World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:9, No:7, 2015

Interaction of Low-Energy Positrons with Mg Atoms: Elastic Scattering, Bound States, and Annihilation

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Open Science Index, Physical and Mathematical Sciences Vol:9, No:7, 2015 publications.waset.org/10002815/pdf

Abstract**—**Annihilations, phase shifts, scattering lengths and elastic cross sections of low energy positrons scattering from magnesium atoms were studied using the least-squares variational method (LSVM). The possibility of positron binding to the magnesium atoms is investigated. A trial wave function is suggested to represent e^+-Mg elastic scattering and scattering parameters were derived to estimate the binding energy and annihilation rates. The trial function is taken to depend on several adjustable parameters, and is improved iteratively by increasing the number of terms. The present results have the same behavior as reported semi-empirical, theoretical and experimental results. Especially, the estimated positive scattering length supports the possibility of positron-magnesium bound state system that was confirmed in previous experimental and theoretical work.

Keywords**—**Bound wave function, Positron Annihilation, scattering phase shift, scattering length.

I. Introduction

POSITRON collisions with atoms and molecules has been the subject of extensive experimental and theoretical work [1], [2]. Only elastic scattering or direct annihilation is possible when the positron incident energy is less than the positronium formation threshold, the possibility of positron bound state had been often invoked to explain the very large annihilation [3]. Positron annihilation is a good tool to give useful information about matter. Positrons offer new ways to study a wide range of phenomena including plasmas [4], atomic clusters and nanoparticles [5], and a new method to ionize molecules, such as those of biological interest, for mass spectrometry [6].

Positron annihilation occurs whenever an electron and positron come into direct contact. If the spin state of the annihilating pair is a singlet ($S = 0$) state, the dominant decay process is the 2γ decay. This signal provides information about the interaction, and it is the basis of many types of measurements. For example, this signal has been used to characterize defects and interfaces in solids [7].

Modified effective range theory is used to extrapolate elastic cross-sections down to thermal energies for positron annihilation rates and positron scattering from atomic and molecular targets [1].

There have been several calculations of elastic scattering to the e^+–Mg system using the distorted-wave polarized orbital method [8], [9]. In addition, there has been an application of many-body perturbation theory (MBPT) with particular emphasis on low-energy elastic scattering [10]. There has also been an application of the close-coupling (CC) method with Ps(1s), Ps(2s) and Ps(2p) channels included [11].

The existence of positron-atom bound states was predicted by many-body theory calculations and proved variationally more than a decade ago [12]. There are accurate theoretical calculations of positron binding to atoms [13].

The least squares variational method (LSVM) was applied successfully for low energy positron scattering from H, He [14], Kr [15] and Xe [16]. It was applied to obtain the wave function of the continuum Auger electron emitted from an ionized Ne atom [17] and developed to study positron-H molecule scattering [18].

In the present work LSVM has been developed to study positron-magnesium interaction at low energy. The annihilation parameter Z_{eff}, phase shift, cross section and scattering length is calculated. Positron binding to of neutral magnesium is investigates.

II. Theory

In non-relativistic time-independent quantum mechanics, Schrodinger's equation is equivalent in form to the conventional eigenvalue problem:

$$(H-E)\,|\,\Psi\,\rangle = |\,0\,\rangle \tag{1}$$

where H and E are the total Hamiltonian and energy, respectively, of a quantum mechanical system described by the vector $|\,\Psi\,\rangle$. The interaction Hamiltonian for positron-magnesium system can be written as

$$H = H_T - \nabla_X^2 + V_{int}(x,r) + V_p(r) \tag{2}$$

where H_T being the Hamiltonian for the target atom, ∇_X^2 is the kinetic energy operator for the incident positron, and $V_{int}(r,x)$ stands for the interaction potential between the positron and the target:

$$V_{int}(r,x) = \frac{2Z}{x} - \sum_i^N \frac{2}{|x-r_i|} \tag{3}$$

where x and r_i are the position vectors of positron and i^{th} electrons respectively. The polarization potential $V_p(r)$ is given the form [19]

$$V_p(r) = -\alpha_d(1-\exp(-r^6/r_c^6)) \,/\, 2r^4 \tag{4}$$

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The dipole polarizability α_d = 72 a_o^3, and the cut-off parameter r_c =3.032 [19]. Large values of α_d ensure that the positron experiences a strong attractive polarization potential outside the atom and the positron binding to neutral magnesium is possible.

The total energy E of the system may be written, in Rydberg, as:

$$E = E_T + k_p^2 , \tag{5}$$

where E_T *and* k_p^2 are the energy of the target and the kinetic energy of the incident positrons, respectively.

