International Journal of Pure and Applied Physics
ISSN 0973-1776 Volume 5, Number 2 (2009), pp. 93–100

http://www.ripublication.com/ijpap.htm

Resonance in Positron – lithium Scattering

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Abstract

The appearance of intermediate states (also referred to as resonant states) in atomic, molecular and nuclear reactions is considered as the most interesting physical phenomena since the development of the quantum theory in the early thirties of the preceding century. The development of femtosecond lasers has tremendously enhanced the experimental identification of these states in chemical reactions. The main objective of the present work is to develop a unified mathematical formalism for the localization of resonant states in physical and chemical reactions. Numerical examples for the validity of this formalism will be demonstrated.

Introduction

Resonance states are quasi bound state occurring in the continuum (positive relative energy region) of different physical and chemical reaction processes. They are rigorously defined as poles of the scattering (as well as the reactance matrix). The resonance state is usually defined in a complex energy plane; the real part of it characterizes the position of the resonant energy on the positive real axis, whilst the imaginary par is a measure of the collapse (or annihilation rate) as well as the lifetime of this state. This time is ranging from few milliseconds to few picoseconds. In chemistry, experimental investigation of intermediate states became possible through the development of femtosecond cameras by Ahmed Zewail [1]. Theoretical investigations of resonant states in chemical reactions are given by different authors, (see e.g. Tucker and Truhlar [2] and Kendrick [3]). Resonant states appear also in nuclear reactions (see e.g. [4] and [5]). Quite extensive theoretical and experimental investigations are given within the frame work of the shell [6] and cluster [7], [8] models are given in the literature. The appearance of the phenomenon in electron- [9], positron- [10] and photon-atom [11] collisions as well as different molecular collision processes [12] was well visited over the last half century.

Most theoretical treatments of resonances in the previously mentioned areas were based on calculations of the differential cross sections (DCS) as functions of the scattering energies using quantum mechanical [13], or semi-classical approaches (see e.g. [14] and [15]). Resonant states are identified in this case as the singular points of the DCS. On the other hand, trials to localize the resonant states by diagonilizing the complex Hamiltonians are given in the literature within the so called Complex coordinate approach, (see e.g. [16] and [17]). The major advantage of this approach comparative to the preceding ones is the use of L^2-wavefunctions for describing collision process.

The aim of this paper is to utilize the complex coordinate method for the investigation of resonances in positron- atom collisions. Apart from the present section, the paper contains other three sections. In section 2, the generalized mathematical foundation of the method is shortly presented. Details of the analyses for arbitrary two interacting systems, as well as the adherent computer code are out of the scope of the present work. Section 3 deals with the collision of positrons with one-valence electron atoms. A test for the approach in case of positron-lithium scattering is demonstrated in sections 4. The same section ends with the main conclusions drawn from the work. The paper ends with the list of reference appearing in the text.

The Complex Coordinate Method

In this section we are trying to familiarize the reader with the main feature of the complex coordinate, (known also as the complex rotational), approach. The mathematical roots of this approach are founded in the works of Aguilar and Combes [18], Balslev and Combes [19] and Simon [20]. For arbitrary collision processes the method could be utilized as follows: Let $A(r_a)$ and $B(r_b)$ are two interacting quantum mechanical systems with r_a and r_b stand for the internal structures and all degrees of freedom of the two systems, respectively.

If $U(r_{ab})$ is the mutual interaction between the two systems, with r_{ab} referring to the relative coordinates of the two systems, the total Hamiltonian can be written as :

