DYNAMICAL EFFECTS IN PIONIC ATOMS

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SUBMITTED TO THE DEPARTMENT OF
PHYSICS
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE OF

DOCTOR OF PHILOSOPHY

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
February 1984

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February, 1984

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This work is dedicated to

Departamento de Fisica
Facultad de Ciencias
Universidad Central de Venezuela

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ABSTRACT

In recent years more accurate measurements of the energy shifts and widths in pionic atoms provide a more stringent test for pion-nucleus optical potentials. Several anomalies have been found throughout the periodic table, calling for a reexamination of the theory. In this work the Doorway State Approach to the Bound State problem is developed in order to study these energy shifts and widths. It is found that within the first doorway truncation the essential physics of this problem is obtained and effects like Pauli-Blocking, nucleon rescattering in the presence of Coulomb forces and absorption are summed up linearly when the first doorway expectation value is considered. The new optical potential takes into account nucleon recoil and finite range effects. In this way the contribution of the first order optical potential is calculated properly. The higher order contributions are considered through a spreading potential. The parameters of this potential are found for the pion-nucleon S_{11} channel and S_{31} channel through an energy shift fitting with ^{4}He and 16_{O} the results of this fitting finally solve the ^{4}He problem and the proper energy shift and width can be obtained with the same set of parameters. The ratio of the imaginary part of the strength and the mass difference is the same as the one for the delta-isobar.

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ACKNOWLEDGEMENT

I would like to thank Professor Ernest J. Moniz for offering me this problem. In the main discussions that led to the development of this work, he always showed patience, dedication and trust.

I should thank the Consejo de Desarrollo Cientifico y Humanistico de la Univeridad Central de Venezuela and Massachusetts Institute of Technology for their financial assistance.

For the untiring assistance in computing problems, I am grateful to Gary Nixon, Jeanne Funk and Eduardo Alvarez. I also thank Jose Martinez, Theodoros Karapiperis, Bekir Karaoglu, Hang Ryu, Giovanni Puddu, Lutz Doehnert and Vidal Alonso for interesting discussions.

For the impecable typing my gratitude to Catherine Lewinson and Carmen Elena Alvarez.

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INTRODUCTION

In recent years more accurate measurements of the energy shifts and widths in pionic atoms put into test the semiphenomenological optical potentials used to describe the pion-nucleus interactions. Now it is clear that several anomalies appear in different regions of the periodic table, calling for a reexamination of these optical potentials. Measurements of the widths of heavy elements, not measured earlier,show a systematic deviation of the predicted widths from the experimental ones, which can not be explained using standard semiphenomenological potentials.All attempts to explain this anomaly have failed to date. There are also problems for very light nuclei like Helium, which is going to be discussed with detail throughout this work, and Sodium.

In chapter I a brief presentation of the general phenomenology and problems in pionic atoms is given, stressing the case of narrower widths of 3d levels of heavy nuclei and the problems of pionic ^{3}He and ^{4}He. As a review, effects like Pauli-blocking, nucleon binding and Ericson-Ericson-Lorentz-Lorenz effects are briefly introduced.

In chapter II the problem of Dynamical Nuclear Polarization is considered. After the successful attempt of Dubach, Moniz and Nixon, explaining the measured x-ray attenuations for several nuclei, it was found that ^{110}Pd can not be explained within the same simple approach. This fact was particularly intriguing for these authors when they compare the

nuclear structure of ^{110}Pd with the one of ^{104}Ru, since they are very similar and the x-ray attenuations are different by a factor of two. This finding led us to think that nuclear structure effects have probably little to do with the essential problem. In their model a mixing between 2^+ one- and two surfon states is considered, and for ^{110}Pd there is a third 2^+ state at 1470,1 Kev which can be a participant in the pionic-nuclear mixing that takes place in the Dynamical Nuclear polarization process. First, the calculation is done with information coming only from the first and second 2^+, with results that agree with the measured x-ray attenuation. Nevertheless, Coulomb excitation experiments were not able to detect the presence of the 1470,1 Kev state as a 2^+. In order to fit the one, two and three surfon model this state should be observable in Coulomb excitation experiments. The data for the quadrupole moment of the first 2^+ and the reduced transition probability from this level to the ground state are quantities measured in a not very accurate way and this allows us to consider the information from the 1470,1 state in $(n,n'\gamma)$ reactions bringing our result to the value predicted by Dubach,Moniz and Nixon, which is nearly half of the experimental one. After that the role of Giant Resonances was also considered, but with negative results. This brings us to the conclusion that the optical potential has to be reexamined.

In chapter III a convenient tool to achieve that objective is developed: The Doorway State Approach to perturbation

theory. This method turns out to be a very efficient one in the handling of perturbations of any size. At the same time the treatment of fully nonlocal interactions is made possible showing in this way a definite edge over other methods when practical numerical calculations are required. The convergence is so good that the essential physics of the problen can be extracted in most cases with one-doorway truncations. The whole procedure is an extension of the one developed by Lenz,Moniz and Yazaki for potential scattering theory. In our discussion we also consider the case of degeneracy. In order to study convergence properties very simple systems, like a harmonic oscillator with a harmonic perturbation, an infinite square well with a delta perturbation and a finite square well with a square barrier as a perturbation, are discussed in detail. The last example mentioned is the most interesting one because a simulation of the pionic atom problem can be made and in this way we can show that for the purpose of the analysis that comes in chapter V, the first doorway truncation is more than enough for the energy shift and widths calculations.

In chapter IV the parameters related to the forces are determined using Yamaguchi form factors. This information is extracted from the phase shifts for the S_{11} and P_{33} channels. In the S_{31} channel case there is a problem with the curvature of the phase shift, and instead information from the energy shift of pionic hydrogen is used. In this way a proper behaviour of the very low energy limit is guaranteed. After that, a plot of the phase shifts for the S_{31} channel is made and we

find that the fit is essentially good up to 50 MeV. The rest of the p-wave channels is not taken into account under the argument of the Δ- isobar dominance. In the case of pionic hydrogen the importance of the Coulomb interaction in the rescattering process is demonstrated.

Once these parameters were determined in a reliable way, the consideration of the $\Delta(A-1)$, $N^*(A-1)$, $\Delta^*(A-1)$ model is done in chapter V. There a static resonance model for s-wave pion-nucleus interaction, already developed in chapter IV, is used to enrich the $\Delta(A-1)$ model for the description of pion-nucleus dynamics. Effects like Pauli-blocking, nucleon binding, nucleon recoil and finite range interactions are considered in detail for the non-relativistic case. In this chapter the way in which an optical potential can be constructed within the Doorway State formalism is just outlined and the nonlocal character of the effective interaction is shown explicitly. The energy shift can be calculated, without going into the calculation of the optical potential first, using the same procedure. In this way we can compare with the experimental data using the energy shifts and go more into the detail of the physical effects by studying the optical potential. Nevertheless, the first doorway truncation of the energy shift is going to provide detailed information about different physical effects without considering the structure of the optical potential, which is the object of future work. In the first doorway expectation value the contribution of effects like Pauli-blocking and Coulomb contributions to the

rescattering and spreading potentials is summed up linearly, making the interpretation easier. One new feature of our optical potential is a "spreading potential" for the s-wave interaction. The "strengths" of this potential were fitted to the energy shifts and widths of ^{4}He and ^{16}O and the recalculated quantities agree very well with the experimental ones when conditions on the signs of the imaginary parts are imposed in order to make the potential consistent with the absorption process. Up to date fittings of a similar kind in ^{4}He were not able to reproduce the energy shift and width for ^{4}He and even less to achieve the same with ^{16}O in a consistent way.

CHAPTER I

LOW ENERGY PION-NUCLEUS INTERACTIONS: PIONIC ATOM STUDIES

After a brief description of the essential physics and quantities to be measured in pionic atoms, a detailed discussion of pion-nucleus semiphenomenological optical potentials will follow including effects like nucleon binding, Pauli-blocking effect, Lorentz - Lorenz and absorption. Special attention is going to be paid to the absorption effects. At the end of the chapter agreement with experimental data is going to be considered.

(1) General features of pionic atoms:

A pionic atom is formed when a low energy negative pion is captured in a Bohr orbit. This initial orbit is not exactly known and an analysis of X-ray intensities observed during the cascade to lower levels indicate that the main quantum number should be a very high one, i.e., $n \gtrsim 20$. During this cascade process Auger electrons are emitted as well and it ends with pion absorption followed by the ejection of nucleons. The emission of nucleons is not a surprise since the absorbed pion provides an enormous amount of energy, its rest mass around 139.6 MeV. For orbits with main quantum numbers $n < (M_\pi/Me)^{\frac{1}{2}}$, where Me is the electron

mass, the pion moves inside the electronic cloud and a pionic atom can be considered a hydrogen -like system as a very good approximation, transforming a many body problem into a simple two body problem. With this system, the electromagnetic properties of the pion-nucleus interaction can be tested. These are the Coulomb potential, vacuum polarization, electronic screening and electromagnetic polarization of the nucleus and the pion. The main interest lies on strong interaction studies and because of the short range of the pion-nucleon forces (around $\sim$ 1fm), this effect can only be seen when the overlap of the pion wavefunction is appreciable in the nuclear region. Unfortunatley, when this overlap is big the pion absorption is enhanced and for very heavy systems, the very internal levels (like the 1S or 2p) can not be seen. The experimental observed quantities are transition X-ray energies and in strong interactions studies the interesting quantities are the "energy shift" and the hadronic width. The energy shifts are defined experimentally as the energy difference for a X-ray transition between the situation where the strong interaction is taken into account fully and the situation where there is total absence of it, i.e., only electromagnetic effects counts. The X-ray lines typically measured are those related with transitions between circular orbits.

From the theoretical point of view the electromagnetic contribution is very well known and be calculated fully. Since the actual energy shift from the upper level is several orders of magnitude less than the energy shift from the lower level, the energy difference can be taken directly as the energy shift (due to strong interaction effects) of the latter. The hadronic width can be obtained by considering a line broadening problem with the same line of reasoning as the one used for the energy shifts. Of course, the energy shifts and widths are not the only available information which can be obtained from pionic atoms. In chapter II X-ray line attenuation is going to be considered to obtain information about the "hidden" levels that can be seen due to pion absorption (see chapter II for details). In most of the pionic atom studies found in the literature, the ground state of nucleus has spin zero. In the case of non-zero spin, the observation of a splitting is also possible. So, in this way we can see a wide variety of phenomena to be studied, which contain valuable information about strong interactions, nuclear structure and atomic phenomena. In the next chapter we are going to consider the essential tool in pion-nucleus interaction studies: the phenomenological optical potentials.

(2) Optical potential phenomenology for pionic atoms:

The repeated scattering of a pion by several nucleons in a nucleus can best be treated in terms of an optical potential and its iteration by the Schroedinger equation. The use of the latter is possible due to the non-relativistic character of the pionic atom problem. In one of the first applications of Watson's multiple scattering theory, Kisslinger[1] in 1955 found the general form of the pion-nucleus coordinate-space optical potential produced by the strong P-wave of the pion nucleon amplitude. Adding the S-wave term, this on-shell amplitude has the form:

$$\langle \vec{k}_o' | t_{\pi N} | \vec{k}_o \rangle = t_s(k_o) + t_p(k_o) k_o^2 \cos\theta_{\vec{k}_o', \vec{k}_o} \qquad \text{(I-1)}$$

and the off-shell amplitude is given by

$$\langle \vec{k}' | t_{\pi N}[E(k_o)] | \vec{k} \rangle = t_s(k_o) + t_p(k_o)\, \vec{k}' \cdot \vec{k} \qquad \text{(I-2)}$$

where $\vec{k}$ is the pion-nucleon relative momentum. From multiscattering theory the lowest order for the optical potential can be obtained through[2]

$$\langle \vec{p}_\pi' | U_{\pi A}^{(1)} | \vec{p}_\pi \rangle = \sum_{i=1}^{A} \int \frac{d\vec{p}_N}{(2\pi)^3} \frac{d\vec{p}_N'}{(2\pi)^3} \phi_i^*(\vec{p}_N') \langle \vec{p}_N', \vec{p}_\pi' | t_{\pi N} | \vec{p}_N, \vec{p}_\pi \rangle \phi_i(\vec{p}_N) \qquad \text{(I-3)}$$

where i stands for the occupied single particle states for nucleons. After a double Fourier transform, the optical potential given by equation (I-3) gives the velocity-dependent pion-nucleus potential: (neglecting recoil)

$$\langle \vec{r}' | U_{\pi A}^{(1)} | \vec{r} \rangle = \delta(\vec{r}-\vec{r}')\, t_s(k_0)\rho(\vec{r}) - t_p(k_0)\vec{\nabla}\cdot\left[\rho(\vec{r})\vec{\nabla}\delta(\vec{r}-\vec{r}')\right] \quad \text{(I-4)}$$

in equation (I-4) we are not making any distinction between protons and neutrons. An expression of the same form of the one given by equation (I-4) can be found for systems with the same number of protons and neutrons and the quantities t_s and t_p should be replaced by the proper ones according to the isospin differences. Potentials of the form given by equation (I-4) fail badly when they are confronted with low energy data. As an improvement, Ericson et al[3] propose a density expansion for these potentials and the isospin differences were also taken into account for the S-wave pion-nucleon contribution:

$$U_{\pi A}^{(s)}(r) = -\frac{4\pi}{2\mu_R}\left\{b_0\rho(r) + b_1\left(\rho_n(r)-\rho_p(r)\right) + B_0\rho^2(r)\right\} \quad \text{(I-5)}$$

where:

$$\mu_R = \frac{M_\pi M_A}{M_\pi + M_A} \quad \text{(I-6)}$$

is the pion-nucleus reduced mass. The coefficients b_0 and b_1 can be found through a spin, isospin and Fermi average for the pion-nucleon free space scattering matrix in the low density limit. The justification for this procedure comes from a theorem in nuclear matter for a density expansion of the pion-nucleus optical potential[4]. The results for the spin-isospin average are:

$$b_0 = \frac{1}{2}\left(a_{\pi^- n} + a_{\pi^- p}\right) = \frac{1}{3}\left(a_{11}^S + 2a_{31}^S\right) \quad \text{(I-7)}$$

$$b_1 = \frac{1}{2}\left(a_{\pi^- n} - a_{\pi^- p}\right) = \frac{1}{3}\left(a_{31}^S - a_{11}^S\right) \quad \text{(I-8)}$$

where $a_{\pi^- n}$ and $a_{\pi^- p}$ are respectively the pion-proton and pion-neutron scattering lengths and a_{11}^S and a_{31}^S are the scattering lengths for the S_{11} and S_{31} channels. The constant coefficient B_0 is complex and contains in principle medium corrections and pion absorption effects and its determination is possible through experiments. The isoscalar term nearly cancels and it has to be corrected taking into account the Pauli

principle:

$$b_o' = b_o - \frac{(a_{11}^s)^2 + 2(a_{31}^s)^2}{3} \langle r^{-1} \rangle_F \qquad \text{(I-9)}$$

where

$$\langle r^{-1} \rangle_F = \frac{2}{\pi} p_F \qquad \text{(I-10)}$$

this correction can be shown in a very simple way using the medium corrected T-matrix, given by

$$T = t + t\,(G_m - G_o)\,T \qquad \text{(I-11)}$$

where G_m is the pion and nucleon propagator in the medium, G_o is the propagator for the same particles in free space and the t-matrix is also given for the free space situation. The expressions for the propagators in nuclear matter are given by[4,5]

$$\langle \vec{p}\,\vec{k} \,|\, G_p^{(+)}(E) \,|\, \vec{p}\,\vec{k} \rangle = \frac{\theta(p - p_F)}{E^+ - \omega_k - \frac{p^2}{2M_N} - M_N} \qquad \text{(I-12)}$$

$$\langle \vec{p}\vec{k} \mid G_o^{(+)}(E) \mid \vec{p}\vec{k} \rangle = \frac{1}{E^+ - \omega_k - \frac{p^2}{2M_N} - M_N} \qquad \text{(I-13)}$$

where equation (I-12) takes into account the Pauli-Blocking effect and equation (I-13) gives the propagator in free space and only forward scattering is considered. The quantity p_F is the Fermi momentum and

$$\omega_k \equiv \sqrt{k^2 + M_\pi^2} \qquad \text{(I-14)}$$

gives the pion energy. At the lowest order we can write:

$$\delta t^{(1)} = t\,(G_m - G_o)\,t \qquad \text{(I-15)}$$

in the pionic atom problem we are interested in the threshold limit:

$$\lim_{E^+ \to M_\pi + M_N} \langle \vec{p}'\vec{k}' \mid t_{\pi N} \mid \vec{p}\vec{k} \rangle = -\frac{4\pi}{2\mu}\, a \qquad \text{(I-16)}$$

and then:

$$\lim_{E^+ \to M_\pi + M_N} \delta t^{(1)} \longrightarrow -\left(\frac{4\pi}{2\mu}\right)^2 a^2 \lim_{E^+ \to M_\pi + M_N} \int \frac{d\vec{p}}{(2\pi)^3} \; \frac{\theta(p_F - p)}{E^+ - \omega_p - \frac{p^2}{2M_N} - M_N}$$

$$\longrightarrow \left(\frac{4\pi}{2\mu}\right)^2 a^2 \, \frac{2\mu}{(2\pi)^3} \int \frac{d\vec{p}}{p^2}\, \theta(p_F - p)$$

$$= \frac{4\,a^2}{\mu}\, p_F \qquad \text{(I-17)}$$

and using equation (I-16), we obtain:

$$\delta t = -\frac{2\pi}{\mu}\,\delta a \qquad \text{(I-18)}$$

leading to the result:

$$\frac{\delta a}{a} = -\frac{2}{\pi}\, a\, p_F \qquad \text{(I-19)}$$

and then:

$$\delta b_0 = \delta\left(\frac{a_{11}^S + 2a_{31}^S}{3}\right) = -\frac{(a_{11}^S)^2 + 2(a_{31}^S)^2}{3}\,\frac{2}{\pi}\, p_F \qquad \text{(I-20)}$$

since the nuclear radius is small compared with the Bohr radius, quantities like $\Delta\mathcal{E}_{1S}$ and Γ_{1S} are mainly determined by $U_{\pi A}^{(S)}$. In reference (5) the values of b_0' and b_1 are kept fixed and $\mathcal{B}_0$ is determined. Except for the very light nuclei the fit is good for values:

$$\mathrm{Re}\,\mathcal{B}_0 \,/\, \mathrm{Im}\,\mathcal{B}_0 = -1.0 \pm 0.1 \qquad \text{(I-21)}$$

$$\mathrm{Im}\, B_0 = 0.042\, M_\pi^{-4} \tag{I-22}$$

The nucleon binding effect can be estimated also by looking into the nuclear matter problem. The pion and nucleon propagator, when the latter is bound, is given by

$$\langle \vec{p}\,\vec{k} | G_B^{(+)}(E) | \vec{p}\,\vec{k} \rangle = \frac{1}{E^+ - \omega_k - \frac{p^2}{2M_N} - U(p) - M_N} \tag{I-23}$$

At threshold, we can obtain for the lowest order of δt :

$$\lim_{E^+ \to M_\pi + M_N} \delta t^{(1)} = \left(\frac{4\pi a}{2\mu}\right)^2 \int \frac{d\vec{p}}{(2\pi)^3} \left\{ \frac{1}{E^+ - \omega_p - \frac{p^2}{2M_N} - M_N - U(p)} - \frac{1}{E^+ - \omega_p - \frac{p^2}{2M_N} - M_N} \right\} \tag{I-24}$$

if the potential is taken as:

$$U(p) = U_0\, \theta\,(p_F - p) \tag{I-25}$$

where U_0 = - 50 MeV, from equation (I-24) the following can be obtained:

$$\delta t^{(1)} = \frac{4a^2}{\mu}\sqrt{2\mu|U_0|}\ \text{arc tg}\ \frac{p_F}{\sqrt{2\mu|U_0|}} \qquad \text{(I-26)}$$

and then expanding equation (I-26) in $\sqrt{2\mu|U_0|}/p_F$ powers and keeping the lowest order of

$$\delta t^{(1)} = \frac{2\pi a^2}{\mu}\sqrt{2\mu|U_0|} - \frac{8a^2|U_0|}{p_F} + \mathcal{O}\left[\frac{\sqrt{2\mu|U_0|}}{p_F}\right]^3 \qquad \text{(I-27)}$$

the following correction can be found:

$$\frac{\delta a}{a} = -a\sqrt{2\mu|U_0|} \qquad \text{(I-28)}$$

and

$$\delta b_0 = \delta\left(\frac{a_{11}^S + 2a_{31}^S}{3}\right) = -\frac{(a_{11}^S)^2 + 2(a_{31}^S)^2}{3}\sqrt{2\mu|U_0|} \qquad \text{(I-29)}$$

The general prescription to improve the potential given by these corrections is the use of the local density approximation[4]

$$p_F \to p_F\left[\frac{\rho(r)}{\rho(0)}\right]^{1/3} \qquad U_0 \to U_0\ \frac{\rho(r)}{\rho(0)} \qquad \text{(I-30)}$$

where $\rho(0)$ is the nuclear matter density. The total contribution from the pion-nucleon S-wave is given by

$$U_{\pi A}^{(S)}(r) = -\frac{4\pi}{2\mu_R}\left\{ b_0 \rho(r) + b_1 (\rho_n(r) - \rho_p(r)) + B_0 \rho^2(r) \right.$$

$$\left. - \frac{(a_{11}^S)^2 + 2(a_{31}^S)^2}{3}\left[\frac{2}{\pi} p_F \left(\frac{\rho(r)}{\rho(0)}\right)^{4/3} + \sqrt{2\mu |U_0|}\left(\frac{\rho(r)}{\rho(0)}\right)^{3/2}\right]\right\} \quad \text{(I-31)}$$

The analog of equation (I-5) for the p-wave pion-nuclear contribution is given by

$$U_{\pi A}^{(p)}(\vec{r},\vec{r}') = \frac{4\pi}{2\mu_R}\vec{\nabla}\cdot\left[\alpha(r)\vec{\nabla}\delta(\vec{r}-\vec{r}')\right] \quad \text{(I-32)}$$

where

$$\alpha(\vec{r}) \equiv c_0 \rho(r) + c_1(\rho_n(r) - \rho_p(r)) + C_0' \rho^2(r) \quad \text{(I-33)}$$

and the quantities c_0 and c_1 are the isoscalar and isovector averages of the p-wave pion-nuclear scattering volumes:

$$c_0 \equiv \frac{1}{3}\left[4a_{33}^P + 2a_{31}^P + 2a_{13}^P + a_{11}^P\right] \quad \text{(I-34)}$$

$$c_1 \equiv \frac{1}{3}\left[(2a_{33}^P + a_{31}^P) - (2a_{13}^P + a_{11}^P)\right] \quad \text{(I-35)}$$

the constant C_o is complex and takes into account the medium corrections and pion absorption. There are also short-range correlation corrections[3] that could be expressed in a manner very similar to the Lorentz - Lorenz effect for the dielectric constant of a crystal. The pion provides a pseudoscalar field ϕ and its gradient $\vec{\nabla}\phi$ gives a vector field coupled to the nucleon according to

$$\mathcal{H}_v = -i \frac{g_{\pi NN}}{2M_\pi} \vec{\sigma} \cdot \vec{\nabla}\phi \qquad \text{(I-36)}$$

where $\vec{\sigma}$ is the nucleonic spin and $g_{\pi NN}$ is the strong interaction coupling constant. The form of the coupling described by equation (I-36) has the same form as the coupling between a dipole and a field and it tends to orient the nucleonic spin in the direction of $\vec{\nabla}\phi$. Due to the Pauli principle a nucleon in a nucleus cannot rotate its spin freely, but if a pion field is applied to a nucleus an induced axial dipole appears. Accordingly to the linear response theory the polarization vector density is proportional to the applied field and the proportionality function is the axial polarizability coefficient per unit volume:

$$\vec{P}(\vec{r}) = \chi(\vec{r})\, \vec{\nabla}\phi(\vec{r}) \qquad \text{(I-37)}$$

with

$$\chi(\vec{r}) = \gamma \rho(\vec{r}) \qquad \text{(I-38)}$$

where γ is the polarizability constant and $\rho(\vec{r})$ is the density of the medium. Actually the axial polarizability $\chi(\vec{r})$ is proportional to $\alpha(\vec{r})$, where higher order terms of the density should be considered, but in order to simplify our derivation the lowest order term proportional to the density is the only one kept in equation (I-38). Taking into account just the pion-nucleus p-wave in the equation of motion for the pion in configuration space, we have:

$$\left(\omega^2 - M_\pi^2 + \nabla^2 - \gamma \vec{\nabla}\cdot\rho(\vec{r})\,\vec{\nabla}\right)\phi(\vec{r}) = 0 \qquad \text{(I-39)}$$

and it can be written as:

$$\vec{\nabla}\cdot\left[\left(1 - \gamma\rho(\vec{r})\right)\vec{\nabla}\phi(\vec{r})\right] = -\left(\omega^2 - M_\pi^2\right)\phi(\vec{r}) \qquad \text{(I-40)}$$

There is a repulsion effect due to Pauli principle between the nucleon and other nucleons, so a volume around the nucleon is cleared of nuclear matter. The normal component of $(1-\gamma\rho(\vec{r}))\,\vec{\nabla}\phi(\vec{r})$ must be continuous across the boundary of this volume and it can

be seen using familiar arguments from electromagnetic theory. Then, we can write:

$$(1-\gamma\rho(\vec{r}))\left[\vec{\nabla}\phi(\vec{r})_{\perp}\right]_{\substack{\text{OUTSIDE THE}\\ \text{VOLUME}}} = \left[\vec{\nabla}\phi(\vec{r})_{\perp}\right]_{\substack{\text{INSIDE THE}\\ \text{VOLUME}}} \qquad \text{(I-41)}$$

If the volume is a spherical one and the angle average is properly taken, we obtain:

$$\left[\vec{\nabla}\phi(\vec{r})\right]_{\text{INSIDE}} = \left[\vec{\nabla}\phi(\vec{r})\right]_{\text{OUTSIDE}} - \frac{4\pi}{3}\gamma\rho(\vec{r})\left[\vec{\nabla}\phi(\vec{r})\right]_{\text{INSIDE}} \qquad \text{(I-42)}$$

and

$$\left[\vec{\nabla}\phi(\vec{r})\right]_{\text{INSIDE}} = \frac{1}{1+\frac{4\pi}{3}\gamma\rho(\vec{r})}\,\vec{\nabla}\phi(\vec{r}) \qquad \text{(I-43)}$$

with the association:

$$\left[\vec{\nabla}\phi(\vec{r})\right]_{\text{OUTSIDE}} = \vec{\nabla}\phi(\vec{r}) \qquad \text{(I-44)}$$

being $\vec{\nabla}\phi(\vec{r})$ the average field of the medium. Then, the corrected pion-nucleus p -wave contribution to the optical potential has the form:

$$U_{\pi A}^{(p)} \phi(\vec{r}) = \gamma \vec{\nabla} \cdot \frac{\rho(\vec{r})}{1 + \frac{4\pi}{3} \xi \gamma \rho(\vec{r})} \vec{\nabla} \phi(\vec{r}) \qquad \text{(I-45)}$$

Equation (I-45) gives the corrected version originally derived by Ericson and Ericson[3] using similar arguments to the ones outlined in this section. From a multiple scattering approach, Eisenberg, Hufner and Moniz[6] were able to obtain the same result. The difference is a new constant ξ given by:

$$\xi \equiv -\int d\vec{x}\, g(x) \int \frac{d\vec{t}}{(2\pi)^3} e^{i \vec{t} \cdot \vec{x}}\, h^2(t^2) \qquad \text{(I-46)}$$

and in reference (3) the value is $\xi = 1$. The function $h(t^2)$ is the pion-nucleon form factor and $g(x)$ is the nucleon-nucleon correlation function. If the following forms are taken:

$$g(x) = -\theta(r_c - x) \qquad \text{(I-47)}$$

and

$$h(k^2) = \frac{1}{1 + \frac{k^2}{\alpha^2}} \qquad \text{(I-48)}$$

If $r_c = 0.5$ fm and $\alpha = 6$ fm^{-1} the constant is evaluated to give $\xi = 0.5$, showing that the pionic Lorentz - Lorenz effect or Ericson - Ericson - Lorentz-Lorenz (EELL) effect is greatly reduced by finite size effects. The fits to the data for the p -wave contribution to the optical potential are performed with the following two conditions:

$U_{\pi A}^{(s)}$ is not varied and $Re\, C_0 = 0$. Then the coefficients C_0, C_1 and $Im\, C_0$ are determined for several values of the parameter ξ, with $0 \leq \xi \leq 1$. Table (I-I) summarizes the result for these parameters and show a strong dependence of $Im\, C_0$. The analyses are not very sensitive to ξ but consistent with $\xi = 1$; however the variety of assumptions eliminate the possibility of microscopic interpretation. The fits are always poor when these potentials are confronted with light nuclei data. This is particularly noticeable for 1S level shift in the ^{3}He case. This will be examined in the next section.

(3) Isotope effects in light pionic atoms

One of the features of the experimental data that can give us direct evidence of non-local pion-nucleus interactions is the change of sign observed when a comparsion is made between 1S level and 2p level shifts. In the 2p level case a change of sign is expected for

TABLE (I-I)

Parameters of the Kisslinger potential from a fit to experimental data of pionic atoms.

	FIT[$\xi=0$]	FIT[$\xi=1$]	Scattering volume averages
$C_0\ (M_\pi^{-3})$	0.17	0.23	0.21
$C_1\ (M_\pi^{-3})$	0.22	0.22	0.19
$Im\ C_0\ (M_\pi^{-6})$	0.036	0.076	

TABLE (I-II) [10]

Energy Shifts and widths of Helium Isotopes

ISOTOPE	ENERGY SHIFT (eV)	WIDTH (eV)
^3He	32±3	28±7
^4He	-75.7±2	45±3
Isotopic Effect ($^4He - ^3He$)	107.7±3.6	17±8

$Z \gtrsim 36$, since the p -wave contributions becomes more important for sufficiently large nuclei. The change of sign is difficult to see due to pion absorption. Using the "trick" explained in Chapter II for ^{110}Pd, Leon et al[8] were able to confirm this theoretical expectation. In the $2p$ level case, the change sign is essentially due to the increase in the size of the system. For $1S$ level a change of sign problem is also reported, although the nature of the problem seems to be different. While all the $1S$ level shifts are repulsive, the level for ^3He is attractive in an anomalous way[9,10]. Although the experiment is complicated, there is a strong confirmation about the sign of this shift. In table (I-II) the experimental values of the recent reference (10) are given. The results for ^3He alone are given in table (I-III). Although the experimental results shown in this table are not very consistent, the isotope effect is still large. In reference (9) the pion-nucleus optical potential is used to calculate the $1S$ level energy shift for comparison with the experimental value. All the established parameters[5,7] are used with the exception of b_o and C_o. In the b_o parameter case the argument is that a strong dependence on the atomic number is expected for this parameter of the isoscalar local

potential. The complete set of parameters used in this calculation is shown in table (I-IV). The calculated energy shift and widths are

$$\Delta\mathcal{E}_{1S} = 30.5\ eV \qquad \Gamma_{1S} = 38.6\ eV \qquad (I\text{-}49)$$

where $C_0 = 0$, as indicated in table (I-IV). According to reference (9) if the pion-nucleon absorption term contribution is included the 1S level reduces the width by 24eV whereas from the physics point of view no dramatic influence of the p -wave potential should be expected on the pionic S -states. The authors claim that the standard optical potential produces the unphysical negative p -wave absorption effect on the S -state and then their experiment suggests that the simplification of including the absorptive p -wave potential part in the gradient structure is not correct for light nuclei and that another form of absorption on the surface may be more appropriate for the p -wave interaction.

In the ^4He case the calculations of the energy shift and width also show problems. The results are presented in table (I-V) Although the order of magnitude is the correct one, it is clear that the shifts and widths calculated with optical potentials are not in good agreement with the experimental value. The stand-

TABLE (I-III)

Energy Shifts and widths of ^{3}He (1S level)

ENERGY SHIFT(eV)	WIDTH (eV)	REFERENCE
50 ± 18	89 ± 67	(11)
44 ± 5	42 ± 14	(12)
27 ± 5	65 ± 12	(9)
32 ± 3	28 ± 7	(10)

TABLE (I - IV)

Parameter set used in reference (9)

$b_0 = -0.015\ m_\pi^{-1}$ $\quad b_1 = -0.09\ m_\pi^{-1}$

$c_0 = 0.21\ m_\pi^{-3}$ $\quad c_1 = 0.18\ m_\pi^{-3}$

$B_0 = i\ 0.04\ m_\pi^{-4}$ $\quad C_0 = 0$

R_{RMS} (^{3}He) = 1.88fm

ard parameter set (not shown in the table) yields a shift which is too large if a harmonic well distribution for the density with r_{RMS} = (1.63 ± 0.03) fm is used. When the r_{RMS} is changed in 1%, the energy changes by 0.3eV and the width by 5%. Treating the isoscalar parameter as an effective quantity, b_0^{eff}, the result is[14]

$$b_0^{eff} = (-0.0235 \pm 0.0008)\, M_\pi^{-1} \qquad \text{(I-50)}$$

as the best fit in table (I-V), making $Re\, B_0 = 0$. Although the energy shift is adjusted to the right value, the width is far off from the experimental value. This problem joins the ^{3}He case to show the inadequacy of the absorption term in standard optical potentials.

In the table (I-VI) the experimental results for the oxygen case are shown. We can see that the isotope effect is roughly given by 25% and it is a large one. Using standard optical potentials there are no reported problems in regards to the widths.

