Theoretical Modeling of Near-Threshold Shape Resonance Behaviour in Photodetachment Experiments

Laurentiu Dan Dumitriu

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THEORETICAL MODELING OF NEAR-THRESHOLD SHAPE RESONANCE
BEHAVIOUR IN PHOTODETACHMENT EXPERIMENTS

by

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A thesis submitted to the Graduate College
in partial fulfillment of the requirements
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THEORETICAL MODELING OF NEAR-THRESHOLD SHAPE RESONANCE BEHAVIOUR IN PHOTODETACHMENT EXPERIMENTS

Laurentiu Dan Dumitriu, M.A.
Western Michigan University, 2013

This thesis attempts to better understand the results obtained from photodetachment experiments of Fe\(^-\), made by the Western Michigan University experimental atomic physics group at the Advanced Light Source (ALS), Lawrence Berkeley National laboratory.

After a relevant description of the quantum mechanics and theoretical atomic physics concepts and formulas involved in this subject, a physically realistic model, based on the square well potential, is developed. Based on this model, the theoretical photodetachment cross section is computed in order to reproduce the qualitative behavior of the experimental photodetachment cross section measured at ALS.

This development, involving programming in Fortran and numerical computing, offers a great opportunity to study and appreciate the interplay between analytical, computational, and experimental aspects of an atomic physics problem. The results of this works show a good qualitative description of the experimental data.
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I would like to express my gratitude and appreciation to all the people from the Department of Physics at Western Michigan University. There will always be a special place in my heart for my professors, but especially for Dr. Thomas Gorczyca, who revealed to me the beauty and elegance of the atomic physics entailed in this project.

Of course, I will not conclude without a special thanks to my wife, Ileana, for a lifetime of support.

Laurentiu Dan Dumitriu
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CHAPTER I

INTRODUCTION

An negative ion is an atom or molecule in which the number of electrons is greater than the number of protons, giving the system a net negative charge. Such systems are more fragile than their positive counterparts.

The study of negative ions is important in a wide range of fields. For instance, in August 2011, University of Gothenburg arranged the symposium ”Negative ions and Molecules in Astrophysics,” bringing together physicists, chemists and astrophysicists with interest in this rapidly increasing interdisciplinary field. Another area influenced by the presence and dynamics of negative ions is radio communications within a range of 30 MHz. Those electromagnetic waves can return to Earth after being reflected by the ionosphere (a region of the upper atmosphere, from about 85 km to 600 km, where the presence of $O^-$ and $O_2^-$ plays an important role). Another interesting area of study is the influence of negative ions in the air on living organisms, especially on the human body, with applications both in hospitals and in other inhabited areas.

The first mention of negative ions was in the the electrolysis experiments conducted by Michael Faraday in 1833 [2]. The term used by him for the electrolyte particles attracted by the positive electrode was anion, from the Greek word meaning ”up.” However, for more than seven decades, negative ions remained to be studied by chemists.

At the beginning of the 20th century, studying the cathode rays, J. J. Thompson mentions the negatively electrified atoms and the negatively electrified molecules [3]. Even if
the main concern of Thompson was positive ions, this work remains the benchmark as the first mention of negative ions in the gas phase. Just a year after H. Massey published the first monograph on negative ions in 1938 [4], R. Wildt suggested that the photodetachment of negative hydrogen ions from the Sun’s photosphere was responsible for the observed absorption in the solar infrared spectrum [5]. After another year, S. Chandrasekhar supported this with calculation [6].

At present, experimentalists have provides new data that theoreticians try to explain as rigorously as possible using complex theories such as R-matrix and Multiconfiguration Dirac-Hartree-Fock method [7], [8], [9].

1.1 Production of negative ions

The nature of the interaction between a neutral atom and an extra electron (which together form the negative ion) is qualitatively different from the interaction between the nucleus and electrons as occurs in the case of atoms or positive ions. While in the latter case, the interaction is the long range Coulomb attractive force, in the case of negative ions, the interactions has a particular behavior, having the shape of a short-range induced dipole potential.

Negative atomic ions are formed when an electron attaches to a neutral atom. As the electron is approaching it polarizes the charge cloud of the atom. The induced electric dipole moment is strong enough to bind the incident electron, which is now trapped in an induced electric dipole potential \( \propto r^{-4} \) [10]. As will be shown later in our model, this value may be neglect compared with the centrifugal potential.
Figure 1.1  Semi-classical picture of negative ion binding: a) the electron is not attracted by the neutral atom; b) the electric field of the electron polarize the atom, and this induces an electric dipole moment.

This weak potential does not support a Rydberg series, but rather only a finite number of states exist. Often this potential supports only a single bound state [11].

Figure 1.2  Semi-classical picture of negative ion binding: The representation of the binding potentials for negative ions (induced dipole potential), with continuous line and for atoms and positive ions (Coulomb potential) with dashed line

The energy the atom gains in this process is the electron affinity (EA) of the neutral atom (or the binding energy of the negative ion). In other words, the electron affinity of an atom is defined as the amount of energy released when an electron is added to an neutral
atom to form a negative ion.

Figure 1.3  Comparative diagram of relative energies of the lowest bound state of the negative ion, \( A^- \) and the neutral atom, \( A \)

1.2 Destruction of negative ions

The reverse process of the formation of the negative ion is its destruction in an energy absorption process. This process occurs with the electron detachment from the bound ground state into a continuum state which consists of the residual neutral atom and the free electron. The energy absorbed in this process may have come from negative ion impact with another particle, from the absorption of a photon, or from application of an external electric field.

The absorption of a photon followed by the expulsion (detachment) of an electron is called photodetachment and the ejected electron is called a photoelectron. Fig. 1.4 shows schematically the photodetachment process.

As can be seen from Fig. 1.4.c, if the incident photon has a lower energy than the EA,
Figure 1.4  Schematic of the photodetachment process. **a)** the photon (with energy $h\nu$) is absorbed by an electron in the negative ion; **b)** the photoelectron (with the kinetic energy $KE$) is ejected; **c)** the corresponding energy level diagram

The negative ion cannot be ionized. For this reason this energy is named *the threshold energy*. 

