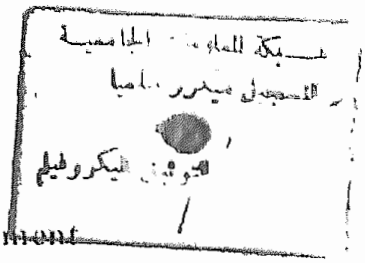
# INVESTIGATION OF RESONANCE IN POSITRON-ALKALI ATOM SCATTERING USING THE METHOD OF COMPLEX COORDINATE





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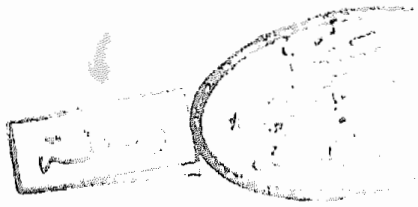



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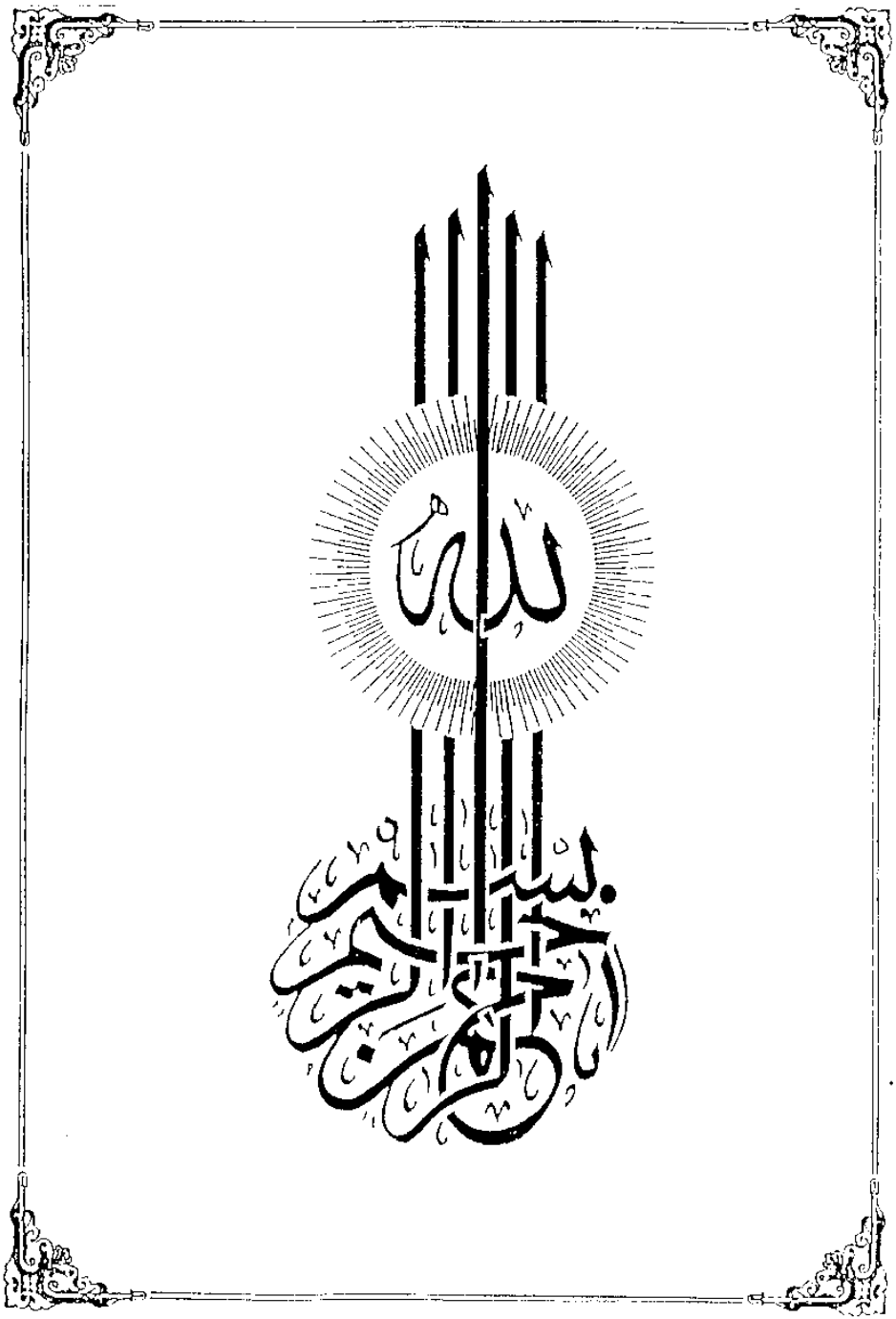

