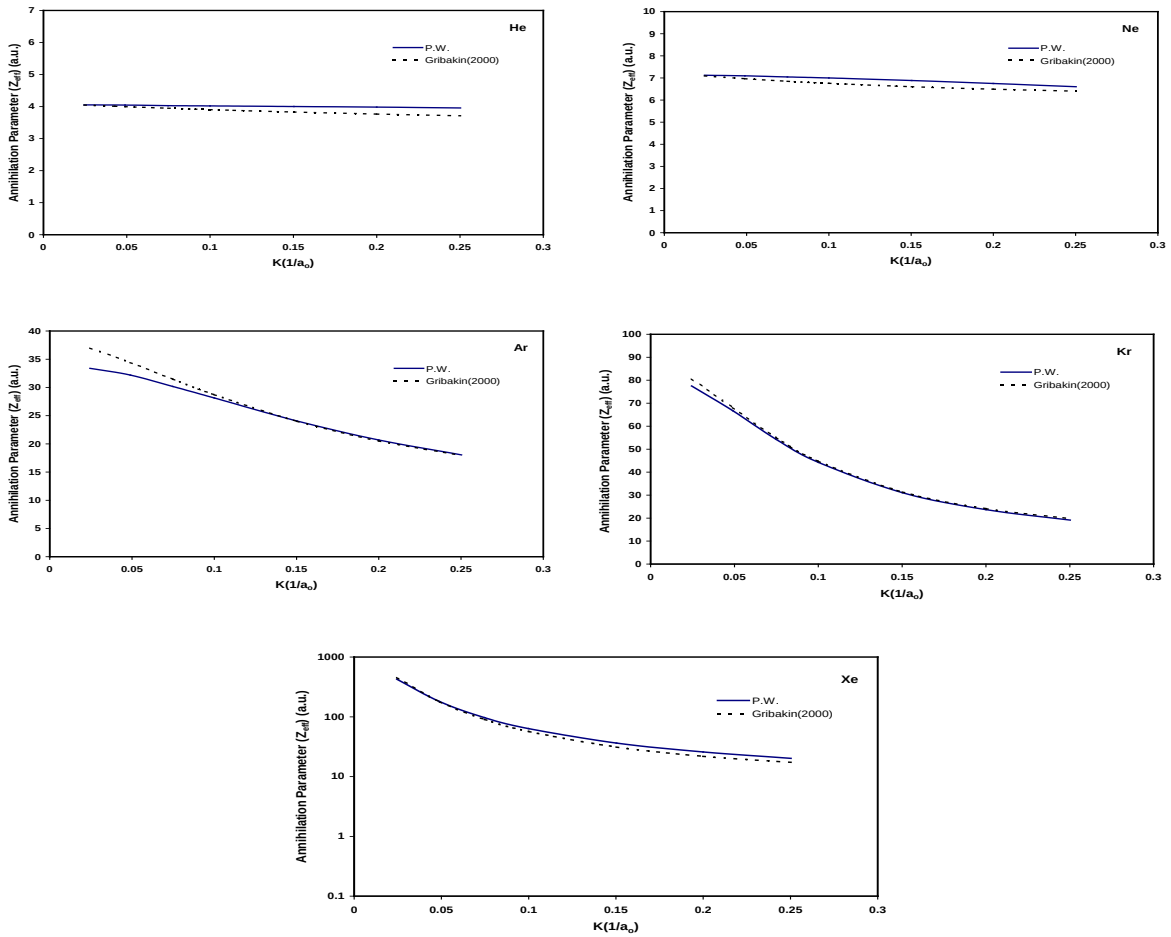
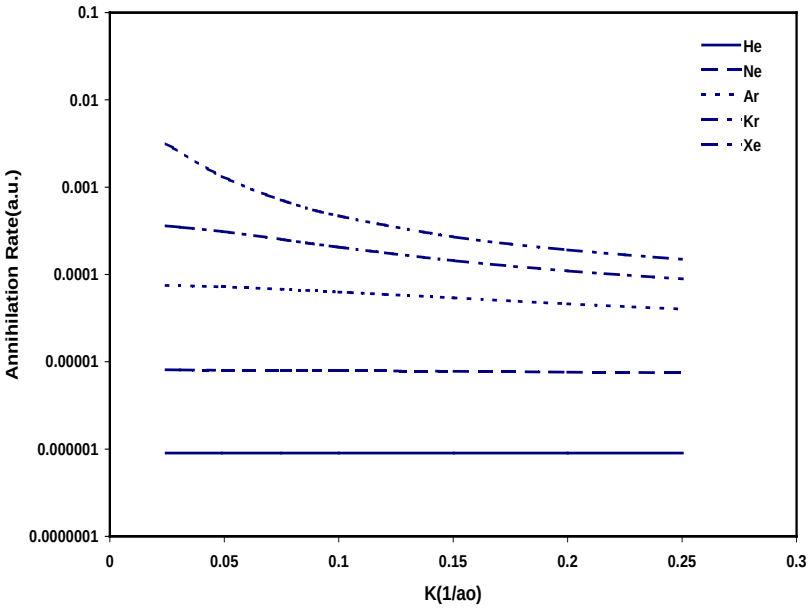
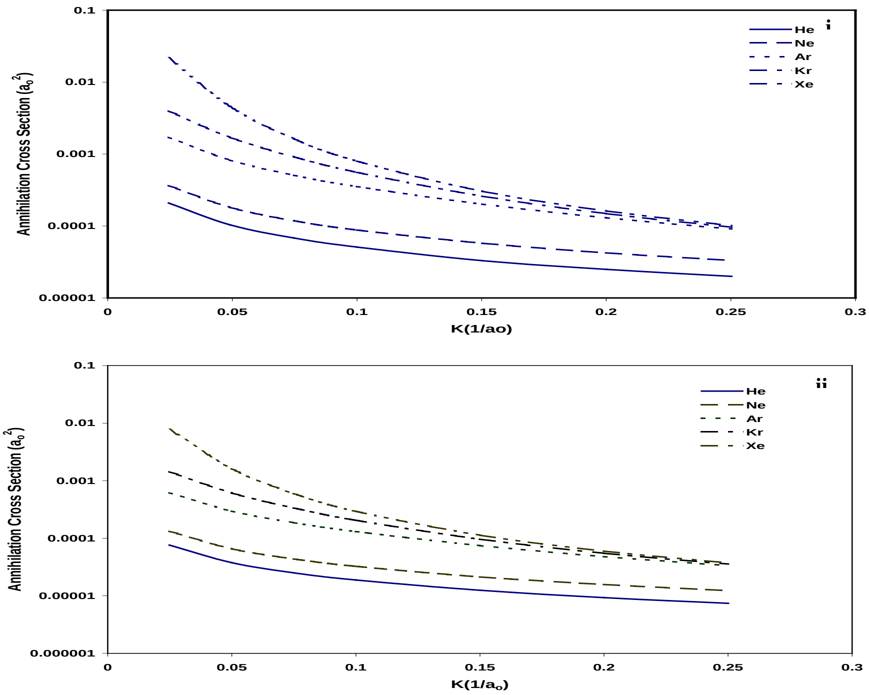