III. The Least-Squares Variational Method and Trial Wavefunction

The variational treatment [19] starts by defining a trial wavefunction $\left| \Psi_t^n \ (x, r_N; k) \right\rangle$, n refers to the dimension of the Hilbert-space part of the trial wavefunction representing all possible virtual states of quantum mechanical system composed of the positron and the target.

The s-wave elastic scattering trial wavefunction for the system may be written in abbreviated form as:

$$\left| \Psi_t^n \right\rangle = \left| S \right\rangle + R_{11} \left| C \right\rangle + \left| \phi_n \right\rangle \tag{6}$$

where *S* is the regular part;

$$S = \frac{1}{\sqrt{4\pi}} \ \frac{Sin(kx)}{kx} . \Phi_T(r_N) \tag{7}$$

the irregular part of the asymptotic solution. It has the form

$$C = \frac{1}{\sqrt{4\pi}} \ (1 - e^{-\alpha x})) (\frac{\cos(kx)}{kx}) \Phi_T(r_N) \ , \tag{8}$$

the cut-off function $(1 - e^{-\alpha x})$ avoid the singularity at the origin. This cut-off function will tend to zero at the origin and to unity at infinity, and the quadratic integrable wavefunction;

$$\left| \phi_n(x, r_N) \right\rangle = \Phi_T(r_N) . \sum_{i=1}^{n} d_i \left| \chi_i(x) \right\rangle \tag{9}$$

$$\chi_i = x^i \ e^{-\alpha x} \tag{10}$$

where α is an adjustable (free) parameter which is selected from the values that give a plateau of R_{11} [14]. In this case the reactance matrix R_{11} contains a single element which is identical with the tangent of the s-wave scattering phase shift η_0 and is calculated by:

$$R_{11} = \tan \eta_0 \ , \tag{11}$$

$\left| \Phi_T(r_N) \right\rangle$ represents the target in its ground-state, which can be determined according to Hartree-Fock-Slater method [20]. The next step in the variational treatment is to select a proper test-wave function $\left| \Psi_S \right\rangle$ and define the functional

$$\left\langle \Psi_S \left| H - E \right| \Psi_t^n \right\rangle = V \tag{12}$$

The linear variational parameters R_{11} and d_i are chosen according to the following variational principle:

$$\delta V^2 = 0 \tag{13}$$

Thus, they are chosen according to a least-squares variational principle in which all projections of the vector $(H - E) \left| \Psi_t^n \right\rangle$ on $\left| \Psi_S \right\rangle$ are minimal. The test wavefunction $\left| \Psi_S \right\rangle$ is constructed [21], [22] by:

$$\left| \Psi_S \right\rangle = \{ \left| S \right\rangle, \left| C \right\rangle, \left| \Psi_j \right\rangle; \ j = 1,2,....n \}. \tag{14}$$

In this case we have the system of projections

$$\begin{aligned} &(S \mid S) + R_{11} (S \mid C) + \sum_{i=1}^{n} d_i \ (S \mid \Psi_i) = V_1 \\ &(C \mid S) + R_{11} (C \mid C) + \sum_{i=1}^{n} d_i \ (C \mid \Psi_i) = V_2 \\ &(\Psi_j \mid S) + R_{11} (\Psi_j \mid C) + \sum_{i=1}^{n} d_i \ (\Psi_j \mid \Psi_i) = V_{j+2} \end{aligned} \tag{15}$$

$$; \ j = 1,2,....n \tag{16}$$

and the LSVM implies:

$$\delta \sum_{j=1}^{n+2} V_j^2 = 0 \tag{17}$$

which means that the sum of the projections of $(H - E) \left| \Psi_t^n \right\rangle$ on the test function space Ψ_s are minimum. The minimization of $\sum_{j=1}^{n+2} V_j^2$ guarantees that the vector $(H - E) \left| \Psi_t^n \right\rangle$ has a minimum length. The variational parameters are obtained by applying this variational principle. The matrix elements required for the employment of the LSVM, namely $(S \mid S)$, $(S \mid C)$, $(S \mid \Psi_i)$, $(C \mid S)$, $(C \mid C)$, $(C \mid \Psi_j)$, $(\Psi_j \mid S)$, $(\Psi_j \mid C)$, and $(\Psi_j \mid \Psi_i)$, have the general form [14]:

$$(g \mid f) = \langle g \mid E - H \mid f \rangle \tag{18}$$

Thus, the final form of the trial expansion space $\left| \Psi_t^n \right\rangle$ can be expressed [14] in terms of vector determinants as

$$\left|\Psi_t^n\right\rangle = \frac{1}{\Delta:n}\left\{ \begin{vmatrix} |S\rangle & |\phi_1\rangle....|\phi_n\rangle. \\ M_:^S & \Delta:n \end{vmatrix} + R_{11} \begin{vmatrix} |C\rangle & |\phi_1\rangle....|\phi_n\rangle. \\ M_:^C & \Delta:n \end{vmatrix} \right\} \quad (19)$$