# Abstract

*Resonance in positron-Lithium scattering is investigated below the first excitation threshold within the framework of the complex coordinate variational method.*

*The Lithium target is described by the One-valence electron frozen core model. An elaborate Hylleraas-type wavefunction is employed for describing the positron-target system. The resonance state is localized using a stabilization technique in which resonance energies are stationary with respect to the nonlinear parameters involved in the wavefunction and the rotational angle in the complex plane.*

*The results support, for the first time the existence of a shape resonance at* $E_R$ = -0.3551 Ry (-4.8294 eV) *with a width* $\Gamma$ = 0.09022 Ry *occurring about* 0.04135 Ry (0.56236 eV) *above the ground-state of the Lithium atom* ( $E_{2s}^{Li}$ = −0.39645 Ry = −5.3917 eV )*and about* -1.2866 eV *below the first excitation threshold of the atom* ($E_{2p}^{Li}$ = -0.2605 Ry = -3.5428 eV). *These results emphasize the employment of the complex coordinate method as a powerful technique for the investigation of resonance processes in positron-atom collisions.*

# contents

# Chapter I

# Introduction

Resonance[1] is one of the most interesting phenomena discovered in collision processes since the establishment of the quantum theory in the thirties of this century. It is a common phenomenon in various areas of Physics and Chemistry. It frequently appears in nuclear scattering processes[2], electron scattering by atoms and molecules[3], particle-antiparticle interactions[4], photo ionization cross section[5] as well as molecular reactions[6].

In the collisions of positrons with atoms and molecules[7], resonance plays an important role among other low energy scattering phenomena, e.g. dissociative attachment, recombination and associative ionization processes, etc. Since the development of the atomic collision theory, the scattering of electrons and positrons by atoms and ions has continuously attracted many experimental and theoretical atomic physicists. This is because the resultant data are very important for the successful development of various directions in modern physics and new technology, e.g. laser technology, plasma physics, quantum chemistry, fusion power, astrophysics, . . etc. In these processes, the target alone, or the system consisting of the target and the incident projectile, gives rise to quasistationary states. The decay of these states lead to a complex resonance structure in the scattering cross section. In other words, the cross section exhibits sharp maxima or minima. Thus resonance can be produced if the energy of the incident projectile is sufficient to excite the target into a long-lived state which decays with a characteristic lifetime. The other possibility is that the projectile may be captured by the target forming together a long-lived "quasistationary" state.

Thus, denoting the projectile (e or $e^+$) by $a$, the target by $x$ and the target in the excited state by $x^*$, different possibilities for resonance can be classified as:

(i) $a + x \rightarrow a + x^* \rightarrow a + x$ (1.1)

(ii) $a + x \rightarrow x^{-*}\,(x^{+*}) \rightarrow a + x$ (1.2)

(iii) $a + x \rightarrow x^{-*}\,(x^{+*}) \rightarrow a + x^* \rightarrow a + x$ (1.3)

In the first case, the target is excited to an intermediate resonant state, then decays to its ground-state with a characteristic lifetime. Experimentally, we look in this case for sharp changes in the cross section as a function of the energy loss of the incident particle, or look for peaks in the spectrum of the ejected electrons in their final state.

In the second case, the projectile and the target form together a compound system in a resonant state, and here we look for a peak in the cross section as a function of the incident electron energy.