(4) Anomalous energy shifts and widths in pionic atoms

Recently shifts and widths have been measured for $3d$ states in nuclei of considerably higher Z than earlier and have been found to be several times smaller

TABLE (I-V)[14]

Calculated Energy Shifts and Widths for ^4He (1S level)

	SHIFT(eV)	WIDTH(eV)
Experimental value[14]	-75.7±2.0	45±3
According to Deser et al.[15] and Brueckner:[16]		
with parameters of ref. (25)	- 75±10	40
with parameters of ref. (26)	- 56 ±4	40
Calculated by Koltun and Reiten[17]		64
Optical Potential Calcultions		
with $b_0^{eff} = -0.029\,M_\pi^{-1}$	- 91	62
with $b_0^{eff} = -0.023\,M_\pi^{-1}$	- 75	65
with $b_0^{eff} = -0.018\,M_\pi^{-1}$	- 61	68

TABLE (I-VI)

Experimental results for Oxygen (1S level)

ISOTOPE	ENERGY SHIFT (eV)	WIDTH (eV)
16_0	-15.43± 0.10 [14]	7.92 ± 0.32 [14]
	-15.73± 0.26 [18]	7.56 ± 0.50 [18]
18_0	-19.92± 0.26	6.33 ± 0.43
	-20.59± 0.26	8.67 ± 0.70
Isotope Effect (18_0 - 16_0)	-4.49 ± 0.14 [14]	-1.59 ± 0.53 [14]
	-4.86 ± 0.37 [18]	+1.11 ± 0.09 [18]

than expected [19]. This tendency was pointed out earlier by Ericson and Krell [13]. Ericson and Tauscher [20] give general indications of the possible origin of the effect:

(a) The origin of the anomaly should be in the local part of the potential, since the heviest 3d states are affected while the 4f states behave normally and it is strongly dominated by the velocity-dependent term.

(b) The anomalous nuclei have strong Coulomb binding of the pion (high Z number) and then electromagnetic binding effects on the strong interactions may be responsible.

(c) The isoscalar scattering length is accidentally small and the local interaction term of the potential is dominated by double-scattering contributions from the Pauli-blocking effect. Any other effect that would prevent the cancellations from being so accurate might hence give large contributions, and must be considered in a careful way.

Ericson and Tauscher[20] propose that the energy dependence of the S-wave pion-nucleon amplitude is mainly responsible for the anomaly since it gives rise to an energy-dependent potential. Another contribution is the gauge condition, i.e., everywhere in the equations momenta p_μ should be replaced by $(p_\mu - e A_\mu)$ in terms of the vector potential A_μ. In the case of

an external Coulomb potential $V_c(r)$ we should everywhere replace the pion energy ω by $[\ \omega - V_c(r)\ ]$ including the potential. This generates an additional potential from the energy dependence of the strong - interaction potential[20]

$$\delta V = -V_c(r)\frac{dV}{d\omega} \simeq 4\pi V_c(r)\left(1+\frac{M_\pi}{M_N}\right)\beta^{(+)}\rho(r) \qquad \text{(I-51)}$$

since $dV/d\omega$ is given by

$$\frac{dV}{d\omega} = -4\pi\left(1+\frac{M_\pi}{M_N}\right)\beta^{(+)}\rho(r) \qquad \text{(I-52)}$$

where $\beta^{(+)}$ can be found through the following expansion for the energy shift:

$$(k_\pi \delta_{L=0}/k)^{(+)} = a^{(+)} + \beta^{(+)}k^2 + \cdots \qquad \text{(I-53)}$$

and $k^2 = \omega^2 - M_\pi^2$. The range of the potential given by equation (I-51) is the nuclear range. If the energy dependence of S -wave pion-nucleon amplitude is attributed to a non-local interaction, to leading order and with a non-locality of short range

$$2\mu V = -4\pi\left(1+\frac{M_\pi}{M_N}\right)\left\{a^{(+)}\rho(r) + \frac{1}{2}\beta^{(+)}\left[\nabla^2\rho(r) + \rho(r)\nabla^2\right]\right\} \qquad \text{(I-54)}$$

The Coulomb field can be generated by using the Laplacion term of pion wavefunction in the Klein-Gordon equation and it is the same as equation (I-51). At this point we may wonder if the new Coulomb contribution to the potential or a non-local character of the interaction are responsible for the results claimed in reference (20). With a standard optical potential with an additional isospin term of the form

$$c_1 (\rho_n + \rho_p)(\rho_n - \rho_p)$$

and the above mentioned Coulomb term, there is good agreement with the energy shift experimental data.[20] With the widths the anomaly persists and Ericson and Tauscher[20] were not able to provide a suggestion about the problem. According to Seki[21] the extra Z (atomic number) dependence of this potential is not a real one, since it is buried in the pion wavefunction through the Klein-Gordon equation as it is also stated in the non-locality discussion around equation (I-54). This result can be written as

$$2\mu V = -4\pi\left(1+\frac{M_\pi}{M_N}\right)\left\{a^{(+)}\rho(r)+\beta^{(+)}\vec{\nabla}\cdot\rho(r)\vec{\nabla}+\frac{1}{2}\beta^{(+)}\nabla^2\rho(r)\right\} \qquad \text{(I-55)}$$

and the third term of equation (I-55) has the same form as the so-called angular transformation terms.

This angular transformation terms arise when nucleon recoil is taken into account in pion-nucleon relativistic problems.[22] Working with the same problem in a non-relativistic approach (adequate for pionic atoms), the result is the same, i.e., the Laplacion term of the density appears. The coefficient of the $\nabla^2\rho(r)$ term is given by

$$-\left(1+\frac{M_\pi}{M_N}\right)\frac{\beta^{(+)}}{2} = -0.020\, M_\pi^{-3} \qquad \text{(I-56)}$$

in the non-locality approach to the problem, while the angular transformation coefficient has a somewhat smaller magnitude, given by

$$\frac{\mu_R}{\left(1+\frac{M_\pi}{M_N}\right)} C_o = -0.013\, M_\pi^{-3} \qquad \text{(I-57)}$$

where C_o is the isoscalar velocity-dependent p-wave potential parameter and μ_R is the pion reduced mass. In equation (I-56) the Pauli-blocking corrected $\beta^{(+)}$ was taken. Based on the same order of magnitude shown in equations (I-56) and (I-57), Seki[21] considered the angular transformation studies for pionic atoms in a previous work[23] and showed that the terms obtained in this way can be replaced by a renormalization of the effective potential parameters. Seki[21] looks into the neutron density distributions and the sensitivity

of the energy shifts and width of ^{209}Bi for the pionic $3d$ level. The results are given in fig (I-I), which is taken from reference (21). The parameter C_n is the neutron radius, C_p is the proton radius and t is the nuclear diffuseness. Although it is possible to obtain the appropriate shift around $C_n \sim 7.0$ fm, there is no practical way to achieve the same thing with the width and then the essential problem of the anomaly remains.

There are more reports about anomalous data[24] in the ^{23}Na case for the 1S width, which joins the Helium cases in the light nuclei group of problems. Seki [21] questions the reliability of the experimental cases and in the ^{23}Na case there is the claim that experimental values have varied by a factor of about 2 in the past. Aside the cases mentioned here, in the next chapter we are going to consider in detail the hidden level problem in ^{110}Pd case and an anomaly related to the width will be found, leading us to the conclusion that the pion-nucleus optical potential requires reexamination. Since the quantities related to the anomalies are the widths, it seems clear that pion absorption is the center of the problem.

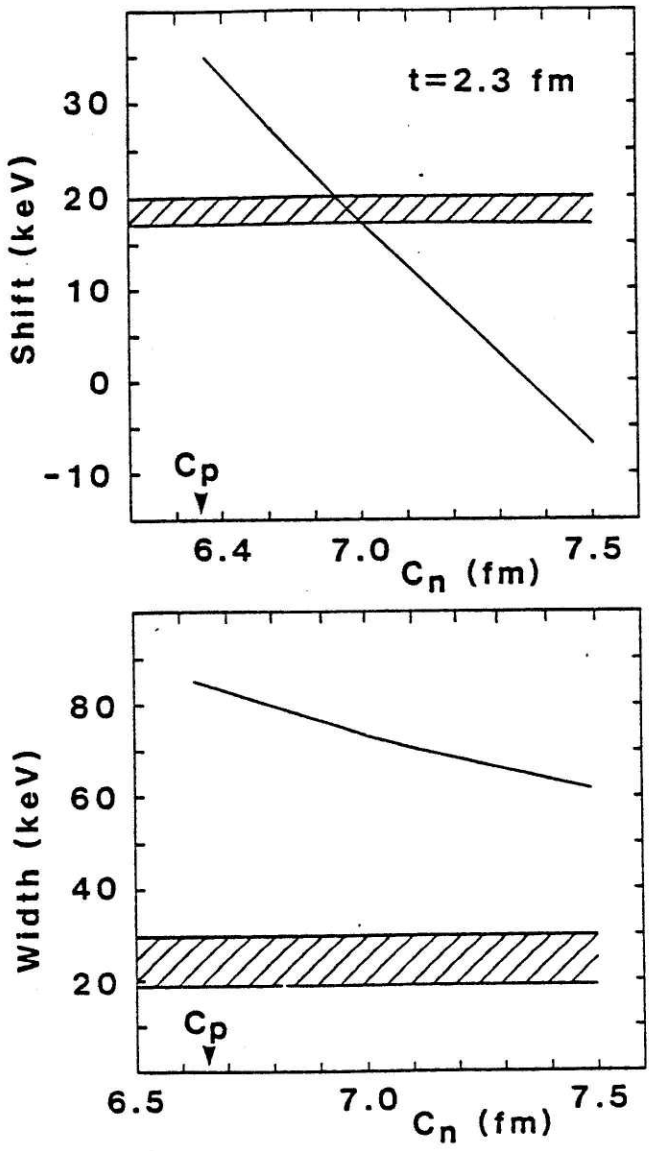
t=2.3 fm
Shift (keV)
30
20
10
0
-10
Cp
6.4
7.0
7.5
Cn (fm)
Width (keV)
80
60
40
20
Cp
6.5
7.0
7.5
Cn (fm)

Fig. (I-1)

REFERENCES FOR CHAPTER I

(1) L.S. Kisslinger, Phys. Rev. vol. 98, p.761, 1955

(2) E.J. Moniz, Nuclear Physics with Heavy Ions and Mesons, vol. 2, p.436, 1977 R. Balin, M. Rho and G. Ripka Eds.

(3) M. Ericson and T.E.O. Ericson, Ann Phys. vol.36, p.323, 1966

(4) J. Hufner, Phys. Reports, vol.21C, 1975

(5) L. Tauscher and W. Schneider, Z. Phys. 271 p. 409, 1974

(6) J.M. Eisenberg, J. Hufner and E.J. Moniz, Phys. Letts., vol. 47B, p.381, 1973

(7) Proc. International Seminar on Pion-nucleus interactions, Strassbourg, France, September 1971, V-1-15 University of Strassbourg

(8) M. Leon, Nucl. Phys., A260, p.461, 1976
M. Leon et al., Phys. Rev. Lett., vol. 37, p. 1135, 1976

(9) G.R. Mason et al., Phys. Lett., vol. 74B, p.179, 1978

(10) I. Schwanner et al., Phys. Lett., vol. 96B, p.268, 1980

(11) B.O. Lapp, Ph.D thesis, The College of William and Mary, VA, USA, 1974

(12) R. Abela et al., Phys. Lett., vol. 68B, p.429, 1977

(13) M. Krell and T.E.O. Ericson, Nucl. Phys. vol.B11, p.521, 1969

(14) G. Backenstoss et al., Nucl. Phys. vol. A232, p.519, 1974

(15) S. Deser et al., Phys. Rev., vol. 96, p.774, 1954

(16) K.A. Brueckner, Phys. Rev., vol. 98, p.769, 1955

(17) D.S. Koltun and A. Reitan, Nucl. Phys., vol. B4, p. 629, 1968

(18) G. Backentoss et al., Phys. Lett., vol. 25B, p.365, 1967

(19) C.J. Batty et al., Nucl. Phys., vol. A355, p.383, 1981

(20) T.E.O. Ericson and L. Tauscher, Phys. Lett., vol. 112B, p. 425, 1982

(21) R. Seki, Phys. Rev. C, vol. 26, p.1342, 1982
R. Seki, Phys. Rec. C to be published, 1983

(22) A.W. Thomas and R.H. Landau, Phys. Reports, vol. 58, p.121, 1980 (specifically p.172)

(23) R. Seki, M. Oka, K. Masut ni and K. Yazaki, Phys. Lett., vol. 97B, p.200, 1980

R. Seki and K. Masutani, Phys. Rev. vol.C27, p.2799, 1983

R. Seki, K. Masutani and K. Yazaki, Phys. Rev., vol. C27, p.2817, 1983

(24) J. Konijn et al., Nucl. Phys., vol. A326, p.401, 1979

J. Konijn et al., Nucl. Phys., vol. A360, p.187, 1981

(25) V.K. Samaranayake and W.S. Woolcock, Phys. Rev. Lett., vol. 15, p. 936, 1965; Nucl. Phys. vol. B48, p. 205, 1972

(26) D.V. Bugg, A.A. Carter and J.R. Carter, Phys. Lett. vol. 44B, p. 278, 1973

CHAPTER II

COLLECTIVE EXCITATIONS AND THE NUCLEAR POLARIZATION

The failure to explain the discrepancy between the theoretical and experimental widths in pionic atoms for several nuclei lead us to consider two possibilities: either the pion-nucleus optical potential has to be reexamined or particular nuclear structure effects present in the bound pion problem are playing a role. An important effect of this kind is dynamical nuclear polarization, where nuclear collective excitations are taken into account. Recently [1] some studies were performed in several nuclei, considering nuclear excitations above the lowest collective quadrupole mode and all the studied cases except ^{110}Pd were understood. In this chapter the ^{110}Pd case is going to be examined again from the nuclear structure point of view, taking into account collective excitations like vibrations with three surfon (phonon) states and Giant Resonances. All these cases are analyzed in detail leading to negative results, i.e., it seems that nuclear structure effects are not going to provide an explanation for the ^{110}Pd case, leaving the optical potential as the only one possible source of the problem.

(1) Two and Three surfon states and dynamical nuclear polarization in pionic atoms: The ^{110}Pd case.

The main interest upon dynamical nuclear polarization comes as a way to obtain information from "hidden" pionic levels. These levels can not be observed directly in experimental measurements due to pion absorption, which is very strong for low angular momentum pionic states. The presence of this absorption process is what makes them interesting for the pion-nuclear structure and strong interactions. With dynamical nuclear polarization [6] the idea is to find pionic atoms in which a nuclear excitation of appropiate multipolarity is nearly degenerate with a de-excitation of a pionic level and a mixing is produced. In order to clarify these ideas, the ^{110}Pd case can be offered as a convenient example, since it is going to be studied in detail throughout this chapter. The level scheme is depicted in fig. (II-1). There we see that there is a near degeneracy in the energy differences between the nuclear ground state and the first excited state (a $0^+ \longrightarrow 2^+$ transition) and the pionic n=4 and n=3 states. These dynamical polarization effects were studied for the first time in muonic atoms where the relevant interaction to be considered is the very well known electromagnetic force, making the extraction of the quadrupole moments of the excited states a simple task. In the ^{110}Pd case it is this

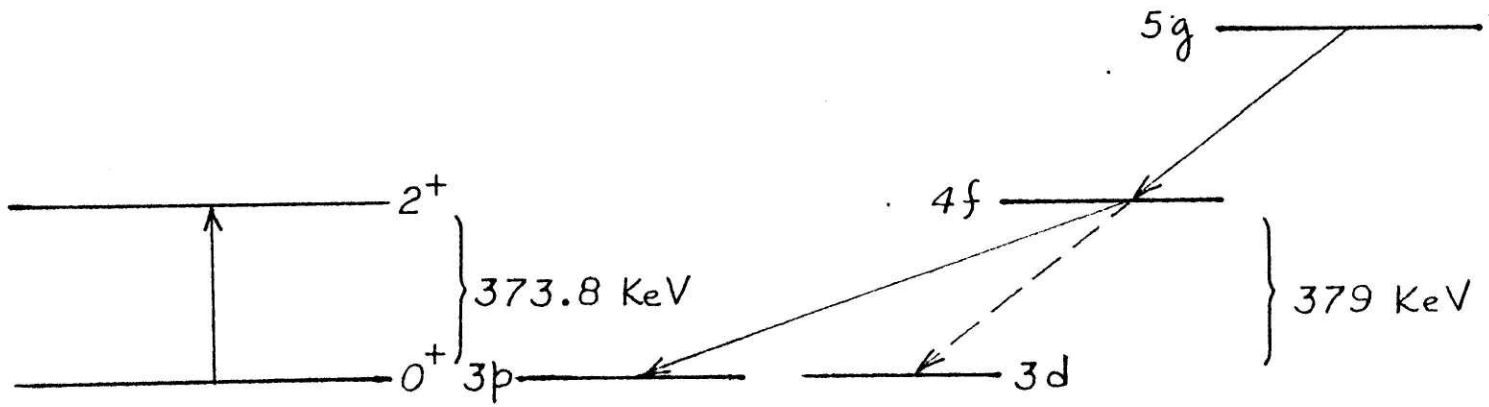

Fig. (II-1)

quadrupole interaction which is going to give us the interesting mixing between the $|0^+; 4f\rangle$ and $|2^+; 3p\rangle$ states, giving the following admixture coefficient:

$$a = \pm \frac{\langle 2^+; 3p | H_Q | 0^+; 4f \rangle}{E(2^+; 3p) - E(0^+; 4f)} \qquad \text{(II-1)}$$

where H_Q is the electric quadrupole interaction between the pion and the nucleus. The pionic 3p level is hidden by the absorption effect. Due to the mixing the induced width for the pionic 4f level is given by

$$\Gamma_{4f}^{ind} \simeq |a|^2 \Gamma_{3p} \qquad \text{(II-2)}$$

and in an approximate way the 3p width is one order of magnitude bigger than the 4f width and if $|a|^2$ is small (say, two orders of magnitude less than unity), the induced width could be comparable to the radiative width of the 4f level and an appreciable attenuation of the 4f $\longrightarrow$ 3d x-ray line should be observed. This transition is represented by a dotted line in fig. (II-1). The experiment is done by comparing the x-ray intensities for ^{108}Pd (which has no degeneracy effect) against those of ^{110}Pd, through the ratio

$$\delta = \frac{R(^{110}Pd)}{R(^{108}Pd)} \qquad \text{(II-3)}$$

where the quantity R is defined as:

$$R(N,Z) \equiv \left[\frac{I\,[(n,\ell) \rightarrow (n-1,\ell-1)]}{I\,[(n+1,\ell+1) \rightarrow (n,\ell)]} \right]_{(N,Z)} \qquad \text{(II-4)}$$

where I represents the x-ray intensity of the pionic transition and (N,Z) are the neutron and proton number of the particular isotope. Translating equation (II-4) to our example, we obtain

$$R(^{110}Pd) = \frac{I\,[4f \rightarrow 3d]}{I\,[5g \rightarrow 4f]} \qquad \text{(II-5)}$$

and a similar expression for $R(^{108}Pd)$. The 5g $\longrightarrow$ 4f x-ray line is not affected by any mixing effect and it is supposed to be equal for both isotopes. The ratio R removes many experimental uncertainties like detector efficiencies, target absorption, etc. Since the isotope ^{108}Pd does not have the degeneracy, the x-ray attenuation given by

$$A \equiv 1 - \delta \qquad \text{(II-6)}$$

is going to be a direct measurement of the induced pion absorption out of the pionic 4f level in ^{110}Pd, and then

$$A = \frac{\Gamma_{ind}}{\Gamma_{tot}} \qquad \text{(II-7)}$$

where the total width of the pionic (n,l) level

is given by

$$\Gamma_{tot} = \Gamma_{\gamma}\left[(n,\ell) \rightarrow (n-1, \ell-1)\right] + \Gamma_{abs}(n,\ell) + \Gamma_{ind} \qquad \text{(II-8)}$$

being Γ_{γ} the width related to the x-ray transition, Γ_{abs} denotes the hadronic width in the absence of dynamical nuclear polarization and Γ_{ind} is the induced width related to the mixing effect and given by equation (II-2). In general this induced width can be rewritten as:

$$\Gamma_{ind} = 2\gamma \left| \frac{\langle I_f, \pi_f | H_Q | I_i, \pi_i \rangle}{\Delta\epsilon - i\gamma} \right|^2 \qquad \text{(II-9)}$$

where $\Delta\epsilon - i\gamma$ is the energy difference between the admixed levels:

$$\Delta\epsilon - i\gamma = \mathcal{E}(I_f, \pi_f) - \mathcal{E}(I_i, \pi_i) \qquad \text{(II-10)}$$

and $I(\pi)$ represents the appropiate nuclear (pionic) state. In the ^{110}Pd case the experiments yield the following values:

$$\delta = 0.811 \pm 0.027 \qquad \text{(II-11)}$$

and then:

$$A = (19.4 \pm 2.8)\,\% \qquad \text{(II-12)}$$

the energy difference is given by

$$\Delta\epsilon = (E_{2+} + E_{3p}) - (E_0 + E_{4f}) \qquad \text{(II-13)}$$

and

$$\gamma = \frac{1}{2}\left(\Gamma_{3p} - \Gamma_{4f}\right) \qquad \text{(II-14)}$$

for a fixed attenuation A, equation (II-9) gives a circular contour in the $(\Delta\epsilon, \gamma)$ plane [7]. The experiment can not specify $\Delta\epsilon$ and γ in a separated way. This circular contour can be seen more clearly if we rewrite equation (II-9) as:

$$(\Delta\epsilon)^2 + \left[\gamma - \xi\left(\frac{1-A}{A}\right)\right]^2 = \left[\xi\left(\frac{1-A}{A}\right)\right]^2 \qquad \text{(II-15)}$$

where

$$\xi \equiv \frac{\left|\langle I_f, \pi_f | H_Q | I_i, \pi_i \rangle\right|^2}{\Gamma_\gamma + \Gamma_{abs}} \qquad \text{(II-16)}$$

With equations (II-15) and (II-16) the plots of fig. (II-2) can be constructed [8]. It is clear from fig. (II-2) that there is a quantitative disagreement with the optical potential prediction, resulting a somewhat larger

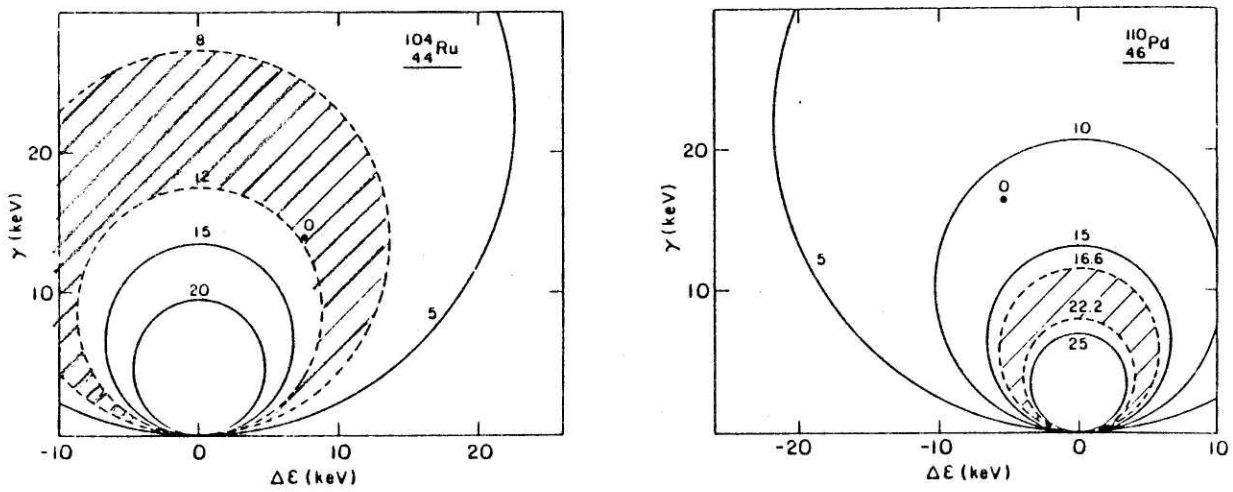

Fig. (II-2) Attenuation contours for ^{104}Ru and ^{110}Pd. The shadowed area represents the experimental measurement and the dot , the predicted value from standard optical potentials.

level shift and a considerably smaller width. This discrepancy needs an explanation. In a second approach to the problem, in addition to the mixing of nuclear and pionic states caused by electromagnetic multipole interactions there is a second mechanism provided by the pion-nucleus interaction. Aside this feature, there is a consideration of nuclear excitations beyond the lowest quadrupole collective mode. This was done first by Dubach, Moniz and Nixon[1]. In the description of these collective states they followed the standard correction which is to mix the one and two quadrupole phonon states. It was possible then to understand cases like ^{48}Ti, ^{104}Ru, ^{112}Cd and ^{150}Sm, but the problem with ^{110}Pd remains. The calculated attenuation for several parameter sets of the pion-nucleus optical potential gives a value which is very close to the one reported in reference (8). A strange feature is that one of the successful cases, ^{104}Ru, has a nuclear structure which is extremely close to ^{110}Pd and the measured attenuation is different by an approximate factor of two. The calculated attenuation in the absence of strong mixing with the Tauscher parameter set [8] is given by:

$$A(^{110}Pd) = 11.0\% \qquad \text{(II-17a)}$$

$$A(^{104}Ru) = 11.0\% \qquad \text{(II-17b)}$$

while in the presence of the strong mixing with the same parameter set, the result is

$$A_{ST}\ (^{110}Pd) = 11.20\% \qquad \text{(II-18a)}$$

$$A_{ST}\ (^{104}Ru) = 11.53\% \qquad \text{(II-18b)}$$

With the Batty parameter set there is some improvement:

$$A_{SB}\ (^{110}Pd) = 12.99\% \qquad \text{(II-19a)}$$

$$A_{SB}\ (^{104}Ru) = 10.12\% \qquad \text{(II-19b)}$$

Finally, based on results of high energy (p,p') elastic scattering experiments which led to differences in neutron and proton root-mean-square radii in semiquantitative agreement with those calculated in mean field theory, Negele's Hartree Fock calculations were used to obtain [1] $\overline{\Delta R}$ = 0.15 fm for ^{104}Ru and 0.16 fm for ^{110}Pd, yielding attenuations of 10.0% and 13.2%, respectively, for the Tauscher parameter set. The only possibility (not related to the optical potential problem) which is left is the consideration of a third state in the mixing which is not present in the ^{104}Ru case. In reference (1) there is a suggestion that the state with energy 1470KeV with the

pionic 2p level is nearly degenerate to the other two, being the problem the unknown structure and spin-parity of this state. The state has been observed in (p,p'γ) experiments [11], in (p,p') experiments and (n,n'γ) experiments[3] and is completely absent in Coulomb excitation tests [2]. Deye, Robinson and Ford [11] made a tentative spin-parity assignment based in three-quadrupole phonon states, in a pure phonon picture, giving 0^+, 2^+, 3^+, 4^+ and 6^+ to the states 1401, 1472, 1576, 1713 and 1933 KeV (we used the reported energies of that moment to identify the states). Their analysis makes the 1470 KeV state a 0^+, based on the model of predictions and the experimental angular distributions for (p,p'). The 3^+ and 4^+ assignments were used for the 1401 and 1576 levels, based upon decay results [12]. The 1713 level was assigned 2^+ because of the similarity between ^{110}Pd and ^{124}Te spectra and the 6^+ assignment for the 1933 level consistent with (p,p'), leaving 0^+ for the 1472 level. It is now clear that this assignment can not be correct because gamma transitions were observed between the 1470 KeV level and the 0^+_g,2 levels [3]. Another kind of information that should be considered is the theoretical spectrum that can be calculated in the interacting boson model. This particular model has been very succesful in reproducing both the spectra and transitions rates. Using his model, Iachello provided the assignments of 3^+, 4^+ and 6^+ to the 1212, 1398 and 1574

KeV levels. Energies predicted by the model in this case are 1200, 1378 and 1630 KeV respectively. The predictions for the 2^+ states are located at 383, 802 and 1360 KeV. If we look at the first two 2^+ in nuclear spectrum of ^{110}Pd, depicted in fig. (II-3), we see that the agreement is quite good. If we try to associate the 1470 KeV level to the third one, it would mean that the model prediction would be off by more than 100 KeV, which is a relatively large error for the usual performance of the model. Based on these considerations we will take an assignment of 2^+ for the 1470 KeV state throughout this chapter. With the transition strengths predicted by the interacting boson model there was no improvement in the attenuation calculated by taking into account a mixing which includes the pionic 2p level.

The first task in this chapter will be the study of dynamical nuclear polarization effect in the particular case of ^{110} Pd using a microscopic model which takes into account three excited states described by

$$|\psi\rangle_{374} = \alpha_1|1\rangle + \alpha_2|2\rangle + \alpha_3|3\rangle \qquad \text{(II-20a)}$$

$$|\psi\rangle_{814} = \beta_1|1\rangle + \beta_2|2\rangle + \beta_3|3\rangle \qquad \text{(II-20b)}$$

$$|\psi\rangle_{1470} = \gamma_1|1\rangle + \gamma_2|2\rangle + \gamma_3|3\rangle \qquad \text{(II-20c)}$$

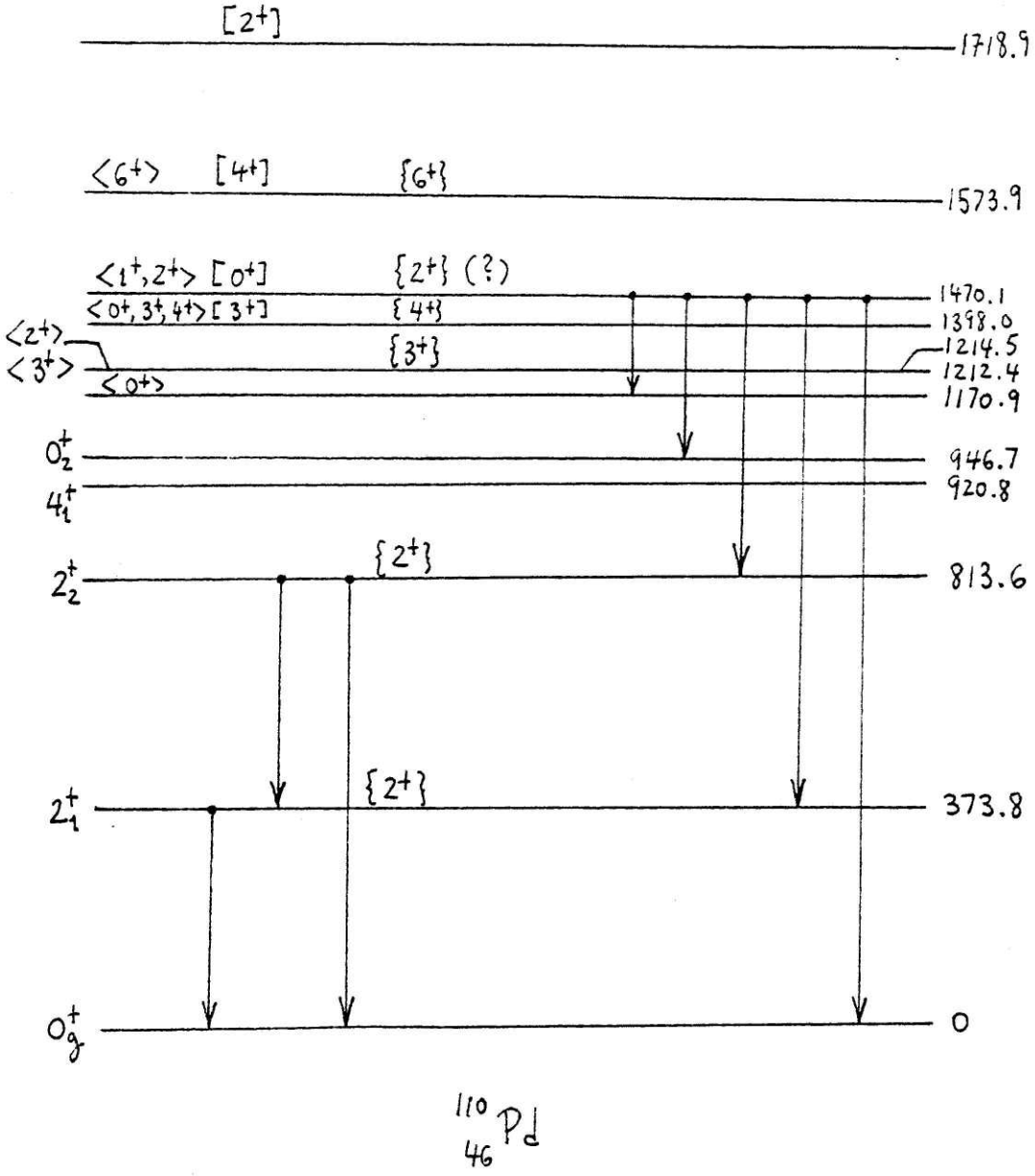

Fig. (II-3) Nuclear Spectrum of ^{110}Pd. The square brackets assignments are from reference (11). The curly brackets are the predictions from the interacting boson model. The sign (?) is used to indicate the association that we are making between the predicted 1360 KeV level and the observed 1470 KeV level. The assignments on the left are in agreement with all the references and the ones in angular brackets are taken from reference (3). All the relevant transitions for the 1470 level were taken from reference (3) also and are shown on the right side of the figure. On the left we show the transitions used in the determination of model parameters.

the subcripts of the $|\psi\rangle$ indicate the appropiate excited state and $|1\rangle$, $|2\rangle$ and $|3\rangle$ are, respectively, states with one, two and three phonons. In a nucleus with a ground state density characterized by a radius parameter a_0 , the vibrational surface waves (surfon) are introduced by allowing the radius parameter to be angle dependent:

$$a(\Omega) = a_0 \left\{ 1 + \sum_{\substack{lm \\ (l\geq 2)}} q_{lm} Y_{lm}(\Omega) - \frac{\Delta}{4\pi} \sum_{\substack{lm \\ (l\geq 2)}} |q_{lm}|^2 \right\} \qquad \text{(II-21)}$$

where Δ is chosen to preserve the normalization to order q^3, so that

$$\int d\vec{x} \langle I\pi | \hat{\rho}(x) | I\pi \rangle = A + \vartheta(q^3) \qquad \text{(II-22)}$$

where $|I\pi\rangle$ is a nuclear eigenstate. If a Woods-Saxon shape for the ground state density is used the parameter is very close to unity. The deformation parameters are treated as quantum mechanical operators and can be written in terms of creation and annihilation operators as:

$$\hat{q}_{lm} \equiv \chi_l \left[\hat{a}_{lm} + (-1)^m \hat{a}^{+}_{l,-m} \right] \qquad \text{(II-23)}$$

with commutation relations:

$$\left[\hat{a}_{\ell m}\,,\,\hat{a}^{+}_{\ell' m'}\right] = \delta_{\ell\ell'}\delta_{mm'} \qquad \text{(II-24a)}$$

$$\left[\hat{a}_{\ell m}\,,\,\hat{a}_{\ell' m'}\right] = \left[\hat{a}^{+}_{\ell m}\,,\,\hat{a}^{+}_{\ell' m'}\right] = 0 \qquad \text{(II-24b)}$$