In the usual way, the photons used for the negative-ions photodetachment studies can have two main sources: lasers (for low energy photons, below 15 eV) and the synchrotron radiation (for photons above 15 eV). But the lasers to be developed in the European Extreme Light Infrastructure Project are designed to create coherent light up to 1000 eV, returning the research of the negative ions photodetachment back to university laboratories.

Starting from the first studies of the photodetachment processes (L. Branscomb et al. [12]), one of the most used representations is the dependency of the photodetachment cross section on the incident photon’s energy. The cross section is zero at the threshold and rises depending only on the angular momentum of the detached photoelectron, while the photoionization cross section of neutral atoms at threshold is non-zero [10].

The aim of this thesis is to fit the shape of the photodetachment cross section, including the positions of the resonances found in Fe$^-$ photodetachment, using a square well potential model. The reference experimental data are the results of Dr. Nora Berah’s team at the
Advanced Light Source at Lawrence Berkeley National Laboratory [1].
CHAPTER II
THEORETICAL APPROACH

The model will be developed in the following chapters is not really new, it has been used for many years in solving of scattering problems (such as neutron scattering [13]). Because of this, some parts of the theory development can be found partly in few books as [14] and [12].

Photodetachment of negative ions is a classic case of a collision between an elementary particle (the photon) and an atomic system (the negative ion). The schematic illustration of the process is represented in Fig. 2.1. When a photon (having an energy $h\nu$ greater than $E_{tre}$, the threshold energy) interacts with a free negative ion in state $i$, an electron is emitted

$$A^- + h\nu \rightarrow A^0 + e^-.$$  

The kinetic energy of the outgoing electron will be $KE = h\nu - E_{tre}$.

![Figure 2.1 Schematic illustration of a photodetachment experiment](image)
2.1 Potential non-relativistic scattering

In order to find the expression of the photodetachment cross section, we first study the cross section for potential non-relativistic scattering. The system is described by time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi (\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 (\vec{r}, t) + V (\vec{r}, t) \right] \Psi (\vec{r}, t). \quad (2.1)$$

The first simplification of the problem comes from the fact that the potential $V(\vec{r})$ is time independent. For this reason, the Schrödinger equation admits stationary state solutions

$$\Psi (\vec{r}, t) = \psi_E (\vec{r}) e^{-iEt/\hbar}, \quad (2.2)$$

where $E$ is a constant and $\psi_E (\vec{r})$ satisfies the time-independent Schrödinger equation

$$\left[ -\frac{\hbar^2}{2m} \nabla + V (\vec{r}) \right] \psi_E (\vec{r}) = E \psi_E (\vec{r}), \quad (2.3)$$

or

$$H \psi_E = E \psi_E. \quad (2.4)$$

Recalling Fig. 2.1, the photons comprise an incident monoenergetic beam traveling in the direction $\hat{k}_i$ (which is parallel to the z axis), hence it will be represented by a wave plane function

$$\psi_{\text{inc}} (\vec{r}) = Ae^{i\hat{k}_i \cdot \vec{r}} = Ae^{ikz}, \quad (2.5)$$

where $A$ is an arbitrary normalization constant and the wave number is related to the total energy by

$$k^2 = \frac{2mE}{\hbar^2}. \quad (2.6)$$
Far from the scatterer, the scattered wave has the form of an outgoing spherical wave

\[ \psi_{sc} (\vec{r}) = A f(k, \theta, \phi) \frac{e^{ikr}}{r}, \]  

where \((\theta, \phi)\) are the polar angles of \(\vec{r}\) with respect to the incident direction \(\vec{k}_i\) (the z-axis) and \(f\) is the \textit{scattering amplitude}. At large distances from the scatterer, in the region where both waves are moving away from the scatterer, the stationary state wave function \(\psi_{ki}^{(+)}\) is the superposition of the incident plane wave and the outgoing spherical wave

\[ \psi_{ki}^{(+)} \xrightarrow{r \to \infty} e^{ikz} + f(k, \theta, \phi) \frac{e^{ikr}}{r}. \]  

For a stationary state, from the expression of the probability current density

\[ \vec{j} = \frac{\hbar}{2m} \left[ \psi^* (\nabla \psi) - (\nabla \psi^*) \psi \right], \]

the radial current is given by

\[ \vec{j} \cdot \hat{r} = \frac{\hbar}{2m} \left[ \psi^* \frac{\partial \psi}{\partial r} - \frac{\partial \psi^*}{\partial r} \psi \right]. \]

Substituting for the scattered outgoing spherical wave (Eq. 2.8) and writing the gradient operator in spherical polar coordinates, one gets

\[ \vec{j} \cdot \hat{r} = \frac{\hbar}{m} \left\{ A^* A \frac{1}{2i} \left[ e^{-ikr \cos \theta} + f^* (\theta, \phi) e^{-ikr} \right] \times \frac{\partial}{\partial r} \left[ e^{ikr \cos \theta} + f(\theta, \phi) e^{-ikr} \right] \right\} + c.c \]

where c.c denotes the complex conjugate. For large \(r\) (terms of higher order in \(1/r\) will be neglected)

\[ \vec{j} \cdot \hat{r} \to A^* A \frac{\hbar k}{m} \frac{|f(\theta, \phi)|^2}{r^2} = |A|^2 \frac{\hbar k}{m} \frac{|f(\theta, \phi)|^2}{r^2} \]
Now let’s focus on the meaning of the cross section of a photodetachment process.

$$A^- + h\nu \rightarrow A^0 + e^- .$$

Considering the above equation, we will define the following values:

- $$F_{phot} = \text{the flux of the incident photons}$$ (defined as the number of photons crossing per unit time a unit area placed perpendicular to the direction of the photon beam)
- $$N_{tot} = \text{the number of electrons detached per unit time in the collision of the incident photons with the target (negative ions)}$$
- $$n_{ion} = \text{the number of negative ions within the target interacting with the incident beam.}$$

In the following equation:

$$N_{tot} = F_{phot} \cdot n_{ion} \cdot \sigma_{tot} \quad (2.13)$$

$$\sigma_{tot}$$ has the meaning of transition probabilities per unit time, per unit target scatterer and per unit flux of the incident photons with the respect of the target and is called the cross section.