IV. Positron-Magnesium Scattering and Bound State

The s-wave elastic scattering cross section (in πa_0^2 units) is related to the phase shift η_0 by [14]

$$\sigma_{el} = \frac{4}{k^2} Sin^2(\eta_0). \quad (20)$$

Also, the determination of the phase shift is useful to calculate the s-wave scattering length which is defined as [14]:

$$A = \lim_{k\to 0}\left\{\frac{-\tan\eta_0}{k}\right\} \quad (21)$$

A positive scattering length would indicate that the potential was strong enough to support a bound state [23]. Accordingly, the scattering lengths, A, defined by the s-wave phase shift $\eta_0 \approx -Ak$ (in the limit that the particle's wave number $k\to 0$), become negative in both case. As a result, the s-wave phase shift now passes through zero at a small but nonzero projectile momentum**.** In this situation, the elastic scattering cross sections enhancement at low energy can be viewed as arising from the existence of a *virtual level* for the projectile at an energy $1/(2A^2)$. These virtual levels also lead to enhanced positron annihilation cross sections.

A bound state occurs when the long-range attractive polarization potential is large enough to overcome the short-range repulsive interaction with the nucleus. Calculations by Dzuba et al. suggested that alkaline earth metals such as Mg, Zn, Cd and Hg could stably bind positrons [24]. Ryzhikh and Mitroy rigorously investigated bound states for a positron and a lithium atom [25]. Their model predicted bound positron-atom with binding energies in the order of 60 meV. Subsequent calculations also predicted positron binding to Be, Na, Mg, Ca, Cu, Zn, Ag and Cd [26]. When the scattering cross section is large the annihilation rate is greatly enhanced. Indeed, if the positron has a virtual or bound state with energy $k^2/2$ close to zero, its binding energy is $-1/A^2$, where A is the positron scattering length. These positron-binding systems decay by electron–positron annihilation with the annihilation rate for e^+-A systems largely determined by the parent atom ionization potential.

Fig. 1 shows the present work s-wave elastic scattering cross sections calculated using LSVM compared to the total cross sections calculated by the many body theory without including positronium formation but with polarization potential [27]. The figure also shows the total cross sections using semi-empirical method [28], and the total cross sections measured by the Detroit group [29]. The figure shows the elastic scattering σ_{el} decreases rapidly as the energy of the incident positron increases but it starts to decrease slowly as the positron energy approach the positronium formation threshold.

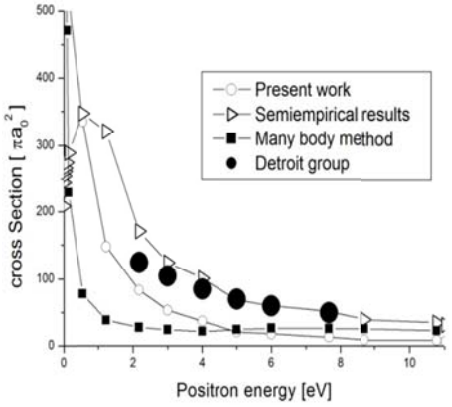


Fig. 1 Comparison of scattering cross section for e^+-Mg scattering as a function of positron energy in (eV). The present work is the s-wave elastic cross section, the total elastic cross-section results in semi-empirical model [27], many body method [28] and the total cross section measured by Detroit group [29]

TABLE I
The Positron Binding Energies (in Hartree), and the Scattering Length (A in a_0) in Different Models for e^+-Mg Ground States

Model	Binding energy [Hartree]	A [a_0]
Present Work	0.0077	8.07
model potential [12]	0.01391	7.4
$FCSVM_{pol}$ [10]	0.0136	--
Coupled DF [30]	0.0074	30.1
MBPT [28]	0.036	4.2

The s-wave positron scattering phase shifts are plotted in Fig. 2. The phase shift increases from -0.0805 rad. at k=0.01 a_o^{-1} until it reaches a maximum at k=0.3 a_o^{-1} with the value 1.955 rad., then starts to decrease. The negative sign of the phase shift means that the scattering length is positive whish support the possibility of a positron-magnesium bound state. The calculated scattering length is A = 8.07 a_o at k = 0.01 a_o^{-1}, the estimated positron binding energy is - 0.21 eV. The positron binding energy (in eV) and scattering length (in a_0) computed in different models are shown in Table I.