Then, the nuclear density as operator can be written, up to order q^2, as:

$$\hat{\rho}(\vec{x}) = \rho(\vec{x}, a_0) + a_0 \left.\frac{\partial \rho(\vec{x}, a)}{\partial a}\right|_{a=a_0} \left\{ \sum_{\ell m} \hat{q}_{\ell m}\, Y_{\ell m}(\Omega_x) \right.$$

$$\left. - \frac{\Delta}{4\pi} \sum_{\ell m} :|q_{\ell m}|^2: \right\} + \frac{1}{2}\, a_0^2 \left.\frac{\partial^2 \rho(\vec{x}, a)}{\partial a^2}\right|_{a=a_0^{\ell m}} :\left| \sum_{\ell m} \hat{q}_{\ell m}\, Y_{\ell m}(\Omega_x) \right|^2: \qquad \text{(II-25)}$$

the symbol : : denotes normal ordering, avoiding in this way vacuum fluctuations. In general, the multipole (collective) operator can be written as:

$$\hat{Q}_{\lambda\mu} = e \int d\vec{r}\; r^{\lambda}\, Y_{\lambda\mu}(\Omega)\, \hat{\rho}_p(\vec{r}) \qquad \text{(II-26)}$$

where $\hat{\rho}_p(\vec{r})$ denotes the proton density. In order to determine the parameters α_i, β_i, and γ_i of equations (II-20) and the parameter X_2 given in equation (II-23) (which are the essential parameters of our nuclear model) measured experimental quantities are used. In an initial approach to this problem the experimental information from the first two excited states plus orthonormalization conditions which include the third excited state ,

are going to give the necessary number of equations for a quantitative determination of the model parameters and in this way try to asses whether or not the presence of a third 2^+ can lead to an explanation of the ^{110}Pd problem. There are reasonable good measurements of the transition probabilities for the lines $(2_1^+ \longrightarrow 0_g^+)$, $(2_2^+ \longrightarrow 0_g^+)$ and $(2_2^+ \longrightarrow 2_1^+)$ summarized in table (II-1). Unfortunely the measurements for the quadrupole moment of the first excited state are not very conclusive. Robinson, Mc Gowan, Stelson, Milner [2] and Sayer reported a value of $Q(2_1^+) = (-83.0 \pm 0.19)$ barns obtained from Coulomb excitation and using a version of the Winther and De Boer Program for the quantitative analysis. The reduced matrix elements for the appropiate multipolar excitation, given by equation (II-33) constitute the input information for this program. Harper, Christy, Hall, Nagib and Wakefield [13] considered the problem of the phase for these matrix elements, i.e., the constructive and destructive interference between the 2_1^+ and the 2_2^+ states, obtaining (-0.72 ± 0.12) barns and (-0.45 ± 0.12) barns. A previous determination due to Beyer, Scharenberg and Thomson[14] gives values of (-0.483 ± 0.049) barns for the constructive interference case and (-0.266 ± 0.049) barns for the destructive one. Due to this experimental situation the variation of the quadrupole moment over a wide range will be considered. Replacing equation (II-25) in equation (II-26) for the quadrupole case, we obtain the

TABLE (II-I)

Experimental Transition Probabilities $B(E2, I_i \longrightarrow I_f)$

Energy (KeV)	Transition	Transition Probability (e^2fm^4)	Reference
373.8 ± 0.3	$2_1^+ \longrightarrow 0_g^+$	1820 ± 120	(2)
		1640 ± 160	(13)
439.9 ± 0.7	$2_2^+ \longrightarrow 2_1^+$	1800 ± 300	(2)
813.7 ± 0.5	$2_2^+ \longrightarrow 0_g^+$	25.6 ± 2.2	(2)

operator:

$$\hat{Q}_{2\mu} = A\,\hat{q}^{+}_{2\mu} + B\sum_{\substack{\ell' m' \\ \ell m}} (-1)^{m}[\ell'][\ell] \otimes \begin{pmatrix} \ell' & 2 & \ell \\ -m' & \mu & m \end{pmatrix}\begin{pmatrix} \ell' & 2 & \ell \\ 0 & 0 & 0 \end{pmatrix} \hat{q}^{+}_{\ell' m'}\,\hat{q}_{\ell m} \qquad \text{(II-27)}$$

where $[\ell] \equiv \sqrt{2\ell+1}$ and

$$A \equiv e\,a_p \int_0^{\infty} dr\; r^4 \frac{\partial \rho_p}{\partial a_p} \qquad \text{(II-28)}$$

$$B \equiv \frac{e}{2}\sqrt{\frac{5}{4\pi}}\; a_p^2 \int_0^{\infty} dr\; r^4 \frac{\partial^2 \rho_p}{\partial a_p^2} \qquad \text{(II-29)}$$

being a_p the proton radius. Using equation (II-27) the quadrupole moment for a excited state is given by:

$$Q \equiv \langle 2^{+}2 \,|\, \hat{Q}_{20} \,|\, 2^{+}2 \rangle \qquad \text{(II-30)}$$

and then, the relevant operator to be used, derived from equation (II-27), is given by:

$$\hat{Q}_{20} = A\,\hat{q}^{+}_{20} - \sqrt{\frac{10}{7}}\; B\sum_{m} \begin{pmatrix} 2 & 2 & 2 \\ -m & 0 & m \end{pmatrix} \hat{q}_{2,-m}\,\hat{q}_{2m} \qquad \text{(II-31)}$$

the transition probabilities are given by:

$$B(EL;\, I_1 \rightarrow I_2) = \frac{1}{2I_1 + 1}\,|M(I_2, I_1)|^2 \qquad \text{(II-32)}$$

where the index L stands for the appropiate multipolarity and $\mathcal{M}(I_2, I_1)$ is the reduced multipole matrix element given by:

$$\mathcal{M}(I_2, I_1) \equiv \langle I_2 \| Q_L \| I_1 \rangle \qquad \text{(II-33)}$$

Using equations (II-30), (II-31) and (II-32), expressions related to experimental quatities are found : (see appendix II-A)

$$Q_{374} = \sqrt{\frac{16\pi}{5}} \left\{ A X_2 \left[\frac{4}{7}\sqrt{7}\,\alpha_1\alpha_2 + \frac{4}{7}\sqrt{2}\,\alpha_2\alpha_3 \right] \right.$$

$$\left. + B X_2^2 \left[-\frac{4}{7}\alpha_1^2 + \frac{12}{49}\alpha_2^2 + \frac{24}{343}\alpha_3^2 + \frac{12}{49}\sqrt{\frac{2}{7}}\alpha_1\alpha_3 \right] \right\} \qquad \text{(II-33a)}$$

$$B(E2; 2_1^+ \to 0_g^+) = \frac{1}{5}\left[\sqrt{5}\, A X_2 \alpha_1 + \frac{3}{7}\sqrt{\frac{5}{7}}\, B X_2^2 \alpha_2 \right]^2 \qquad \text{(II-33b)}$$

$$B(E2; 2_2^+ \to 0_g^+) = \frac{1}{5}\left[\sqrt{5}\, A X_2 \beta_1 + \frac{3}{7}\sqrt{\frac{5}{7}}\, B X_2^2 \beta_2 \right]^2 \qquad \text{(II-33c)}$$

$$B(E2; 2_2^+ \to 2_1^+) = \frac{1}{5} \left\{ \left[-\frac{4}{7}\sqrt{\frac{35}{2}}\,\alpha_1\beta_1 + \frac{6}{49}\sqrt{5}\,\alpha_1\beta_3 \right.\right.$$

$$\left. + \frac{12}{49}\sqrt{\frac{35}{2}}\,\alpha_2\beta_2 + \frac{6}{49}\sqrt{5}\,\alpha_3\beta_1 + \frac{24}{343}\sqrt{\frac{35}{2}}\,\alpha_3\beta_3 \right] B X_2^2$$

$$\left. + \left[\sqrt{10}\,\alpha_1\beta_2 + \sqrt{10}\,\beta_1\alpha_2 + \frac{2}{7}\sqrt{35}\left(\alpha_2\beta_3 + \alpha_3\beta_2\right) \right] A X_2 \right\}^2 \qquad \text{(II-33d)}$$

In order to solve this nonlinear set of equations a computer program was developed, taking into account the experimental allowances for each of the quanti-

ties described in equations (II-33). In the particular case of the quadrupole moment the range of values to be considered is very wide due to the phase problem discussed already. In spite of that, the solutions were found around two values: -50.0 and -70.0 barns. Due to the fact that we are considering experimental errors, the number of solutions for this problem is, in principle, infinite. Nevertheless the allowances can be tightened to reduce the solution set to the representative ones, i.e., the solution set associated with the absence of allowances. It was verified that in a given neighborhood the parameters related to every solution, change very little and they were very close to the representative solution. Using the experimental values of table (II-I) and this tightening procedure lead us to a finite number of solutions. We note in table (II-I) that the value for the transition probability $B(E2, 2_1^+ \longrightarrow 0_g^+)$ is given in a wide range ranking from 1480 e^2fm^4 to 1940 e^2fm^4, being the average around 1710 e^2fm^4. With the tightening procedure several points can be explored throughout the range with the result that below 1820 e^2fm^4 only solutions with $Q(2_1^+) = -50.0$ barns were found. Looking at the experimental data we see that, in general, low values for the quadrupole moment of the first 2^+ should be the adopted ones [10]. Then, we are going to explore the value range for $B(E2, 2_1^+ \longrightarrow 0_g^+)$ from 1480 e^2fm^4 to 1820 e^2fm^4 with fixed values for $B(E2, 2_2^+ \rightarrow 0_g^+)$

and $B(E2, 2_2^+ \longrightarrow 2_1^+)$ given in table (II-I) and $Q(2_1^+) = -50$ barns, but before this exploration, it is good to see how the attenuation is going to be calculated. Following reference (1) the basic procedure is diagonalization of the pion-nucleus Hamiltonian $H_{\pi A}$ in the model basis given by nearly degenerate states with total angular momentum J and parity π , i.e., the determinantal equation is given by:

$$let \left\{ < [I' \pi_N' ; \widetilde{n' \ell'}] J \pi \mid (E - H_{\pi A}) \mid [I \pi_N ; n \ell] J \pi > \right\} = 0 \qquad \text{(II-34)}$$

these nearly degenerate states, as it was mentioned before, are direct products of nuclear and pionic states coupled to total angular momentum J and parity π , , then

$$H_N \mid I \pi_N > = \epsilon_{I \pi_N} \mid I \pi_N > \qquad \text{(II-35)}$$

$$\left\{ k_\pi + < 0^+ \mid H_{em}^\pi + H_s^\pi \mid 0^+ > \right\} \mid n \ell > = E_{n \ell} \mid n \ell > \qquad \text{(II-36)}$$

where H_N is the nuclear Hamiltonian, $\mid I \pi_N >$ is a nuclear state with spin (parity) $I(\pi_N)$ and $\epsilon_{I \pi_N}$ its energy, H_{em} and H_s represent the pion-nucleus electromagnetic and strong interaction, respectively, and $\mid 0^+ >$ is the nuclear ground state. In equation (II-36), the matrix element $< 0^+ \mid H_{em} + H_s \mid 0^+ >$ gives us the pion-nucleus interaction when the nucleus is in its ground state. The elec -

tromagnetic part of this interaction represents the Coulomb potential and the strong interaction part represents the pion optical potential

$$V_{opt} \equiv \langle o^+ | H_s^{\pi} | o^+ \rangle \qquad \text{(II-37)}$$

which is non-Hermitian due to the presence of a strong absorption channel, making E_{nl} complex and the meaning of the "tilde" over the pionic states in equation (II-34) is that a bi-orthogonal basis $|\tilde{nl}\rangle$ should be used. These states can be obtained through the equation:

$$(\hat{k}_{\pi} + V_{COUL}^{\pi} + V_{opt}^{\pi}) \, |\tilde{n\ell}\rangle = E_{n\ell}^{*} \, |\tilde{n\ell}\rangle \qquad \text{(II-38)}$$

the matrix element for the pion-nucleus total Hamiltonian can be written as:

$$\langle [I'\pi_N', \tilde{n'\ell'}]J\pi \, | H_{\pi A} | \, [I\pi_N ; n\ell]J\pi \rangle$$

$$= (\epsilon_{I\pi_N} + E_{n\ell}) \, \delta_{I'I} \, \delta_{\pi_N'\pi_N} \, \delta_{nn'} \delta_{\ell\ell'}$$

$$+ \langle [I'\pi_N', \tilde{n'\ell'}]J\pi \, | \, (\Delta H_{em}^{\pi} + \Delta H_s^{\pi}) \, | \, [I\pi_N ; n\ell]J\pi \rangle \qquad \text{(II-39)}$$

where:

$$\Delta H_{em}^{\pi} \equiv H_{em}^{\pi} - \langle o^+ | H_{em}^{\pi} | o^+ \rangle \qquad \text{(II-40)}$$

$$\Delta H_S^{\pi} \equiv H_S^{\pi} - \langle 0^+ | H_S^{\pi} | 0^+ \rangle \qquad \text{(II-41)}$$

the operator ΔH_{em}^{π} can be calculated, considering a multipole expansion of

$$\Delta H_{em}^{\pi} = \sum_L \Delta H_{em}^{\pi(L)} \qquad \text{(II-42)}$$

where the L-th term is given by

$$\Delta H_{em}^{\pi(L)} = -\frac{4\pi e^2}{2L+1} \sum_{M=-L}^{+L} \int d\vec{r}' \hat{\rho}(\vec{r}') \frac{r_<^L}{r_>^{L+1}} Y_{LM}(\Omega') Y_{LM}^*(\Omega) \qquad \text{(II-43)}$$

for $L \neq 0$, and

$$\Delta H_{em}^{\pi(0)} = -e^2 \int d\vec{r}' \left[\hat{\rho}(\vec{r}') - \rho(\vec{r}', a_0) \right] \frac{1}{r_>} \qquad \text{(II-44)}$$

for L =0. Replacing the density given by equation (II-25) in equation (II-43), we obtain:

$$\Delta H_{em}^{\pi(L)} = \frac{e^2}{2} a_p \Delta_p \delta_{oL} \left\{ \frac{1}{r} \int_0^r R^2 dR \frac{\partial \rho_p}{\partial a_p} + \int_r^\infty dR \left[R - \frac{R^2}{r} \right] \frac{\partial \rho_p}{\partial a_p} \right.$$

$$\otimes \sum_{\ell m} : \hat{q}_{\ell m}^+ \hat{q}_{\ell m} : - \frac{4\pi e^2 a_p}{2L+1} \left\{ \frac{1}{r^{L+1}} \int_0^r R^{L+2} dR \frac{\partial \rho_p}{\partial a_p} + \int_r^\infty dR \left[\frac{r^L}{R^{L-1}} - \frac{R^{L+2}}{r^{L+1}} \right] \frac{\partial \rho_p}{\partial a_p} \right\}$$

$$\otimes \sum_M \hat{q}_{LM}^+ Y_{LM}^*(\Omega) - \sqrt{\frac{\pi}{2L+1}} e a_p^2 \left\{ \frac{1}{r^{L+1}} \int_0^r R^{L+2} dR \frac{\partial^2 \rho_p}{\partial a_p^2} + \int_r^\infty dR \left[\frac{r^L}{R^{L-1}} - \frac{R^{L+2}}{r^{L+1}} \right] \frac{\partial^2 \rho_p}{\partial a_p^2} \right\}$$

$$\otimes \sum_{M} Y^{*}_{LM}(\Omega) \sum_{\substack{\ell m \\ \ell' m'}} [\ell][\ell'] \begin{pmatrix} \ell & \ell' & L \\ m & m' & M \end{pmatrix} \begin{pmatrix} \ell & \ell' & L \\ 0 & 0 & 0 \end{pmatrix} : \hat{q}_{\ell m} \hat{q}_{\ell' m'} : \qquad \text{(II-45)}$$

where: $\Delta_p \equiv \dfrac{1 + (t/a_p) \log\left(1 + e^{-a_p/t}\right)}{1 + \frac{\pi^2}{3}\frac{t^2}{a_p^2} + 2\frac{t^2}{a_p^2} \sum_{n=1}^{\infty} (-1)^n \frac{e^{-n a_p/t}}{n^2}}$

being t the radius diffusiness and a_p the proton radius. For the strong interaction part a prescription based upon the collective model is going to be used, considering variations in the nuclear radius parameter 'a' as it was done for the nuclear density, being the pion-nucleus optical potential the object of the expansion:

$$\Delta H_S^{\pi} = a_o \left(\frac{\partial}{\partial a} V_{opt}^{\pi}\right)\Big|_{a=a_o} \left\{ \sum_{\ell m} \hat{q}_{\ell m} Y_{\ell m} - \frac{\Delta}{4\pi} \sum_{\ell m} : |\hat{q}_{\ell m}|^2 : \right\}$$

$$+ \frac{1}{2} a_o^2 \left(\frac{\partial^2}{\partial a^2} V_{opt}^{\pi}\right)\Big|_{a=a_o} : \Big| \sum_{\ell m} \hat{q}_{\ell m} Y_{\ell m} \Big|^2 : + \vartheta(q^3) \qquad \text{(II-46)}$$

V_{opt}^{π} is described as the standard version of the semiphenological Kisslinger pion-nucleus optical potential, considering just the first two partial waves:

$$V_{opt}^{\pi} = V_S + V_p \qquad \text{(II-47)}$$

where the S-wave contribution is given by:

$$V_S = -\frac{4\pi}{2\mu} \left\{ \left(1 + \frac{M_\pi}{M_N}\right) b_o \rho(x) + \left(1 + \frac{M_\pi}{M_N}\right) b_1 \left[\rho_n(x) - \rho_p(x)\right] + \left(1 + \frac{M_\pi}{2M_N}\right) B_o \rho^2(x) \right\} \qquad \text{(II-48)}$$

with M_π, M_N and μ standing for the pion, nuclear

and reduced mass, respectively. The reduced mass was taken as:

$$\mu = \frac{M_\pi M_A}{M_\pi + M_A} \qquad \text{(II-49)}$$

being M_A the nuclear mass. The p-wave contribution is given by:

$$V_p = \frac{4\pi}{2\mu} \vec{\nabla} \cdot \frac{\alpha(x)}{1 + \frac{4\pi}{3} \xi \alpha(x)} \vec{\nabla} \qquad \text{(II-50)}$$

where:

$$\alpha(x) \equiv \frac{c_0}{1 + \frac{M_\pi}{M_N}} \rho(x) + \frac{c_1}{1 + \frac{M_\pi}{M_N}} \left[\rho_n(x) - \rho_p(x)\right] + \frac{C_0}{1 + \frac{M_\pi}{M_N}} \rho^2(x) \qquad \text{(II-51)}$$

and $\rho(x) = \rho_n(x) + \rho_p(x)$ is the total nuclear density. The relevant parameters for the optical potential were already discussed in Chapter I. The Tauscher parameter set is going to be used throughout this chapter. Up to now we were discussing all the elements presented in equation (II-34) and models to be used in the calculation of attenuation. The matrix elements used in actual calculation are given in appendix (II-B). At the begining of this section we used the induced width and total

width to find the attenuation and now, in order to find the width in the absence of dynamical nuclear polarization, equation (II-36) is solved using a version of the PIATOM computer program provided by Nixon [15]. A small modification allowed the calculation of all the necessary overlap integrals related to pionic wavefunctions. The total width is calculated through equation (II-34). The original program which gives us the nuclear model parameters was extended to include the attenuation calculation and all the relevant quadrupole matrix elements for a verification with Coulomb excitation. The discussion of the results for pionic 4f level in ^{110}Pd, including this verification is the subject of the next section.

(2) Predicted Attenuations for the (4f $\longrightarrow$ 3d) line and Coulomb excitation tests for the three surfon state model:

As it was said in the previous section we are going to explore a range of values for the $B(E2, 2_1^+ \longrightarrow 0_g^+)$ from 1480 e^2fm^4 to 1820 e^2fm^4 with fixed values for $B(E2, 2_2^+ \longrightarrow 0_g^+)$ and $B(E2, 2_2^+ \longrightarrow 2_1^+)$ given in table (II-I) and taking -50 barns as the quadrupole moment value for the first excited state with 2^+. For the $B(E2, 2_1^+ \longrightarrow 0_g^+)$ = 1820 e^2fm^4 case several solutions were found, but only four fall within the experimental allowances for the attenuation as it is summarized in table (II-II). Using experimental information about excitation probabilities for the

first 2^+ in ^{110}Pd [13] we can test the parameter sets (I) and (II) related to a quadrupole moment value closer to the adopted one [10]. The results are given in table (II-III). Sets I and II are taken from table (II-II). The set I* is obtained from set I cancelling all the contributions from the 2_3^+ and set I** is also obtained from set I, making this time $Q(2_2^+) = 0$. From these results it is clear that the choice of the relative phases is sensitive and a better agreement is obtained with the set II. Looking at the set I*, it seems the role played by the 2_3^+ state is an insignificant one and in that sense is in agreement with the general experimental observation that the 1470 KeV state is not present in Coulomb excitation [2]. Also taking into account results from the set I**, we can see that the particular structure of the 2_2^+ state seems to be not very relevant when the Coulomb excitation process is studied. The set II corresponds to the destructive interference case between the one phonon and two phonon states in the 2_1^+. The required matrix elements for the calculation of the attenuation are given in table (II-IIA) and the reduced quadrupole matrix elements needed in the Coulomb excitation analysis in table (II-IIB). The atomic level information is provided in table (II-IIC). The induced width in reference (1) is 1.84 eV and in this work the result was 3.067 eV for the set II. In order to test the sensitivity of these results in terms of the $B(E2, 2_1^+ \longrightarrow 0_g^+)$ value, it was

TABLE (II-II)

Calculated Model Nuclear Parameters for

$B(E2, 2_1^+ \longrightarrow 0_g^+) = 1820\ e^2fm^4$

	Attenuation: 17.28%		Attenuation: 21.54%	
	Set I	Set II	Set III	Set IV
α_1	-0.9747	-0.9747	+0.9402	+0.9402
α_2	-0.2963	+0.2063	-0.2841	+0.2841
α_3	-0.0861	-0.0861	+0.1880	+0.1880
β_1	-0.1057	+0.1057	-0.1012	+0.1012
β_2	+0.7648	+0.7648	-0.7599	-0.7599
β_3	-0.6355	+0.6355	-0.6421	+0.6421
γ_1	+0.1969	+0.1969	+0.3253	+0.3253
γ_2	-0.6104	+0.6104	+0.5847	-0.5847
γ_3	-0.7673	-0.7673	-0.7432	-0.7432
X_2	-0.0948	+0.0948	+0.0948	-0.0948
$Q(2_1^+)$	-50 barns	-50 barns	-70 barns	-70 barns

TABLE (II-IIA)

Matrix Elements related to Dynamical Polarization in ^{110}Pd for the set II.

We define $|1\rangle \equiv |4f,0^+\rangle, |2\rangle \equiv |3p,2^+_1\rangle, |3\rangle \equiv |2p,2^+_3\rangle$

and

$$\Delta H \equiv \Delta H_{em} + \Delta H_s$$

(energy units:KeV)

$\langle 1|\Delta H_{em}|2\rangle = -0.1292 - i0.0116$ $\langle 1|\Delta H_s|2\rangle = -0.0299 + i0.0068$

$\langle 1|\Delta H_{em}|3\rangle = -0.1237 - i0.0011$ $\langle 1|\Delta H_s|2\rangle = 0.0101 - i0.0029$

$\langle 2|\Delta H_{em}|3\rangle = -1.8150 - i0.5577$ $\langle 2|\Delta H_s|3\rangle = 2.1187 - i0.3483$

$\langle 2|\Delta H_{em}|2\rangle = -0.7617 - i0.2372$ $\langle 2|\Delta H_s|2\rangle = 0.9213 - i0.1456$

$\langle 3|\Delta H_{em}|3\rangle = -1.4635 - i0.3979$ $\langle 3|\Delta H_s|3\rangle = 1.3857 - i0.2409$

TABLE (II-IIB)

Reduced Quadrupole Matrix elements used in the Coulomb Excitation Analysis for the set II (in barns). We define

$|1\rangle \equiv |0^+\rangle, |2\rangle \equiv |2^+_1\rangle, |3\rangle \equiv |2^+_2\rangle$ and $|4\rangle \equiv |2^+_3\rangle$

$\langle 1\|Q\|2\rangle = -0.954$ $\langle 1\|Q\|3\rangle = 0.113$ $\langle 1\|Q\|4\rangle = 0.201$

$\langle 2\|Q\|2\rangle = -0.660$ $\langle 2\|Q\|3\rangle = -0.948$ $\langle 2\|Q\|4\rangle = -0.898$

$\langle 3\|Q\|3\rangle = 0.971$ $\langle 3\|Q\|4\rangle = 0.161$ $\langle 4\|Q\|4\rangle = -0.348$

TABLE (II-IIC)

Atomic level inforation for pionic ^{110}Pd(1)

Level	Energy (KeV)	Width (KeV)
4f	-493.27	1.88×10^{-3}
3p	-873.62	32.50
2p	-1962.40	94.55

$\Gamma_\gamma(4f \rightarrow 3d) = 12.8$ eV

TABLE (II-III)

Excitation Probabilities for the First 2^+ in ^{110}Pd for a $\theta_{LAB} = 162^\circ$ ($P(2_1^+) \times 10^4$).

Proj.	E(MeV)	Exp.[13]	SET I	SET I*	SET I**	SET II
^4He	7.00	48.5 ± 5.3	53.5	53.6		51.97
^4He	8.00	87.3 ± 9.3	97.8	98.1		94.92
^{16}O	27.96	454.0 ± 47	557	562	561	499
^{16}O	31.96	819.0 ± 86	994	1007	1006	890
^{16}O	35.97	1310.0 ± 140	1551	1583	1581	1389
^{16}O	39.98	1810.0 ± 194	2191	2256	2251	1966

TABLE (II-IV)

Tauscher Parameter Set used for the pion-nucleus optical potential.

$$b_0 = (-0.0293 \pm 0.0005) M_\pi^{-1} \qquad b_1 = (-0.078 \pm 0.007) M_\pi^{-1}$$

$$B_0 = (0.0428 \pm 0.0015) i M_\pi^{-4} \qquad C_0 = (0.076 \pm 0.013) i M_\pi^{-6}$$

$$c_0 = (0.227 \pm 0.008) M_\pi^{-3} \qquad c_1 = (0.18 \pm 0.03) M_\pi^{-3}$$

$$\xi = 1.0 \pm 0.1$$

increased until we reached 1480 e^2fm^4 (the lowest possible experimental value according to the allowances) and the results are summarized in table (II-V). For certain values of transition probabilities there is only one solution and it is denoted in the table by (U), i.e., "unique". In the rest of cases the closest attenuation theoretical value to the experimental one was chosen. We can see that the overall agreement is good, specially for the first three values of the $B(E2, 2_1^+ \longrightarrow 0_g^+)$ in table (II-V), which are associated to unique solutions. The entry "Reference (2)" in this table is related to a calculation of the Excitation Probabilities for the first 2^+ with the parameters given in reference (2) in order to verify the agreement between the reported experimental values (2,13) and then we can say that they are consistent , at least from the Coulomb Excitation point of view. To proceed further with our test, the Yields and total Cross sections can be calculated for the attenuation cases 21.17%, 20.93% and 20.26%. The Calculated Yields can be compared with the measured ones [2] in table (II-VIA) for the 2_2^+ state, which provides an independent verification. The calculated Cross Sections constitute a prediction of the model. All the Coulomb Excitation calculations were carried out using a computer code named COULEX and provided by Steadman [16]. This program is an Updated and expanded version of the Winther- De Boer program for Coulomb Excitation calcula -

TABLE (II-V)

Excitation Probabilities for the First 2^+ in ^{110}Pd (13) for a $\theta_{LAB} = 162°$

($P(2_1^+) \times 10^4$)

Projectile	^4He	^4He	^{16}O	^{16}O	^{16}O	^{16}O	
Energy (MeV)	7.00	8.00	27.96	31.96	35.97	39.98	
Exp. value	48.5	87.3	454	819	1310	1810	$B(E2, 2_1^+ \rightarrow 0_g^+)$
	±5.3	±9.3	±47	±86	±140	±194	(e^2fm^4 units)
Reference (2)	51.4	93.9	480	852	1325	1868	1820
Attenuations:							
21.17% (U)	43.8	80.2	464	832	1306	1854	1480
20.93% (U)	45.0	82.2	476	851	1331	1884	1520
20.26% (U)	45.7	83.6	480	861	1355	1934	1550
17.81%	46.2	84.5	484	868	1365	1945	1570
22.74%	46.9	85.8	492	884	1391	1984	1590
16.31%	48.3	88.3	504	903	1414	2006	1640
28.10%	50.9	93.5	543	980	1548	2215	1720

tions, developed by the MIT Heavy Ion Group. Another interesting test is to predict the Yields for the 2_3^+ and try to estimate if this state can be observed in a Coulomb Excitation experiment. In order to do that, calculated Yields and Total Cross Sections are provided for the 2_1^+ and 2_3^+ states in tables (II-VIB)and (II-VIC).

In reference (2) there is no report of a 1470 KeV state and a 30 cm^3 Ge(Li) detector was used. We are going to estimate the heights of the observed peaks in the 20.26% attenuation case, which has the lowest yields and then is closer to the experimental fact of absence of peaks. The behavior of the experimental peak height to total ratio versus gamma ray energy is given in fig (II-4) [17] for a detector like the one used in reference (2). In table (II-VII) this ratio is given for the relevant transitions in ^{110}Pd. In table (II-VIII) the experimental information of the $(2_1^+ \longrightarrow 0_g^+)$ and $(2_2^+ \longrightarrow 0_g^+)$ lines [2] is considered in order to obtain the total number of counts which lead to the estimation of the relative efficiency, given by the functional form:

$$\log \xi = 1 + \alpha \log(E/E_o) \qquad \text{(II-52)}$$

where $\alpha = -1.1580$ and $E_o = 373.8$ KeV. Now we can estimate the peak height of the $(2_3^+ \longrightarrow 0_g^+)$ line taking into account the information from the $(2_2^+ \longrightarrow 0_g^+)$line,

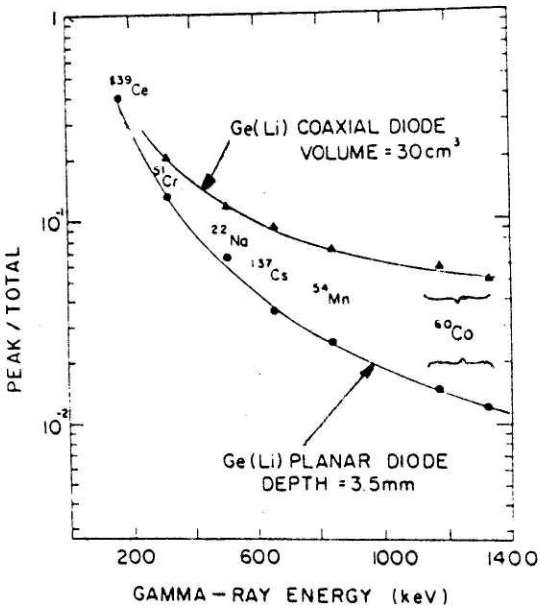
1
10^{-1}
10^{-2}
PEAK / TOTAL
^{139}Ce
Ge(Li) COAXIAL DIODE
VOLUME = 30cm^3
^{51}Cr
^{22}Na
^{137}Cs
^{54}Mn
^{60}Co
Ge(Li) PLANAR DIODE
DEPTH = 3.5mm
200
600
1000
1400
GAMMA-RAY ENERGY (keV)

Fig. (II-4)

TABLE (II-VIA)

Yields* (μCoulomb per O^{+6} ions) and Total Cross Sections (mb) for the 2_2^+ state in ^{110}Pd.

Energy (MeV)	Y	σ_T	Y	σ_T	Y	σ_T	Exp. Y[2]
42.0	13.4	8.72	13.2	8.58	13.8	8.97	13.8 $\pm$1.4
45.5	22.9	12.07	22.3	11.72	23.5	12.36	22.7 $\pm$2.5
49.0	36	15.47	36	15.37	38.4	16.36	37.0 $\pm$4.0
Attenuation:	21.17%		20.93%		20.26%		

*Y x 10^{-4}

TABLE (II-VIB)

Yields* (μCoulomb per O^{+6} ions) and Total Cross Sections (mb) for the 2_3^+ state in ^{110}Pd.

Energy (MeV)	Y	σ_T	Y	σ_T	Y	σ_T
42.0	60.0	38.92	12.8	8.31	8.1	5.23
45.0	56.0	29.38	50.2	26.34	31.2	16.37
49.0	50.1	21.32	45.0	19.16	27.6	11.77
Attenuation:	21.17%		20.93%		20.26%	

*Y x 10^{-4}

TABLE (II-VIC)

Yields* (μCoulomb per O^{+6} ions) and Total Cross Sections (mb) for the 2_1^+ state in ^{110}Pd.

Energy (MeV)	Y	σ_T	Y	σ_T	Y	σ_T
42.0	479.7	311.35	486.1	315.49	500.0	324.42
45.5	1262.0	662.35	1285.2	674.50	1327.2	696.55
49.0	859.0	365.80	879.0	374.16	910.5	387.58
Attenuation:	21.17%		20.93%		20.26%	

*Y x 10^{-4}

TABLE (II-VII)

Transition	Peak/Total
$2_1^+ \longrightarrow 0_g^+$	0.1532
$2_2^+ \longrightarrow 0_g^+$	0,0711
$2_3^+ \longrightarrow 0_g^+$	0,0500
$2_3^+ \longrightarrow 2_2^+$	0,0918
$2_3^+ \longrightarrow 2_1^+$	0,0550

TABLE (II-VIII)*

Estimated Experimental information from reference (2).