From the definition of flux, if $$N$$ is the number of particles and $$S$$ is the area, one immediate result is the expression for the incident flux of the photon beam (the number of incident particles that flows through a unit cross-section per second):

$$F_{phot} = \frac{N}{S} \frac{1}{\Delta t} = \frac{N}{V} \frac{l}{\Delta t} = |A^2| v = |A^2| \frac{\hbar k}{m}. \quad (2.14)$$

Now, if one defines the differential cross section as

$$\frac{d\sigma}{d\Omega} = \frac{\text{scattered flux / unit solid angle}}{\text{incident flux / unit area}}, \quad (2.15)$$
or

\[
\frac{d\sigma}{d\Omega} = \frac{\vec{j} \cdot \hat{r} / d\Omega}{F/r^2 d\Omega},
\]  

(2.16)

and using the relationships (Eq. 2.12), (Eq. 2.14), and (Eq. 2.16), it’s easy to see that

\[
\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2,
\]  

(2.17)

where \( f(\theta, \phi) \) is the potential amplitude.

The total cross section over all scattering angles is obtained after integration

\[
\sigma_{\text{tot}} = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta |f(\theta, \phi)|^2.
\]  

(2.18)

On the other hand, the total number of particles entering into the scattering region per unit time must be equal to the number leaving per unit time, or

\[
r^2 \int (\vec{j} \cdot \hat{r}) d\Omega = 0,
\]  

(2.19)

which, together with (2.11), we can solve for \( \theta = 0 \) as

\[
\text{Im} f(k, \theta = 0) = \frac{k}{4\pi} r^2 \int |f(\theta, \phi)|^2.
\]  

(2.20)

Using (Eq. 2.17), we can find the relationship that express the conservation of the probability flux (also known as optical theorem)

\[
\sigma_{\text{tot}} = \frac{4\pi}{k} \text{Im} f(k, \theta = 0).
\]  

(2.21)

### 2.2 Central force: separation of variables in polar coordinates

We already found that, because the potential is time independent, the Schrödinger equation admits stationary state solutions (Eq. 2.2)

\[
\Psi (\vec{r}, t) = \psi_E(\vec{r}) e^{-iEt/\hbar}.
\]
Since the potential is spherically symmetric, it is natural to use spherical polar coordinates. The Hamiltonian of the system becomes

\[
H = -\frac{\hbar^2}{2m} \nabla^2 + V(r)
\]

\[
= -\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] + V(r) .
\]

(2.22)

Taking into consideration that

\[
\vec{L}^2 = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] ,
\]

(2.23)

the Hamiltonian (Eq. 2.22) may be written as

\[
H = -\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \vec{L}^2 \right] + V(r) .
\]

(2.24)

With this expression, the time-independent Schrödinger equation (Eq. 2.3) becomes

\[
\left\{ -\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) \right] + V(r) \right\} \psi(\vec{r}) = E \psi(\vec{r}) .
\]

(2.25)

A particular solution for the Schrödinger equation (Eq. 2.25) can be expressed in terms of spherical harmonics \( Y_{l,m}(r, \theta, \phi) \) (because the spherical harmonics \( Y_{l,m}(\theta, \phi) \) are simultaneous eigenfunction of \( \vec{L}^2 \) and \( L_z \))

\[
\psi_{E,l,m}(r, \theta, \phi) = R_{E,l}(r) Y_{l,m}(\theta, \phi) .
\]

(2.26)

Substituting (Eq. 2.26) into (Eq. 2.25) and using the spherical harmonics proprieties

\[
\vec{L}^2 Y_{l,m}(\theta, \phi) = l(l + 1) \hbar^2 Y_{l,m}(\theta, \phi) ,
\]

(2.27)

we can find an equation for the radial function \( R_{E,l}(r) \)

\[
-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) - \frac{\hbar^2}{2m} l(l + 1) \frac{1}{r^2} + V(r) R_{E,l}(r) = E R_{E,l}(r) .
\]

(2.28)
Now, with the new radial functions

\[ u_l(k, r) = r R_l(k, r) , \]  

we can find for \( u_l(k, r) \) the radial equation:

\[ - \left\{ \frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} + V(r) \right\} u_l(k, r) = Eu_l(k, r). \]  

(2.30)

We see that the above equation is identical in form with the one-dimensional Schrödinger equation, where instead of the potential \( V(r) \) we have an effective (reduced) potential:

\[ V_{\text{eff}}(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr^2}. \]  

(2.31)

The second term of (Eq. 2.31) is called the centrifugal potential, since its negative gradient is equal to the fictitious centrifugal force. Fig. 2.2 shows the effective potential for the case of square well potential and \( l \neq 0 \).

### 2.3 Central force: the free particle

The free particle is moving in a potential-free environment \((V(r) = 0)\). In this case, from (Eq. 2.28) we obtain

\[ - \frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} R = ER. \]  

(2.32)

Recalling the relationship between the wave number \( k \) and the total energy \( E \) (Eq. 2.6), the previous equation (Eq. 2.32) may be simplified as

\[ - \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{l(l+1)}{r^2} R = k^2 R. \]  

(2.33)
Figure 2.2 The effective potential (for \( l \neq 0 \))

The expression of radial equation is a Bessel differential equation (after a convenient change of variable \( \rho = kr \))

\[
\frac{d^2}{d\rho^2} + \frac{2}{\rho} \frac{d}{d\rho} + \left[ 1 - \frac{l(l+1)}{\rho^2} \right] R = 0 .
\] (2.34)