$$H(r_a,r_b,r_{ab}) = Ha(r_a) + Hb(r_b) + U(r_{ab}) ; \tag{1}$$

The time-independent reaction processes are governed by the Schrödinger equation

$$H\,\Psi = E\,\Psi \tag{2}$$

where Ψ and E characterize the total wavefunction and total energy, respectively, of the system considered. Expressing the scattering matrix in terms of relative complex momentum k, we see that the scattering matrix, S(k) , has the following properties: (1) Its poles at $k = i\,K$ (where $K .> 0$) specify the exact bound states of the system composed of A and B at energies $- K^2$. Remembering that $S(k) = f\,(-k)/ f(k)$, where f is called the Jost function, the bound states are also defined as the zeros of f (2) The excitation channels of A or B are localized at the zeros of f when $k = K^{2,}$, $K > 0$. (3) The zeros of f at $k = K_i– K_{im}$, (K_r, $K_{im} > 0$) identify the resonant states of the two interacting systems.. On the other hand, the transformation from the k complex plane to the complex energy plane shows that the the first two cases are located on the upper (physical) part of the complex plane, whilst the resonances are located at the lower (negative) part of the plane.. The complex coordinate approach makes use of the preceding characteristic of the scattering matrix. By rotating the coordinated of the problem in the complex plane., (i.e replacing a coordinate r by r $e^{i\theta}$ and calculating the eigenvalues of the complex Hamiltonian.. Cases where the eigenvalues posse only negative real parts are bound states, they are not affected by the rotation of the coordinates. The thresholds should also occur at the physical energy sheet and would not be affected by rotation. Resonant states, however, would be affected; rotation should show their places in the unphysical s sheet. Of the energy plane. Their true positions, however, should be located in the regions where their values are stationary with respect to their variation. The main goal of the complex coordinate method is to find those places. The real parts of the energies give the resonant energies. The imaginary parts of these energies provide the annihilation rates or the life time of the corresponding state.

Collisions of Positrons With One-Valence-Electron Atoms

The investigation of the collisions of positrons with one-valence electron atoms has gained increasing interest over the last two decades. Many theoretical and experimental groups distributed world wide are looking for resonances in these scattering processes, e.g. the theoretical group at York University (CANADA), the experimental groups at Detroit, Texas and Michigan Universities (USA), and at Max Planck Institute in Stuttgart (GERMANY). Following, Abdel-Raouf [21], one-valence electron atom can be treated as an electron moving in the field of a frozen and a nucleus. As a consequence, the system can be considered as an effective three-body system dominated by Coulomb forces in addition to a screening potential. Thus, the total Hamiltonian can be written (in Ry) as

$$H = H_T - \nabla_x^2 + U \tag{3}$$

Where H_T is the Hamiltonian of the target and has the following form

$$H_T = - \nabla_r^2 - 2/r + V_c(r) \tag{4}$$

R is the position vector of the valence electron relative to a fixed nucleus.

- 2/r represents the Coulomb interaction between the valence electron and the unscreened unit nuclear charge. The core potential $V_c(r)$ is split into Coulomb part and exchange part.

$$V_c(r) = V_{cCoul}(r) + V_{cex}(r) \tag{5}$$

$$\text{where } V_{cCoul}(r) = \sum_j^{M} N_j < \varphi_j (r_i) \mid 2/\mid r - r_i \mid - 2/r \mid \varphi_j (r_i) > \tag{6}$$

$$\text{and } V_{cex}(r) = \sum_j^{M} < \varphi_v (r_i) \mid 2/\mid r - r_i \mid \mid \varphi_j (r_i) > \tag{7}$$

M and N_j are the number of orbitals and the number of electrons occupying the orbital j, respectively. -2/r is repeated for each j. The wavefunction φ_j (r_i) is taken to be a Cleminti-Roetti wavefunction representing the i^{th} electron in the j^{th} orbital of the lithium target. The closed forms of V_{cCoul}(r) and V_{cex}(r). The last term U of the total Hamiltonian H given at eq. (3) represents the interaction potential between the incident positron and the target atom. It is expressed as

$$U = 2/x - 2/ \left| r - x \right| + V_{cCoul}(x) \qquad (8)$$

2/x represents the interaction between the positron and the unscreened part of the nucleus, $- 2/\left| r - x \right|$ represents the Coulomb interaction between the positron and the valence electron and V_{cCoul}(x) is the interaction between the positron and the electrons of the core as well as the second part of the nucleus. V_{cCoul}(x) is determined by eq. (6) after replacing r with x. and changing the sign to become positive.

The employment of the complex coordinates approach starts by introducing the following replacement.

$r_j \rightarrow r_j\, e^{i\theta}$ to the Hamiltonian described at eq. (3) and obtaining the H(θ) . Considering Schrödinger's equation (2) for the system under consideration we may express the trial wavefunction of the system via Hylleraas-type basis such that

$$\Psi = \sum_{mn\ell}^{n} C_{mb\ell}\, \chi_{mn\ell} \;, \qquad (9)$$

$$\text{where } \chi_{mn\ell} = x^m r^n \rho^\ell \, Exp\{-\gamma(x + r + \rho)\} \;. \qquad (10)$$

x, r and ρ are the internal coordinates of the system. The first two stand for the distances between the positron and the valence-electron from the nucleus, respectively. The latter describes the relative distance between the positron and the valence electron.