Transition	$(2_1^+ \longrightarrow 0_g^+)$	$(2_2^+ \longrightarrow 0_g^+)$
Measured Peak (including Background) (in counts)	316000 ± 20000	473 ± 27
Background (in counts)	2700 ± 450	240 ± 40
Peak (without Background) (in counts)	313300 ± 20000	232 ± 68
Total Counts (after Peak/Total correction)	2045000 ± 130000	3270 ± 960
Yields (μC per O^{+6} ions)	1327,2**	22,7***
Total Count/Yield Ratio	1540	626
Relative efficiency	1	0,4062
Energy (KeV)	373,8 (2)	813,7 (2)

* For 45 MeV Oxygen Ions, ** From table (II-VIC), ***Taken from reference (2),(x0,23 from branching ratio)

branching ratios [3], the predicted yield given in table (II-VIB) and the relative efficiency given by equation (II-43). This estimation gives a peak which is approximately the same size of the one for the $(2_2^+ \longrightarrow 0_g^+)$ line, above the background level. In the energy region intended for the $(2_3^+ \longrightarrow 0_g^+)$ transition this means a peak of about three times the background level and the conclusion is that it should be observable. Since this result is in direct contradiction with the experimental measurement of reference [2], there is the necessary motivation for a repetition of the experiment. Taking into account this experimental information in a rigourous way, the propo sal is that the 2_3^+ state of the microscopic theory developed in the previous section is not the 1470 KeV state and unfortunely there is no candidate to replace it. In order to test this propo - sal the experimental information from reference (3) was taken into account, particularly the reduced transition probabilities ratios. From the branching ratios given in table (II-IX) the following relations can be extracted:

$$B(E2;2_3^+ \longrightarrow 2_2^+) \;/\; B(E2,2_3^+ \longrightarrow 2_1^+) = 8.84 \quad \text{(II-53a)}$$

$$B(E2,2_3^+ \longrightarrow 0_2^+) \;/\; B(E2,2_3^+ \longrightarrow 2_1^+) = 194.19 \quad \text{(II-53b)}$$

$$B(E2,2_3^+ \longrightarrow 0_g^+) \;/\; B(E2,2_3^+ \longrightarrow 2_1^+) = 0.026 \quad \text{(II-53c)}$$

with 20% error. Using equations (II-53), the particular features of the 1470 KeV are incorporated in

TABLE (II-IX)[3]

Branching Ratios for (1470 KeV $\longrightarrow I_f$)* transitions

(20 % error)

Transition	Fraction	Energy (KeV)
$2_3^+ \longrightarrow 2_1^+$	0,458	1096,3
$2_3^+ \longrightarrow 2_2^+$	0,325	656,4
$2_3^+ \longrightarrow 0_g^+$	0,140	1470,1
$2_3^+ \longrightarrow 0_2^+$	0,077	298,8

* Assuming the 1470,1 KeV state a 2^+ state,

the determination of the nuclear model parameters. For that purpose a new computer program was developed and only negative results were found, i.e., there was no solution for the nonlinear system of equations, which is obtained with the inclusion of equations (II-44a) and (II-44c) replacing equations (II-33a) and (II-33b) as conditions for this determination. A solution was found by relaxing the orthogonality conditions through small allowances on the grounds that, in principle, the three states considered do not span the whole space. The predicted attenuation is close to 12%, a value already obtained in reference (1) and using Coulomb Excitation as a test, the intensity of the $(2_3^+ \longrightarrow 0_g^+)$ line is so small that observation is impossible. All the quantities related to this calculation are given in table (II-X). Then, it seems that collective excitations like vibrations are not going to provide the explanation for the ^{110}Pd problem and the only collective phenomena which are left are going to be considered in the next section.

(3) Estimation of the Giant resonance role:

In order to estimate the importance of Giant Resonances, the starting point is the isoscalar sum rule, given by

$$S_{T=0}^{E_L} = \sum_i B(EL, 0 \rightarrow i)\,(E_i - E_0)$$

$$= \frac{L(2L+1)}{4\pi} \frac{\hbar^2}{2M_N} \frac{Z^2}{A} \langle r^{2L-2} \rangle_{00} \qquad \text{(II-54)}$$

where Z is the proton number, A is the nuclear mass number, M_N is the nuclear mass and $\langle \rangle_{00}$ means that the average is taken over the nuclear ground state. In the ^{110}Pd case, we can list these sum rules up to the hexadecapole as:

$$S^{E2}_{T=0} = 318.89 \langle r^2 \rangle_{00} \; e^2 MeV fm^4 \qquad \text{(II-55a)}$$

$$S^{E3}_{T=0} = 669.68 \langle r^4 \rangle_{00} \; e^2 MeV fm^6 \qquad \text{(II-55b)}$$

$$S^{E4}_{T=0} = 1148.02 \langle r^6 \rangle_{00} \; e^2 MeV fm^8 \qquad \text{(II-55c)}$$

In order to estimate the sum rule in equation (II-55a), we make the association

$$\langle r^2 \rangle_{00} = r^2_{RMS} \qquad \text{(II-56)}$$

in ^{110}Pd the r_{RMS} experimental value is 5.75 fm and the sum rule for the quadrupole isoscalar resonance takes the 90% of the sum rule as the highest percentage . We are going to follow this assumption and write:

$$E^{T=0}_{G2} \; B(E2, 0^+ \longrightarrow G2, T=0) = (0.90) \, S^{E2}_{T=0} \qquad \text{(II-57)}$$

where $E_{G2}^{T=0}$ is giving the effective location of the resonance and $B(E2,0^+ \longrightarrow G2,T=0)$ is the effective transition probability. If perturbation theory is used for the calculation of the energy shift, the quadrupole interaction makes a contribution in the second order term as the lowest possible. For the estimation intended in this section our attention is going to be concentrated in this term. This contribution in second order will be maximum if we take the maximum percentage (already taken) with the minimum possible energy $E_{G2}^{T=0}$. For the isoscalar E2 we have

$$E = \frac{k}{A^{1/3}} \qquad \text{(II-59)}$$

which describes the position of the resonance in terms of the energies as a function of the mass number A. The quantity k is a constant ranking between 63 and 65 MeV and we take the energy in equation (II-59) as the effective location $E_{G2}^{T=0}$ for the resonance:

$$E_{G2}^{T=0} = 13.15 \text{ MeV} \qquad \text{(II-60)}$$

and then the effective transition probability is given by

$$B(E2,0^+ \longrightarrow G_2;\ T=0) = 721.60\ e^2 fm^4 \qquad \text{(II-61)}$$

The purpose now is to compare the second order contribution from this resonance with the contribution from the nearly degenerate states which up to this point was the leading one.

Defining:

$$S_1 \equiv \frac{|\langle \widetilde{4f}\ 0^+\ 3 \,|\, \Delta H_{em}^{\pi(2)} \,|\, 3p\ 2_1^+\ 3\rangle|^2}{\mathcal{E}_{4f} - \mathcal{E}_{3p} - E_{2_1^+}} \qquad \text{(II-62)}$$

and

$$S_2 \equiv \frac{|\langle \widetilde{4f}\ 0^+\ 3 \,|\, \Delta H_{em}^{\pi(2)} \,|\, 3p\ G_2^{T=0}\ 3\rangle|^2}{\mathcal{E}_{4f} - \mathcal{E}_{3p} - E_{G_2}^{T=0}} \qquad \text{(II-63)}$$

where the relevant quantities used in equations (II-62) and (II-63) are given in table (II-XI) and the general form of the matrix elements is given by:

$$\langle \tilde{n}\ell\ I\ J \,|\, \Delta H_{em}^{\pi(2)} \,|\, n'\ell'I'J\rangle$$

$$= -\sqrt{\frac{4\pi}{5}}\, e^2\, (-1)^{J+\ell'+\ell+I}\, (2\ell+1)(2I+1)\left[\frac{2\ell'+1}{2J+1}\right]^{1/2}$$

$$\otimes \left[B(E2, I\to I')\right]^{1/2} \begin{pmatrix} \ell & 2 & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \ell & \ell' & 2 \\ I' & I & J \end{Bmatrix} \qquad \text{(II-64)}$$

The numerical evaluation of the absolute ratio gives

$$\left|\frac{S_2}{S_1}\right| = \left|\frac{\mathcal{E}_{4f} - \mathcal{E}_{3p} - E_{2_1^+}}{\mathcal{E}_{4f} - \mathcal{E}_{3p} - E_{G_2}^{T=0}}\right| \left|\frac{B(E2, 0^+\to G_2^{T=0})}{B(E2, 0^+\to 2_1^+)}\right| = 10^{-4} \qquad \text{(II-65)}$$

and defining:

$$S_4 \equiv \frac{|<\widetilde{4f}\ 0^+ 3 \mid \Delta H_{em}^{\pi(2)} \mid 2p\ G_2^{T=0}\ 3>|^2}{\varepsilon_{4f} - \varepsilon_{2p} - E_{G_2}^{T=0}} \qquad (II-66)$$

and

$$S_3 \equiv \frac{|<\widetilde{4f}\ 0^+ 3 \mid \Delta H_{em}^{\pi(2)} \mid 2p\ 2_3^+\ 3>|^2}{\varepsilon_{4f} - \varepsilon_{2p} - E_{2_3^+}} \qquad (II-67)$$

with an absolute ratio in this case given by

$$\left| \frac{S_4}{S_3} \right| = 0.1 \qquad (II-68)$$

Then the possibility of any role for the isoscalar quadrupole resonance is eliminated since the contribution is at most one order of magnitude less than the leading one . The next case to study is the octupole resonance and we have to consider matrix elements of the form:

$$<\widetilde{n\ell}\ IJ \mid \Delta H_{em}^{\pi(3)} \mid n'\ell' I' J>$$

$$= -\sqrt{\frac{4\pi}{7}}\ e^2 (-1)^{J+\ell'+\ell+I}\ (2\ell+1)(2I+1)\left[\frac{2\ell'+1}{2J+1}\right]^{1/2}$$

$$\otimes \left[B(E3, I \to I')\right]^{1/2} \begin{pmatrix} \ell & 3 & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \ell & \ell' & 3 \\ I' & I & J \end{Bmatrix}$$

$$\otimes \int_0^\infty \frac{1}{r^2} R_{n\ell} R_{n'\ell'}\, dr \qquad (II-69)$$

TABLE (II-X)

Results for the three phonon model in ^{110}Pd taking into account experimental information from the 1470 KeV state.

Define: $\vec{A} \equiv (\alpha_1, \alpha_2, \alpha_3)$ $\vec{B} \equiv (\beta_1, \beta_2, \beta_3)$ $\vec{C} \equiv (\gamma_1, \gamma_2, \gamma_3)$

$\alpha_1 = 0,9965$	$\beta_1 = 0,1220$	$\gamma_1 = 0,0622$
$\alpha_2 = -0,1600$	$\beta_2 = 0,9635$	$\gamma_2 = -0,0100$
$\alpha_3 = -0,1600$	$\beta_3 = 0,1300$	$\gamma_3 = 0,975$
	$\chi_2 = 0,0835$	
$\lvert\vec{A}\rvert = 1,0442$	$\lvert\vec{B}\rvert = 0,9601$	$\lvert\vec{C}\rvert = 0,9644$
$\vec{A}.\vec{B} = -0,0534$	$\vec{A}.\vec{C} = -0,0780$	$\vec{B}.\vec{C} = 0,0380$

(in e^2fm^4 units)

$B(E2, 2_1^+ \longrightarrow 0_g^+) = 1480$

$B(E2, 2_2^+ \longrightarrow 2_1^+) = 2100$

$B(E2, 2_2^+ \longrightarrow 0_g^+) = 26,4$

$B(E2, 2_3^+ \longrightarrow 0_g^+) = 5,58$

$B(E2, 2_3^+ \longrightarrow 2_1^+) = 99,72$

$B(E2, 2_3^+ \longrightarrow 2_2^+) = 878,8$

Ratios

$B(E2, 2_3^+ \longrightarrow 2_2^+)/B(E2, 2_3^+ \longrightarrow 2_1^+) = 8,813$

$B(E2, 2_3^+ \longrightarrow 0_g^+)/B(E2, 2_3^+ \longrightarrow 2_1^+) = 0.026$

(in barns units)

$Q_{374} = -32,47$ $Q_{814} = 36,67$ $Q_{1470} = -10.34$

Predicted Attenuation: 12 %

TABLE (II-XI)

Energies:

$\mathcal{E}_{4f} = (-493{,}27 - i\ 0{,}94\times10^{-3})$ KeV

$\mathcal{E}_{3p} = (-873{,}62 - i\ 16{,}25)$ KeV

$\mathcal{E}_{2p} = (-1962{,}40 - i\ 47{,}28)$ KeV

$E_{2_1^+} = 373{,}8$ KeV $\qquad E_{2_3^+} = 1470{,}1$ KeV

Transition Probabilities:

$B(E2, 0^+ \longrightarrow 2_3^+) = 28{,}5\ e^2fm^4$

$B(E2, 0^+ \longrightarrow 2_1^+) = 8600\ e^2fm^4$

$B(E2, 0^+ \longrightarrow 3^+) = 85402\ e^2fm^6$

Overlap Integrals:

$$\int_0^\infty \frac{1}{r} R_{4f}\, R_{3p}\, dr = (-2{,}5991\times10^{-6} - i\ 2{,}254\times10^{-7})\ fm^{-3}$$

$$\int_0^\infty \frac{1}{r^2} R_{4f}\, R_{1s}\, dr = (0{,}8403\times10^{-6} + i\ 0{,}8452\times10^{-7})\ fm^{-4}$$

$$\int_0^\infty \frac{1}{r^2} R_{1s}\, R_{1s}\, dr = (0{,}4566\times10^{-3} + i\ 0{,}3602\times10^{-2})\ fm^{-4}$$

$$\int_0^\infty \frac{1}{r} R_{3p}\, R_{3p}\, dr = (1{,}1356\times10^{-4} + i\ 3{,}536\times10^{-5})\ fm^{-3}$$

(the Overlap Integrals were calculated with the PIATOM code)

All the relevant quantities related to the calculation of the matrix elements are given in table (II-XI) and the results are:

$$\langle 4f\ 0^+3|\Delta Hem^{\pi}(2)|\ 3p\ 2_1^+3\rangle = 0.1248 + i0.0112\ KeV \qquad (II\text{-}70a)$$

$$\langle 4f\ 0^+3|\Delta Hem^{\pi}(3)|\ 1S\ 3^-3\rangle = -0.0677 + i0.0068\ KeV \qquad (II\text{-}70b)$$

and finally if we consider the ratio:

$$\left|\frac{\langle \widetilde{4f}\ 0^+3|\Delta H_{em}^{\pi(2)}|3p\ 2_1^+3\rangle}{\mathcal{E}_{4f0^+}-\mathcal{E}_{3p2_1^+}}\right|^2 \Big/ \left|\frac{\langle \widetilde{4f}\ 0^+3|\Delta H_{em}^{\pi(3)}|1S\ 3^-3\rangle}{\mathcal{E}_{4f0^+}-\mathcal{E}_{1S3^-}}\right|^2 = 113.1 \qquad (II\text{-}71)$$

Then even in this case the contribution from the isoscalar resonance is two orders of magnitude less than the leading contribution.

The conclusion at this point is that nuclear structure is not going to offer a possible explanation, for the phenomenon observed with attenuation (and then the widths) in ^{110}Pd. In consequence our strategy has to run to the issue of the optical potential, as it seems that the cause of the problem is located there.

REFERENCES FOR CHAPTER II

(1) J.F.Dubach,E.J.Moniz,G.D.Nixon,Phys.Rev.C,Vol.20, p.725,1979

(2) R.L.Robinson,F.K.Gowan,P.H.Stelson,W.T.Milner,R.O. Sayer,Nuc.Phys. A124.p.553,1969

(3) L.I.Govor,A.M.Demidov,I.B.Shukalov,Nuc.Phys.A245,p.13, 1975

(4) I.N.Borzov,S.P.Kamerdzhiev,Izvestiya Akademii Nauk SSSR.Seriya Fizicheskaya Vol.41,p.4,1977

(6) M.Leon,Nuc.Phys. A260,p.461,1976

(7) M.Leon,Proceedings of the LAMPF Summer School on Nuclear Structure with pions and protons 1977,R.L.Burman and B.F.Gibson Eds.(LAMPF,Los Alamos,N.M.,1977)

(8) M.Leon et al.,Phys.Rev.Lett.,Vol.37,p.1135,1976

(9) R.L.Robinson et al.,Phys.Rev.Lett.,Vol.187,p.1609,1969

(10) Nuclear Data Sheets,Vol.22,p.163,1977

(11) J.A.Deye,R.L.Robinson,J.L.C.Ford,Nuc.Phys.A204,307,1973

(12) J.A.Pinston,F.Schussler,Nuc.Phys.A144,P.42,1970

(13) R.P.Harper,A.Christy,I.Hall,I.M.Naqib,B.Wakefield,Nuc. Phys,A162,p.161,1971

(14) R.Beyer,R.P.Scharenberg,J.Thomson,Phys.Rev.C2,1469,1970

(15) G.D.Nixon (private communication)

(16) S.Steadman (private communication)

(17) G.Bertolini,A.Coche,Semiconductor Detectors,Wiley 1968

CHAPTER III

DOORWAY STATE APPROCH TO BOUND STATE PERTURBATION THEORY

The Doorway State Approach to optical potential scattering developed in reference (1) is going to give us an alternative treatment of the energy shifts and widths in pionic atoms, putting the strong interaction dynamics and the rescattering process on the same footing. With this method the essential physics of the problem can be obtained with few doorway states and sometimes with just the first one. The original formalism was applied to problems with asymtotic boundary conditions for the energy and it should be modified and extended in order to treat bound state problems, like the pionic atom case. This modification is going to be considered in this chapter and in order to test and demonstrate the power of the method, some simple examples will be studied at the end.

(1) A different approach to bound state perturbation theory

It is useful at this point to review perturbation theory and the first step is the consideration of the eigenvalue problem:

$$H|\psi_\tau\rangle = E_\tau|\psi_\tau\rangle \qquad \text{(III-1)}$$

where H is the Hamiltonian operator given by

$$H = H_o + V_2 \qquad \text{(III-2)}$$

where V_2 is a perturbation and

$$H_o = T + V_1 \qquad \text{(III-3)}$$

is the unperturbed or model Hamiltonian related to the eigenvalue problem that can be solved exactly, being T the kinetic energy operator and V_1 the basic interaction. The eigenvalue problem

$$H_o|\tau\rangle = \epsilon_\tau|\tau\rangle \qquad \text{(III-4)}$$

is known and V_2 is taken in such a way that there is a one-to-one correspondence between the states $|\tau\rangle$ and the states $|\psi_\tau\rangle$. For the moment, degenerate cases are set aside. From equation (III-1) the energy shift can be obtained, with the result

$$\Delta\mathcal{E}_\tau = \frac{\langle\tau|V_2|\psi_\tau\rangle}{\langle\tau|\psi_\tau\rangle} \qquad \text{(III-5)}$$

In order to provide an expression for this energy shift in terms of the information from the unperturbed system and the exact energy, a formal solution for $|\psi_\tau\rangle$ has to be given. Using the closure relation for the unperturbed states, $|\psi_\tau\rangle$ can be written as

$$|\psi_\tau\rangle = \langle\tau|\psi_\tau\rangle|\tau\rangle + \sum_{m\neq\tau} |m\rangle\langle m|\psi_\tau\rangle \qquad \text{(III-6)}$$

From equation (III-1) it can be seen that

$$\langle m|\psi_\tau\rangle = \frac{1}{E_\tau - \epsilon_m}\langle m|V_2|\psi_\tau\rangle \qquad \text{(III-7)}$$

and

$$\sum_{m\neq\tau} |m\rangle\langle m|\psi_\tau\rangle = \sum_{m\neq\tau} |m\rangle \frac{1}{E_\tau - \epsilon_m}\langle m|V_2|\psi_\tau\rangle \qquad \text{(III-8)}$$
$$= G_o(E_\tau) Q_\tau V_2 |\psi_\tau\rangle$$

where Q_τ projects out the eigenstate $|\tau\rangle$ and the Green's Function $G_o(E_\tau)$ is given by

$$G_o(E_\tau) \equiv \sum_m \frac{|m\rangle\langle m|}{E_\tau - \epsilon_m} = \frac{1}{E_\tau - H_o} \qquad \text{(III-9)}$$

Replacing (III-8) in (III-6) and assuming that inverses exist, $|\psi_\tau\rangle$ can be written as

$$|\psi_\tau\rangle = \frac{1}{1 - G_o(E_\tau) Q_\tau V_2}|\tau\rangle\langle\tau|\psi_\tau\rangle \qquad \text{(III-10)}$$

Now equation (III-10) can be replaced in (III-5) with the result

$$\Delta\mathcal{E}_\tau = \langle\tau| V_2 \frac{1}{1 - G_o(E_\tau) Q_\tau V_2} |\tau\rangle \qquad \text{(III-11)}$$

And it should be noted that the quantity $\langle\tau|\psi_\tau\rangle$ cancels exactly. The state $|\psi_\tau\rangle$ is not normalized and equation (III-10) can be written as

$$|\psi_\tau\rangle = N_\tau \frac{1}{1 - G_o(E_\tau) Q_\tau V_2} |\tau\rangle \qquad \text{(III-12)}$$

is the normalization constant to be determined, provided the formal problem given by equation (III-12) can be solved.

Equations (III-10) and (III-12) give us, in a compact form, the Brillouin-Wigner perturbation theory results [2,3]. The energy shift is usually expressed in terms of a perturbation series, which can be obtained by expanding equation (III-11) in

$$\Delta\mathcal{E}_\tau = \langle\tau| V_2 |\tau\rangle + \langle\tau| V_2 G_o(E_\tau) Q_\tau V_2 |\tau\rangle + \ldots \qquad \text{(III-13)}$$

At the same time equation (III-11) has a structure that can be treated adequately using the Doorway State Formalism [1], since it can be written as

$$\Delta\mathcal{E}_\tau = \langle\tau|\sqrt{V_2}\ \frac{1}{1-\sqrt{V_2}\,G_o(E_\tau)\,Q_\tau\sqrt{V_2}}\sqrt{V_2}\,|\tau\rangle \qquad \text{(III-14)}$$

and we can speak about doorway states in the same sense as in reference[1], being the main difference the rescattering operator given by

$$W \equiv \sqrt{V_2}\,G_o(E_\tau)\,Q_\tau\sqrt{V_2} \qquad \text{(III-15)}$$

where the Green's Function was replaced by the Reduced Green's Function:

$$\vartheta(E_\tau) \equiv G_o(E_\tau)\,Q_\tau = G_o(E_\tau) - \frac{|\tau\rangle\langle\tau|}{\Delta\mathcal{E}_\tau} \qquad \text{(III-16)}$$

The starting vectors in the doorway basis are naturally given by[1]

$$|\mathcal{D}_o\rangle \equiv N_o\sqrt{V_2}\,|\tau\rangle \qquad |\widetilde{\mathcal{D}_o}\rangle \equiv \widetilde{N}_o\,(\sqrt{V_2})^\dagger|\tau\rangle \qquad \text{(III-17)}$$

and the biorthogonal basis is constructed in the following way[1]:

$$|\mathcal{D}_n\rangle \equiv N_n\left\{W|\mathcal{D}_{n-1}\rangle - \sum_{j=o}^{n-1}\langle\widetilde{\mathcal{D}_j}|W|\mathcal{D}_{n-1}\rangle|\mathcal{D}_j\rangle\right\} \qquad \text{(III-18)}$$

$$|\tilde{\mathcal{D}}_n\rangle \equiv \tilde{N}_n \left\{ W^+ |\tilde{\mathcal{D}}_{n-1}\rangle - \sum_{j=0}^{n-1} \langle \mathcal{D}_j | W^+ |\tilde{\mathcal{D}}_{n-1}\rangle |\tilde{\mathcal{D}}_j\rangle \right\}$$

This construction is also known as the Lanczos construction or Lanczos method[4] for matrix diagonalization. The W operator is tridiagonal in this basis, i.e.,

$$\langle \tilde{\mathcal{D}}_n | W | \mathcal{D}_m \rangle \neq 0 \quad \text{if} \quad |n-m| \leq 1 \qquad \text{(III-19)}$$

and this property allows us to write the energy shift as a continued fraction:

$$\Delta\mathcal{E}_\Gamma = (\tilde{N}_0^* N_0)^{-1} \sigma_{00} = \cfrac{(\tilde{N}_0^* N_0)^{-1}}{1 - W_{00} - \cfrac{W_{01} W_{10}}{1 - W_{11} - \cdots}} \cdots \qquad \text{(III-20)}$$

where the following definitions were used:

$$W_{nm} \equiv \langle \tilde{\mathcal{D}}_n | W | \mathcal{D}_m \rangle \qquad \text{(III-21)}$$

$$\sigma_{nm} \equiv \langle \tilde{\mathcal{D}}_n | \frac{1}{1-W} | \mathcal{D}_m \rangle \qquad \text{(III-22)}$$

The first order perturbation theory term is related to the first doorway state normalization through the equation:

$$(\tilde{N}_o^* N_o)^{-1} = \langle T | V_2 | T \rangle \qquad \text{(III-23)}$$

In this representation the perturbed wavefunction has a simple structure when it is calculated in the interaction region. Using equation (III-12), the result is

$$N_o \sqrt{V_2} |\psi_T\rangle = N_T N_o \sqrt{V_2} \frac{1}{1 - \vartheta(E_T) V_2} |T\rangle$$

$$= N_T N_o \frac{1}{1 - \sqrt{V_2}\, \vartheta(E_T) \sqrt{V_2}} \sqrt{V_2} |T\rangle = N_T \sum_n G_{no} |D_n\rangle \qquad \text{(III-24)}$$

Up to now, we were working under the assumption that the perturbation V_2 can be factorized as a product of two square roots. In the case of non-local interactions this kind of factorization may be difficult since the solution of a nonlinear integral equation is required:

$$V(\vec{r}, \vec{r}') = \int d\vec{r}'' \, \psi(\vec{r}, \vec{r}'') \psi(\vec{r}'', \vec{r}') \qquad \text{(III-25)}$$

this problem can be solved [1] by noting that the square root is not needed and a simple product representation can be taken for the same purpose:

$$V \equiv \tilde{\mathcal{J}} \cdot \mathcal{J} \qquad \text{(III-26)}$$

In this case, the doorway basis and its dual can be built from two different starting vectors

$$|\mathcal{D}_0\rangle \equiv N_0 \mathcal{J} |T\rangle \qquad |\tilde{\mathcal{D}}_0\rangle \equiv \tilde{N}_0 \tilde{\mathcal{J}}^+ |T\rangle \qquad \text{(III-27)}$$

With the rescattering operator

$$W = \mathcal{J} \vartheta(E_T) \tilde{\mathcal{J}} \qquad \text{(III-28)}$$

The method developed so far in this section for the calculations of the energy shifts and wavefunctions assumes that E_T, the exact energy, is known. In standard problems this is not the case and all the previous formalism can be useful if a self-consistent calculation is practical in terms of computer time. This is possible when the convergence is very strong and with few doorways the required accuracy is achieved. If the convergence is such that many doorways have to be used to achieve the required accuracy then the calculation turns to be inpractical and a different approach should be called for. This approach can be based on the Rayleigh-Schroedinger perturbation theory where the

energy shift and wavefunction can be obtained from information coming only from the unperturbed system. This will be the topic of the next section.

(2) Rayleigh-Schroedinger perturbation theory and the Doorway State Approach

The Rayleigh-Schroedinger perturbation theory can be obtained in a compact form by noting that equation (III-7) can be rewritten as

$$\langle m|\psi_\tau\rangle = \frac{1}{E_\tau - \epsilon_m}\langle m|V_2|\psi_\tau\rangle = \frac{1}{\epsilon_\tau - \epsilon_m}\langle m|(V_2 - \Delta\mathcal{E}_\tau)|\psi_\tau\rangle \quad \text{(III-29)}$$

which is essentially a shift in the energies. Using equation (III-29) in (III-6), the perturbed wavefunction is given by

$$|\psi_\tau\rangle = \langle\tau|\psi_\tau\rangle \frac{1}{1 - \vartheta(\epsilon_\tau)(V_2 - \Delta\mathcal{E}_\tau)}|\tau\rangle \quad \text{(III-30)}$$

where

$$\vartheta(\epsilon_\tau) \equiv \sum_{m\neq\tau} \frac{|m\rangle\langle m|}{\epsilon_\tau - \epsilon_m} = G_o(\epsilon_\tau)Q_\tau \quad \text{(III-31)}$$

is the reduced Green's Function. Replacing (III-30) in (III-5), the result is

$$\Delta\mathcal{E}_\tau = \langle\tau|V_2 \frac{1}{1 - \vartheta(\epsilon_\tau)(V_2 - \Delta\mathcal{E}_\tau)} |\tau\rangle \qquad \text{(III-32)}$$

and we can rewrite (III-30) as

$$|\psi_\tau\rangle = N_\tau \frac{1}{1 - \vartheta(\epsilon_\tau)(V_2 - \Delta\mathcal{E}_\tau)} |\tau\rangle \qquad \text{(III-33)}$$

Equations (III-32) and (III-33) give us the Rayleigh-Schroedinger perturbation theory. It should be noted that the self-consistency in the calculation of the energy shift $\Delta\mathcal{E}_\tau$ is still present. An expansion in powers of $\Delta\mathcal{E}_\tau$ can be performed on the right hand side of equations (III-32) and (III-33) and the coefficients of such expansion are going to be functions of the information related to the unperturbed system and they can be found once, making the self-consistent calculation trivial. The expansion of equation (III-32) in powers of $\Delta\mathcal{E}_\tau$ is completely equivalent to the expansion of equation (III-14) around ϵ_τ and evaluated for the energy E_τ:

$$\Delta\mathcal{E}_\tau = (\tilde{N}_o^* N_o)^{-1} \left\{ \sigma_{oo}(\epsilon_\tau) + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n \sigma_{oo}(\mathcal{E})}{\partial \mathcal{E}^n} \Big|_{\mathcal{E}=\epsilon_\tau} \Delta\mathcal{E}_\tau^n \right\} \qquad \text{(III-34)}$$

or for better convergence:

$$\Delta\epsilon_T = \frac{(\tilde{N}_o^* N_o)^{-1}\ \sigma_{oo}(\epsilon_T)}{1 - (\tilde{N}_o^* N_o)^{-1} \sum_{n=1}^{\infty} \frac{1}{n!} \left.\frac{\partial^n \sigma_{oo}(\varepsilon)}{\partial \varepsilon^n}\right|_{\varepsilon=\epsilon_T} \Delta\epsilon_T^{\,n-1}} \qquad \text{(III-35)}$$

and $\sigma_{oo}(\varepsilon)$ is given by

$$\sigma_{oo}(\varepsilon) \equiv \langle \tilde{D}_o | \frac{1}{1 - \sqrt{V_2}\,\vartheta(\varepsilon)\sqrt{V_2}} | D_o \rangle \qquad \text{(III-36)}$$

It is convenient to introduce the definitions:

$$w(\varepsilon) \equiv \sqrt{V_2}\,\vartheta(\varepsilon)\sqrt{V_2} \equiv w^{(1)}(\varepsilon) \qquad \text{(III-37)}$$

$$w^{(k)}(\varepsilon) \equiv \sqrt{V_2}\,\vartheta^k(\varepsilon)\sqrt{V_2} \qquad \text{(III-38)}$$

$$\sigma^{(1)} \equiv \frac{1}{1 - w(\varepsilon)} \qquad \text{(III-39)}$$

$$S^{(k)} \equiv w^{(k)}\,\sigma^{(1)} \qquad \text{(III-40)}$$

and from equation (III-38) we obtain

$$\left.\frac{\partial^n w(\varepsilon)}{\partial \varepsilon^n}\right|_{\varepsilon=\epsilon_T} = (-1)^n w^{(n+1)}(\epsilon_T) \qquad \text{(III-41)}$$

Using equations (III-36) through (III-41) we can see that higher derivatives of $\sigma_{oo}(\varepsilon)$ can be found by means of recursion relations. For example, the first derivative is obtained from:

$$\sigma^{(2)} \equiv \sigma' = -\sigma^{(1)} w^{(2)} \sigma^{(1)} = -\sigma^{(1)} S^{(2)} \qquad \text{(III-42)}$$

and in the same way:

$$\sigma^{(3)} \equiv \frac{1}{2!}\sigma'' = \sigma^{(1)} w^{(2)} \sigma^{(1)} w^{(2)} \sigma^{(1)} + \sigma^{(1)} w^{(3)} \sigma^{(1)}$$

$$= -\sigma^{(2)} S^{(2)} + \sigma^{(1)} S^{(3)} \qquad \text{(III-43)}$$

$$\sigma^{(4)} \equiv \frac{1}{3!}\sigma''' = -\Big\{ \sigma^{(1)} w^{(2)} \sigma^{(1)} w^{(2)} \sigma^{(1)} w^{(2)} \sigma^{(1)}$$

$$+ \sigma^{(1)} w^{(3)} \sigma^{(1)} w^{(2)} \sigma^{(1)} + \sigma^{(1)} w^{(2)} \sigma^{(1)} w^{(3)} \sigma^{(1)} + \sigma^{(1)} w^{(4)} \sigma^{(1)} \Big\}$$

$$= -\sigma^{(3)} S^{(2)} + \sigma^{(2)} S^{(3)} - \sigma^{(1)} S^{(4)} \qquad \text{(III-44)}$$

$$\sigma^{(5)} = -\sigma^{(4)} S^{(2)} + \sigma^{(3)} S^{(3)} - \sigma^{(2)} S^{(4)} + \sigma^{(1)} S^{(5)} \qquad \text{(III-44a)}$$

and in general

$$\sigma^{(N)} \equiv \frac{1}{(N-1)!} \left. \frac{\partial^{N-1} \sigma(\varepsilon)}{\partial \varepsilon^{N-1}} \right|_{\varepsilon = \epsilon_T} \qquad \text{(III-45)}$$

$$= \sum_{M=2}^{N} (-1)^{M+1} \sigma^{(N+1-M)} S^{(M)} \qquad \text{(III-46)}$$

Equation (III-35) can be rewritten as:

$$\Delta\mathcal{E}_\tau = \frac{(\tilde{N}_o^* N_o)^{-1}\ \sigma_{oo}^{(1)}(\epsilon_\tau)}{1 - (\tilde{N}_o^* N_o)^{-1} \sum_{n=2}^{\infty} \sigma_{oo}^{(n)}(\epsilon_\tau)\ \Delta\mathcal{E}_\tau^{n-2}} \qquad \text{(III-47)}$$

In the construction of the doorway basis the matrix elements $w_{nm}^{(1)}$ are found and σ_{oo} can be calculated as a continued fraction[1]. To obtain all the $\sigma_{nm}^{(1)}$ the following recursion relation has to be used[1]

$$\sigma^{(1)} = \frac{1}{1-w} = 1 + w\,\frac{1}{1-w} = 1 + w\,\sigma^{(1)} \qquad \text{(III-48)}$$

If we have the doorway basis, the calculation of the matrix elements:

$$w_{nm}^{(k)} \equiv \langle \tilde{\mathcal{D}}_n \mid w^{(k)} \mid \mathcal{D}_m \rangle \qquad \text{(III-49)}$$

is necessary to obtain the $S_{nm}^{(k)}$ matrix elements. At this point the calculation could be expensive in terms of computer time, and it is therefore important to keep the $\Delta\mathcal{E}_\tau$ powers to a minimum. Fortunately in most practical applications very high powers in the energy shifts are not needed. Once the $S_{nm}^{(k)}$ matrix elements are calculated, equation (III-46) can be used to generate all the necessary $\sigma_{nm}^{(N)}$. As a byproduct, the wavefunction in the interaction region can be found through a similar expansion:

$$N_o \sqrt{V_2}\, |\psi_T\rangle = N_T \sum_{n=0}^{\infty} \sum_{m=1}^{\infty} \Delta\mathcal{E}_T^{m-1}\, \sigma_{no}^{(m)}(\epsilon_T)\, |\mathcal{D}_n\rangle \qquad \text{(III-50)}$$

in terms of both powers of the energy shift and the doorway basis $\{|\mathcal{D}_n\rangle\}$. The only one quantity that has to be determined a posteriori is the normalization N_T and this can be done through equation (III-50), giving

$$|N_T|^2 \equiv \left[\sum_{n=0}^{\infty} |\vartheta_n(\epsilon_T)|^2\right]^{-1} \qquad \text{(III-51)}$$

and

$$\vartheta_n(\epsilon_T) \equiv \sum_{m=1}^{\infty} \Delta\mathcal{E}_T^{m-1}\, \sigma_{no}^{(m)}(\epsilon_T) \qquad \text{(III-52)}$$

Standard perturbation theory fails in providing a good representation for the perturbed wavefunction and it will be interesting to study what equation (III-50) has to offer in that respect. This will be done at the end of this chapter with simple examples where the exact solution is known.