The general solution of the above equation is a linear combination of the spherical Bessel function

\[
j_l(\rho) = \sqrt{\frac{\pi}{2\rho}} J_{l+1/2}(\rho) ,
\] (2.35)

and the spherical Neumann function

\[
n_l(\rho) = (-1)^{l+1} \sqrt{\frac{\pi}{2\rho}} J_{-l-1/2}(\rho) ,
\] (2.36)

where \( J_n(\rho) \) is a Bessel function of order \( n \). The behavior of the functions \( j_l \) and \( n_l \) for small \( \rho \) is given by

\[
j_l(\rho) \sim_{\rho \to 0} \frac{\rho^l}{(2l+1)!!} \left[ 1 - \frac{\rho^2/2}{1!(2l+3)} + \frac{(\rho^2/2)^2}{2!(2l+3)(2l+5)} - \ldots \right] ,
\] (2.37)
and
\[ n_l(\rho) \sim \frac{(2l - 1)!!}{\rho^{l+1}} \left[ 1 - \frac{\rho^2/2}{1!(1-2l)} + \frac{(\rho^2/2)^2}{2!(1-2l)(3-2l)} - \cdots \right] . \] (2.38)

For larger \( \rho \) we have the asymptotic relationships
\[ j_l(\rho) \to \frac{1}{\rho} \sin \left( \rho - \frac{l\pi}{2} \right) , \] (2.39)

and
\[ n_l(\rho) \to -\frac{1}{\rho} \cos \left( \rho - \frac{l\pi}{2} \right) . \] (2.40)

These are the only solutions that are acceptable (non-singular at the origin).

If we consider the region in which the particle moves freely (\( V_0 = 0 \)), the solution of the radial equation (Eq. 2.33) is a linear combination of \( j_l(kr) \) and \( n_l(kr) \)
\[ R_l(k, r) = \frac{u_l(k, r)}{r} = B_l(k) j_l(kr) + C_l(k) n_l(kr) , \] (2.41)
with \( B_l(k) \) and \( C_l(k) \) are real constant of integration, independent of \( r \).

For \( r \to \infty \) we can use the asymptotic formulas (Eq. 2.39, 2.40) and the previous equation becomes
\[ R_l(k, r) = \frac{u_l(k, r)}{r} \to \frac{1}{r} B_l(k) \sin(kr - l\pi/2) - C_l(k) \cos(kr - l\pi/2) . \] (2.42)

With a convenient notations
\[ A_l(k) = \sqrt{B_l^2(k) + C_l^2(k)} , \] (2.43)

and
\[ \tan \delta_l(k) = -\frac{C_l(k)}{B_l(k)} , \] (2.44)
the (Eq. 2.42) can be rewritten

\[ R_l(k, r) = \lim_{r \to \infty} \frac{A_l(k)}{kr} \sin \left[ kr - \frac{l\pi}{2} + \delta_l(k) \right]. \quad (2.45) \]

The quantities \( \delta_l(k) \) is called phase shift and it measures the difference between the phase of the radial wave function for angular momentum \( l \) and the non-scattering case \( (\delta_l = 0) \). The phase shift is a function of energy (or wave number \( k \)).

If we expand the wave function which correspond to the incoming wave plane and which we call \( \psi^{(+)}_{k_i} \) (Eq. 2.8) in a series of Legendre polynomials as

\[ \psi^{(+)}_{k_i}(k, r, \theta) = \sum_{l=0}^{\infty} R_l(k, r) P_l(\cos \theta), \quad (2.46) \]

and replace them properly in the (Eq. 2.45), we obtain

\[ \psi^{(+)}_{k_i}(k, r, \theta) = \sum_{l=0}^{\infty} \frac{A_l(k)}{kr} P_l(\cos \theta) \sin \left[ kr - \frac{l\pi}{2} + \delta_l(k) \right]. \quad (2.47) \]

After the sine function is expanded using Euler’s formula, finally we find

\[ \psi^{(+)}_{k_i}(k, r, \theta) = \sum_{l=0}^{\infty} \frac{A_l(k)}{kr} P_l(\cos \theta) \frac{1}{2i} \left( e^{i(kr - \frac{l\pi}{2} + \delta_l)} - e^{-i(kr - \frac{l\pi}{2} + \delta_l)} \right). \quad (2.48) \]

### 2.4 Spherical wave expansion of a vector plane wave

We have two alternative complete sets of eigenfunction of a free particle Hamiltonian: the plane waves (Eq. 2.5) and the spherical waves (Eq. 2.26). These two sets of eigenfunctions are related by the expression

\[ e^{ikr} = \sum_{l=0}^{\infty} \sum_{m=-1}^{l} c_{l,m} j_l(kr) Y_{l,m}(\theta, \phi), \quad (2.49) \]

with expansion coefficients \( c_{l,m}(k) \) to be determined.
The general expression of spherical harmonics in terms of the associated Legendre functions is

$$Y_{l,m}(\theta, \phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_{l,m}(\cos \theta) e^{im\phi}. \quad (2.50)$$

For the particular case of $\phi = 0$ (because of rotational symmetry) the previous formula is simplified as

$$Y_{l,0}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta), \quad (2.51)$$

and as a result, we have

$$e^{ikr \cos(\theta)} = \sum_{l=0}^{\infty} \sqrt{\frac{(2l+1)}{4\pi}} A_l j_l(kr) P_l(\cos \theta). \quad (2.52)$$

From the orthogonality relation of the Legendre polynomials, we have

$$\int_{-1}^{1} d\cos \theta P_l(\cos \theta) P_{l'}(\cos \theta') = \frac{2\delta_{ll'}}{2l+1}. \quad (2.53)$$

Multiplying (Eq. 2.52) by $P_l \cos(\theta)$ and integrating over $\theta$, we will find

$$A_l j_l(kr) = \frac{1}{2} \sqrt{\frac{(2l+1)}{4\pi}} \int_{-1}^{1} dz P_l(z) e^{ikrz}. \quad (2.54)$$

Using the Taylor expansion of the exponential function, the previous integral becomes

$$\int_{-1}^{1} dz P_l(z) e^{ikrz} = \int_{-1}^{1} dz P_l(z) \left[ \ldots + \frac{(ikr z)^l}{l!} + \frac{(ikr z)^{l+1}}{(l+1)!} + \ldots \right]$$

$$= (ikr)^l \frac{2^l l!}{(2l)!} \int_{-1}^{1} dz P_l(z) + O((kr)^{l+1}) \quad (2.55)$$

$$= \frac{i^l(kr)^l}{(2l+1)!} \frac{2^{l+1} l!}{(2l+1)!} + O((kr)^{l+1}).$$
with

$$A_l = i^l \sqrt{4\pi(2l + 1)}.$$  \hspace{1cm} (2.56)