Substitution from eqs (3) – (10) into eq. (2) and Diagonalizing the Hamiltonian in the basis defined at eq. (10), we end up with the following matrix equation

$$H(\theta)\, c(\theta) = E(\theta)\, S\, c(\theta) \;, \qquad (11)$$

where H(θ) and S are the Hamiltonian and overlap matrices, respectively. c(θ) contains the set of complex eigenvectors corresponding the complex eigenvalues E(θ). Equation (11) has been solved in the present paper using one of the licensed computer packages available.

Localization of Resonant States

In order to test our mathematical and computational algorithm we first consider the collision of positions with lithium atoms taking the elastic channel as the only open channel while all other

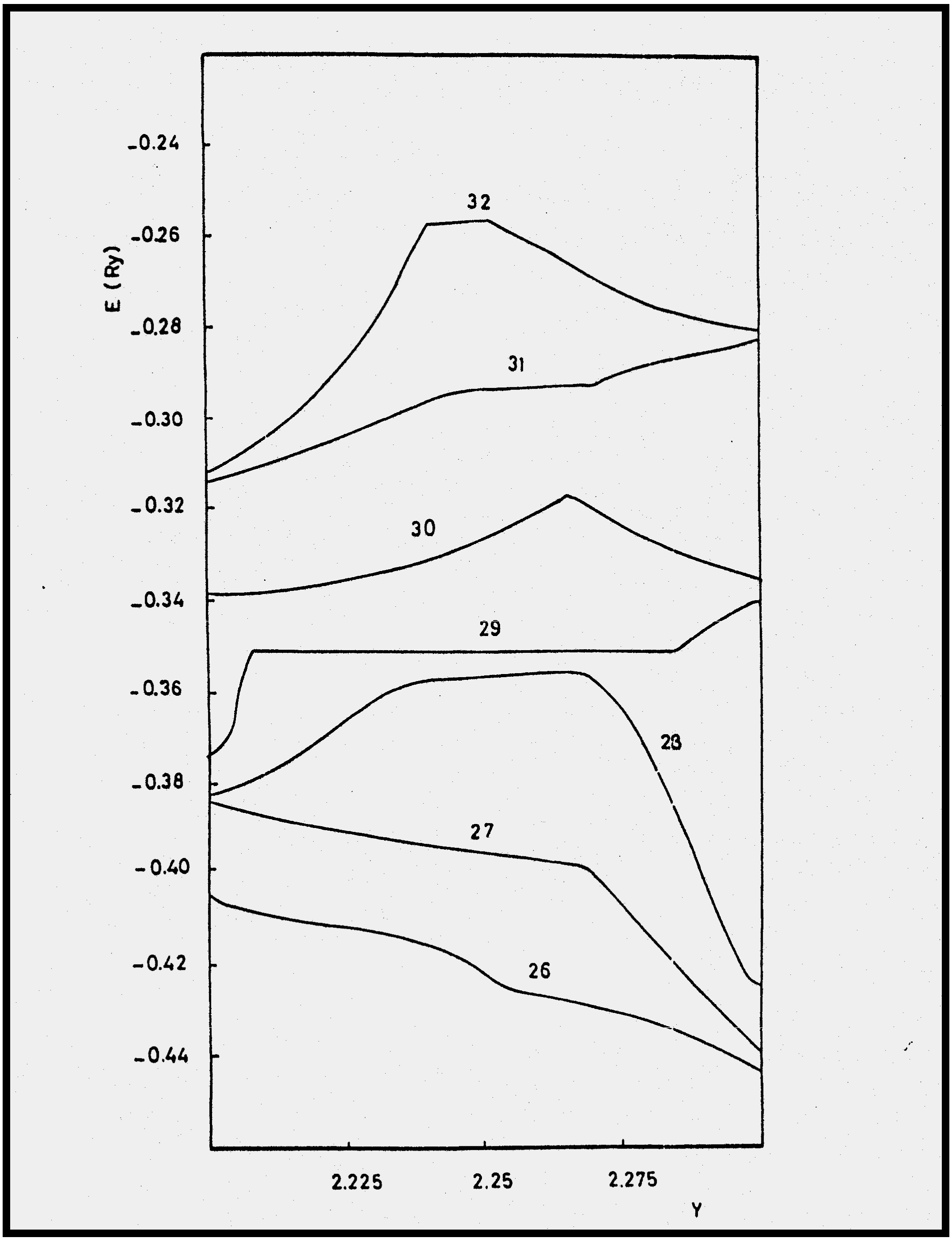

Figure 1: Variation of E with the nonlinear parameter γ for positron scattering by lithium atoms below the first excitation threshold obtained by the Complex Coordinate Method.