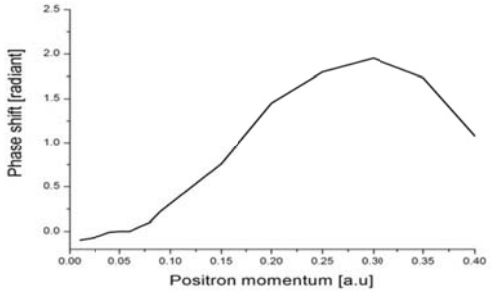


Fig. 2 The elastic scattering phase shifts η_0 for e^+- Mg as a function of momentum k (in a_o^{-1} units).

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V. Positron Annihilation in Magnisium

Annihilation into two γ-rays is far more probable than into three γ-rays [30], in such case, the annihilation rate in a gas is:

$$\lambda = \pi r_0^2 c \rho Z_{eff}(k), \quad (22)$$

where $r_o = e^2 / (mc^2)$ is the classical radius of the electron, c the speed of light, ρ is the density of electrons per atom available to the positron for annihilation and k is the positron momentum. Z_{eff} is the effective annihilation parameter. The value of Z_{eff}, which varies with positron momentum, is a measure of the probability of the positron being at the same position as one of the target electrons. It is calculated from the elastic scattering wavefunction for the positron-target system as;

$$Z_{eff}(k) = \langle \Psi(x, r_N; k) | \sum_{i=1}^{N} \delta(r_i - x) | \Psi(x, r_N; k) \rangle \quad (23)$$

where $\Psi(x, r_N; k)$ is the scattering wavefunction, including all partial waves, for a system made up of the incident positron with wave vector k and the target atom, x and r_N stand for the position vectors of the positron and the target (composed of N electrons), respectively. A good agreement between the calculated value of Z_{eff} and an experimental value, derived from measurements of the annihilation rate, is therefore an important measure for the quality of the scattering wavefunction.

The cross section for positron annihilation in a many-electron target is obtained by [31]:

$$\sigma_{ann} = r_0^2 (\pi / k) Z_{eff} \quad (24)$$

Since $r_0 \approx 10^{-4}\ a_0$, the Bohr radius, the cross section for annihilation is thus expected to be much smaller than that for a typical atomic scattering process. The annihilation parameter Z_{eff} is computed numerically. It is found that it is sensitive to the chosen wavefunction. When positrons interact with atoms they annihilate predominantly with valance electrons, since the repulsive force between the positrons and nucleus keeps the positrons away from inner electrons. However, small fraction of positrons can tunnel into inner electrons and annihilate with some of them [16].

The dependence of the Z_{eff} on the positron energy, over the range 0 eV to 2 eV is plotted in Fig. 3. The figure shows that our calculations have the same behavior as that calculated by the semi-empirical model [27]. Our calculation is smaller than that of the semi-empirical model because we computed the s-wave scattering only. At low energies, the annihilation parameter Z_{eff} reveals an initial decrease as positron energy increases. Instead of Z_{eff} continue to decrease, as expected; it starts to increase at positron energies ≈ 0.3 eV to make resonance with peak at energy ≈ 0.85 eV.

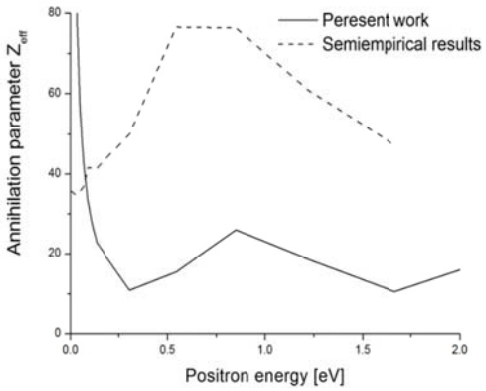


Fig. 3 The energy dependence of annihilation parameters Z_{eff} of positron. The sold line is the present results. The dashed lines are the semiemperical results calculated by [27]

Detection of the resonances can thus provide the first evidence of positron binding to neutral atom. The annihilation parameters Z_{eff} is about 77 while it is about 35 for semiempirical model at room temperature 293K (thermal energy ~ 0.024 eV, momentum ~ 0.042 a^{-1}) which means that positrons annihilate is large at room temperature.

VI. Conclusion

The annihilation parameters, scattering length, phase shifts and cross sections for low energy positron scattering from Mg were obtained using the least-squares variational method (LSVM). Hartree-Fock-Slater method is used to generate the orbital wavefunctions for target atoms. The estimated positive scattering length supports the possibility of existing a positron-magnesium bound state system, which was confirmed in previous experimental and theoretical work. The calculation of the present work for cross section and annihilation parameters show the same behavior as the reported theoretical, semi-empirical and experimental data of the Detroit group.

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