The expansions then becomes

$$e^{ikr \cos(\theta)} = \sum_{l=0}^{\infty} i^l (2l + 1) j_l(kr) P_l(\cos \theta),$$  \hspace{1cm} (2.57)

which can be used for the partial wave expansion of the unperturbed plane wave (Eq. 2.5) as

$$\psi(\vec{r}) = \psi_{inc}(\vec{r}) = A e^{ikz} = A \sum_{l=0}^{\infty} i^l (2l + 1) j_l(kr) P_l(\cos \theta).$$  \hspace{1cm} (2.58)

Using the above formula in (eq. 2.8)

$$\psi_{k_i}^{(+)}(r) \rightarrow_{r \rightarrow \infty} A \left[ \sum_{l=0}^{\infty} \frac{i^l (2l + 1)}{kr} \sin(kr - l\pi/2) P_l \cos(\theta) + f(k, \theta) \frac{e^{ikr}}{r} \right],$$  \hspace{1cm} (2.59)

and expanding the sine function we obtain

$$\psi_{k_i}^{(+)}(r) \rightarrow_{r \rightarrow \infty} A \frac{e^{ikr}}{r} \left[ f(k, \theta) - \sum_{l=0}^{\infty} \frac{i}{2k} P_l \cos(\theta) \right]$$

$$+ A \frac{e^{-ikr}}{r} \left[ \sum_{l=0}^{\infty} (-1)^l \frac{i}{2k} P_l \cos(\theta) \right].$$  \hspace{1cm} (2.60)

Because (Eq. 2.48) and (Eq. 2.60) are equivalent, we can find the expression for the scattering amplitude $f(k, \theta)$ by matching the coefficients of $e^{ikr}$

$$f(k, \theta) = \frac{1}{2i} \sum_{l=0}^{\infty} (2l + 1) e^{i\delta_l(k)} P_l(\cos \theta)$$

$$= \frac{1}{i} \sum_{l=0}^{\infty} (2l + 1) e^{i\delta_l(k)} \sin \delta_l(k) P_l(\cos \theta).$$  \hspace{1cm} (2.61)
It is immediately clear that the scattering amplitude does not depend on the choice of the normalization coefficient $A_l(k)$. If we identify the partial wave amplitudes as

\[ f_l(k) = \frac{2l + 1}{2i k} \left[ e^{2i\delta_l(k)} - 1 \right] = \frac{2l + 1}{k} e^{i\delta_l(k)} \sin \delta_l(k), \]  

then the differential cross section (Eq. 2.17) is given by

\[ \frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2 = \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} (2l + 1)(2l' + 1) e^{i[\delta_l(k) - \delta_{l'}(k)]} \times \sin \delta_l(k) \sin \delta_{l'}(k) P_l(\cos \theta) P_{l'}(\cos \theta). \]  

(2.63)

Considering the orthogonality relation

\[ \int_{-1}^{1} P_l(x) P_{l'}(x) dx = \frac{2}{2l + 1} \delta_{ll'}, \]  

(2.64)

the total cross section is obtained after the integration of the differential cross section

\[ \sigma_{tot}(k) = 2\pi \int_{0}^{\pi} \frac{d\sigma}{d\Omega}(k, \theta) \sin \theta d\theta = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l(k). \]  

(2.65)

Expanding the above relation for each individual value $l$, we obtain

\[ \sigma_l(k) = \frac{4\pi}{k^2} (2l + 1) \sin^2 \delta_l(k), \]  

(2.66)

and the total cross section is given by

\[ \sigma_{tot}(k) = \sum_{l=0}^{\infty} \sigma_l(k). \]  

(2.67)

It is immediately obvious that the maximum contribution of each partial wave to the total cross section occurs when $\sin \delta_l(k) = \pm 1$, or $\delta_l(k) = (2n + 1)\pi/2$, where $n$ is an integer. Under these conditions,

\[ \sigma_l(k) = \frac{4\pi}{k^2} (2l + 1). \]  

(2.68)
CHAPTER III

SQUARE WELL POTENTIAL

The square well is a central potential defined as:

\[ V(r) = \begin{cases} 
-V_0, & r < a \\
0, & r > a, 
\end{cases} \]  

(3.1)

that shown in Fig 3.1.

![Figure 3.1 Spherical potential square well](image)

We now study the motion of an spineless electron of mass \( m \). Depending on its total energy, the electron may have

- a bound state (when \(-V_0 < E < 0\)) or

- a free state or a continuum (when \( E > 0 \)), when the electron is scattered by the potential \( V(r) = -V_0 \), where \( r < a \)
3.1 The continuum solutions for the square well

We already found the radial time independent Schrödinger equation for a particle in a central force potential (Eq. 2.28),

\[
\left\{ -\frac{\hbar^2}{2m} \left[ \frac{d^2}{r^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} \right] + V(r) \right\} R(r) = E R(r) .
\]

With particular values of the potential energy (Eq. 3.1) the radial wave equation for a state of angular momentum \(l\) we can separate two equations, corresponding to the two regions (inside and outside the well)

\[
\left\{ -\frac{\hbar^2}{2m} \left[ \frac{d^2}{r^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} \right] \right\} R(r) = (E + V_0) R(r) , \text{ if } r < a , \tag{3.2}
\]

and

\[
\left\{ -\frac{\hbar^2}{2m} \left[ \frac{d^2}{r^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} \right] \right\} R(r) = (E) R(r) , \text{ if } r > a . \tag{3.3}
\]

We will consider first the region inside of the square well (\(r < a\)), where (Eq. 3.2) can be rewritten as

\[
\left[ \frac{d^2}{r^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2 \right] R(r) = 0 , \tag{3.4}
\]

with

\[
k = \sqrt{\frac{2m(E + V_0)}{\hbar^2}} . \tag{3.5}
\]

(Eq. 3.4) is now similar with (Eq. 2.34) (with \(\rho = kr\)) which gives us a regular solution

\[
R_l(k, r) = \frac{u_l(k, r)}{r} = B_l(k) j_l(kr) + C_l(k) n_l(kr) , \tag{3.6}
\]

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where $B_l(k)$ and $C_l(k)$ are real constants of integration, independent of $r$.