Another interesting byproduct is the perturbed Green's Function in the interaction region. To see this we consider the equation for the full Green's Function:

$$G(\varepsilon) = G_o(\varepsilon) + G_o(\varepsilon) V_2 G(\varepsilon) \qquad \text{(III-53)}$$

Multiplying from the left by $Q_\tau \equiv 1 - P_\tau$, (P_τ projects onto the state $|\tau\rangle$, eigenstate of H_o)

$$H_o |\tau\rangle = \epsilon_\tau |\tau\rangle \qquad \text{(III-54)}$$

and

$$G_o(\varepsilon) = \frac{1}{\varepsilon - H_o} \qquad \text{(III-55)}$$

we obtain

$$Q_\tau G(\varepsilon) = \vartheta(\varepsilon) + \vartheta(\varepsilon) V_2 G(\varepsilon) \qquad \text{(III-56)}$$

where $\vartheta(\varepsilon)$ is the Reduced Green's Function:

$$\vartheta(\varepsilon) \equiv Q_\tau G_o(\varepsilon) = \sum_{m \neq \tau} \frac{|m\rangle\langle m|}{\varepsilon - \varepsilon_m} \qquad \text{(III-57)}$$

Solving equation (III-56) from the formal point of view we get

$$G(\varepsilon) = \frac{1}{1 - P_\tau - \vartheta(\varepsilon) V_2} \vartheta(\varepsilon) \qquad \text{(III-58)}$$

Expanding $G(\varepsilon)$ in terms of $P_\tau + \vartheta(\varepsilon)V_2$ we see that

$$G(\varepsilon) = \frac{1}{1 - \vartheta(\varepsilon)\, V_2}\, \vartheta(\varepsilon) \qquad \text{(III-59)}$$

As in the case of the energy shift and the wave-function, we can expand (III-59) around ϵ_τ and evaluate it for arbitrary ε such that

$$\Delta\varepsilon \equiv \varepsilon - \epsilon_\tau$$

and

$$G(\varepsilon) = \frac{1}{1 - \vartheta(\epsilon_\tau)\, V_2}\, \vartheta(\epsilon_\tau) - \frac{1}{1 - \vartheta(\epsilon_\tau)\, V_2}\, \vartheta(\epsilon_\tau) \frac{1}{1 - \vartheta(\epsilon_\tau) V_2}\, \vartheta(\epsilon_\tau)\Delta\varepsilon$$

$$+ \frac{1}{1 - \vartheta(\epsilon_\tau) V_2}\, \vartheta(\epsilon_\tau) \frac{1}{1 - \vartheta(\epsilon_\tau)\, V_2}\, \vartheta(\epsilon_\tau) \frac{1}{1 - \vartheta(\epsilon_\tau)\, V_2}\, \vartheta(\epsilon_\tau)\, \Delta\varepsilon^2 + \cdots$$

(III-60)

In the interaction region we have two alternative expressions:

$$\sqrt{V_2}\, G(\varepsilon) = \sum_{n=1}^{\infty} 6^{(n)}(\epsilon_\tau)\, \Delta\varepsilon^{n-1}\, \sqrt{V_2}\, \vartheta(\epsilon_\tau) \qquad \text{(III-61)}$$

$$\sqrt{V_2}\, G(\varepsilon) \sqrt{V_2} = \left[\sum_{n=1}^{\infty} \sigma^{(n)}(\epsilon_\tau)\, \Delta\varepsilon^{n-1} \right] \mathcal{W} \qquad \text{(III-62)}$$

We are going to explore equation (III-62) in a simple example where the full Green's Function is well known: Harmonic oscillator with a harmonic perturbation. This will be done at the end of this chapter.

(3) Representations of the Reduced Green's Function and methods for its calculation in applications

The Reduced Green's Function is defined by

$$\vartheta(\varepsilon) \equiv \sum_{m \neq \tau} \frac{|m\rangle\langle m|}{\varepsilon - \epsilon_m} = G_0(\varepsilon) - \frac{|\tau\rangle\langle\tau|}{\varepsilon - \epsilon_\tau} \qquad \text{(III-63)}$$

Equation (III-63) is the form used in Brillouin-Wigner Theory for the self-consistent calculations. When we follow the approach based on the Schroedinger-Rayleigh Theory, equation (III-63) becomes a limit:

$$\vartheta(\epsilon_\tau) \equiv \lim_{\varepsilon \to \epsilon_\tau} \left\{ G_0(\varepsilon) - \frac{|\tau\rangle\langle\tau|}{\varepsilon - \epsilon_\tau} \right\} \qquad \text{(III-64)}$$

From the operational point of view, equation (III-64) can be rewritten in a more convenient form as

$$\vartheta(\epsilon_\tau) = \lim_{\varepsilon \to \epsilon_\tau} \frac{d}{d\varepsilon} \left\{ (\varepsilon - \epsilon_\tau)\, G_0(\varepsilon) \right\} \qquad \text{(III-65)}$$

to the equation (III-65) we give the special name of differential representation. It is also possible to obtain an Integral representation:

$$\vartheta(\epsilon_\tau) \equiv \frac{1}{2\pi i} \oint_{C_\tau} \frac{G_o(\mathcal{E})}{\mathcal{E} - \epsilon_\tau} \, d\mathcal{E} \qquad \text{(III-66)}$$

where the closed contour contains the point $\mathcal{E} = \epsilon_\tau$. Our choice of the particular representation will depend on the particular problem at hand.

An alternative method to the previous two, which is going to be used in the next chapters, is based on the fact that once we have the unperturbed state and the corresponding eigenvalue ϵ_τ, we have all the necessary information required in the calculation of the Reduced Green's Function. This feature can be shown by looking at the simple case of a spherical local potential. There the differential equation for the radial part of the Reduced Green's Function is given by

$$\left\{ \mathcal{E}_{n\ell} + \frac{1}{2\mu}\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{2\mu r^2} + V_1(r) \right\} \widetilde{\vartheta}_{n\ell}(r,r') = \delta(r-r') - r\phi_{n\ell}(r)\phi_{n\ell}(r')r' \qquad \text{(III-67)}$$

At the same time the Schroedinger equation gives us

$$\left\{ \varepsilon_{n\ell} + \frac{1}{2\mu} \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{2\mu r^2} + V_1(r) \right\} \phi_{n\ell}(r) = 0 \qquad \text{(III-68)}$$

In equation (III-67) and (III-68) we will write the radial parts in the following way:

$$\vartheta_{n\ell}(r,r') = \frac{\tilde{\vartheta}_{n\ell}(r,r')}{rr'} \qquad \text{(III-69)}$$

$$\phi_{n\ell}(r) = \frac{u_{n\ell}(r)}{r} \qquad \text{(III-70)}$$

Now the Reduced Green's Function is factorized in the following way:

$$\tilde{\vartheta}_{n\ell}(r,r') = r\, \phi_{n\ell}(r)\, m_{n\ell}(r,r')\, \phi_{n\ell}(r')\, r' \qquad \text{(III-71)}$$

Replacing equation (III-71) in equation (III-67) and using equation (III-68) we get:

$$\frac{1}{\mu} \frac{d}{dr} \left(r\, \phi_{n\ell}(r) \right) \frac{d}{dr} m_{n\ell}(r,r')\, \phi_{n\ell}(r')\, r' + r\, \phi_{n\ell}(r) \frac{d^2}{dr^2} m_{n\ell}(r,r')\, \phi_{n\ell}(r')\, r' = \delta(r-r') - r\, \phi_{n\ell}(r)\, \phi_{n\ell}(r')\, r' \qquad \text{(III-72)}$$

If we multiply equation (III-72) on the left by $r\, \phi_{n\ell}(r)$, the factor $\phi_{n\ell}(r')\, r'$ can be cancelled due to the presence of the Dirac's Delta Function and

$$\frac{1}{2\mu}\frac{d}{dr}\left\{r^2\phi_{n\ell}^2(r)\frac{d}{dr}m_{n\ell}(r,r')\right\} = \delta(r-r') - r^2\phi_{n\ell}^2(r) \qquad \text{(III-73)}$$

Equation (III-73) can be decomposed in two equations that can be solved in sequence:

$$\frac{d}{dr}h_{n\ell}(r,r') = 2\mu\,\delta(r-r') - 2\mu\, r^2\phi_{n\ell}^2(r) \qquad \text{(III-74)}$$

$$r^2\phi_{n\ell}^2(r)\frac{d}{dr}m_{n\ell}(r,r') = h_{n\ell}(r,r') \qquad \text{(III-75)}$$

Equation (III-74) has the following boundary condition:

$$h_{n\ell}(0,r') = 0 \qquad \text{(III-76)}$$

and solving for $h_{n\ell}(r,r')$, the result is:

$$h_{n\ell}(r,r') = 2\mu\,\theta(r-r') - 2\mu\int_0^r t^2\phi_{n\ell}^2(t)\,dt \qquad \text{(III-77)}$$

from equation (III-75) we obtain:

$$\frac{d}{dr}m_{n\ell}(r,r') = \frac{2\mu}{r^2\phi_{n\ell}^2(r)}\theta(r-r') - \frac{2\mu}{r^2\phi_{n\ell}^2(r)}\int_0^r t^2\phi_{n\ell}^2(t)\,dt \qquad \text{(III-78)}$$

We introduce the following definitions

$$m_{ne}(r,r') = \begin{cases} m_{ne}^{>}(r,r') & \text{if} \quad r > r' \\ m_{ne}^{<}(r,r') & \text{if} \quad r < r' \end{cases} \qquad \text{(III-79)}$$

and from equation (III-78) by integrating between and and conversely, we get

$$m_{ne}^{>}(r,r') - m_{ne}^{>}(r,r')$$

$$= 2\mu \int_{r'}^{r} \frac{dt}{t^2 \phi_{ne}^2(t)} - 2\mu \int_{r'}^{r} \frac{dy}{y^2 \phi_{ne}^2(y)} \int_0^y t^2 \phi_{ne}^2(t)\, dt \qquad \text{(III-80)}$$

$$m_{ne}^{<}(r',r') - m_{ne}^{<}(r,r')$$

$$= -2\mu \int_{r}^{r'} \frac{dy}{y^2 \phi_{ne}^2(y)} \int_0^y t^2 \phi_{ne}^2(t)\, dt \qquad \text{(III-81)}$$

From the continuity condition for the Reduced Green's Function, i.e.,

$$\tilde{\theta}_{ne}(r,r')\Big|_{r=r'^{+}} = \tilde{\theta}_{ne}(r,r')\Big|_{r=r'^{-}} \qquad \text{(III-82)}$$

where $r'^{+} = r' + \delta$ and $r'^{-} = r' - \delta$ with $\delta \to 0$ Equation (III-82) is equivalent to

$$m_{ne}^{>}(r',r') = m_{ne}^{<}(r',r') = C_0(r') \qquad \text{(III-83)}$$

Using the normalization condition for $\phi_{ne}(r)$:

$$\int_0^y t^2 \phi_{n\ell}^2(t)\, dt = 1 - \int_y^\infty t^2 \phi_{n\ell}^2(t)\, dt \qquad \text{(III-84)}$$

and equation (III-83) in equation (III-80), we obtain:

$$M_{n\ell}^{>}(r,r') = C_0(r') + 2\mu \int_{r'}^{r} \frac{dy}{y^2 \phi_{n\ell}^2(y)} \int_y^\infty t^2 \phi_{n\ell}^2(t)\, dt \qquad \text{(III-85)}$$

$$M_{n\ell}^{<}(r,r') = C_0(r') + 2\mu \int_{r}^{r'} \frac{dy}{y^2 \phi_{n\ell}^2(y)} \int_0^y t^2 \phi_{n\ell}^2(t)\, dt \qquad \text{(III-86)}$$

Finally using the projection condition:

$$\vartheta_{n\ell} \, |n\ell\rangle = 0 \qquad \text{(III-87)}$$

which can be translated as:

$$\int_0^\infty r^2 \phi_{n\ell}^2(r)\, M_{n\ell}(r,r')\, dr = 0 \qquad \text{(III-88)}$$

the function $C_0(r')$ can be obtained through

$$C_0(r') = -2\mu \int_0^{r'} \frac{dx}{x^2 \phi_{n\ell}^2(x)} \int_0^x y^2 \phi_{n\ell}^2(y)\, dy$$
$$-2\mu \int_0^\infty x^2 dx\, \phi_{n\ell}^2(x) \int_{r'}^{x} \frac{dy}{y^2 \phi_{n\ell}^2(y)} \int_y^\infty t^2 \phi_{n\ell}^2(t)\, dt \qquad \text{(III-89)}$$

The complete radial contribution to the Reduced Green's Function will be given by

$$\mathcal{G}_{n\ell}(r,r') = \phi_{n\ell}(r)\, \mathcal{M}_{n\ell}(r,r')\, \phi_{n\ell}(r') \qquad \text{(III-90)}$$

Equations (III-85), (III-86), (III-89) and (III-90) will be applied to the study of pionic atoms in the forthcoming chapters. This set of equations gives us the possibility of immediate numerical applications for realistic cases. It should be noted that the input information is coming in its entirety from the state $|n\ell\rangle$.

(4) Degenerate Cases:

One natural question is what to do in case of degeneracy. In such a case we see that:

$$H_o|s\rangle = \epsilon_s|s\rangle = \epsilon_{\mathcal{D}}|s\rangle \qquad \text{(III-91)}$$

where $\mathcal{D}$ is a set of states with the feature:

$$\epsilon_s = \epsilon_{\mathcal{D}} \qquad \text{for any } |s\rangle \text{ in } \mathcal{D} \qquad \text{(III-92)}$$

being $\epsilon_{\mathcal{D}}$ a constant. The set forms a degenerate set of states. This property makes the application of our formalism impossible. In this section, a method is

going to be developed in order to solve this problem and it will be based on standard projection techniques. The use of these techniques to consider degenerate cases in perturbation theory is not new[3], being the essential difference between previous approaches an ours, the use of the Doorway State Formalism. The first step is the introduction of projectors:

P_D which projects onto the space

(III-93)

$Q_D = 1 - P_D$ which is just the complement

Using equations (III-78) the perturbation can be rewritten as:

$$V_2 = P_D V_2 P_D + P_D V_2 Q_D + Q_D V_2 P_D + Q_D V_2 Q_D \qquad \text{(III-94)}$$

and the following definitions are introduced:

$$U \equiv V_2 - P_D V_2 P_D \qquad \text{(III-95)}$$

$$H_1 \equiv H_0 + P_D V_2 P_D \qquad \text{(III-96)}$$

$$G_1(\varepsilon) \equiv (\varepsilon - H_1)^{-1} \qquad \text{(III-97)}$$

the eigenvalue problem for the Hamiltonian H_1 can be solved using standard diagonalization techniques and

in practice it is a simple problem, since usually a few states should be considered. Once this is done, a new set of states $\tilde{\mathcal{D}}$ is generated with the result

$$H_1 |\tau\rangle = \epsilon_\tau |\tau\rangle \qquad |\tau\rangle \in \tilde{\mathcal{D}} \tag{III-98}$$

where the degeneracy is removed. If in a given case the degeneracy is not removed then the prescription is to apply projection techniques a second time or n times until it is achieved.

Assuming that in the first step the remotion is achieved, which is the common case, the state $|\tau\rangle$ is a linear combination of the states $|s\rangle \in \mathcal{D}$ and

$$P_{\mathcal{D}} |\tau\rangle = P_{\tilde{\mathcal{D}}} |\tau\rangle = |\tau\rangle \tag{III-99}$$

$$Q_{\mathcal{D}} |\tau\rangle = Q_{\tilde{\mathcal{D}}} |\tau\rangle = 0 \tag{III-100}$$

Now, equation (III-1) can be written as:

$$(H_0 + P_{\mathcal{D}} V_2 P_{\mathcal{D}} + \mathcal{U}) |\psi_\tau\rangle = (H_1 + \mathcal{U}) |\psi_\tau\rangle = E_\tau |\psi_\tau\rangle \tag{III-101}$$

and then the energy shift is given by:

$$\Delta\mathcal{E}_\tau = \frac{\langle\tau|\mathcal{U}|\psi_\tau\rangle}{\langle\tau|\psi_\tau\rangle} = \frac{\langle\tau|V_2 Q_{\mathcal{D}}|\psi_\tau\rangle}{\langle\tau|\psi_\tau\rangle} \qquad \text{(III-102)}$$

equations (III-94) and (III-95) were used in order to obtain the right hand side of (III-102). Following a similar procedure to the one outlined by equations (III-6), (III-7), (III-8) and (III-9), we get:

$$|\psi_\tau\rangle = \langle\tau|\psi_\tau\rangle \frac{1}{1 - G_1(E_\tau) Q_\tau \mathcal{U}} |\tau\rangle \qquad \text{(III-103)}$$

replacing equation (III-103) in (III-102), the energy shift can be written as:

$$\Delta\mathcal{E}_\tau = \langle\tau|V_2 Q_{\mathcal{D}} \frac{1}{1 - G_1(E_\tau) Q_\tau \mathcal{U}} |\tau\rangle \qquad \text{(III-104)}$$

by expanding equation (III-104) and using equations (III-99) and (III-100) in addition to

$$Q_{\mathcal{D}} Q_\tau = Q_{\mathcal{D}} = Q_{\tilde{\mathcal{D}}} \qquad \text{(III-105)}$$

the energy shift can be rewritten as:

$$\Delta\mathcal{E}_\tau = \langle\tau|V_2 \frac{1}{1 - G_1(E_\tau) Q_{\tilde{\mathcal{D}}} V_2} |\tau\rangle - \langle\tau|V_2|\tau\rangle \qquad \text{(III-106)}$$

and taking into account the important result:

$$G_1(E_\tau)\, Q_{\tilde{\mathcal{D}}} = G_0(E_\tau)\, Q_{\mathcal{D}} \qquad \text{(III-107)}$$

which essentially is a consequence of the diagonalization procedure and allows us to simplify even further equation (III-106) to give

$$\Delta\mathcal{E}_\tau = \langle\tau|V_2 \frac{1}{1 - G_0(E_\tau) Q_{\mathcal{D}} V_2}|\tau\rangle - \langle\tau|V_2|\tau\rangle \qquad \text{(III-108)}$$

This equation has a convenient structure for the application of the Doorway State Formalism and the interesting feature is that, aside the state $|\tau\rangle$ (obtained through the first order diagonalization) and the unperturbed energy E_τ, all the required information comes from the original unperturbed problem. The new object here is a Reduced Green's Function given by

$$\vartheta_{\mathcal{P}}(E_\tau) \equiv G_0(E_\tau) Q_{\mathcal{D}} = G_0(E_\tau) - \sum_{m\in\mathcal{D}} \frac{|m\rangle\langle m|}{E_\tau - \epsilon_m} \qquad \text{(III-109)}$$

and the associated rescattering operator is given by

$$W(E_\tau) \equiv \sqrt{V_2}\, \vartheta_{\mathcal{P}}(E_\tau) \sqrt{V_2} \qquad \text{(III-110)}$$

At this point, the approach based on the Brillouin-Wigner Perturbation Theory outlined in section (1) can

be applied without difficulties. In this Rayleigh-Schroedinger case, equation (III-108) is expanded in terms of the energy shift $\Delta\epsilon_\tau$ and the structure is formally the same as the one outlined in section (2), being the difference a Reduced Green's Function given by

$$\vartheta_p(\epsilon_\tau) \equiv G_o(\epsilon_\tau) Q_D = G_o(\epsilon_\tau) - \sum_{m \epsilon D} \frac{|m><m|}{\epsilon_\tau - \epsilon_m}$$

$$= G_o(\epsilon_\tau) - \frac{1}{\epsilon_\tau - \epsilon_D} P_D \qquad \text{(III-111)}$$

where $\epsilon_\tau \neq \epsilon_D$ and the expansion is done around the energy value ϵ_τ. In an alternative way the expansion can be done around ϵ_D and in this case a differential representation for the Reduced Green's Function can be obtained:

$$\vartheta(\epsilon_D) \equiv G_o(\epsilon_D) Q_D = \lim_{\epsilon \to \epsilon_D} \left\{ G_o(\epsilon) - \frac{1}{\epsilon - \epsilon_D} \sum_{m \epsilon D} |m><m| \right\}$$

$$= \lim_{\epsilon \to \epsilon_D} \frac{d}{d\epsilon} \left[(\epsilon - \epsilon_D) G_o(\epsilon) \right] \qquad \text{(III-112)}$$

From the formal point of view there is no difference between the calculation of this Reduced Green's Function and the standard Reduced Green's Function applicable to the nondegenerate case and that is the

essential advantage of this alternative approach.

Up to now, the guidelines for a general structure in the Doorway State Approach to Bound State Peturbation Theory were given and the task to be continued is the application of this theory to simple cases (which can be solved exactly) in order to examine and to test its features, in particular convergence as the most important one.

(5) Simple Cases to study:

In this section the approach outlined in section (2) based on the Rayleigh-Schroedinger Theory is going to be studied through simple cases that can be considered analytically and with detail. Our attention is going to be concentrated in energy shifts, wavefunctions and Green's Functions. The functions are found in the perturbation region with relatively few doorway states, being this a success of the method. We are going to see that usually less doorways are needed for a good approximation to the energy shifts. In standard perturbation theory a good representation of the wavefunctions is, in general, not possible due to the fact that the truncation is done in terms of the perturbation higher orders. In the Doorway State Approach, the contribution from higher order terms in the perturbation is kept at every level of truncation, which is the origin of strong

convergence that leads to a good representation of the wavefunction and a good approximation to the energy shift. Next, we are going to consider the examples:

(a) <u>One dimensional Harmonic Oscillator and a Harmonic Perturbation</u>:

In this case the unperturbed Hamiltonian is considered to be:

$$H_0 = \frac{p^2}{2M} + \frac{1}{2} M\omega^2 x^2 \qquad \text{(III-113)}$$

and the perturbation has a harmonic form also:

$$V_2 \equiv \frac{1}{2} \beta M\omega^2 x^2 \qquad \text{(III-114)}$$

where ω is the natural oscillator frequency and β is a size parameter for the perturbation. The combination of equations (III-113) and (III-114) gives us a new Hamiltonian which is a new Harmonic Oscillator with a natural frequency given by:

$$\tilde{\omega} \equiv \sqrt{1+\beta}\ \omega \qquad \text{(III-115)}$$

At this point it is useful to introduce second quantization language in order to make the handling of problem simpler and then, the position and momentum

operators can be defined as:

$$p \equiv i\sqrt{\frac{M\omega}{2}}\,(a^{\dagger} - a) \qquad \text{(III-116)}$$

$$x \equiv \frac{1}{\sqrt{2M\omega}}\,(a^{\dagger} + a) \qquad \text{(III-117)}$$

using the commutation rule for the position and momentum operators

$$[x, p] = i \qquad \text{(III-118)}$$

the commutation rule for a and $a^{\dagger}$ is found to be

$$[a, a^{\dagger}] = 1 \qquad \text{(III-119)}$$

and then

$$a\,|n\rangle = \sqrt{n}\;|n-1\rangle \qquad \text{(III-120)}$$

$$a^{\dagger}\,|n\rangle = \sqrt{n+1}\;|n+1\rangle \qquad \text{(III-121)}$$

and the unperturbed Hamiltonian can be written in normal form as:

$$H_o = \left[\, a^{\dagger}a + \frac{1}{2} \,\right]\omega \qquad \text{(III-122)}$$

To find the rescattering operator, we use the square root of the perturbation given by

$$\sqrt{V_2} = \frac{1}{2}\sqrt{\beta\omega}\,(a^+ + a) \qquad \text{(III-123)}$$

and the Reduced Green's Function:

$$\vartheta(\epsilon_s) = \sum_{m\neq s} \frac{|m\rangle\langle m|}{\epsilon_s - \epsilon_m} = \frac{1}{\omega}\sum_{m\neq s} \frac{|m\rangle\langle m|}{s-m} \qquad \text{(III-124)}$$

with the result:

$$W^{(k)} \equiv \sqrt{V_2}\,\vartheta^k(\epsilon_s)\sqrt{V_2} = \frac{\beta}{4}(a^+a)\sum_{m\neq s}\frac{|m\rangle\langle m|}{(s-j)^k}(a^+a) \qquad \text{(III-125)}$$

where $|s\rangle$ is the unperturbed state to be considered, such that

$$H_0|s\rangle = \epsilon_s|s\rangle \qquad \text{(III-126)}$$

and

$$\epsilon_s = \left(s + \tfrac{1}{2}\right)\omega \qquad \text{(III-127)}$$

To proceed with the construction of the Doorway basis it is convenient to write the rescattering operator $W^{(k)}$ and the starting vectors $|\mathcal{D}_0\rangle$ and $|\tilde{\mathcal{D}}_0\rangle$ in the

Harmonic Oscillator basis:

$$W_{nm}^{(k)} = \frac{\beta}{4}\left\{\frac{(1-\delta_{s,n+1})}{(s-n-1)^k}\left[\sqrt{(n+1)(n+2)}\,\delta_{m,n+2} + (n+1)\,\delta_{m,n}\right.\right.$$
$$\left.\left. + \frac{(1-\delta_{s,n-1})}{(s-n+1)^k}\left[n\,\delta_{nm} + \sqrt{n(n-1)}\,\delta_{m,n-2}\right]\right\} \qquad \text{(III-128)}$$

$$N_o^{-1}|\mathcal{D}_o\rangle = \tilde{N}_o^{-1}|\tilde{\mathcal{D}}_o\rangle = \frac{\sqrt{\beta(s+1)}}{2}|s+1\rangle + \frac{\sqrt{\beta s}}{2}|s-1\rangle \qquad \text{(III-129)}$$

and

$$(\tilde{N}_o^{\dagger} N_o)^{-1} = \frac{\beta}{4}(2s+1) \qquad \text{(III-130)}$$

The rest of this basis can be constructed with equations (III-18). Equations (III-128) and (III-129) are particularly convenient for computer calculations. We begin our numerical studies with $\beta = 1$ (the original interaction and the perturbation have the same size) and the state to be considered in detail will be the ground state. The results for energy shifts calculated through equation(III-47) and the wavefunction coefficients in the Doorway Basis given by equation (III-52) are summarized in table (III-I). In that table $N_{\mathcal{D}}$ represents the number of Doorway States used and M is the maximum order in the energy shift expansion, to be considered for truncation, which gives stable numerical values with seven figures. The first observation is that convergence for the energy shift $\Delta\mathcal{E}^{(n)}$ is very good. At the

TABLE (III-I)

Results for the Harmonic Oscillator With a Harmonic Perturbation With $\beta = 1$ for the Ground State

$\Delta\mathcal{E}$ (Exact) = 0.2071068 ω
$\Delta\mathcal{E}$ (First Order Perturbation Theory) = 0.25 ω

N_D	M	ϑ_0	ϑ_1	ϑ_2	ϑ_3
1	5	0.7830095	0	0	0
2	4	0.9040504	0.4601959	0	0
3	5	0.8307469	0.1829259	0.0809657	0
4	4	0.8285029	0.1743676	0.0349413	0.0146797
5	5	0.8284296	0.1740891	0.0334427	0.0064620
6	5	0.8284272	0.1740802	0.0333943	0.0061917
7	4	0.8284274	0.1740797	0.0333927	0.0061886
8	4	0.8284274	0.1740797	0.0333927	0.0061883
9	4	0.8284274	0.1740797	0.0333927	0.0061883

N_D	M	ϑ_4	ϑ_5	ϑ_6	ϑ_7
1	5	0	0	0	0
2	4	0	0	0	0
3	5	0	0	0	0
4	4	0	0	0	0
5	5	0.0026419	0	0	0
6	5	0.0011744	0.0004722	0	0
7	4	0.0011277	0.0002111	0.0000839	0
8	4	0.0011262	0.0002029	0.0000377	0.0000149
9	4	0.0011262	0.0002027	0.0000362	0.0000067

N_D	M	ϑ_8	$\Delta\mathcal{E}^{(0)}$ (ωunits)	$\Delta\mathcal{E}^{(M)}$ (ωunits)
1	5	0	0.2	0.1957524
2	4	0	0.2277580	0.2260126
3	5	0	0.2105047	0.2076867
4	4	0	0.2100259	0.2071257
5	5	0	0.2100112	0.2071074
6	5	0	0.2100108	0.2071068
7	4	0	0.2100108	0.2071068
8	4	0	0.2100108	0.2071068
9	4	0.0000026	0.2100108	0.2071068

second Doorway level of truncation there is a $\sim 10\%$ deviation from the exact value. The exact shift can be reproduced up to third figure at the third Doorway State level and up to the seventh figure at the sixth Doorway State level for an "intermediate" size perturbation. By intermediate size we mean that the perturbation is about the same size as the original interaction, like the one that we are considering. With the first Doorway and $M = 5$ we see a 6% deviation while in the same case with $M = o$ (the simplest truncation) there is a 3.5% deviation. This behaviour is what makes the truncation at the first Doorway level interesting in physical applications. The second observation is that a relatively low order in the energy shift expansion is required for accurate results. If we are interested in few percent is probable that there is no need in going beyond the zeroth order in the energy shift. In the example that we are considering for seven figures, the saturation value is reached within the fourth and fifth orders. Of course, this is an extreme case which is unusual in practical cases. In the case of a Third Doorway truncation to obtain the energy shift up to the third figure is possible at the first order in the energy shift as it is shown in table (III-II). In that table the sixth Doorway truncation is also shown in

TABLE (III-II)

Convergence according to the energy shift order for the third and sixth Doorway truncations in the ground state case with $\beta = 1$.

Third Doorway Truncation:

M	$\Delta\mathcal{E}^{(M)}$(ω units)
0	0.2105047
1	0.2078735
2	0.2076993
3	0.2076876
4	0.2076868
5	0.2076867
6	0.2076867

Sixth Doorway Truncation:

M	$\Delta\mathcal{E}^{(M)}$(ω units)
0	0.2100108
1	0.2073029
2	0.2071203
3	0.2071077
4	0.2071069
5	0.2071068
6	0.2071068

TABLE (III-III)

Results for the Harmonic Oscillator with a Harmonic Perturbation with $\beta = 0.1$ for the Ground State.

$\Delta\mathcal{E}$ (Exact) = 0.02440442 ω $\Delta\mathcal{E}$(First Order Perturbation Theory) = 0.025 ω

N_D	M	$\Delta\mathcal{E}^{(0)}$(ω units)	$\Delta\mathcal{E}^{(M)}$(ω units)
1	3	0.02439024	0.02438290
2	2	0.02441397	0.02440718
3	2	0.02441127	0.02440443
4	2	0.02441127	0.02440442

detail and we see that it is not necessary to go beyond the first order to obtain a result with three figures. So with little effort reasonably accurate numbers can be obtained for the energy shifts in the presence of perturbations of intermediate size. For small perturbations is clear that the demands are much less as it is evidenced in table (III-III) and for most physical applications this is a very interesting case. If we try a truncation at the first Doorway level in that particular example we get good results up to the third figure and just keeping the zeroth order term in the energy shift expansion. A comparison of the relevant numerical values in table (III-III) shows that the approximation is very good and performs much better than the first order perturbation theory. The real effort has to be done when the perturbation is a large one as it is shown in table (III-IV) where a value with three figures can be obtained at the 8-th Doorway truncation level. The calculated M values are for saturation with seven figures and the three figure accuracy can be kept with four orders in the energy shift. A few percent accuracy can be achieved at the fourth Doorway level with zeroth order in the energy shift, which is remarkable if we realize that the perturbation has a strength five times than the one of the original interaction.

TABLE (III-IV)

Results for the Harmonic Oscillator with a Harmonic Perturbation with $\beta = 5$ for the Ground State.

$\Delta\mathcal{E}$(Exact) = 0.7247449 ω, $\Delta\mathcal{E}$(First Order Perturbation Theory = 1.25 ω

N_D	M	$\Delta\mathcal{E}^{(0)}$ (ω units)	$\Delta\mathcal{E}^{(M)}$ (ω units)
1	7	0.5555556	0.4738284
2	7	-0.2685097	-0.09032234
3	11	0.4229153	0.2276600
4	23	0.7100424	0.5193817
5	23	0.7741272	0.6766929
6	17	0.7862582	0.7164256
7	12	0.78894938	0.7233197
8	9	0.7889031	0.7244950
9	8	0.7889777	0.7247004
10	9	0.7889913	0.7247369
11	8	0.7889937	0.7247434

Although there is more effort, we can see that results are guaranteed. Another important item presented in table (III-I) is the wavefunction coefficients in the Doorway basis, denoted by ϑ_n. They are calculated jointly to the energy shifts to show a general feature of any perturbation theory: Convergence for energy shifts is faster than convergence for wavefunctions. In this example when the energy shift is stable within seven figures at the sixth Doorway truncation, the first coefficient stabilizes at the seventh Doorway truncation. This is also the case with the second and the third coefficients. Looking at these coefficients the suggestion is that a good representation of the wavefunction in the perturbation region (same as the interaction region in this case) is possible. In order to answer that question, table (III-V) was prepared. In that table the comparison is made using the normalized perturbed state given in equation (III-50) with the state in the perturbation region, given by $N_E\sqrt{V_2}|\psi_{EXACT}\rangle$, and the unperturbed state in the region, $N_0\sqrt{V_2}\,|\psi_0\rangle$, which is the first Doorway State. The normalization constant for the exact state

TABLE (III-V)

Unperturbed, Perturbed and Exact Wavefunctions for the Harmonic Oscillator with a Harmonic Perturbation with = 1 for the Ground State in 9th Doorway truncation.