Figure(1): Z_{eff} for different values of *k*: the solid curve denote to the present work, the dash curve denote to the data of Gribakin(2000)



Figure(2): The rate of positronium atom annihilation vs *k*



Figure(3): The annihilation cross section for (i) $2\gamma - ray$ & (ii) $3\gamma - ray$ for positron

حساب معاملات الفناء من تفاعل البوزترونات مع الأنظمة النبيلة

علاء عبد الحسن خلف

فزلطهويئ؟ ّتيبطعكهل ً جذلعبطكا شبنطكا شبنطكعف

طكلخش

تعتبر عملية الفناء لذرة البوزترونيوم (الكترون+بوزترون) واحدة من أهم الأحداث التي تجري عند تفاعل البوزترونات مع الذرات، والتي تتولد خلال التفاعل. لقد قمنا بتوسيع عملنا السابق على طريقة الموجة المجزئة بمعالجة عملية الفناء لنظام بوزترون–ذرة في منطقة الاستطارة المرنة. لقد قمنا بالاستعانة بصيغة معامل الفناء (Z_{eff}) المقترحة بواسطة الباحث Gribakin معتمدا في الصيغة العامة لهذا المعامل على إزاحة الطور والذي بدوره قد تم حسابه باستخدام طريقة المدار المستقطب، بينما كانت الطريقة التي اعتمدناها في حساب هذا العامل هي طريقة الموجة المجزئة. تم الحصول على توافق جيد بين نتائجنا لهذا المعامل ونتائج الباحث Gribakin، كذلك قمنا بحساب كل مع معدل الفناء (λ_a) والمقطع العرضي للفناء (σ_a) حيث يعتمد كلاهما عل قيمة (Z_{eff}) في علاقات رياضية صريحة.