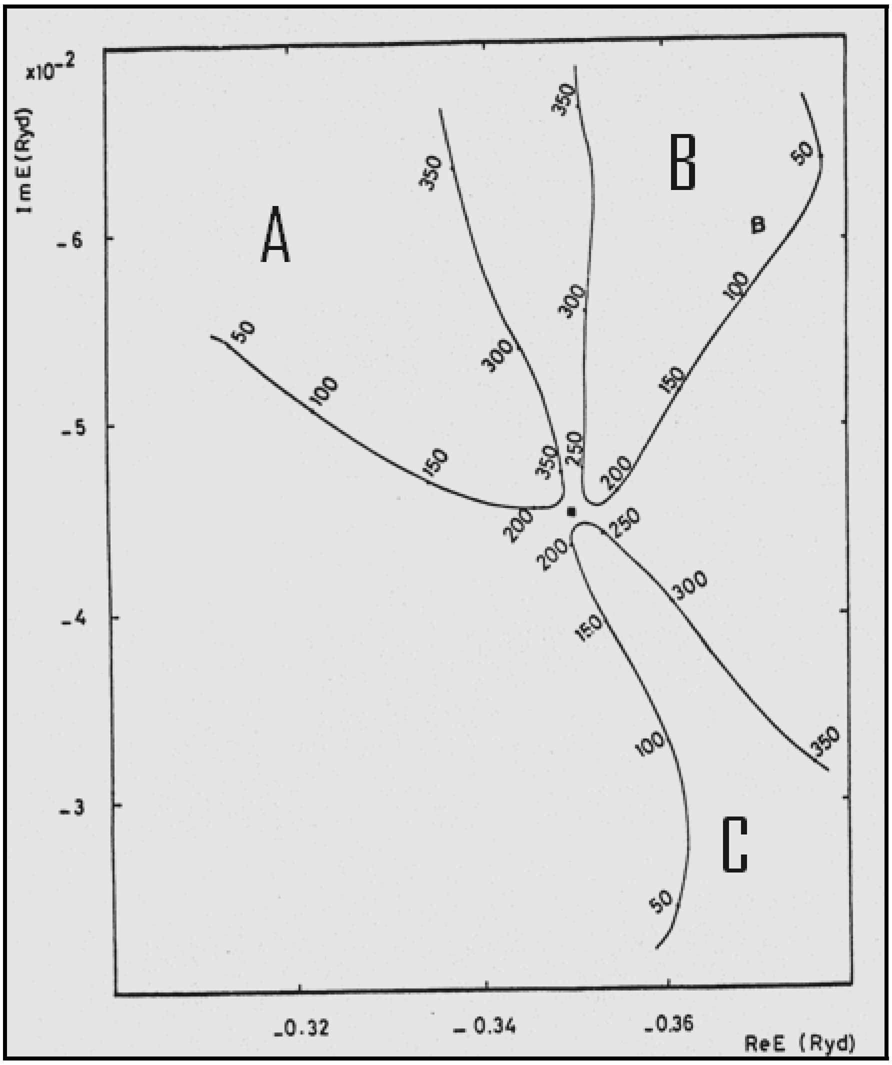

Figure 2: The eigenvalues plotted as functions of the rotational angle θ (in rad) for different values of γ (2.3, 2.5 and 2.7, corresponding to the curves A, B and C, respectively)

channels (positronium formation, excitation and ionization) are closed. This means that we are seeking resonant states occurring below the 2p threshold of the target (-0.2605 Ry or -3.54eV) The powers m_i, n_i and ℓ_i are chosen such that $m_i+n_i+\ell_i \leq 7$ which allows us to use up to 120 terms in the wavefunction which leads to 120 eigenvalues and 120 eigenvectors. For the localization of the resonant energies E_r we have to fulfill the following three conditions

$$(\partial E_r/ \partial\gamma)_{\theta=0} = 0 \ , \ (\partial E_r/ \partial\theta)_{\gamma=\mathrm{opt}} = 0 \ , \ (\partial E_r/ \partial n)_{\gamma=\mathrm{opt}\,,\ \theta=\mathrm{opt}} = 0 \qquad (12)$$

n is the number of basis functions used to expand the wavefunction at eq. (9).