ξ	$\langle\xi\|\bar{0}\rangle$	$\langle\xi\|\bar{2}\rangle$	$\langle\xi\|\bar{3}\rangle$	$\langle\xi\|\bar{4}\rangle$	$\langle\xi\|\bar{5}\rangle$	$\langle\xi\|\bar{6}\rangle$	$\langle\xi\|\bar{7}\rangle$	$\langle\xi\|\bar{8}\rangle$	$\langle\xi\|\bar{9}\rangle$	EXACT
0.25	0.2573925	0.3664322	0.3455604	0.3329042	0.3301382	0.3296178	0.3295238	0.3295072	0.3295039	0.3295039
0.50	0.4687170	0.6347283	0.5996579	0.5813059	0.5778223	0.5772719	0.5772915	0.57718051	0.5771792	0.5771792
0.75	0.6013724	0.7447589	0.7098957	0.6957187	0.6941401	0.6940834	0.6941090	0.6941185	0.6941215	0.6941215
1.00	0.6442884	0.6935005	0.6771193	0.6769788	0.6786062	0.6791118	0.6792164	0.6792340	0.6792368	0.6792368
1.25	0.6079180	0.5276924	0.5502862	0.5658687	0.5697309	0.5703481	0.5704151	0.5704176	0.5704159	0.5704159
1.50	0.5172941	0.3172990	0.3914789	0.4173289	0.4208615	0.4240322	0.4209858	0.4209695	0.4209657	0.4209657
1.75	0.4.20242	0.1256053	0.2506816	0.2762262	0.2770580	0.2766179	0.2765059	0.2764914	0.2764909	0.2764909
2.00	0.28752033	-0.100108	0.1514028	0.1660472	0.1635807	0.1628949	0.1628357	0.1628414	0.1628446	0.1628446
2.25	0.1901525	-0.0814552	0.0932142	0.0910036	0.0867081	0.0863457	0.0864033	0.0864230	0.0864252	0.0864252
2.50	0.1166802	-0.1013039	0.0632405	0.0447044	0.0410727	0.0413390	0.0414607	0.0414713	0.0414692	0.0414692
2.75	0.0665862	-0.0901822	0.0474606	0.0182049	0.172513	0.0179749	0.0180474	0.0180364	0.0180326	0.0180326
3.00	0.0354017	-0.0667965	0.0366965	0.0041678	0.0064840	0.0071848	0.0071408	0.0017793	0.0071187	0.0071187
3.25	0.0175587	-0.0432922	0.0272287	-0.0023357	0.0024521	0.0026903	0.0025615	0.0025514	0.0025547	0.0025547
3.50	0.0081328	-0.0251355	0.0186710	-0.00446831	0.0013154	0.0009390	0.0008193	0.0008309	0.0008343	0.0008343
3.75	0.0035207	-0.0132447	0.116727	-0.0043224	0.0010981	0.0002529	0.0002243	0.0002482	0.0002481	0.0002481
4.00	0.0014254	-0.0063852	0.0066378	-0.0032707	0.00099407	-0.0000304	0.0000530	0.0000708	0.0000673	0.0000673
4.25	0.0005400	-0.0028315	0.0034400	-0.0021125	0.0008048	-0.0001385	0.0000217	0.0000206	0.0000166	0.0000166
4.50	0.0001915	-0.0011594	0.0016297	-0.0012032	0.0005655	-0.0001553	0.0000252	0.0000049	0.0000037	0.0000037
4.75	0.0000636	-0.0004396	0.0007080	-0.0006142	0.0003479	-0.0001273	0.0000291	-0.0000015	0.0000008	0.0000008
5.00	0.0000198	-0.0001546	0.0002829	-0.0002836	0.0001897	-0.0000863	0.0000263	-0.0000044	0.0000001	0.0000001

$\langle\xi|\bar{n}\rangle \equiv \langle\xi|\sqrt{V_2}|\psi\rangle^{(n)}$ EXACT $\equiv \langle\xi|\sqrt{V_2}|\psi_{EXACT}\rangle$

is given by

$$|N_E|^2 \equiv \frac{\Delta\mathcal{E}_{FOPT}}{\langle \psi_{EXACT} | V_2 | \psi_{EXACT} \rangle} \qquad \text{(III-131)}$$

where

$$\Delta\mathcal{E}_{FOPT} \equiv \left(\tilde{N}_o^* N_o\right)^{-1} \qquad \text{(III-132)}$$

is just the first order perturbation theory energy shift. In the Harmonic Oscillator case we obtain:

$$\langle \psi^{(n)}_{EXACT} | V_2 | \psi^{(n)}_{EXACT} \rangle = \frac{\beta}{2\sqrt{1+\beta}} \left(n + \tfrac{1}{2}\right) \omega \qquad \text{(III-133)}$$

then the normalization constant is given by

$$N_E = 2\, N_o^{-1} \frac{(1+\beta)^{1/4}}{\sqrt{\beta(2n+1)}} \qquad \text{(III-134)}$$

and the normalized exact wavefunction in the perturbation region is given by

$$\langle \zeta | \sqrt{V_2} | \psi^{(n)}_{EXACT} \rangle = N_E \left(\frac{M\omega}{\pi}\right)^{1/4} \sqrt{\frac{\beta\omega}{2}} \frac{(1+\beta)^{1/8}}{\sqrt{2^n n!}}$$
$$\otimes\, \zeta\, H_n\left(\sqrt{1+\beta}\,\zeta\right) e^{-\frac{1}{2}\sqrt{1+\beta}\,\zeta^2} \qquad \text{(III-135)}$$

where

$$\zeta \equiv \sqrt{M\omega}\, x \qquad \text{(III-136)}$$

and the unperturbed wavefunction (First Doorway wavefunction) can be written as:

$$\langle \zeta | \sqrt{V_2} | \psi_0^{(n)} \rangle = N_0 \left(\frac{M\omega}{\pi}\right)^{1/4} \sqrt{\frac{\beta\omega}{2}} \frac{\zeta}{\sqrt{2^n n!}} H_n(\zeta) e^{-\frac{1}{2}\zeta^2} \qquad \text{(III-137)}$$

since we are working with the ground state $n=0$ is taken. In the construction of table (III-V) the mass M and frequency ω were taken as unity. If we examine the convergence process closely, the immediate observed feature is that the representation of the wavefunction is getting poorer as we go farther from the origin where oscillations appear. With the increasing number of Doorway States the oscillation region is pulled away from the origin region where the representation is good. Within few percent accuracy and for a region close to the origin , a good representation can be obtained at the third Doorway truncation. At the level of the nineth Doorway truncation there is no distinction between the perturbed and exact wavefunctions within seven significant figures. Another interesting point to examine is the Green's Function representation and in order to do that, table (III-VIA) was prepared. In this table the

TABLE (III-VIA)

Green's Function in the Perturbation Region Evaluated at $E = E_0 + \frac{1}{2}\Delta E_0$ for the Harmonic Oscillator with a Harmonic Perturbation Up to the Nineth Doorway Truncation and $\beta = 1$. The Symbol (i,j) stands for the i-th Doorway and j-th Doorway Coefficient

N_D	(1,1)	(2,1)	(2,2)	(3,1)	(3,2)	(3,3)
1	-0.1979627	0	0	0	0	0
2	-0.08711197	0.4308044	-0.9725796	0.	0	0
3	-0.1549363	0.1678514	-0.2936387	0.073792	0.2991220	-0.8652418
4	-0.1569223	0.1601230	-0.3250252	0.0314632	.1275410	-0.2830438
5	-0.1569850	0.1598788	-0.3260169	0.0301258	0.1219486	-0.3127861
6	-0.1569870	0.1598711	-0.3260482	0.0300836	0.1219432	-0.3137248
7	-0.1569871	0.1598709	-0.3260492	0.0300822	0.1219430	-0.3137542
8	-0.1569871	0.1598709	-0.3260492	0.0300822	0.1219430	-0.3137552
9	-0.1569871	0.1598709	-0.3260492	0.0300822	0.1219430	-0.3137552
Exact	-0.1569871	0.1598709	-0.3260492	0.0300822	0.1219430	-0.3137552

N_D	(5,3)	(5,4)	(5,5)	(6,1)	(6,2)	(6,3)
5	0.0520619	0.2894153	-0.7914290	0	0	0
6	0.0230069	0.1278969	-0.2737404	0.0041481	0.0016815	0.0092247
7	0.0220963	0.1228349	-0.3020752	0.0001846	0.0007484	0.0041056
8	0.0220680	0.1226773	-0.309572	0.0001774	0.0007193	0.0039462
9	0.0220671	0.1226725	-0.3029844	0.0001772	0.0007184	0.0039413
Exact	0.0220671	0.1226725	-0.3029844	0.0001772	0.0007184	0.0039411

N_D	(7,4)	(7,5)	(7,6)	(7,7)	(8,1)	(8,2)
7	0.0090524	0.0506708	0.2852930	-0.7716220	0	0
8	0.0040479	0.0226582	0.1275129	-0.2710307	0.1275129	0.0000522
9	0.0038930	0.0217914	0.1226924	-0.2986357	0.0000058	0.0000234
Exact	0.0038881	0.0217638	0.1225373	-0.2995126	0.0000056	0.0000225

N_D	(9,1)	(9,2)	(9,3)	(9,4)	(9,5)	(9,6)
9	0.0000023	0.0000092	0.0000503	0.0002796	0.0015652	0.0088125
Exact	0.00000	0.0000040	0.0000217	0.0001209	0.0006768	0.0038104

N_D	(4,1)	(4,2)	(4,3)	(4,4)	(5,1)	(5,2)
4	0.0131577	0.053337	-0.8114672	0	0	0
5	0.0057460	0.0232923	0.1277826	-0.2767047	0.2341060	0.0094899
6	0.0055121	0.0223441	0.1225807	-0.3056224	0.0103455	0.0041937
7	0.0055047	0.0223143	0.1224177	-0.3065287	0.0009936	0.0040277
8	0.0055045	0.0223134	0.1224126	-0.3065569	0.0009923	0.0040226
9	0.0055045	0.0223134	0.1224124	-0.3065578	0.0009923	0.0040224
Exact	0.0055045	0.0223134	0.1224124	-0.3065578	0.0009923	0.0009923

N_D	(6,4)	(6,5)	(6,6)	(7,1)	(7,2)	(7,3)
5	0	0	0	0	0	0
6	0.0512806	0.2870434	-0.7795151	0	0	0
7	0.0228231	0.1277526	-0.2720822	0.0000732	0.0002968	0.0016284
8	0.0219373	0.1227945	-0.2999982	0.0000327	0.0001327	0.0007282
9	0.0219099	0.1226411	-0.3008620	0.0000315	0.0001277	0.0007003
Exact	0.0219091	0.1226362	-0.3008895	0.0000315	0.0001275	0.0006994

N_D	(8,3)	(8,4)	(8,5)	(8,7)	(8,7)	(8,8)
7	0	0	0	0	0	0
8	0.0002866	0.0015930	0.0089170	0.0502056	0.2839711	-0.7660093
9	0.0001286	0.0007147	0.0400073	0.0225254	0.1274073	-0.2703076
Exact	0.0001236	0.0006868	0.0384456	0.0216461	0.1224338	-0.2985391

N_D	(9,7)	(9,8)	(9,9)
9	0.0498450	0.2829425	-0.7618093
Exact	0.0215522	0.1223399	-0.2978115

Green's Function in the perturbation region is given in terms of the Doorway basis, i.e., the coefficients of such expansion are the tabulated quantities. It can be observed that the convergence properties are quite similar to the wavefunction ones. It can be shown that these convergence properties are not altered by the particular energy where the Green's Function is evaluated and that is the purpose of tables (III-VIB) and (III-VIC) where the evaluation is done at $\mathcal{E} = \mathcal{E}_0 + \frac{1}{10}\Delta\mathcal{E}_0$ and $\mathcal{E}_0 + \Delta\mathcal{E}_0$. The results for a very large perturbation $\beta = 10$, are given in table (III-VII) where a good result for the energy shift can be obtained within three significant figures at the nineth Doorway truncation. It should be noted that after an apparent breakdown at the second Doorway truncation, the sequence recovers its way towards the correct values. In this case it is clear that a big effort has to be done in order to obtain the adequate information, although considering perturbation theory in its standard form this will be merely impossible. Then we can conclude that in the Harmonic Oscillator case with a Harmonic Perturbation the Approach outlined in this chapter works in a very adequate fashion and in what follows the main features are going to be verified for other simple examples.

TABLE (III-VIB)

Green's Function in the Perturbation Region Evaluated at $E = E_0 + \frac{1}{10}\Delta E_0$ for the Harmonic Oscillator with a Harmonic Perturbation Up to the Nineth Doorway Truncation and $\beta = 1$. The Symbol (i,j) stands for the i-th Doorway and j-th Doorway Coefficient

N_D	(1,1)	(2,1)	(2,2)	(3,1)	3,2)	(3,3)	(4,1)	(4,2)	(4,3)	(4,4)	(5,1)	(5,2)
1	-0.1996034	0	0	0	0	0	0	0	0	0	0	0
2	-0.0886079	0.4487997	-1.0087664	0	0	0	0	0	0	0	0	0
3	-0.1573883	0.1708208	-0.2985022	0.0747006	0.3044970	-0.865242	0	0	0	0	0	0
4	-0.1593174	0.1630187	-0.3303168	0.0315424	0.1285746	-0.2850557	0.0131429	0.0535736	0.2964602	-0.8197564	0	0
5	-0.1593770	0.1627780	-0.3312982	0.0302111	0.1231479	-0.3150854	0.0057034	0.0232486	0.1286508	-0.2780503	0.00231737	0.0094462
6	-0.1593788	0.1627705	-0.3313286	0.0301697	0.1229795	-0.3160173	0.0056726	0.0223076	0.1234633	-0.3071683	0.0010193	0.0041548
7	-0.1593789	0.1627703	-0.3313296	0.0301685	0.1229743	-0.3160462	0.0056654	0.0222785	0.1232822	-0.3080690	0.0009791	0.0039912
8	-0.1593789	0.1627703	-0.3313296	0.0301684	0.1229741	-0.3160470	0.0056652	0.0222776	0.1232773	-0.3080968	0.0009779	0.0039861
9	-0.1593789	0.1627703	-0.3313296	0.0301684	0.1229741	-0.3160470	0.0056652	0.0222775	0.1232771	-0.2080976	0.0009779	0.0039860
Exact	-0.1593789	0.1627703	-0.3313296	0.0301684	0.1229741	-0.3160471	0.0056652	0.0222775	0.1232771	-0.3080977	0.0009779	0.0039860

N_D	(5,3)	(5,4)	(5,5)	(6,1)	(6,2)	(6,3)	(6,4)	(6,5)	(6,6)	(7,1)	(7,2)	(7,3)
5	0.0522722	0.2922842	-0.7934763	0	0	0	0	0	0	0	0	0
6	0.0229916	0.1285595	-0.2747558	0.0004078	0.0016623	0.0091584	0.0514336	0.2893245	-0.7842811	0	0	0
7	0.0220859	0.1234950	-0.3032447	0.0001508	0.0007370	0.0040786	0.0228056	0.1282859	-0.2726971	0.0000716	0.0002918	0.0016148
8	0.0220580	0.1233390	-0.3041221	0.0001738	0.0007085	0.0039209	0.0219239	0.1233266	-0.3009388	0.0000319	0.0001301	0.0007198
9	0.0220572	0.1233343	-0.3041790	0.0001736	0.0007078	0.0039161	0.0218969	0.1231745	-0.3017987	0.0000307	0.0001251	0.0006924
Exact	0.0220571	0.1233341	-0.3041798	0.0001736	0.0007076	0.0039159	0.0218961	0.1231697	-0.3018238	0.0000307	0.0001250	0.0006915

N_D	(7,4)	(7,5)	(7,6)	(7,7)	(8,1)	(8,2)	(8,3)	(8,4)	(8,5)	(8,6)	(8,7)	(8,8)
7	0.0050230	0.0307900	0.2871859	-0.7755570	0	0	0	0	0	0	0	0
8	0.0040249	0.0226406	0.1280188	-0.2717113	0.0000125	0.0000511	0.0002828	0.0015815	0.0088963	0.0503030	0.2855887	-0.7693612
9	0.0038714	0.0217774	0.1231378	-0.2994225	0.0000056	0.0000229	0.0001266	0.0007077	0.0039808	0.0225087	0.1277903	-0.2708919
Exact	0.0038666	0.0217502	0.1229840	-0.3002957	0.0000054	0.0000220	0.0001216	0.0006801	0.0038259	0.0216329	0.1228178	-0.2992121

N_D	(9,1)	(9,2)	(9,3)	(9,4)	(9,5)	(9,6)	(9,7)	(9,8)	(9,9)
9	0.0000022	0.0000089	0.0000494	0.0002765	0.0015553	0.0087941	0.0499273	0.2843548	-0.7647292
Exact	0.0000009	0.0000039	0.0000213	0.0001193	0.0006710	0.0037940	0.0215397	0.1226767	-0.2984010

TABLE (III-VIC)

Green's Function in the Perturbation Region Evaluated at $E = E_0 + E_0$ for the Harmonic Oscillator with a Harmonic Perturbation Up to the Nineth Doorway Truncation and = 1. The Symbol (i,j) stands for the i-th Doorway and the j-th Doorway Coefficient

N_D	(1,1)	(2,1)	(2,2)	(3,1)	(3,2)	(3,3)	(4,1)	(4,2)	(4,3)	(4,4)	(5,1)	(5,2)
1	-0.1957524	0	0	0	0	0	0	0	0	0	0	0
2	-0.0851070	0.4081912	-0.9271538	0	0	0	0	0	0	0	0	0
3	-0.1516773	0.1639303	-0.2872470	0.0725579	0.2924936	-0.8352402	0	0	0	0	0	0
4	-0.1537368	0.1563099	-0.3180910	0.0313228	0.1262705	-0.2804755	0.0131595	0.0530493	0.2877866	-0.8010575	0	0
5	-0.1538037	0.1560616	-0.3190955	0.0299796	0.1208559	-0.3098510	0.0057928	0.0233525	0.1266851	-0.274997	0.0023683	0.0095473
6	-0.1538059	0.1560536	-0.3191279	0.0299362	0.1206813	-0.3107981	0.0055553	0.0223951	0.1214911	-0.3036611	0.0010528	0.0042442
7	-0.1538061	0.1560534	-0.3191291	0.0299349	0.1206757	-0.3108283	0.0055478	0.0223646	0.1213256	-0.3045744	0.0010109	0.0040752
8	-0.1538061	0.1560534	-0.3191291	0.1206755	0.1206755	-0.3108293	0.0055475	0.0223636	0.1213204	-0.3046032	0.0010096	0.0040700
9	-0.1538061	0.1560534	-0.3191291	0.0299349	0.1206755	-0.3108293	0.0055475	0.0223636	0.1213202	-0.3046041	0.0010095	0.0040697
Exact	-0.1538059	0.1560533	-0.3139290	0.0299348	0.1206756	-0.3108293	0.0055475	0.0223636	0.1213202	-0.3046041	0.0010095	0.0040697

N_D	(5,3)	(5,4)	(5,5)	(6,1)	(6,2)	(6,3)	(6,4)	(6,5)	(6,6)	(7,1)	(7,2)	(7,3)
5	0.0517934	0.2858227	-0.7838403	0	0	0	0	0	0	0	0	0
6	0.0230244	0.1270604	-0.2724565	0.0004233	0.0017064	0.0092571	0.0510855	0.2841870	-0.7735377	0	0	0
7	0.0221078	0.1220021	-0.3005961	0.0001893	0.0007631	0.0041395	0.0228440	0.1270805	-0.2710539	0.0000752	0.0003033	0.0016456
8	0.0220788	0.1218425	-0.3014839	0.0001819	0.0007333	0.0039781	0.0219531	0.1221241	-0.298111	0.0000838	0.0001361	0.0007388
9	0.0220779	0.1218375	-0.3015116	0.0001817	0.0007324	0.0039730	0.0219252	0.1219690	-0.2996799	0.0000325	0.0001309	0.0007104
Exact	0.0220779	0.1218373	-0.3015125	0.0001817	0.0007323	0.0039729	0.0219243	0.1219640	-0.2997077	0.0000324	0.0001308	0.0007095

N_D	(7,4)	(7,5)	(7,6)	(7,7)	(8,1)	(8,2)	(8,3)	(8,4)	(8,5)	(8,6)	(8,7)	(8,8)
7	0.0090814	0.0505193	0.2829227	-0.7666888	0	0	0	0	0	0	0	0
8	0.0040769	0.0226795	0.1270115	-0.2701732	0.0000133	0.0000537	0.0002913	0.0016076	0.0089428	0.0500821	0.2819458	-0.7618085
9	0.0039202	0.0218081	0.1221318	-0.2976443	0.0000060	0.0000242	0.0001311	0.0007237	0.0040258	0.022548	0.1269254	-0.2695772
Exact	0.0039152	0.0217802	0.1219752	-0.2985258	0.0000058	0.0000232	0.0001260	0.0006953	0.0038680	0.0216622	0.1219510	-0.2976919

N_D	(9,1)	(9,2)	(9,3)	(9,4)	(9,5)	(9,6)	(9,7)	(9,8)	(9,9)
9	0.0000023	0.0000095	0.0000514	0.0002836	0.0015777	0.0088355	0.0497408	0.2811746	-0.7581509
Exact	0.0000010	0.0000041	0.0000223	0.0001230	0.0006841	0.0038310	0.0215675	0.1219167	-0.2970697

TABLE (III-VII)

Results for the Harmonic Oscillator With a Harmonic Perturbation With $\beta = 10$ for the Ground State

$\Delta\mathcal{E}$ (Exact) = 1.158312 ω
$\Delta\mathcal{E}$ (First Order Perturbation Theory = 2.5 ω

N_D	M	ϑ_0	ϑ_1	ϑ_2	ϑ_3
1	7	0.2236945	0	0	0
2	4	-0.0091527	-0.3408318	0	0
3	10	0.1549323	-0.0960450	-0.4513739	0
4	14	0.3083534	0.1129463	-0.1110140	-0.4035197
5	12	0.4052915	0.2350880	0.0784918	-0.0729190
6	10	0.4453037	0.2832662	0.1510896	0.0518822
7	8	0.4580210	0.2983051	0.1734846	0.0901557
8	8	0.4617709	0.3027147	0.1800267	0.1013158
9	8	0.4628680	0.3040027	0.1819354	0.1045699

N_D	M	ϑ_4	ϑ_5	ϑ_6	ϑ_7
1	7	0	0	0	0
2	4	0	0	0	0
3	10	0	0	0	0
4	14	0	0	0	0
5	12	-0.2610387	0	0	0
6	10	-0.0365490	-0.1418721	0	0
7	8	-0.0320615	-0.0172838	-0.0742780	0
8	8	-0.0520461	0.0189756	-0.0082730	-0.0390871
9	8	-0.0578714	0.0295422	0.0109577	-0.0040451

N_D	M	ϑ_8	$\Delta\mathcal{E}^{(0)}$ (ω units)	$\Delta\mathcal{E}^{(M)}$ (ω units)
1	7	0	0.7142857	0.5592363
2	4	0	-0.0387785	-0.0228818
3	10	0	0.6737387	0.0387331
4	14	0	1.115731	0.7708834
5	12	0	1.272837	1.013229
6	10	0	1.320414	1.113259
7	8	0	1.334325	1.145035
8	8	0	1.338371	1.154427
9	8	-0.0207601	1.339548	1.157170

(b) <u>One dimensional infinite square well with a delta function perturbation</u>:

Now we are going to consider an unperturbed Hamiltonian given by

$$H_0 = \frac{p^2}{2\mu} + V(x) \qquad \text{(III-138)}$$

where

$$V(x) = \begin{cases} 0 & -a \leq x \leq a \\ \infty & \text{otherwise} \end{cases} \qquad \text{(III-139)}$$

and a perturbation given by

$$V_2(x) \equiv \beta V_0 \, a \, \delta(x) \qquad \text{(III-140)}$$

where V_0 has energy units and jointly to a, which has units of length, plays the role of the potential strength. The quantity β is just a dimensionless size parameter for the perturbation. For the unperturbed problem a purely discrete spectrum is going to be found, with states of well defined parity as it is the case for Harmonic Oscillator also. The new ingredient is a highly singular and localized perturbation represented by the

delta function interaction. As it was done for the previous case, our concentation will rest upon the ground state, described by the wavefunction:

$$\psi_0(x) = \frac{1}{\sqrt{a}} \cos \frac{\pi}{2a} x \qquad \text{(III-141)}$$

the delta function can be replaced by any representation in a limit form (i.e., gaussions, heavyside functions, etc.) and we can take the square root of it. Once all the operations necessary for the construction of the Doorway basis and related quantities are performed, the proper limit can be taken. Another possible approach to this problem is an asymmetrical choice in the factorization of the perturbation. For example, the following starting vectors can be taken:

$$|D_0\rangle = N_0 |\psi_0\rangle \qquad |\tilde{D}_0\rangle = \tilde{N}_0 V_2 |\psi_0\rangle \qquad \text{(III-142)}$$

and the result for the normalization of the states will be:

$$(\tilde{N}_0^* N_0)^{-1} = \langle \psi_0 | V_2 | \psi_0 \rangle = \beta V_0 \qquad \text{(III-143)}$$

as it will be the case if the limit procedure would be followed. The rescattering operator is defined in this

case by

$$W \equiv \vartheta_0 V_2 \qquad \text{(III-144)}$$

where ϑ_0 is the Reduced Green's Operator, given by

$$\vartheta_0 \equiv \sum_{n\neq 0} \frac{|n\rangle\langle n|}{\mathcal{E}_0 - \mathcal{E}_n} \qquad \text{(III-145)}$$

With equations (III-144) and (III-145) it is possible to find the first Doorway expectation value for the rescattering operator: (the result is the same in the limit procedure)

$$W_{00} \equiv \langle \tilde{\mathcal{D}}_0 | W | \mathcal{D}_0 \rangle = -\frac{2\mu a^2}{\pi^2}\beta V_0 \qquad \text{(III-146)}$$

where specific use of the Reduced Green's Function, evaluated at the origin, was made:

$$\vartheta_0(0,0) = -\frac{2\mu a}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n(n+1)} = -\frac{2\mu a}{\pi^2} \qquad \text{(III-147)}$$

The second Doorway state is given by

$$\langle x | \mathcal{D}_1 \rangle \equiv N_1\left\{\sqrt{\beta V_0 a}\;\vartheta_0(x,0) + \frac{2\mu a}{\pi^2}\sqrt{\beta V_0 a}\cos\frac{\pi}{2a}x\right\} \qquad \text{(III-148)}$$

an expression for the Reduced Green's function can be

found by solving the appropriate differential equation, as it was done in section (3), with the result:

$$\vartheta_0(\zeta,\zeta') = -\frac{2\mu a}{\pi}\left\{\frac{1}{\pi}\cos\frac{\pi}{2}\zeta\cos\frac{\pi}{2}\zeta' + \zeta\sin\frac{\pi}{2}\zeta\cos\frac{\pi}{2}\zeta'\right.$$
$$\left. + \zeta'\cos\frac{\pi}{2}\zeta\sin\frac{\pi}{2}\zeta' + \sin\frac{\pi}{2}(\zeta_< - \zeta_>)\right\} \qquad \text{(III-149)}$$

where:

$$\zeta \equiv \frac{x}{a} \qquad \text{(III-150)}$$

and $\zeta_<$ ($\zeta_>$) means that the lesser (greater) between ζ and ζ' has to be taken. An interesting feature of equation (III-148) is the discontinuity of the origin of the first term with $\vartheta_0(x,0)$, when equation (III-149) is used, and it is a natural consequence of using a singular and localized perturbation. When it is attempted to proceed further with the construction of the Doorway basis, the following results:

$$W_{01} = W_{10} = 0 \qquad \text{(III-151)}$$

As it can be verified from equations (III-148) and (III-142), using as intermediate result:

$$\langle x | W^+ | \tilde{\mathcal{D}}_0 \rangle = -(\beta V_0 a)^{3/2}\,\frac{2\mu a}{\pi^2}\,\delta(x) \qquad \text{(III-152)}$$

in that case the energy shift in zeroth order is given by:

$$\Delta\mathcal{E}_o^{(0)} = \frac{\beta V_o}{1 + \frac{2\mu a^2}{\pi^2}\beta V_o} \qquad \text{(III-153)}$$

and interesting test for this number is provided by the limit $\beta \to \infty$, where our initial problem of one dimensional box is converted in two adjacent boxes. The ground state energy in the one box problem is given by

$$\mathcal{E}_o(\text{ONE BOX}) = \frac{\pi^2}{8\mu a^2} \qquad \text{(III-154)}$$

and when this box of length $2a$ is splitted in two boxes of length a, the new ground state energy is given by

$$\mathcal{E}_o(\text{TWO BOXES}) = \frac{\pi^2}{2\mu a^2} \qquad \text{(III-155)}$$

and consequently the shift will be

$$\Delta\mathcal{E}_o = \frac{3}{8}\frac{\pi^2}{\mu a^2} \qquad \text{(III-156)}$$

taking the limit $\beta \to \infty$ in equation (III-153) the result is

$$\lim_{\beta\to\infty} \Delta\varepsilon_o^{(0)} = \frac{\pi^2}{2\mu a^2} \qquad \text{(III-157)}$$

Although $\frac{1}{2}$ is close to $\frac{3}{8}$, is clear that higher order terms in the energy shift expansion are needed to provide a better accuracy. Considering the first order term in the energy shift, the result is (for arbitrary β):

$$\Delta\varepsilon_o^{(1)} = \Delta\varepsilon_o^{(0)} - \left[\Delta\varepsilon_o^{(0)}\right]^2 \frac{4\mu^2 a^4}{\pi^4} S_2 \, \Delta\varepsilon_o^{(1)} \qquad \text{(III-158)}$$

which is derived from (III-34) and where

$$S_2 \equiv \sum_{n=1}^{\infty} \frac{1}{n^2 (n+1)^2} = 0.289868133696\ldots \qquad \text{(III-159)}$$

to obtain equation (III-158) the square of the Reduced Green's Function evaluated at the origin was also required:

$$\vartheta_o^2(0,0) \equiv \frac{4\mu^2 a^3}{\pi^4} S_2 \qquad \text{(III-160)}$$

equation (III-158) can be rewritten as

$$\Delta\varepsilon_o^{(1)} = \frac{\Delta\varepsilon_o^{(0)}}{1 + \left[\Delta\varepsilon_o^{(0)}\right]^2 \frac{4\mu^2 a^4}{\pi^4} S_2} \qquad \text{(III-161)}$$

Taking the limit $\beta \to \infty$:

$$\lim_{\beta \to \infty} \Delta\varepsilon_0^{(1)} = \frac{1}{2\,(1+S_2)} \frac{\pi^2}{\mu a^2} \qquad \text{(III-162)}$$

where

$$\frac{1}{2(1+S_2)} = 0.3876365... \qquad \text{(III-163)}$$

up to seven significant figures, which compares good with the exact value of 0.375. So, even if the premature Doorway truncation is taken into account, the procedure has its way towards the correct value through higher order terms in the energy shift expansion. We can examine also if for finite values of the size parameter β the behaviour is the same. The exact energies in the perturbed case are given by the solutions of the following trascendental equation

$$\frac{tg\, ka}{ka} = -\frac{1}{\beta \mu V_0 a^2} \qquad \text{(III-164)}$$

which are summerized in table (III-VIII). Using equation (III-153) the energy shifts in zeroth order are given by:

$$\Delta\varepsilon_0^{(0)}(\text{SET I}) = 4.555368 \text{ MeV} \quad \Delta\varepsilon_0^{(0)}(\text{SET II}) = 25.302851 \text{ MeV} \qquad \text{(III-165)}$$

and we see that equations (III-165) are giving to us a good representation of the energy shift that can be improved in a considerably way when the first order term in the energy shift is considered using equation (III-161):

$$\Delta\mathcal{E}_0^{(1)}(\text{SET I}) = 4.555298\ \text{MeV} \quad \Delta\mathcal{E}_0^{(1)}(\text{SET II}) = 23.631580\ \text{MeV} \qquad \text{(III-166)}$$

so it is clear that for arbitrary β the behaviour of the procedure is the same, i.e., there is convergence towards the correct energy shift value. The particular choice of the starting vectors is not going to affect the energy shift values but it is very sensitive in regards to the wavefunction. In this particular example, the choice described by equation (III-142) is given a wavefunction proportional to the unperturbed one as the perturbed wavefunction and this is obviously not correct. Working with the limit procedure

TABLE (III-VIII)

Exact results for the Infinite Square Well with a Delta Function perturbation with =150MeV, V_0 = 50 MeV and a = 5 fm

β	ka	$\mathcal{E}$ (MeV)	$\Delta\mathcal{E}_0$ (MeV)	SET
0.1	1.8283829	17.351110	4.544543	I
1	2.64018301	36.179370	23.372800	II

outlined at the beginning, the energy shift results can be kept in their entirety, the premature truncation is still observed when the limit is taken and the wavefunction is going to be obtained in the interaction region. The odd feature of the interaction region in this case is that it is given by a single point: $\chi = o$. Then contributions from higher Doorway states are still possible through a complicated limit procedure that we are not going to consider here and in that sense this example has been useful to show the importance of the proper choice for our Doorway basis. Next, we are going to consider a simple case which is closer to the kind of applications intended in forthcoming chapters.