Because the radial function $R_l(k, r)$ must be finite everywhere (including at the origin), the spherical Neumann functions are not acceptable, so that the solution is expressed only in terms of spherical Bessel functions:

$$R_{l}^{\text{in}}(k, r) = \frac{u_{l}(k, r)}{r} = B_l(k) j_l(kr), \text{ for } r < a, \quad (3.7)$$

where $B_l(k)$ is a normalization constant.

For the outer region, considering the notation (Eq. 2.44)

$$\tan \delta_l(\tilde{k}) = -\frac{C_l(\tilde{k})}{\tilde{B}_l(\tilde{k})},$$

we have

$$R_{l}^{\text{out}}(\tilde{k}, r) = \frac{u_{l}(\tilde{k}, r)}{r} = \tilde{B}_l(\tilde{k}) \left[ j_l(\tilde{kr}) - \tan \delta_l(\tilde{k}) n_l(\tilde{kr}) \right], \text{ for } r > a. \quad (3.8)$$

The continuity of the radial function $R_l$ and its first derivative $R_{l}^{\prime}$ at $r = a$ gives

$$B_l(k) j_l(ka) = \tilde{B}_l(\tilde{k}) \left[ j_l(\tilde{ka}) - \tan \delta_l(\tilde{k}) n_l(\tilde{ka}) \right], \quad (3.9)$$

and

$$k B_l(k) j_{l}^{\prime}(ka) = k \tilde{B}_l(\tilde{k}) \left[ j_{l}^{\prime}(\tilde{ka}) - \tan \delta_l(\tilde{k}) n_{l}^{\prime}(\tilde{ka}) \right] \quad (3.10)$$

The ratio of the last two equations gives the equation for the partial phase shift:

$$\tan \delta_l = \frac{k j_{l}^{\prime}(ka) j_l(ka) - \tilde{k} j_{l}(ka) j_{l}^{\prime}(\tilde{ka})}{k n_{l}^{\prime}(ka) j_l(ka) - \tilde{k} n_{l}(ka) j_{l}^{\prime}(\tilde{ka})}, \quad (3.11)$$

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which for $ka \to 0$ behave as:

$$\tan \delta_l(k) \propto k^{2l+1} \propto E^{l+\frac{1}{2}}, \quad (3.12)$$

In (Eq. 3.11), we are looking for values where the denominator will vanish, which implies that for small variations of the energy (and therefore of $k$), $\tan(\delta_l)$ rises rapidly to infinity. As the tangent function is infinity at $\pi/2$, the partial wave cross section has the largest possible value (Eq. 2.66) and we have resonant scattering

$$\sigma_l(k) = \frac{4\pi}{k^2} \left(2l+1\right) \sin^2 \delta_l(k)_{|\delta_l=\pi/2} = \frac{4\pi}{k^2} \left(2l+1\right).$$

The behavior of this resonant scattering may be represented graphically as in (Fig. 3.2)

This representation can be modeled mathematically as

$$\tan \delta_l^r \simeq \frac{\Gamma/2}{E - E_r}, \quad (3.13)$$
where $E_r$ is the resonance energy, $\Gamma$ is the width of the resonance, and $\delta_r^\prime$ is the resonant phase shift.

Taking into consideration that

\[
\sin^2 \delta_l = \frac{\sin^2 \delta_l}{\cos^2 \delta_l + \sin^2 \delta_l} = \frac{\tan^2 \delta_l}{1 + \tan^2 \delta_l},
\]

(Eq. 2.66) can be expressed as

\[
\sigma_l(k) = \frac{4\pi}{k^2 (2l + 1)} \sin^2 \delta_l(k) = \frac{4\pi}{k^2 (2l + 1)} \frac{\tan^2 \delta_l}{1 + \tan^2 \delta_l} = \frac{4\pi}{k^2 (2l + 1)} \frac{(\Gamma/2)^2}{(E - E_r)^2 - (\Gamma/2)^2}.
\]

This relationship is known the Breit-Wigner resonance formula, or the pure resonance total cross section, and has a Lorenzian shape.

3.2 The bound states for the square well

The radial wave equations for a state of angular momentum $l$, (Eq. 3.2) and (Eq. 3.3) have the same appearance, and also their solutions should be similar.

In the inner region, noting that

\[
k = \sqrt{\frac{2m(E + V_0)}{\hbar^2}},
\]

(Eq. 3.4) has a regular solution at the origin that is similar to (Eq. 3.7)

\[
R^\text{in}_l(k, r) = \frac{u_l(k, r)}{r} = B_l(k) j_l(kr), \text{ for } r < a,
\]

where $B_l(q)$ is a normalization constant.

In the outer region, by noting that

\[
\kappa = \sqrt{\frac{-2mE}{\hbar^2}},
\]
the solution is

\[ R_{L}^{\text{out}}(\kappa, r) = B[j_{l}(i\kappa r) + i n_{l}(i\kappa r)] . \]  

(3.16)

The radial functions (Eq. 3.15) and (Eq. 3.16) and their first derivative (or the logarithmic derivative) must be continuous at \( r = a \).

For the particular case \( l = 0 \), the solution is

\[ u(r) = r R(r) = \begin{cases} A \sin(qr) & \text{for } r < a \\ Ce^{-\kappa r} & \text{for } r > a. \end{cases} \]  

(3.17)

A square well potential may have a bound state only if

\[ V_{0}^{\text{min}} = \frac{\pi^2}{8} \frac{h^2}{m a^2}. \]  

(3.18)

This bound state is represented graphically as in (Fig. 3.3).