The last case is similar to the second one except that the resonant state does not decay to the initial one directly, but with the target left excited.

Of course, there is a possibility of elastic scattering of the incident projectile with the target, which is called the "direct scattering" or the scattering through an "open channel", while the possibility of scattering with one of the above mentioned cases are called scattering through a "closed channel".

When a projectile is incident on an ion target (positive or negative) they may form together a short-lived state which is one of the excited states of a neutral atom in the continuum region. These states are called "autoionizing states", since any of these may spontaneously decay into an electron (or positron) and an ion in the ground state or in an excited state. If the target is a neutral atom, the formed states are states of a negative

or positive ion, which can also decay into an electron or a positron and an atom. These states are usually called "self-detaching states". Nevertheless, to simplify the terminology they can be called "autoionizing states" too.

As mentioned before, the autoionizing states are unstable, thus they are characterized by a certain width $\Gamma$. This width specifies the uncertainty in the energy of these states, and, on the other hand, it represents the probability that this state will decay in a unit time, because the auto ionizing states decay in a time $\tau = 1 / \Gamma$ into an atom (ion) and an electron or a position. When the projectile collides with the target, it may form low-energy autoionizing states, by excitation of an electron from the outer shell of the target, with a subsequent capture of the projectile, also it may form high energy autoionizing states which arise through the formation of vacancies in inner shells of the target, or excitation of several electrons from the outer shell. It is well known that the incident projectile is the main factor that determine the possible scattering process which may be elastic, simultaneous excitation or ionization. The processes which are allowed at this given energy determine the "open channel", while those which are forbidden at the same energy determine the "closed channel". Resonances are classified according to those open and closed channels.

That is, if the incident projectile is captured by the target in an autoionizing state through one of the closed channels, giving rise to resonance in the cross section, those resonances are interchangeably called "Feshbach resonances, closed-channel resonances or type I resonances", (see Taylor et al., [8] and Taylor[9] ). This type takes place when the interaction potential between the projectile and the excited state of the target is strong enough to support a bound state, usually lie approximately 0-0.5 eV below the state from which they derive the "parent". When the excitation takes place near the centre of the resonance, decay into the parent is energetically forbidden, but decay into some other states (non parents) is allowed, and because this means a change in the configuration of the atoms, this type of resonance is usually long-lived and consequently its width is narrow. If these resonances are excited in high-energy

range, decay into the parent may become energetically possible and becomes a favored decay (Taylor[9], 1970).

If the projectile is captured temporarily by the target in an open channel, i.e. forming resonance lying above their parents, these types are interchangeably called "shape resonances", "open channel resonances", or "type II" (Taylor[8] et al.). In this type of resonance, the potential forms a penetrable barrier which traps the incident particle near the target. The barrier is formed by the angular momentum of the projectile, consequently one excepts p-, d-, f- wave resonances but not the s-wave one, since in this case $l = 0$.

Shape type of resonances prefer to decay into their parents directly, thus have a shorter lifetime i.e. larger width compared with those of Feshbash resonance. An exception takes place only when a sharp resonance exists barely above an inelastic threshold (Macek and Burk[10] 1967), such that the barrier can be viewed as being very thick, giving rise to a long-lived resonance and a narrow width.

In fact the theoretical and experimental studies on resonance are concerned with determining the parameters of the autoionizing states (energies and widths),which is the main goal here, and their effects on the cross sections for the scattering processes under consideration.

The first discovery of a quasistationary state was made in 1921, by accident when J. Frank and his colleagues[11] were studying certain aspects of discharge processes in Neon atoms. As explanation, Frank suggested that when an outer-shell electron of a Neon atom is excited into a vacant orbital, the incident electron may be captured, and an excited negative Neon ion may be formed. After few years, Auger[12] obtained another indication for resonance lying above the first continuum threshold, where the electrons were ejected from rare gases due to the radiation less reorganization of an

atom ionized in an inner shell, where an outer electron is transited into the shell vacancy and the excess energy is removed by the ejection of a second outer electron. Further experimental investigations and more observations took place, Compton and Boyce[13], and Kruger[14] observed emission lines in the vacuum ultra-violet spectrum of Helium associated with transitions from initially doubly excited states of Helium lying in the continuum to normal bound-states. Attempts to interpret these lines theoretically were given by Fender and Vinti[15], Wu[16], Wilson[17], and more recently by Bransden and Dalgarno[18]. However their estimation of the width and position was incompatible with the experimental results.