(c) Three - dimensional square well with a square barrier as a perturbation:

The unperturbed Hamiltonian is considered to be:

$$H_o = \frac{p^2}{2\mu} + V_1(r) \qquad \text{(III-167)}$$

where $V_1(r)$ is a square well potential given by:

$$V_1(r) = -V_c\,\theta(a-r) \qquad \text{(III-168)}$$

being V_c the well depth and a the well radius. The perturbation to be considered in this case is a square barrier:

$$V_2(r) = V_S\,\theta\,(R-r) \qquad \text{(III-169)}$$

where V_S is the barrier height and R is the barrier radius. All the numerical treatment in this subsection will be done for the ground state case where the orbital angular momentum ℓ is taken as zero, i.e., S -wave problem. The ground state wavefunction to be pertubed is given by:

$$\psi_o(r) = A_o\,\frac{\sin kr}{r} \qquad \text{(III-170)}$$

where:

$$k^2 \equiv 2\mu\,(V_c - |E|) \qquad \text{(III-171)}$$

with $E<0$ and

$$A_o \equiv \left\{ \frac{a}{2} - \frac{1}{4k}\sin 2kR + \frac{\sin^2 ka}{2K} \right\}^{-1/2} \qquad \text{(III-172)}$$

The starting wavefunctions are given by

$$\langle x | D_o \rangle = N_o \sqrt{V_S}\;\theta\,(R-r)\,\psi_o(r) \qquad \text{(III-173)}$$

and

$$(\tilde{N}_o^* N_o)^{-1} = V_s \frac{R}{a} \frac{\left\{ \frac{1}{2} - \frac{1}{4kR} \sin 2kR \right\}}{\left\{ \frac{1}{2} - \frac{\sin 2ka}{4ka} + \frac{\sin^2 ka}{2ka} \right\}} \qquad \text{(III-174)}$$

the Reduced Green's Function can be found using the methods described in section (3) (see appendix (III-A)) with the result

$$\tilde{\theta}(r,r') = \begin{cases} -\frac{2\mu}{k_o} \left\{ \cos k_o r_< \sin k_o r_> + \tilde{R}_o \sin k_o r \sin k_o r' \right. & r,r'<a \\ \left. \quad + \tilde{R}_1 (r \cos k_o r \sin k_o r' + r' \sin k_o r \cos k_o r') \right\} & \\ -\frac{2\mu}{k_o} \left\{ \tilde{R}_2 e^{-k_o r} r \sin k_o r' + \tilde{R}_3 r' e^{-k_o r} \cos k_o r' \right. & \\ \left. \quad + \tilde{R}_4 e^{-k_o r} \sin k_o r' \right\} & r>a \end{cases} \qquad \text{(III-175)}$$

and

$$\tilde{\theta}(r,r') = \begin{cases} -\frac{2\mu}{k_o} \left\{ \tilde{R}_2 e^{-k_o r'} r' \sin k_o r + \tilde{R}_3 r e^{-k_o r'} \cos k_o r \right. & \\ \left. \quad + \tilde{R}_4 e^{-k_o r'} \sin k_o r \right\} & r<a \\ -\frac{2\mu}{k_o} \left\{ \frac{1}{2} e^{-k_o (r_> - r_<)} + \tilde{R}_5 e^{-k_o (r+r')} \right. & \\ \left. \quad + \tilde{R}_6 (r+r') e^{-k_o (r+r')} \right\} & r',r>a \end{cases} \qquad \text{(III-176)}$$

where:

$$k_o^2 \equiv 2\mu\,(V_c - |\varepsilon_o|) \qquad K_o^2 \equiv 2\mu\,|\varepsilon_o| \tag{III-177}$$

being ε_o the ground state energy for the unperturbed problem, obtained through the transcendental equation:

$$tg\,ka - \frac{K}{k} = 0 \tag{III-178}$$

the coefficients $\tilde{R}_i$ are given by

$$\tilde{R}_0 \equiv \frac{c_0}{\tilde{a}} - \frac{\tilde{b}}{\tilde{a}^2} W_- \tag{III-179}$$

$$\tilde{R}_1 \equiv \frac{W_- \mu}{\tilde{a}\, k_o} \tag{III-180}$$

$$\tilde{R}_3 \equiv \frac{\mu K_o}{\tilde{a}\, k_o} e^{K_o a} \tag{III-181}$$

$$\tilde{R}_4 \equiv -\frac{\tilde{b}}{\tilde{a}^2} K_o e^{K_o a} - a\tilde{R}_2 \tag{III-182}$$

$$\tilde{R}_2 \equiv \frac{\mu}{\tilde{a}} e^{K_o a} \tag{III-183}$$

$$\tilde{R}_5 \equiv \frac{c_1}{2\tilde{a}} e^{2K_o a} - \frac{\mu W_1 a}{\tilde{a} K_o} e^{2K_o a} - \frac{\tilde{b} W_1}{2\tilde{a}^2} e^{2K_o a} \tag{III-184}$$

$$\tilde{R}_6 \equiv \frac{\mu W_1}{2\tilde{a} K_o} e^{2K_o a} \tag{III-185}$$

and other quantities are:

$$W_+ \equiv k_o \cos k_o a + K_o \sin k_o a \qquad \text{(III-186)}$$

$$W_- \equiv k_o \sin k_o a - K_o \cos k_o a \qquad \text{(III-187)}$$

$$W_1 \equiv K_o \sin k_o a - k_o \cos k_o a \qquad \text{(III-188)}$$

$$\tilde{a} \equiv \mu \sin k_o a \left\{ -\frac{1}{k_o}\left[(1+K_o a)\frac{K_o}{k_o} + k_o a\right] - \frac{1}{K_o} \right\} \qquad \text{(III-189)}$$

$$\tilde{b} \equiv -\frac{\mu}{2k_o^2}\left\{\tilde{a} + \frac{\mu}{K_o}\sin k_o a\right\} + \frac{\mu^2}{2k_o}\left\{-(2+K_o a)\, a \sin k_o a \right.$$

$$\left. - k_o a^2 \cos k_o a \right\} - \frac{\mu^2 a}{k_o K_o}\cos k_o a - \frac{\mu^2}{2K_o^2}\sin k_o a \qquad \text{(III-190)}$$

$$C_o \equiv -\frac{\mu}{k_o^2} W_- + \left.\frac{dW_-}{d\varepsilon}\right|_{\varepsilon=\varepsilon_o} \qquad \text{(III-191)}$$

$$\left.\frac{dW_-}{d\varepsilon}\right|_{\varepsilon=\varepsilon_o} \equiv \frac{\mu}{K_o}\cos k_o a + \frac{\mu}{k_o}\left[(1+K_o a)\sin k_o a + k_o a \cos k_o a\right] \qquad \text{(III-192)}$$

$$C_1 \equiv \frac{\mu}{K_o^2} W_1 + \left.\frac{dW_1}{d\varepsilon}\right|_{\varepsilon=\varepsilon_o} \qquad \text{(III-193)}$$

$$\left.\frac{dW_1}{d\varepsilon}\right|_{\varepsilon=\varepsilon_o} = \frac{\mu}{k_o}\left[(K_o a - 1)\cos k_o a + k_o a \sin k_o a\right] - \frac{\mu}{K_o}\sin k_o a \qquad \text{(III-194)}$$

and the full radial Reduced Green's Function is given by

$$\vartheta(r,r') = \frac{\tilde{\vartheta}(r,r')}{rr'} \qquad \text{(III-195)}$$

The radius R of the barrier is always considered to be less than the well radius a. For $r<R$ the momentum is given by

$$\zeta^2 \equiv 2\mu\,(V_s - V_c - E) \qquad \text{(III-196)}$$

and a transcendental equation for the energy eigenvalues in the full problem is obtained:

$$\begin{aligned} &Sh\zeta R\,[aW_+ \sin kR - aW_- \cos kR] \\ &+ \frac{\zeta}{R}\, Ch\zeta R\,[aW_- \sin kR + aW_+ \cos kR] = 0 \end{aligned} \qquad \text{(III-197)}$$

Using equations (III-178) and (III-197) the results are summarized in tables (III-IX) and (III-X). In the case of the set I we have a relatively weak perturbation and still there the standard perturbation theory has problems to obtain a good answer. The results for the energy shifts are summarized in table (III-XI). There, the First order Perturbation Theory result is off by an approximated factor of two while with our perturbation theory, the result is within 0.4% the correct one with the simplest product of this approach, i.e., the first

TABLE (III-IX)

Parameters for the Exact and unperturbed cases for the Finite Square Well with a Square Barrier as perturbation.

	μ (MeV)	V_c (MeV)	a (fm)	V_S (MeV)	R (fm)
SET I	140	5	50	10	5
SET II	940	30	5	200	3

TABLE (III-X)

Results for the Exact and unperturbed energies for the Finite Square Well with a Square Barrier as Perturbation.

	$\mathcal{E}_o$ (Unperturbed, MeV)	$\mathcal{E}$ (Exact, MeV)	$\Delta\mathcal{E}$ (Exact, MeV)
SET I	-4.5522039984	-4.5227800415	0.029423957
SET II	-24.0509337249	-11.084767681	12.96616604

TABLE (III-XI)

Energy shift results for the Finite Square Well with a Square Barrier as a perturbation in the set I case.

$\Delta\mathcal{E}$ (First Order Perturbation) = 0.04756713 MeV

$\Delta\mathcal{E}$ (Exact) = 0.029423957 MeV

N_D	M	$\Delta\mathcal{E}^{(H)}$ (MeV)	$\Delta\mathcal{E}^{(O)}$ (MeV)
1	1	0.02932351	0.02931341
	2	0.02932125	
	3	0.02932128	
	4	0.02932128	
2	1	0.02944480	0.02943524
	2	0.02944250	
	3	0.02944253	
	4	0.02944252	
	5	0.02944252	
3	1	0.02942742	0.02941778
	2	0.02942513	
	3	0.02942516	
	4	0.02942515	
	5	0.02942515	

Doorway truncation and the zeroth order in the energy shift expansion. Of course, if more effort is done results with four correct significant figures can be obtained at the third Doorway truncation. In this example the features of the potentials involved are entirely different from the previous ones and in spite of that, the convergence properties of the Doorway-State-based Perturbation Theory behaves in a similar fashion. For the square well potential the spectrum can be separated in a continuum and a discrete part with finite number of bound states. The role of all these states is taken into account through the Reduced Green's Function that we can provide in a close form. The parameters selected for the Set I try to resemble in a very crude way the essential characteristics of the potentials related to the pionic atom problem, which is our aim in forthcoming chapters. The well is shallow and long ranged in an attempt to stimulate the Coulomb potential role and the height and radius of the square barrier were inspired by the repulsive part of the pion-nucleon S -wave interaction. According to the results in table (III-XI) it seems that with little effort in the Doorway State Calculation is possible to obtain good numbers with two or three significant figures (that is the limit of accuracy for any of the

experimental numbers available in the literature) using the most simple tools of the approach in the pionic atom case and probably in any physical problem where the perturbation is relatively weak. In order to examine the situation with the wavefunctions the table (III-XII) was prepared. The first Doorway truncation is just the unperturbed wavefunction multiplied by the square root of the perturbation. As it was observed in the Harmonic Oscillator case the quality of the approximation gets poorer as we go away from the origin, although if we compare with the unperturbed wavefunction the improvement is remarkable in that region. Now the set II can be considered and for that purpose table (III-XIII) was constructed. In that table the energy shift values are obtained for different Doorway truncations for a fixed expansion in the energy shift up to the first order until saturation and afterwards the energy shift order is increased. We can see a repetition of the features already learned in the Harmonic Oscillator case, specially the breakdown the second Doorway level for a large perturbation.

The conclusion at this point is that the Doorway State Approach to bound state perturbation theory is a powerful tool in a wide range of problems which allows in a cheap way (from the calculations point of view) to get the relevant information from the physical system

TABLE (III-XII)

Wavefunction Results for the Square Well Case With a Square Barrier as a Perturbation for the Set I. The Wavefunctions are Normalized to 1 for the First Point of this Table

r(fm)	2 Doorway Truncation	1 Doorway Truncation	Exact
0.01203	1	1	1
0.06318	5.251042	2.250893	5.251135
0.15431	12.828820	12.825158	12.828797
0.28396	23.625720	23.599575	23.622353
0.45000	37.506130	37.395945	37.486731
0.64969	54.326250	53.984796	54.258312
0.87977	73.951150	73.088768	73.768814
1.13645	96.265700	94.386914	95.855340
1.41552	121.117620	117.519954	120.364280
1.71239	148.60090	142.096596	147.147573
2.02220	178.44860	167.700721	176.050785
2.33986	210.58860	193.899319	206.893788
2066014	244.81440	220.250967	239.445818
2.97779	280.80750	246.314418	273.397866
3.28761	318.10710	271.657109	308.336296
3.58448	356.09050	295.863218	343.722042
3.86355	393.97130	318.540950	378.880101
4.12023	430.81460	339.328862	413.003574
4.35031	465.57390	357.901105	445.175104
4.55001	497.14370	373.971503	474.406964
4.71604	524.42650	387.296583	499.697821
4.84569	546.40610	397.677623	520.101876
4.93682	562.22030	404.962062	534.802914
4.98797	571.22960	409.045493	543.186566

TABLE (III-XIII)

Energy Shift Results for the Finite Square Well With a Square Barrier as a Perturbation in the Set II Case

$\Delta\mathcal{E}$(First Order Peturbation Theory) = 103.5592 MeV

$\Delta\mathcal{E}$(Exact) = 12.9661 MeV

N_D	M	$\Delta\mathcal{E}^{(M)}$ (MeV)	$\Delta\mathcal{E}^{(0)}$ (MeV)
1	1	11.40463	14.88294
2	1	-2.233632	-5.230289
3	1	20.30162	26.40256
4	1	12.05307	17.94561
5	1	11.98220	17.84205
6	1	11.98057	17.83972
7	1	11.98054	17.83968
8	1	11.98.53	17.83968
	2	13.72197	
	3	12.66118	
	4	13.17334	
	5	12.87392	
	6	13.03043	
	7	12.94175	
	8	12.98953	
	9	12.96292	

under study. This information is given in the form of energy shifts as the essential products and wavefunctions and Green's Functions as byproducts. In the forthcoming chapters the detailed analysis of pionic atoms will be based entirely in this formalism using just the information from the energy shifts and hoping in a future to exploit in a full scale the possibilties now open with the "byproducts".

REFERENCES FOR CHAPTER III

(1) F. Lenz, E.J. Moniz and K. Yazaki, Ann. Phys. Vol. 129, p.84, 1980

(2) N. H. March, W. H. Young and S. Sampathar, The Many-Body Problem in Quantum Mechanics, Cambridge Press, 1967

(3) I. Lindgren and J. Morrison, Atomic Many-Body Theory, Springer-Verlog, 1982.

(4) R.R. Whitehead, A. Watt, B.J. Cole and I. Morrison, Advances in Nuclear Physics, Vol.9, p.123, 1977 Press.

CHAPTER IV

PION-NUCLEON FORCES AND PIONIC HYDROGEN.

In the models that are going to be used in the next chapter, in order to study the energy shifts and widths, the forces involved have parameters which should be determined as reliably as possible for the low energy range. From the phase shift information, these parameters can be extracted in a very simple fashion for the S_{11} and P_{33} channels of the pion-nucleon interaction using the standard Yamaguchi vertex functions. Due to the behavior of the phase shift for the S_{31} channel, the same parameters are going to be determined from available data for pionic hydrogen. The importance of Coulomb interaction in the rescattering process will be demonstrated. These parameters are used in the calculation of the phase shifts for the comparison with experimental data showing good agreement in the low energy region.

(1) The S_{11} and P_{33} channels in the pion-nucleon interaction:

The pion-nucleon interaction is described in a separable form with vertex functions:

$$\vartheta(K^2) \equiv \frac{1}{\alpha^2 + K^2} \qquad \text{(IV-1)}$$

where α is the cut off parameter related to the interaction range. In phase shift analysis for a separable interaction problem the relevant quantity is the Fredholm Determinant:

$$\mathcal{D}(E) = |\mathcal{D}(E)| \; e^{-i\,\delta(E)} \qquad \text{(IV-2)}$$

which in a relativistic treatment of this problem is given by:

$$\mathcal{D}(E) = E^2 - M_R^2 - G_0^2 \int \frac{d\vec{q}}{(2\pi)^3} \frac{f(q^2)}{(E-\epsilon_q)^2 - \omega_q^2 + i\eta} \qquad \text{(IV-3)}$$

where $f(q^2)$ contains the vertex functions of the particular channel and M_R is the bare mass for the resonance. The energies ϵ_q and ω_q are, respectively, the nuclear and the pion energies given by:

$$\epsilon_q \equiv \frac{q^2}{2M_N} + M_N \qquad \text{(IV-4)}$$

$$\omega_q \equiv \sqrt{q^2 + M_\pi^2} \qquad \text{(IV-5)}$$

Now we follow the semi-relativistic treatment of this problem by Moniz and Sevgen[1], introducing:

$$\xi \equiv E - M_N \qquad \text{(IV-6)}$$

and ignoring terms of order $1/M_N^2$, a simple form for equation (IV-3) can be obtained:

$$D(E) = E^2 - M_R^2 - \frac{G_0^2}{1+\frac{\xi}{M_N}} \int \frac{d\vec{q}}{(2\pi)^3} \frac{f(q^2)}{K^2 - q^2 + i\eta} \qquad \text{(IV-7)}$$

where:

$$K^2 \equiv \frac{\xi^2 - M_\pi^2}{1+\frac{\xi}{M_N}} \qquad \text{(IV-8)}$$

the quantity K^2 in equation (IV-8) behaves like the squared relative momentum and it can be approximated in that way up to $\Theta(1/M^2)$. In the next chapter when the S-wave pion-nucleon channels will be considered, a renormalization procedure will be required in order to eliminate the dependence of our model on the resonance masses. The reason for this is given by the fact that these resonances are located in an energy region where particle formation processes may occur and should be taken into account in the bare mass determination. This complication is not necessary for low energy range and can be avoided by factoring out $(E^2-M_R^2)$ in equation (IV-7) and renormalizing the coupling constant G^2 in the following way:

$$\tilde{G}^2(E) \equiv \frac{G_o^2}{E^2 - M_R^2} = \frac{G_o^2}{(E+M_R)(E-M_R)} \qquad \text{(IV-9)}$$

and taking the low energy limit, the result is:

$$\lim_{E \to M} \tilde{G}^2(E) = G^+G = \frac{G_o^2}{(M+M_R)\,\Delta M_R} \equiv \lambda g^2 \qquad \text{(IV-10)}$$

where $\lambda = \pm 1$ accordingly to the attractive or repulsive character of the interaction and

$$M \equiv M_N + M_\pi \qquad \text{(IV-11)}$$

$$\Delta M_R \equiv M - M_R \qquad \text{(IV-12)}$$

this procedure yields the following Fredholm Determinant for the channels of the S-wave pion-nucleon interaction:

$$D_R(E) \equiv 1 - \frac{\lambda g^2}{1 + \frac{\xi}{M_N}} \int \frac{d\vec{q}}{(2\pi)^3} \frac{f(q^2)}{K^2 - q^2 + i\eta} \qquad \text{(IV-13)}$$

Equation (IV-13) can be applied to the S_{11} channel case, where the vertex form factor is taken to be:

$$h(\vec{q}) \equiv \frac{G}{\sqrt{3}} \frac{\tilde{\tau} \cdot \tilde{\phi}}{\alpha^2 + q^2} \qquad \text{(IV-14)}$$

where $\tilde{\tau}$ is the nucleon isospin operator and $\tilde{\phi}$

is the pion isospin wavefunction given by:

$$\phi_+ \equiv \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\\0\end{bmatrix}, \phi_- \equiv \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\\0\end{bmatrix}, \quad \phi_o \equiv \begin{bmatrix}0\\0\\1\end{bmatrix} \tag{IV-15}$$

the coupling constant G is rewritten in terms of

$$G^+ G = -g^2 \tag{IV-16}$$

where $\lambda = -1$ was taken for the S_{11}, due to its attractive nature and

$$\tilde{\tau}^+ \cdot \tilde{\tau} = 3 \tag{IV-17}$$

The Fredholm Determinant is given by

$$D(E) = 1 - \frac{g^2}{1+\frac{\xi}{M_N}} \frac{1}{8\pi\alpha} \frac{1}{(\alpha - iK)^2} \tag{IV-18}$$

where K is given by equation (IV-8) and ξ by equation (IV-6). From equation (IV-18) the phase shift can be obtained:

$$tg\,\delta(K) = \frac{g^2 K}{4\pi\left(1+\frac{\xi}{M_N}\right)\left(K^2+\alpha^2\right)^2 - \frac{g^2}{2\alpha}\left(\alpha^2-K^2\right)} \tag{IV-19}$$

and the scattering length:

$$a_{11}^{S} = \lim_{K \to 0} \frac{tg\,\delta(K)}{K} = \frac{2\beta_2 g^2}{8\pi\alpha - \beta_2 g^2 \alpha} \qquad \text{(IV-20)}$$

where $\beta_2 \equiv M_N/M$ and M is given by equation (IV-11). In our problem we have essentially two parameters to be determined, the coupling constant g^2 and the cut off parameter α. Since we are primarily interested in very low energies, a way to assure the proper behavior in that limit is to replace g^2 as a parameter by the scattering length a_{11}^{S} using equation (IV-20):

$$g^2 = \frac{1}{\beta_2} \frac{4\pi\alpha^4\, a_{11}^{S}}{1 + a_{11}^{S}\alpha/2} \qquad \text{(IV-21)}$$

then the experimental value for a_{11}^{S} can be used, reducing our problem to one parameter. This experimental value is given by[2]

$$a_{11}^{S} = (0.170 \pm 0.004)\, M_{\pi}^{-1} \qquad \text{(IV-22)}$$

the results of our fit are shown in table (IV-I). The R.M.S. deviation for the fit was 0.35 degrees and the experimental standard deviation was 0.78 degrees, for the phase shifts. Under these conditions the parameters are:

$$g^2(S_{11}) = 11735.46\, fm^{-3} = 108.86\, M_N^3 \qquad \text{(IV-23)}$$

and

$$\alpha_{11}^S = 9.2\, fm^{-1} = 1815.16\ MeV/c \qquad \text{(IV-24)}$$

the scattering length is bound within the experimental allowances:

$$a_{11}^S = 0.168\ M_\pi^{-1} \qquad \text{(IV-25)}$$

and we can see that the fit is quite good. The experimental values given in table (IV-I) are taken from references (2,3). Since our main interest lies in the low energy region, from now on in this work we will consider the low energy limit for equation (IV-18), with the result:

$$D(E) = 1 - \frac{\beta_2 g^2}{8\pi\alpha} \frac{1}{(\alpha - iK)^2} \qquad \text{(IV-26)}$$

and the coupling constant is conveniently redefined once more as:

$$G^+G \equiv \frac{\lambda g^2}{2M_\pi} \qquad \text{(IV-27)}$$

the factor of $2M_\pi$ is introduced in equation

TABLE (IV-I)

Phase Shifts fit for the S_{11} channel. Pion momentum measured in the Center of Mass System.

Pion Momentum (Me V/c)	Experimental Phase Shift (degrees)	Calculated Phase Shift (degrees)
146.90	7.33 ± 0.40	7.92
173.80	8.59 ± 0.34	8.88
193.70	9.68 ± 0.29	9.50
207.10	9.91 ± 0.34	9.87
228.70	10.31 ± 0.69	10.42
247.60	11.34 ± 0.52	10.83
259.50	13.35 ± 1.60	11.07
275.90	11.69 ± 1.89	11.36
292.90	13.87 ± 0.92	11.64

(IV-27) to obtain the proper factors in equation (IV-26). The same form for the coupling constant will be used in the S_{31} channel case, which will be considered later in this chapter.

For the P_{33} channel the analysis is already

done[1] and our requirement is to translate the result to the very low energy case. In this channel the Fredholm Determinant is given by:

$$\mathcal{D}(E) = E^2 - M_\Delta^2 - \frac{g^2}{3\left[1+\frac{\xi}{M_N}\right]}\int\frac{d\vec{q}}{(2\pi)^3}\frac{q^2}{(\alpha^2+q^2)^2(K^2-q^2)} \qquad \text{(IV-28)}$$

where the semi-relativistic treatment is followed and K and ξ are given by equations (IV-6) and (IV-8) and the vertex form factor are taken to be

$$h(\vec{q}) \equiv G\,\frac{\vec{S}\cdot\vec{q}\;\;\tilde{T}\cdot\Phi}{\alpha^2+q^2} \qquad \text{(IV-29)}$$

where $\vec{S}$ is the spin transition operator between spin 1/2 and spin 3/2 defined by the matrices (6):

$$S_x \equiv \begin{bmatrix} -1/\sqrt{2} & 0 \\ 0 & -1/\sqrt{6} \\ 1/\sqrt{6} & 0 \\ 0 & 1/\sqrt{2} \end{bmatrix} \qquad \text{(IV-30)}$$

$$S_y \equiv i\begin{bmatrix} 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{6} \\ 1/\sqrt{6} & 0 \\ 0 & 1/\sqrt{2} \end{bmatrix} \qquad \text{(IV-31)}$$

$$S_z \equiv \begin{bmatrix} 0 & 0 \\ \sqrt{\frac{2}{3}} & 0 \\ 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{bmatrix} \qquad \text{(IV-32)}$$

An useful relation is the product:

$$S_i^+ S_j = \frac{2}{3}\delta_{ij} - \frac{1}{3} i \epsilon_{ijk} \sigma_k \qquad \text{(IV-33)}$$

and it behaves like a J = 3/2 projection operator. This formalism is identical for the isospin transition operator $\widetilde{T}$ given in equation (IV-29).

In the non-relativistic limit equation (IV-28) can be written as:

$$D(E) = (E-M_\Delta)(E+M_\Delta) - \frac{g^2}{6M_T}\int \frac{d\vec{q}}{(2\pi)^3} \frac{q^2}{(\alpha^2+q^2)^2\left(E-\frac{q^2}{2\mu}\right)} \qquad \text{(IV-34)}$$

where μ is the pion-nucleon reduced mass given by

$$\mu = \frac{M_\pi M_N}{M_\pi + M_N} \qquad \text{(IV-35)}$$

and in order to obtain equation (IV-34) the following replacement was taken:

$$\frac{1}{1+\frac{\xi}{M_N}} \xrightarrow[\text{LIMIT}]{\text{NON-RELATIVISTIC}} \beta_2 = \frac{M_N}{M_\Delta} = \frac{\mu}{M_\pi} \qquad \text{(IV-36)}$$

the coupling constant can be renormalized to:

$$g_R^2 = \lim_{\varepsilon \to M} \frac{g^2}{\varepsilon + M_\Delta} = \frac{g^2}{M + M_\Delta} \qquad \text{(IV-37)}$$

and we consider the Fredholm Determinant in the non-relativistic limit to be:

$$D_{NR}(E) = E - M_\Delta - \frac{1}{3} \frac{g_R^2}{2M_\pi} \int \frac{d\vec{q}}{(2\pi)^3} \frac{q^2}{(\alpha^2 + q^2)^2 \left(E - \frac{q^2}{2\mu}\right)} \qquad \text{(IV-38)}$$

with

$$G^+G \equiv \frac{g^2}{2M_\pi \ (M + M_\Delta)} \qquad \text{(IV-39)}$$

In order to verify these results with experi - mental information at low energies, the scattering volume a_{33}^P is calculated using equation (IV-39):

$$a_{33}^P = \frac{2\beta_2 g^2}{24\pi (M + M_\Delta) \alpha^4 \Delta M - \beta_2 g^2 \alpha^3} \qquad \text{(IV-40)}$$

where:

$$\Delta M \equiv M_\Delta - M \qquad \text{(IV-41)}$$

and according to reference [1] the parameters obtained in the semi-relativistic treatment are:

$$M_\Delta = 1370 \text{ MeV} = 6.94 \text{ fm}^{-1} \qquad \text{(IV-42a)}$$

$$\alpha_{33}^{P} = 300 \text{ MeV/c} = 1.52 \text{ fm}^{-1} \qquad \text{(IV-42b)}$$

$$g^2(P_{33}) = 11.38\, M_N^3 = 1226.75 \text{ fm}^{-3} \qquad \text{(IV-42c)}$$

with this set of parameters a phase shift is calculated and compared in table (IV-II) in order to show the quality of the fit. Using these quantities in equation (IV-37) the result is:

$$a_{33}^{P} = 0.589 \text{ fm}^3 = 0.209\, M_\pi^{-3} \qquad \text{(IV-43)}$$

In reference[1] the value $0.2133\ M^{-3}$ is obtained from the model and the experimental value is $(0.215 \pm 0.005)\ M^{-3}$. So we can see that the renormalization procedure presented in this section for the treatment of the very low energies case is consistent with the low energy information. In this point, our discussion about the parameters for the forces in the S_{11} and P_{33} channel cases is completed and in order to consider the S_{31} channel case, the pionic hydrogen information is studied first in the next section.

TABLE (IV-II)

Phase Shifts fit for the P_{33} channel

E(MeV)	Calculated Phase Shift (Degrees)	Experimental Phase Shift (Degrees)
1089	0.5	0.6
1099	1.6	1.8
1110	3.3	3.5
112	7.3	7.8
1148	14.6	15.2
1172	27.7	28.3
1186	38.4	38.3
1202	53.6	53.6
1221	74.2	74.6
1235	89.0	89.4
1253	105.1	105.1
1275	119.7	119.6
1292	128.0	126.8
1320	138.0	135.6
1337	142.5	139.5
1362	147.9	144.7
1390	152.6	149.3
1416	156.1	153.4

(2) Energy Shift for pionic hydrogen

The pionic hydrogen is the simplest pionic atom that can be considered. First, we have a two body system in which the orbital angular momentum is equal to the relative angular momentum between the pion and the nucleon, allowing us to look directly on particular channels of pion-nucleon interaction. For instance, the 1S level has contributions only from the S_{11} and S_{31} channels. Unfortunately the available experimental data is not going beyond this pionic level so far, but this will be enough for our purposes. Second, the absorption phenomenon is not present due to the fact that a nucleon can not absorb a pion with conservation of energy and momentum. Then, pionic hydrogen is an excellent testing ground for S wave pion-nucleon interaction studies in the low energy limit. Now we are going to develop a formalism to calculate the energy shift using separable interactions. This model will be fully justified and developed in the next chapter. Then, for the particular channel of interest the interaction can be described in the following form:

$$\mathcal{V} \equiv g\, g^{+} \qquad \text{(IV-36)}$$

In chapter III it was shown that for cases like

the pionic atom problem perturbation theory in the Doorway State Approach can be applied without going beyond the zeroth order in the energy shift and the approximation is very good, i.e., for practical purposes we are going to replace the exact energy by the unperturbed value $\mathcal{E}_s$ in equation (III-14), giving the following energy shift:

$$\Delta\mathcal{E}_s = \langle s | g \frac{1}{1 - g^+ \vartheta(\mathcal{E}_s)\, g} g^+ | s \rangle \quad \text{(IV-47)}$$

or

$$\Delta\mathcal{E}_s = \frac{N_V^* N_V}{1 - R(\mathcal{E}_s)} \quad \text{(IV-48)}$$

where:

$$N_V \equiv \int \frac{d\vec{q}}{(2\pi)^3} h^+(q^2)\, \phi_s(\vec{q}) = \int d\vec{r}\, h^+(\vec{r})\, \phi_s(\vec{r}) \quad \text{(IV-49)}$$

and:

$$R(\mathcal{E}_s) \equiv \int h^+(\vec{r})\, \vartheta(\mathcal{E}_s; \vec{r}, \vec{r}')\, h(\vec{r}')\, d\vec{r}\, d\vec{r}' \quad \text{(IV-50)}$$

the function $\vartheta(\mathcal{E}_s; \vec{r}, \vec{r}')$ is the Reduced Green's Function calculated for the pionic state S and the $h(q^2)$ (or $h(\vec{r})$) is the vertex function for the interaction. The pion wavefunction in the state S is symbolized by $\phi_s(\vec{q})$. The quantity $R(\mathcal{E}_s)$, given by equation (IV-50), is given to

us a measure of the rescattering effect and in particular for the pionic 1S state we have:

$$R(\varepsilon_s) = f^+ f \; W \qquad \text{(IV-51)}$$

where:

$$f \equiv \frac{G}{4\pi}, \qquad G^+G \equiv \frac{\lambda g^2}{2M_\pi} \qquad \text{(IV-52)}$$

and:

$$h(\vec{r}) \equiv f \frac{e^{-\alpha r}}{r}, \quad h(\vec{q}) \equiv \frac{G}{\alpha^2 + q^2} \qquad \text{(IV-53)}$$

and:

$$W \equiv \int_0^\infty r^2 dr \int_0^\infty r'^2 dr' \frac{e^{-\alpha r}}{r} \vartheta_0^1(r,r') \frac{e^{-\alpha r'}}{r'} \qquad \text{(IV-54)}$$

The Reduced Green's Function is given by

$$\vartheta_0^1(r,r') = -4\mu^2 Z \alpha_{FS} e^{-K_1(r+r')} \qquad \text{(IV-55)}$$

$$\otimes \left\{ \frac{5}{2} - \gamma - K_1(r+r') + G_0^1(K_1 r_<) + \frac{1}{2K_1 r_>} - \log 2K_1 r_> \right\}$$

where Z is the atomic number, $\alpha_{FS} = 1/137$ is the fine structure constant and

$$G_o^1(x) \equiv \sum_{n=1}^{\infty} \frac{2^n x^n}{n(n+1)!} \qquad \text{(IV-56)}$$

In order to obtain $\vartheta_o^1(r,r')$ the results of section (III-3) were used and the details of the tion are given in appendix (IV-A). The calculation of W is very lengthy.