**Figure 3.3** The shape of the radial wave function for the bound states case (\( l=0 \)). **a)** one bound state; **b)** two bound states

For \( l = 0 \), one bound state exists if

\[ \frac{\pi}{2} < \sqrt{\frac{2m V_{0} a^2}{h^2}} < \frac{3\pi}{2}, \]  

(3.19)
and two states exist if

\[
\frac{3\pi}{2} < \sqrt{\frac{2m V_0 a^2}{\hbar^2}} < \frac{5\pi}{2}.
\] (3.20)

3.3 The photodetachment cross section

In the photodetachment process, as shown in (Fig. 1.2), one photon is absorbed by a negative ion and an electron is ejected, if the photon energy is greater than the bound electron energy. The photodetachment cross section, as a measure of the probability of photodetachment process, is a function of photon energy.

*Fermi’s Golden Rule* for a transition for initial state \( |\psi_i\rangle \) to a final state \( \langle \psi_f | \) gives the transition rate from an initial eigenstate \( |\psi_i\rangle \) into a continuum state \( \langle \psi_f | \), due the electric dipole momentum

\[
w = \frac{2\pi}{\hbar} |\langle \psi_f | D | \psi_i \rangle|^2 \rho_e ,
\] (3.21)

where \( D \) is the electric dipole operator and \( \rho_e \) is the density of states. When a magnetic field is absent, the density of states is proportional to the energy of the detached electron

\[
\rho_f \propto \sqrt{\varepsilon} ,
\] (3.22)

and the photodetachment cross section can be described (see [15]) by

\[
\sigma_p \propto |\langle \psi_f | D | \psi_i \rangle|^2 ,
\] (3.23)

or, for atomic photoionization

\[
\sigma_p = N |\langle \psi_f | r | \psi_i \rangle|^2 ,
\] (3.24)

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If there are more than one transition involved,

$$\sigma_p = \sum_{j=1}^{n} N_j^2 |\langle \psi_f^j | r^j | \psi_i^j \rangle|^2,$$

(3.25)

where the summation is over all resonances and the normalization constant $N_j$ will be optimized for the best fit of each shape resonance feature.

Considering (Eq. 3.24) in which the wave function of the photoelectron is given by (Eq. 3.8),

$$\sigma_p \propto \left| \left[ \frac{1}{\sqrt{k}} (j_l(kr) - \tan \delta_l(k)n_l(k)) \right] r \psi_i \right|^2,$$

(3.26)

where $1/\sqrt{k}$ is a factor from the energy-normalization of the free photoelectron.

For small energies $(E - E_{tr}) \to 0$, $k \to 0$, $\tan \delta_l(k) \to 0$ and $j_l(kr) \sim (kr)^l+1$. After replacing the terms, we obtain that

$$\sigma_p \propto \left| \frac{k^{l+1}}{k^{1/2}} \right|^2 = k^{2l+1} \sim (E - E_{tr})^{l+1/2},$$

(3.27)

The general relationship for the cross section has the expression

$$\begin{cases} 
\sigma_l(E) \propto (E - E_{tr})^{l+1/2} & \text{when } E > E_{tr} \\
\sigma_l(E) = 0 & \text{when } E < E_{tr} 
\end{cases}$$

(3.28)

which is known as the Wigner threshold law [16].

For a wide range of photon energies, $\sigma_{tot}(k) = \sum_{l=0}^{\infty} \sigma_l(k)$.

The effective potential (Eq. 2.31) has now an additional term, which is related to the induced dipole potential

$$V_{eff}'(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr} - \frac{\alpha}{r^4}.$$ 

(3.29)
Figure 3.4  The photodetachment cross section near threshold for a s-wave and a p-wave

For the asymptotic behavior of this effective potential, it is easy to see that the dominant term is the centrifugal barrier with $1/r^2$ dependence (as long as $V_0$ is null and the dipole potential term vanishes as $1/r^4$).
CHAPTER IV

THE COMPUTATIONAL METHOD

The code uses the computing power provided by FORTRAN language. FORTRAN is a high-level programming language mostly used for scientific application that require extensive mathematical computation. Being used for more than 50 de years, there are many public code libraries for scientific computation. Subroutine RICBES used for calculate the spherical Bessel and spherical Neumann functions may be found on http://www.fresco.org.uk/programs/barnett/.

The code divides configuration space in two regions for both initial and final states:

- the inner region \((r < a)\)
- the outer region \((r > a)\)

Rydberg atomic units are used, where the electron charge \(e = 1\), the reduced Planck constant \(\hbar = 1\), and the energy is measured in Rydberg units (1 Ry = 13.605 eV).

The sequence of steps in determining the photodetachment cross section is:

1. with the bound state parameters \((a^b, V_0^b)\), performing an iterative calculation based on (Eq. 3.7) and (Eq. 3.8), using the continuity conditions (Eq. 3.9) and (Eq. 3.10), until the bound energy is found;

2. from the electron configurations of the negative ion and of the neutral atom, the
channels through which photodetachment occurs and the corresponding energies are determined;

3. the parameters found above ($a^b$ and $V^b_0$) become constant values for the next step of the code;

4. with the free state parameters ($a^f$ and $V^f_0$), performing an iterative calculation based on (Eq. 3.7) and (Eq. 3.8), using the continuity conditions (Eq. 3.9) and (Eq. 3.10), until the shape of the photodetachment cross section (described by Eq. 3.21) and the position of the resonance energy ($E_r$) are identical with the values measured on the experiment [1].

The trapezoidal method was used to solve (Eq. 3.25). Having determined the numerical values for the bound state wave function and for the free state wave function for $N$ equidistant intervals, we found first the product for each node $r_i$

$$g_i = \left( \psi^i_f r_i \psi^i_b \right)^2,$$  \hspace{1cm} (4.1)

corresponding to (Eq. 3.26). Using a quadrature formula as

$$\int_0^r g(x) \, dx = \sum_{i=1}^{N-1} \frac{g_i + g_{i+1}}{2} (r_{i+1} - r_i)$$  \hspace{1cm} (4.2)

A brief flowchart of the code is shown below (Fig. 4.1).
Figure 4.1  Flowchart of the code
CHAPTER V

RESULTS AND DISCUSSIONS

As mentioned previously, the purpose of this work is to reproduce theoretically the qualitative nature seen experimentally. In this chapter, will be presented the context in which the problem was formulated (as shown in [1]), the steps in solving the problem, and the result and few comments about them.