Thus, we started our calculations by localizing the stationary values of E_r with respect to the nonlinear parameter γ at zero rotation. From Fig. 1 we notice the stationary behavior of the eigenvalues at n = 29 which leads to the resonance position E_r = - 0.3551 Ry (-4.829 eV) in the range of γ lying in the interval {2.20,2.28}. Consequently, the first of conditions (12) is satisfied. The next step towards the localization of resonance is to set n =29, select a set of values of γ from the stationarity region, (namely γ = 2.3, 2.5 and 2.7), and vary the rotational angle θ within a wide range between 50 and 350 milliard. In Fig. (2) we find the result of this experiment. The resultant rotational paths slow down at the position of resonance pole yielding the values

$E_r = 0.3551 \pm 0.00025$ Ry

$\Gamma = -0.022\text{x}10^{-2} \pm 0.00025$ Ry

From the Figure we notice that the three paths do not meet at the same position, this attributed to estimation errors.

The last step in our test calculations is to stabilize the resonant parameters against the variation of the number of components of the basis set.. In this case we have increased the number up to 165 terms which means that $m_i+n_i+\ell_i \leq 8$.. In this case the resonance parameters are improved to

E_r = 0.3551 Ry = -4.82936 eV

Γ = 0.09022 Ry = 1.22699 eV

Thus, the values here correspond to the fulfillment of all conditions presented at eqs. (12).

From the Figure we notice that the three paths do not meet at the same position, this could be attributed to estimation errors.

Conclusion

The existence of a resonant state in positron-lithium scattering at E_r = -4.82936 eV with a width Γ = 1.22699 eV has been confirmed for the first time. This state lies 056236 eV above the ground state (E 2s = -5.391 eV) of the lithium atom and -1.2866 eV below the first excited state of the atom (E2p = -3.5428eV). The resonance is very close to the $\ell = 0$ resonance found several years ago by Abdel-Raouf and Wood [22] using frozen core approximation.

The present work is a first step in our way to utilizing a rigorous mathematical formalism as well as a generalized computer code for the treatment of resonance in arbitrary reaction processes. Further developments are under consideration.

References

[1] A. H. Zewail, J. Phys. Chem. **A10**4, 5660, (2000).

[2] S. C. Tucker and D. G. Truhlar, Journal of Chemical Physics **88**, 3667, (1988).

[3] B. K. Kendrick, Los Alamos NL, Theo. Chem. & Mol. Phys., T-12, (2000).

[4] R. B. Wiringa, Phys. Rev. **C 43**, 1585, (1991).

[5] B.V.Danilin, et al Bull.Rus.Acad.Sci.Phys. **60**, 21, (1996).

[6] P. Kleinwachter and I Rotter, Printed publications, ZKR, Dresden, Issue **7**, (1998).

[7] A. J. Buchmann, U. Meyer, E. Hemandez and A Faessler, Acta Physica Pol., **B27**, 3161, (1996).

[8] A. Valcarce, H. Garcilazo, F. Femandez, Physical Review **C54**, 1010, (1996).

[9] N J Mason, *Rep. Prog. Phys.* **56**, 1275, (1993).

[10] W.E. Kauppila, C.K. Kwan, D. Przybyla and T.S. Stein, in Photonic, Electronic and Atomic Collisions, edited by F. Aumayr and H.P. Winter (World Scientific, Singapore), 373, (1998)

[11] N. J. Mason, Phys, Rev. A 36, 2633, (1987).

[12] M Berman *et al* , *J. Phys.* ***B*** **17,** L453, (1984).

[13] S. K. Adlukari, Phys. Rev. **A63**, 54501, (2001).

[14] M. Grifoni, Phys. Rev. **E 53**, 2210, (1996).

[15] I. Goychuck, Phys. Rev. **E 69**, 21104, (2004).

[16] K. Deguchi and K. Kishikawa, J. Phys. **B13**, L511, (1980).

[17] N. Moisezer, J. Phzs. **B31**, 1431, (1998)

[18] J. Aguilar and J. M. Combes, Commun. Math. Phys. **22,** 280, (1971).

[19] E. Balslev and J.M Combes, Commun. Math. Phys. **22,** 280, (1971).

[20] B. Simon Commun. Math. Phys. **27**, 1, (1972).

[21] M. A. Abdel-Raouf, J. Phys**. B21**, 12331, (1988).

[22] M. A. Abdel-Raouf and R. F. Wood, Phys. Rev. **A42**, 5, (1990)