The first direct observation of resonance states in atomic Helium were made by Whiddington and Priestly[19]. They observed two resonance states lying at 59.25 eV and 62.27 eV above the ground state by means of an inelastic electron-Helium scattering experiment. These two states were studied theoretically by Massey and Mohr[20].

Evidence for resonant states in photon absorption in Argon, Krypton and Xenon has been observed by Beutler[21] and interpreted qualitatively by Fano[22].

The same work was carried out by Rice[23]. These studies were stopped for sometime because of the experimental difficulties such as that of producing monoenergetic electrons, as well as the lack of wide interesting applications at that time.

The revival of widespread interest in resonance experimentally were resumed in the early sixties, which can be attributed to the development of several new techniques with a sufficiently small energy spread and a very high current, also the electron resolution that was obtained using electrostatic analyzer has been reduced to $\cong$ 20 mV at currents up to $10^{-7}$ A (Simon et al.,[24] ). According to that increasing interest,

Schulz[25] detected narrow resonances in the elastic scattering of electrons by atomic Hydrogen, which was also detected by Kleinpoppen and Raible[26]. He also discovered $S^2$ resonance[25] while observing the elastic scattering electrons by Helium atoms.

Later on, further resonances were found in the scattering of electrons by atoms and ions of inert gases (Kuyatt et al.,[27] and Imre et al.,[28] ), alkali metals (Zapensochnyi et al.,[29] Hafner[30], Andrick et al.,[31] ), alkali earths (Burrow et al.,[32] and Romanyuk et al.,[33] ) and also molecules (Bardsley and Mandle[34] ).

In the late fifties, studies concerning positron-atom collisions started, the first work in which the prediction of an infinite sequence of resonances in positron-Hydrogen scattering below the excitation thresholds was carried out by Mittelman[35]. Then there were several attempts to locate such lower lying resonances by Wakid[36], and hence the interest in localizing resonances has been continuously increasing and many excellent theoretical works have been published determining the resonance parameters in different collisions of positrons with atoms. For example, Doolen et al.,[37] found evidences for resonances occurring in $e^+$-Hydrogen s-wave scattering using the coordinate rotation method, and Doolen[38] gave some new results for $e^+$ -H resonances. Several studies concerning the doubly excited state resonances in $e^+$ -H scattering just below the Hydrogen N=2 thresholds took place and gave evidence for its existence as in the work of Choo et al.,[39] and Pelikan and Klar[40]. Ho and Greene[47] have investigated some lower-lying s-wave resonances in $e^+$ -H scattering associated with the positronium (Ps) N=2 and Hydrogen N=3 thresholds using the complex coordinate method. Further investigations of resonances in $e^+$ -H collisions were carried out by Archer et al.,[42], who used a method of hyperspherical coordinates which is commonly used to investigate resonances. Ho[43] has investigated resonances in $e^+$ -H associated with the positronium N=3 and Hydrogen

N=4 thresholds and he determined the resonance parameters at these thresholds, and locate a shape resonance just above the Ps (N=3) threshold at E= -0.7540 eV.

Ward et al.,[44] have investigated resonances in low-energy positron scattering from Li, Na and K, and carried out five-state close-coupling calculations in which the positronium formation channel was ignored. The results gave rise to a number of resonances in the $l$=0,1 channels. Abdel-Raouf and Wood[45] have studied the inelastic collisions of parameters with Lithium atoms at energies below 5 eV. They assumed that only elastic and rearrangement channels are opened while the excitation ones are closed, and showed the possible appearance of resonances in both channels at $l = 0, 1$ may occur.