5.1 The experiment

(as is described in [1])

The inner-shell photodetachment of Fe\(^-\) was conducted in the beamline 10.0.1 of the Advanced Light Source, Lawrence Berkeley National Laboratory. The energy of the incident photons has been in the range of 48 to 72 eV. Because of this energy range, much higher than the electron affinity (0.151(3) eV [17]), the incoming photon has sufficient energy to detach an electron from an inner shell (therefore it is called ”inner-shell photodetachment“).

The complete sequence of the processes observed in the experiment can be written as in the (Eq. 5.1). The analysis is focused only on the first step, so that the results will differ from the total cross section measured in the experiment. Because there are only three representative transition for a good qualitative description of the experiment, we consider only three peaks of the \(3p \rightarrow (\epsilon d)\) transitions. The first one was measured at 51.6 eV and represents the \(3p^63d^74s^2\ \left(^4F_{9/2}\right) \rightarrow 3p^53d^84s^2\ \left(^4G_{7/2}\right)\) transition, the second one was
measured at 53.62 eV and represents the $3p^63d^74s^2 \left(^4F_{9/2}\right) \rightarrow 3p^53d^84s^2 \left(^4F_{9/2}\right)$ transition, an the third one 55.07 eV and represents the $3p^63d^74s^2 \left(^4F_{9/2}\right) \rightarrow 3p^53d^8 \left(^3F\right)4s^2\left(^4D_{7/2}\right)$ transition.

$$h\nu + Fe^- \left(3p^63d^74s^2 \left(^4F_{9/2}\right)\right)$$

$$\rightarrow Fe^-\left(3p^53d^8\right)4s^2 \left[^4D, \ ^4F, \ ^4G\right]$$

↓ first step

$$Fe^{**} + e_{\text{photoelectron}}$$

↓ second step

$$Fe^{**} + e_{\text{Auger}}$$

↓ third step

$$Fe^{2+} + e_{\text{Auger}}$$

The relevant states in the negative ion (whose transitions have been described above) and in the neutral atom are presented below (Fig. 5.1).

The photodetachment cross sections measured under the experiment (as presented in Fig. 5.1) contain both the contributions from the first step ($h\nu + Fe^- \left(3p^63d^74s^2 \left(^4F_{9/2}\right)\right) \rightarrow Fe^-\left(3p^53d^8\right)4s^2 \left[^4D, \ ^4F, \ ^4G\right]$), but also of the second and the third steps (which include the emission of additional electrons, called Auger electrons). This means that as additional electrons are detached, their presence influences the comparison of our results with the data collected in the experiment. Consequently, they will be different. Because of this, we will focus only on the position of the resonances and the shape of the photodetachment cross
5.2 Running the code: results and conclusions

The code first finds the wave function for the bound state. By varying the width and depth of the square well model ($a_b$ and $V_0$), the wave functions of the negative ion (bound)
state are determined such that the calculated binding energy is equal to the electron affinity of the 4d electron (50.5 eV).

The values founded for the two parameters are:

- \( a^b = 2 \)
- \( V^b_0 = 55.05 \text{ eV} \).

With the inner dimensions determined, we find the values of the well width and for the find the continuum state \( E > 0 \).

This part is of high complexity because it involves the following constraints:

- the photodetachment cross section involves the composition of two wave functions through the electric dipole operator, as in (Eq. 3.21);

- the position of the resonances must align with experiment;

- the exact position of the resonances are hard to predict, especially since the definition of resonances implies that the variation of the cross section varies widely over a small variation of the energy;

- the shapes of the cross sections for the transitions shown in (Fig. 5.1) must have a qualitative description as in the article of reference [1] (evaluation which introduces a high level of subjectivity).

To identify the pairs of values \( a^f \) and \( V^f_0 \) corresponding to the free state, all the shapes of the photodetachment cross section, with an increment of 0.1 for both width and depth
of the square well, were generated. On the energy axis zero is corresponds to the threshold (50.5 eV) and the maximum value to 60 eV (the range of the energies where the photodetachment cross section has been observed in the experiment). Therefore, the position of the resonances sought correspond to 51.68 eV, 53.62 eV, and 55.07 eV.

The photodetachment cross sections are presented and shown a very good concordance of the position of the resonances (Fig. 5.2 - 5.4) and a qualitative description for the shape of the total photodetachment cross sections (5.5).

![Figure 5.2](image)

**Figure 5.2** The theoretical photodetachment cross section for the $3p^63d^74s^2 \, (^4F_{9/2}) \rightarrow 3p^53d^84s^2 \, (^4G_{7/2})$ transition, with $a_f = 2$, $V_0^f = 4.90$ eV.
Physicist often find simple models to describe complex phenomena. But what is really important is to find models that not only describe qualitatively but may even predict quantitatively the behavior of complex phenomena.

The results obtained for the photodetachment cross section of Fe$^-$ using the square well
Figure 5.5  The total theoretical photodetachment cross section obtained by summation over all three transitions analyzed potential model contain the essential physics seen experimentally.

A. The Wigner threshold

Our results show the near-threshold shape predicted by the Wigner Threshold Law (Eq. 3.28), in accordance as also seen in the experiment.

B. Breit-Wigner resonances (pure resonance) behavior at the resonance energies

Our results show a Lorentzian behavior of the photodetachment cross section at the resonance shape energy (Eq. 3.14), for each of the transition considered, as also seen in the experiment.

Comparing the results from the summing the photodetachment cross sections of the three dominant shape resonances with the experimental results (Fig. 5.6), is obtained a qualitative description of the experimentally observed phenomena.
Figure 5.6  a) (Upper panel): The cross section of Fe$^+$ ions following photodetachment of Fe$^-$ obtained in experiment. b) (lower panel) The total cross section of Fe atoms following photodetachment of Fe$^-$ obtained in this work, for the three dominant shape resonances [1].
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