Now, we discuss briefly the general backgrounds of different methods employed for determining atomic resonances. Later on we deal with two of the most common methods used for calculating resonance parameters and discuss briefly their mathematical aspects. The complex coordinate method, its mathematical and computational aspects and its application to our problem is discussed in the following chapters.

From the computational point of view there are four methods concerning with the study of resonance, which are classified as follows:

*(i) Briet-Wigner Profile*

From the scattering point of view, resonance is defined as a complex energy pole of the scattering matrix S at $E_n = E_r(n) - \frac{1}{2} i \Gamma(n)$, where $E_r$ and $\Gamma$ are the position and width of the nth resonant state, respectively[46] which is connected with the lifetime $\tau$ by

$\tau = h/\Gamma$.

The expression of the S-matrix in terms of these poles is not obvious. However, a common product expansion[46] was suggested in the form

$$S(k) = \exp[2i\bar{\eta}(k)] \prod_{\nu=0}^{\infty} \frac{1 - k/k_\nu^*}{1 - k/k_\nu} \qquad (1.4)$$

where the product runs over all poles of S, i.e., bound-states on the positive imaginary axis,antibound states on the negative imaginary axis, decaying (resonance) states in the lower half of the complex momentum k-plane (distributed symmetrically about the imaginary axis) [47].The phase $\bar{\eta}(k)$ is related to the phaseshift $\eta(k)$, (connected with S through the relation S = exp (2i $\eta$)), by

$$\eta(k) = \bar{\eta}(k) + \sum_{n=0}^{\infty} \tan^{-1} \frac{2k\,|\mathrm{Im}\,k_n|}{|k_n|^2 - k^2} - \sum_{p=0}^{\infty} \tan^{-1} \frac{k}{\pm|k_p|}, \qquad (1.5)$$

where the contributions from the poles $k_p$ on the imaginary axis ( + $|k_p|$ for bound, - $|k_p|$ for antibound states) and from the resonances $k_n$ have been separated.(Remember that the resonance occurs in pairs ( $k_n$ , - $k_n^*$) because of the analytic properties of the Jost function f(+$k$) and S ($k$) = f(-$k$)/ f(+$k$) ). Particularly the case $\Gamma << E_\gamma$, i.e. at very sharp resonances, is distiguished by the well known Breit-Wigner's formula

$$\eta(E) = \tan^{-1} \frac{\Gamma}{2(E_r - E)}, \qquad (1.6)$$

for energies in the neibourhood of $E_r$. Thus, the resonance parameters can be obtained once the scattering wavefunctions in the vicinity of resonance is calculated. It is interesting to mention here that quite important semiclassical approaches for treating resonance, on the basis of the phaseshift analysis at resonance energies have been developed over the years, (for a review, see Korsch [48] ).

*(ii) Quasi-bound state*

Assuming that resonance is a quasi-bound state in the scattering continuum, Feshbach[49] has very elegantly developed a formalism which sees resonance phenomena as a part of the formal scattering theory. This formalism was applied to atomic processes and led to very fruitful results. The computational aspects of this theory will be discussed later in this chapter.

In the above two methods, calculations of the width require the use of continuum wavefunctions.

*(iii) Exponentially decaying states:*

The relation between resonances and exponentially decaying states from the time dependent point of view[50], has attracted relatively less attention. It is not clear yet the advantages and disadvantages of this method, specially from its computational aspects point of view.

*(iv) Eigenvalues of the Hamiltonian:*

The dependence of resonance on the structures of the cross sections leads to the calculation of the resonance eigenvalues of the Hamiltonian. This method was not widely used before the development of the complex coordinate rotation method. This is because the resonance wavefunction (the so called Sigert[51] wavefunction) diverges at the complex resonance eigenvalue, which seemed to have a great computational difficulty.

Unfortunately this method was interpreted as "tried and rejected" (see Ref. [52] for more details). We will see later how the complex coordinate method was able to overcome this divergence.