Here we offer the final result:

$$W = -4\mu^2 Z\alpha_{FS} \left\{ \frac{5-2\gamma-2\log 2-\log\left(1+\frac{\alpha}{K_1}\right)}{(K_1+\alpha)^4} \right.$$

$$-\frac{17}{4}\frac{K_1}{(K_1+\alpha)^5} - \frac{27}{4K_1(K_1+\alpha)^3} - \frac{1}{2\alpha(K_1+\alpha)^3}$$

$$\left. + \log\left(1+\frac{K_1}{\alpha}\right)\left[\frac{1}{K_1(K_1+\alpha)^3} - \frac{\alpha}{K_1(K_1+\alpha)^4} - \frac{\alpha}{K_1^3(K_1+\alpha)^2}\right]\right\} \qquad \text{(IV-57)}$$

where K_1 in equations (IV-54) and (IV-56) is given by

$$K_1 \equiv \mu Z \alpha_{FS} \qquad \text{(IV-58)}$$

and then:

$$R(\varepsilon_s) = \frac{\lambda g^2}{32\pi^2 M_\pi} W \qquad \text{(IV-59)}$$

The vertex functions are given by

$$N_V \equiv \int d\vec{r}\; h^{\dagger}(\vec{r})\,\phi_s(\vec{r}) = 4\pi f\, C_{1S}\int_0^{\infty} r\, e^{-(\alpha+K_1)r}\, dr$$

$$= \frac{4\pi f\, C_{1S}}{(\alpha+K_1)^2} \qquad \text{(IV-60)}$$

where C_{1S} is the normalization constant for the pionic wavefunction given by:

$$|C_{1S}|^2 = \frac{K_1^3}{\pi} \qquad \text{(IV-61)}$$

the energy shift is finally given by:

$$\Delta\varepsilon_{1S} = \frac{\lambda g^2 K_1^3}{2\pi M_{\pi}\,(\alpha+K_1)^4}\;\frac{1}{1-R(\varepsilon_s)} \qquad \text{(IV-62)}$$

Equation (IV-62) is the energy shift for a particular channel and the total one is obtained by adding the contributions from the S_{11} and S_{31} channels. In order to combine them, we have to take into account:

$$(\tilde{\tau}\cdot\phi_-)\left|\tfrac{1}{2}\, m_\tau\right\rangle = \frac{1}{\sqrt{2(m_\tau+1)}}\left|\tfrac{3}{2}, m_\tau-1\right\rangle \qquad \text{(IV-63)}$$

for the S_{31} channel, and:

$$\frac{1}{\sqrt{3}}(\tilde{\tau}\cdot\tau_-)\left|\tfrac{1}{2}\, m_\tau\right\rangle = \frac{1}{\sqrt{6}}(1+2m_\tau)\left|\tfrac{1}{2}, -m_\tau\right\rangle \qquad \text{(IV-64)}$$

for the S_{11} channel. The ket $\left|\frac{1}{2}\, m_\tau\right\rangle$ is just the nucleon isospin state and the kets on the rigth re -

present the isospin states of the particular channels. Using equations (IV-62), (IV-63) and (IV-64), the combined (total) energy shift is given by:

$$\Delta\mathcal{E}_{1S} = \frac{K_1^3 g_{31}^2}{6\pi M_\pi (\alpha_{31}+K_1)^4}\ \frac{1}{1-R_{31}(\mathcal{E}_s)} - \frac{K_1^3 g_{11}^2}{3\pi M_\pi (\alpha_{11}+K_1)^4}\ \frac{1}{1-R_{11}(\mathcal{E}_s)} \qquad \text{(IV-65)}$$

Equation (IV-65) is going to be used to find the parameters for the S_{31} channel and to test the effect of the rescattering process in the energy shift in the next section. This will be possible thanks to a reported experimental value for the 1S energy shift in pionic hydrogen, given by:

$$\Delta\mathcal{E}_{1S} = (5.5 \pm 1.5)\ eV \qquad \text{(IV-66)}$$

(3) Force parameters for the S_{31} channel.

In the simplest possible approach to the problem the S_{31} channel interacion can be described through vertex functions of simple structure like the ones for the S_{11} and P_{33} channels:

$$h(\vec{q}) = G\,\frac{\bar{\Gamma}\cdot\Gamma}{\alpha^2+q^2} \qquad \text{(IV-67)}$$

where $\approx{T}$ is the transition isospin operator used in the P_{33} channel, then:

$$\approx{T} \cdot \approx{T}^{+} = 1 \qquad \text{(IV-68)}$$

and the coupling constant is given by:

$$G^{+}G = \frac{g^2}{2M_{\pi}} \qquad \text{(IV-69)}$$

following the non-relativistic treatment already outlined in this chapter. The Fredholm Determinant is given by:

$$D(K) = 1 + \frac{\beta_2 g^2}{8\pi\alpha} \frac{1}{(\alpha - iK)^2} \qquad \text{(IV-70)}$$

and then the phase shift can be extracted from

$$tg\,\delta(K) = - \frac{g^2 K}{\frac{4\pi}{\beta_2}(\alpha^2 + K^2)^2 + \frac{g^2}{2\alpha}(\alpha^2 - K^2)} \qquad \text{(IV-71)}$$

and the scattering length is obtained through the limit:

$$a_{31}^{S} = \lim_{K \to 0} \frac{tg\,\delta(K)}{K} = - \frac{g^2}{\frac{4\pi}{\beta_2}\alpha^4 + \frac{g^2\alpha}{2}} \qquad \text{(IV-72)}$$

Using equations (IV-71) and (IV-72) a fit similar to the one obtained for the S_{11} channel can be at-

tempted, but difficulties appear at intermediate energies due to the curvature of $\delta(K)$. It is possible to understand the problem looking at the expansion of:

$$K \operatorname{cotg} \delta(K) = \pm \frac{1}{a} + \frac{1}{2} r K^2 + \cdots \qquad \text{(IV-73)}$$

where a is the scattering length and r is the effective range. For the S-wave interaction the experimental measurements of quantities related to the effective range are given in the table (IV-III) and defined through the following equation:

$$r_{2I} \equiv -2 \left(a_{2I} + \frac{\beta_{2I}}{a_{2I}^2} \right) \qquad \text{(IV-74)}$$

all the quantities reported here are given in pion Compton wavelengths. In equation (IV-74) the index I is the isospin channel with values 1/2 and 3/2 . From refer-

TABLE (IV-III)

Effective range parameters for the S-wave interaction

$\beta_1 + 2\beta_3$	$\beta_1 - \beta_3$	References
-0.15 ± 0.06	0.027 ± 0.015	7
-0.133 ± 0.02	0.040 ± 0.018	8

[This values are taken from "Compilation of Coupling Constants and low Energy Parameters" (1978- edition), reference (5) which leads us to references (7) and (8)]

ence [7] the effective ranges are given by

$$r_1 = (1.91 \pm 1.87)\ M_\pi^{-1} \qquad r_3 = (12.0 \pm 5.6)\ M_\pi^{-1} \qquad \text{(IV-75)}$$

and from reference [8]:

$$r_1 = (0.92 \pm 1.00)\ M_\pi^{-1} \qquad r_3 = (11.8 \pm 3.1)\ M_\pi^{-1} \qquad \text{(IV-76)}$$

Then we can see that the effective ranges are positive as they are extracted from the experimental data, giving a positive curvature to K cotg $\delta(K)$. With the simple vertex function given by (IV-67) the curvature has opposite sign for reasonable values of the parameters, degrading in this way the quality of the fit at low and intermediate energies. It is easy to prove this by looking at the explicit form of Kcotg $\delta(K)$, according to equation (IV-71):

$$K \operatorname{cotg} \delta(K) = -\frac{4\pi}{\beta_2 g^2}(K^2+\alpha^2)^2 - \frac{1}{2\alpha}(\alpha^2 - K^2) \equiv f(K) \qquad \text{(IV-77)}$$

making the expansion given by (IV-73), we get:

$$-\frac{1}{|a|} = -\frac{\alpha}{2} - \frac{4\pi}{\beta_2 g^2}\alpha^4 \qquad \text{(IV-78)}$$

$$r = \frac{1}{\alpha} - \frac{16\pi\alpha^2}{\beta_2 g^2} \qquad \text{(IV-79)}$$

Combining equations (IV-78) and (IV-79) the result is:

$$\alpha r = 3 - \frac{4}{\alpha|a|} \qquad \text{(IV-80)}$$

Positive effective ranges can be obtained for:

$$\alpha \geq \frac{4}{3|a|} \qquad \text{(IV-81)}$$

and then this sets a lower bound around $10 fm^{-1}$ for the cut-off constant α, which is very high value for a realistic description of the S_{31} interaction. On the other hand the error allowances for the reported values of the effective ranges are too wide to give us any reasonable value for the interaction parameters. Our only choice in this point is to consider the information obtained from pionic hydrogen, which can be extracted using the expressions derived in the previous section and after that, try to verify our results by looking at the behavior of phase shifts at low energies. The interaction parameters of the S_{11} Channel are supposed to be known and by just fitting equation (IV-65) to the expe-

rimental value given by equation (IV-66), using equation (IV-72) to remove one parameter (the coupling constant in this case) the result for the cut-off parameter can be obtained to give:

$$\alpha_{31}^{S} = 3.482\, fm^{-1} = 687\ MeV/c \qquad \text{(IV-82)}$$

and in equation (IV-72) for the scattering length, we use the experimental value:

$$a_{31}^{S} = -(0.100 \pm 0.020)\ M_{\pi}^{-1} \qquad \text{(IV-83)}$$

during the fitting procedure we allowed the scattering length to vary within the experimental allowances, in order to meet the 1S energy shift value and the proper behavior for the phase shifts in the low energy limit. In this sense the scattering length that we have to report is

$$a_{31}^{S} = -0.112\ M_{\pi}^{-1} \qquad \text{(IV-84)}$$

the corresponding coupling constant is given by

$$g^2(S_{31}) = 463.84\, fm^{-3} = 4.30\, M_N^3 \qquad \text{(IV-85)}$$

The calculated phase shift is shown in table

(IV-IV) for purposes of comparison. In spite of the initial problem, we can see that the fit at low energies up to 50 MeV (or 126 MeV/c for the pion momentum) is fairly good. In this way we have a reliable tool that can be used in the study of low energy phenomena.

TABLE (IV-IV)

Phase shift fit for the S_{31} channel. Pion momentum is measured in the Center of Mass System.

Pion Momentum (MeV/c)	Experimental Phase Shifts (Degrees)	Calculated Phase Shifts (Degrees)
67.60	-2.92 ± 0.17	-3.07
82.60	-3.55 ± 0.23	-3.73
94.70	-4.41 ± 0.29	-4.25
109.20	-4.76 ± 0.17	-4.86
126.40	-5.84 ± 0.34	-5.57
140.50	-7.62 ± 0.46	-6.13
152.40	-8.48 ± 0.34	-6.59

(4) Rescattering process and Coulomb interaction effects:

The pionic hydrogen system is a very good play-

ground to study the effects of the Coulomb interaction of rescattering process in isolation from many effects present in heavier systems. In order to consider this problem, we can rewrite equation (IV-65) in the following way:

$$\Delta\varepsilon_s = \left(N_V^* N_V\right)_{31} \frac{1}{1-R_{31}} + \left(N_V^* N_V\right)_{11} \frac{1}{1-R_{11}} \qquad \text{(IV-86)}$$

where

$$\left(N_V^* N_V\right)_{31} \equiv \frac{K_1^3 g_{31}^2}{6\pi M_\pi (\alpha_{31}+K_1)^4} \qquad \text{(IV-87)}$$

and

$$\left(N_V^* N_V\right)_{11} \equiv -\frac{K_1^3 g_{11}^2}{3\pi M_\pi (\alpha_{11}+K_1)^4} \qquad \text{(IV-88)}$$

In order to see the effect of the Coulomb interaction, we just consider the energy shift in the absence of it, i.e., the denominators in equation (IV-86) are going to be replaced by a Fredholm Determinant of the form:

$$D(\varepsilon_s) = 1 - f^+ f \int r\,dr\,r'dr' e^{-\alpha r} G_o(r,r') e^{-\alpha r'} \qquad \text{(IV-89)}$$

equation (IV-89) is the analogous to equation (IV-50), where the Reduced Green's Function has been replaced by the Green's Function for a free particle, re-

presented by $G_0(r,r')$. The quantities $(N_V^* N_V)$ represent the energy shift in first order perturbation thery and in the particular case of the pionic 1S state for hydrogen, they are given by:

$$\Delta\mathcal{E}_{1S}\,(S_{11}, F.O.P.T.) = (N_V^* N_V)_{11} = -4.3945\,eV \quad \text{(IV-90)}$$

and

$$\Delta\mathcal{E}_{1S}\,(S_{31}, F.O.P.T.) = (N_V^* N_V)_{31} = 4.2180\,eV \quad \text{(IV-91)}$$

the full rescattering contributions are

$$R_{11} = -3.6150 \qquad R_{31} = 0.3464 \quad \text{(IV-92)}$$

and the Fredholm Determinants in the absence of Coulomb interaction are:

$$\mathcal{D}_{11} = 0.4784 \qquad \mathcal{D}_{31} = 1.3796 \quad \text{(IV-93)}$$

If we define the combined energy shift in the absence of Coulomb interaction as:

$$(\Delta\mathcal{E}_S)_{free} \equiv (N_V^* N_V)_{31}\,\mathcal{D}_{31}^{-1} + (N_V^* N_V)_{11}\,\mathcal{D}_{11}^{-1} \quad \text{(IV-94)}$$

Then the final results for our comparison are:

$$(\Delta\mathcal{E}_S)_{free} = -6.13\,eV \qquad \Delta\mathcal{E}_S = 5.50\,eV$$

then, the elimination of the Coulomb interac - tion in the rescattering term has a violent effect and can not be neglected. Based on these results, we should include Coulomb interaction in our studies of more complex systems in the next chapter. This will be done using the Doorway State Formalism to bound state perturbation theory already developed in chapter III. There the inclusion of this effect will come through the exact calculation of the Reduced Green's Function, using the procedures of section (III-3), making the whole analysis possible quantitatively.

REFERENCES FOR CHAPTER IV.

(1) E.J. Moniz, A. Sevgen, Phys. Rev. C vol. 24, no. 1, p. 224, 1981.

(2) D.V. Bugg. A.A. Carter, J.R. Carter, Phys. Lett. 44B, p.278, 1973.

(3) J.R. Carter, D.V. Bugg. A.A. Carter, Nucl. Phys B58, p. 378, 1973.

(4) H. Pilkuhn et al., Nucl. Phys. B65, p. 460, 1973.

(5) N.M. Nagels et al., Nucl. Phys. B147 , p. 189, 1979.

(6) E.J. Moniz, Nuclear Physics with Heavy Ions and Mesons, vol. 2, p. 466, 1978.

(7) G.Hohler , H.P. Jakov, R. Strauss, Nucl. Phys. vol. B39, p. 237, 1972.

(8) G. Hohler, F. Kaiser, R. Koch, E. Pietcriner, Korlsruhe preprint TKP 78-11, to appear in ZAED Physics Data.

CHAPTER V

PION-NUCLEUS OPTICAL POTENTIAL IN THE PIONIC ATOM PROBLEM

The [$\Delta(A-1), N^*(A-1), \Delta^*(A-1)$] model will be developed as an extension of the $\Delta(A-1)$ model for the pionic atom problem. The natural separable structure of the model allows an immediate application of the Doorway State Method to the bound state problem already considered in Chapter III. The non-local properties of the effective potential can be treated adequately from the quantitative point of view in contrast with the difficulties encountered by standard methods used to date. The convergence of the procedure allows the study of the essential physical effects using just the first doorway expectation value. At the same time the study of the resultant pion-nucleus optical potential can be done with the same tools as it is outlined in section (2). Being our main interest to study the role of the pion-nucleon S-wave interaction, the 1S levels of ^{4}He and ^{16}O will be considered quantitatively in order to obtain the strengths of the spreading potentials for the S_{11} and S_{31} channels. This spreading potential is the new ingredient related to pion absorption in the optical potential. Due to the renormalization considered for

the N^* and Δ^*, the imaginary part of these strengths is given in terms of a ratio $W_o / \Delta M^*$, which turns out to be the same as the ratio $W_\Delta / \Delta M_\Delta$ for the Δ-isobar. In the ^{4}He case the new parameters allow to obtain good agreement with the data in contrast with similar two parameter fitting attempted to date.

(1) The $[\Delta(A-1), N^*(A-1), \Delta^*(A-1)]$ model

. For p-wave absorption a $\Delta(A-1)$ model[1] was already considered and an extension of this model in order to include the S-wave pion-nucleon interaction is required for the treatment of the pionic atom problem due to the fundamental role of this partial wave at very low energies. In parallel to the formation of the Δ-isobar (spin $\frac{3}{2}$, isospin $\frac{3}{2}$) related to the P_{33} channel, the "intermediate particles" N^* (spin ½, isospin ½) and Δ^* (spin ½, isospin $\frac{3}{2}$) related to the S_{11} and S_{31} channels, respectively, should be considered. Within the framework of this model, the Hilbert Space can be spanned through states with A nucleons and one pion, a Δ and A-1 nucleons, a (Δ^* or N^*) and A-1 nucleons and finally, A nucleons to include the possibility of absorption. This statement can be written in the form of a closure relation:

$$P_\pi + P_\Delta + P_{N^*} + P_{\Delta^*} + P_A = 1 \qquad \text{(V-1)}$$

where P_i is a projector onto the i-th space. The remain-

ing p-wave channels can be ignored due to our interest in very low energy phenomena where the P_{33} channel is clearly the dominant one. This low energy region allows the use of non-relatvistic quantum mechanics throughout all the formalism, including the pion case where relativistic effects can be treated as corrections.

The Hamiltonian for the whole system is given by

$$H = K_\pi + \left\{ K_N + K_\Delta + K_{N^*} + K_{\Delta^*} + V(NN \to NN) + V(N\Delta \to N\Delta) \right.$$

$$\left. + V(NN^* \to NN^*) + V(N\Delta^* \to N\Delta^*) \right\}_A + V_c + V \qquad \text{(V-2)}$$

where K_i is the kinetic energy of the i-th particle and V_c is the pion-nucleus Coulomb interaction when the nucleus is in its ground state. The symbols $V(NN \to NN)$ and $V(N\Delta \to N\Delta)$ denote fundamental processes described by the diagrams in fig. (V-1). In these diagrams the "wiggled" line means that the specific exchange is unknown and a phenomenological approach is going to be followed to describe these interactions. Similar considerations can be applied to the N^* and Δ^* cases. The remaining V term can be represented by

$$V = P_o V_{EM} Q_o + Q_o V_{EM} P_o + Q_o V_{EM} Q_o$$

$$+ V(\pi N \rightleftarrows N^*) + V(\pi N \rightleftarrows \Delta^*) + V(\pi N \rightleftarrows \Delta) \qquad \text{(V-3)}$$

$$+\left\{V(N\Delta \rightleftarrows NN) + V(NN^{*} \rightleftarrows NN) + V(N\Delta^{*} \rightleftarrows NN)\right\}_{A}$$

The first three terms in V represent the pion-nucleus electromagnetic interactions when the nucleus is excited or a transition takes place. These terms take into account all the nuclear polarization effects. The next three terms represent the creation and decay for the N^{*}, Δ^{*} and Δ particle described by means of diagrams in fig. (V-2). The absorption process is represented in the last line of equation (V-3) and is graphically described by the diagrams of fig. (V-3). Again, a wiggled line symbolizes our lack of knowledge about the relevant exchanges.

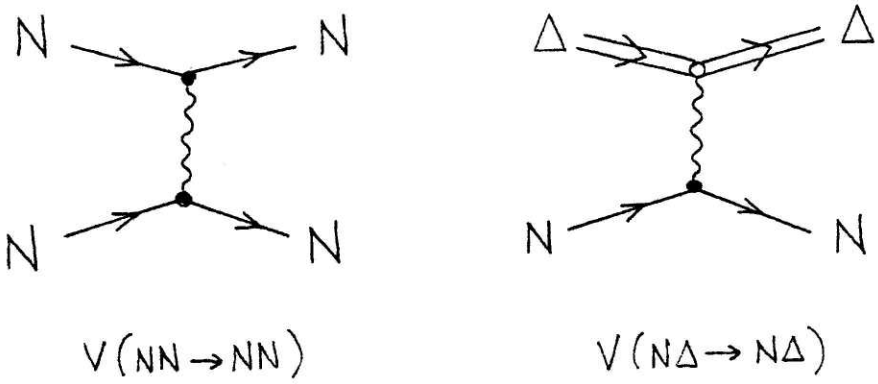

Fig. (V-1)

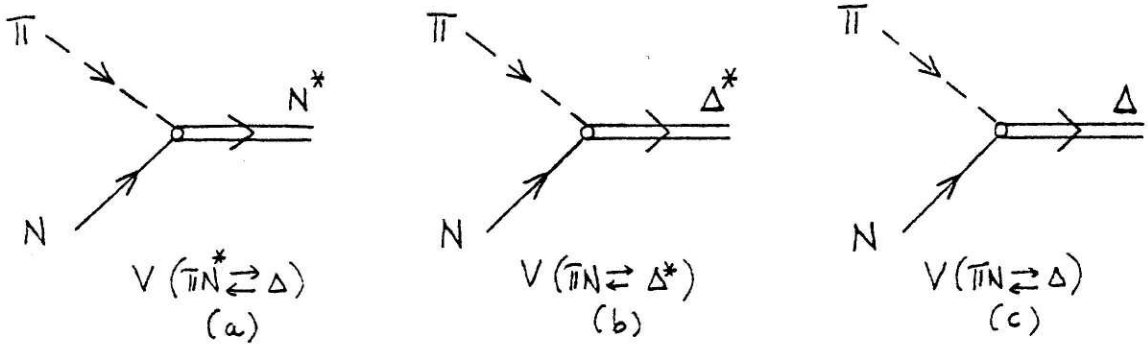

Fig. (V-2)

In order to find an effective interaction for the pion-nucleus problem, a T matrix projection onto the one pion and A nucleons subspace of the Hilbert Space is needed. Our starting point is the Lippmann - Schwinger equation:

$$T(\mathcal{E}) = V + V\,G(\mathcal{E})\,T(\mathcal{E}) \qquad \text{(V-4)}$$

where V is the interaction described by equation (V-3) and G ($\mathcal{E}$) is the Green's Function related to the rest of the Hamiltonian H. Defining:

$$\vartheta_{\pi}^{Em} \equiv P_{\pi}\left(P_o V_{Em} Q_o + Q_o V_{Em} P_o + Q_o V_{Em} Q_o\right) P_{\pi}$$

$$= P_o V_{Em} Q_o + Q_o V_{Em} P_o + Q_o V_{Em} Q_o \qquad \text{(V-5)}$$

and using the projectors given in equation (V-1), the

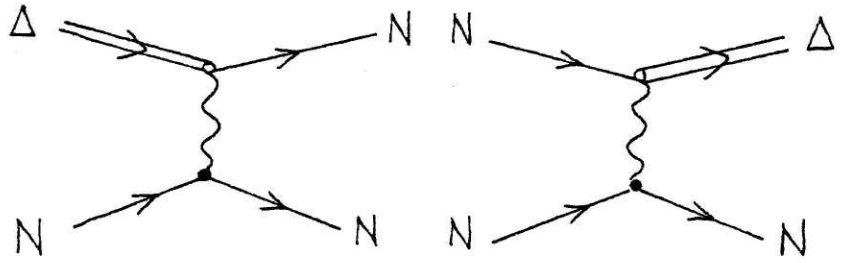

Fig. (V-3)

following set of coupled equations is obtained

$$T_{\pi\pi} = \vartheta_{\pi}^{EM} + \vartheta_{\pi}^{EM} G_{\pi} T_{\pi\pi} + g_{\pi\Delta} G_{\Delta} T_{\Delta\pi}$$

$$+ g_{\pi N^*} G_{N^*} T_{N^*\pi} + g_{\pi\Delta^*} G_{\Delta^*} T_{\Delta^*\pi} \qquad \text{(V-6a)}$$

$$T_{\Delta\pi} = g^{\dagger}_{\Delta\pi} + g^{\dagger}_{\Delta\pi} G_{\pi} T_{\pi\pi} + V_{\Delta A} G_A T_{A\pi} \qquad \text{(V-6b)}$$

$$T_{N^*\pi} = g^{\dagger}_{N^*\pi} + g^{\dagger}_{N^*\pi} G_{\pi} T_{\pi\pi} + V_{N^*A} G_A T_{A\pi} \qquad \text{(V-6c)}$$

$$T_{\Delta^*\pi} = g^{\dagger}_{\Delta^*\pi} + g^{\dagger}_{\Delta^*\pi} G_{\pi} T_{\pi\pi} + V_{\Delta^*A} G_A T_{A\pi} \qquad \text{(V-6d)}$$

$$T_{A\pi} = V_{A\Delta} G_{\Delta} T_{\Delta\pi} + V_{AN^*} G_{N^*} T_{N^*\pi} + V_{A\Delta^*} G_{\Delta^*} T_{\Delta^*\pi} \qquad \text{(V-6e)}$$

where the following notation is used:

$$T_{ij} \equiv P_i T(\varepsilon) P_j \qquad G_i \equiv P_i G(\varepsilon) P_i \tag{V-7}$$

The i and j indices stand for π, A, Δ, N^* and Δ^*. In the interaction case the projectors are the following:

$$P_i V P_j = \begin{cases} g^{\dagger}_{ij} & i = \Delta, N^*, \Delta^* \quad j = \pi \\ g_{ij} & i = \pi \quad j = \Delta, N^*, \Delta^* \\ V_{ij} & i,j = A, N^*, \Delta^*, \Delta \end{cases} \tag{V-8}$$

where the first line involves creation of Δ, N^* or Δ^*, the second line gives the decay of some particles and V_{ij} denotes the absorption process. The next task is the formal solution of the system of equations given by (V-6). Defining:

$$\Omega_\pi \equiv 1 + G_\pi T_{\pi\pi} \tag{V-9a}$$

and

$$\sum_{ij}^{k} \equiv V_{ik} G_k V_{kj} \tag{V-9b}$$

equation (V-6e) can be replaced in equations (V-6b),

(V-6c) and (V-6d), and using equations (V-9) we get

$$T_{\Delta^*\pi} = \frac{1}{1-\sum^{A}_{\Delta^*\Delta^*} G_{\Delta^*}} \left[g^{\dagger}_{\Delta^*\pi}\, \mathcal{R}_{\pi} + \sum^{A}_{\Delta^*\Delta} G_{\Delta}\, T_{\Delta\pi} + \sum^{A}_{\Delta^*N^*} G_{N^*}\, T_{N^*\pi} \right] \quad \text{(V-10)}$$

$$T_{N^*\pi} = \frac{1}{1-\sum^{A}_{N^*N^*} G_{N^*}} \left[g^{\dagger}_{N^*\pi}\, \mathcal{R}_{\pi} + \sum^{A}_{N^*\Delta} G_{\Delta}\, T_{\Delta\pi} + \sum_{N^*\Delta^*} G_{\Delta^*}\, T_{\Delta^*\pi} \right] \quad \text{(V-11)}$$

$$T_{\Delta\pi} = \frac{1}{1-\sum^{A}_{\Delta\Delta} G_{\Delta}} \left[g^{\dagger}_{\Delta\pi}\, \mathcal{R}_{\pi} + \sum^{A}_{\Delta N^*} G_{N^*}\, T_{N^*\pi} + \sum^{A}_{\Delta\Delta^*} G_{\Delta^*}\, T_{\Delta^*\pi} \right] \quad \text{(V-12)}$$

But due to the pion-nucleon S and p-wave spin-isospin channels projectors involved, there are cancellations of

$$\sum^{A}_{i\,j} = 0 \qquad \text{if} \qquad i \neq j \quad \text{(V-13)}$$

and then, a simplified version of equations (V-10), (V-11) and (V-12) can be obtained:

$$T_{\Delta^*\pi} = \frac{1}{1-\sum^{A}_{\Delta^*\Delta^*} G_{\Delta^*}}\, g^{\dagger}_{\Delta^*\pi}\, \mathcal{R}_{\pi} \quad \text{(v-14)}$$

$$T_{N^*\pi} = \frac{1}{1 - \sum^A_{N^*N^*} G_{N^*}} g^+_{N^*\pi} \Omega_\pi \qquad \text{(V-15)}$$

$$T_{\Delta\pi} = \frac{1}{1 - \sum^A_{\Delta\Delta} G_\Delta} g^+_{\Delta\pi} \Omega_\pi \qquad \text{(V-16)}$$

Equations (V-14), (V-15) and (V-16) can be replaced in (V-6a) to give:

$$T_{\pi\pi} = \left\{ v^{EM}_\pi + g_{\pi\Delta} \frac{1}{G^{-1}_\Delta - \sum^A_{\Delta\Delta}} g^+_{\pi\Delta} + g_{\pi N^*} \frac{1}{G^{-1}_{N^*} - \sum^A_{N^*N^*}} g^+_{\pi N^*} \right.$$

$$\left. + g_{\pi\Delta^*} \frac{1}{G^{-1}_{\Delta^*} - \sum^A_{\Delta^*\Delta^*}} g^+_{\Delta^*\pi} \right\} \left(1 + G_{\pi\pi} T_{\pi\pi} \right) \qquad \text{(V-17)}$$

In equation (V-17), the "intermediate particles" N^*, Δ^* and Δ are treated on the same footing. Following the renormalization procedure outlined in Chapter IV, where N^* and Δ^* are taken as static resonances and it yields the result:

$$T_{\pi\pi} = \left\{ v^{EM}_\pi + \tilde{g}_{\pi N^*} \frac{1}{1 - \tilde{\sum}^A_{N^*N^*}} \tilde{g}^+_{N^*\pi} \right. \qquad \text{(V-18)}$$

$$\left. + \tilde{g}_{\pi\Delta^*} \frac{1}{1 - \tilde{\sum}^A_{\Delta^*\Delta^*}} \tilde{g}^+_{\Delta^*\pi} + g_{\pi\Delta} \frac{1}{G^{-1}_\Delta - \sum^A_{\Delta\Delta}} g^+_{\Delta\pi} \right\} \left(1 + G_{\pi\pi} T_{\pi\pi} \right)$$

where the tilde means that these quantities have been

renormalized. Then in equation (V-18), separable interactions for the S_{11} and S_{31} channels are provided in a natural way. This was already done in Chapter IV, where the parameters of the forces were determined. From equation (V-18) the isolation of an effective interaction V is possible and the result is:

$$\vartheta \equiv \vartheta_{\pi}^{EM} + \tilde{g}_{\pi N^*} \frac{1}{1 - \tilde{\Sigma}^{A}_{N^*N^*}} \tilde{g}^{\dagger}_{N^*\pi} \qquad \text{(V-19)}$$

$$+ \tilde{g}_{\pi\Delta^*} \frac{1}{1 - \tilde{\Sigma}^{A}_{\Delta^*\Delta^*}} \tilde{g}^{\dagger}_{\Delta^*\pi} + g_{\pi\Delta} \frac{1}{G_{\Delta}^{-1} - \Sigma^{A}_{\Delta\Delta}} g^{\dagger}_{\Delta\pi}$$

The Shift Matrix for the combined nuclear and pionic states is given by

$$\mathcal{M}^{IS}_{\pi\pi} = \vartheta + \vartheta G_{\pi} Q_{IS} \mathcal{M}^{IS}_{\pi\pi} \qquad \text{(V-20a)}$$

where S is the pionic state and I is the nuclear state. The energy shift is given by

$$\Delta\mathcal{E}_S = \langle I,S| \mathcal{M}^{IS}_{\pi\pi} |I,S\rangle \qquad \text{(V-20b)}$$

Equation (V-20b) can be expressed in a convenient way using the formalism developed in chapter III and exploiting the separable nature of the effective interaction given in equation (V-19), with the exception of

the electromagnetic term ϑ_{π}^{EM}. In the calculation of the energy shifts, the nuclear ground state is combined with the pionic state of interest and a projection of $\mathcal{M}_{\pi\pi}^{OS}$ onto this ground state is adequate, yielding the following system of coupled equations:

$$P_o \mathcal{M}_{\pi\pi}^{OS} P_o = P_o \vartheta_s P_o + P_o \vartheta_s P_o Q_s G_\pi P_o \mathcal{M}_{\pi\pi}^{OS} P_o$$

$$+ P_o (\vartheta_s + V_{EM}) Q_o G_\pi Q_o \mathcal{M}_{\pi\pi}^{OS} P_o \qquad \text{(V-21)}$$

$$Q_o \mathcal{M}_{\pi\pi}^{OS} P_o = Q_o V_{EM} P_o + Q_o (\vartheta_s + V_{EM}) P_o Q_s G_\pi P_o \mathcal{M}_{\pi\pi}^{OS} P_o$$

$$+ Q_o (\vartheta_s + V_{EM}) Q_o G_\pi Q_o \mathcal{M}_{\pi\pi}^{OS} P_o + Q_o \vartheta_s P_o \qquad \text{(V-22)}$$

where ϑ_s gathers all the contributions related to the strong interaction part. From equations (V-21) and (V-22) an equation for $P_o \mathcal{M}_{\pi\pi}^{OS} P_o$ can be obtained:

$$P_o \mathcal{M}_{\pi\pi}^{OS} P_o = \mathcal{U} + \mathcal{U} G_\pi Q_s P_o (P_o \mathcal{M}_{\pi\pi}^{OS} P_o) \qquad \text{(V-23)}$$

where $\mathcal{U}$ is the full optical potential (electromagnetic and strong interaction), given by:

$$\mathcal{U} = P_o \vartheta_s P_o + P_o (\vartheta_s + V_{EM}) Q_o G_\pi Q_o \frac{1}{1 - Q_o (\vartheta_s + V_{EM}) Q_o G_\pi Q_o}$$

$$\otimes Q_o (\vartheta_s + V_{EM}) P_o \qquad \text{(V-24)}$$

Nuclear polarization is considered through the electromagnetic contributions in equation (V-24). These contributions are not going to be studied throughout this work under the grounds that they constitute a second order effect in comparison with the strong interaction contribution and the optical potential to be considered in this chapter is given by:

$$U = P_0 v_s P_0 + P_0 v_s Q_0 G_\pi Q_0 \frac{1}{1 - Q_0 v_s Q_0 G_\pi Q_0} Q_0 v_s P_0 \qquad \text{(V-25)}$$

the structure of v_s is fully separable and the formalism of Chapter III is completely applicable. To do the same separation with the v_π^{En} interaction, appropriate factorizations have to be found and linear combinations of electromagnetic and strong interactions terms will appear in the construction of the Doorway basis. At this point only strong interactions are considered and it makes the choice for the vectors in the Doorway basis a direct and unambigious one, due to its natural separable structure. To show explicitly the details of this construction in the next section the optical potential in the Doorway State approach will be considered.

(2) Pion-Nucleus Optical Potential in the Doorway State Approach

The optical potential of equation (V-25) can be

written more explicitly using equation (V-19). The result is:

$$U = P_0 \Big\{ \tilde{g}_{\pi N^*} \frac{1}{1 - \tilde{\Sigma}^A_{N^*N^*} - \tilde{g}^+_{N^*\pi} G_\pi Q_0 \tilde{g}_{\pi N^*}} \tilde{g}^+_{N^*\pi}$$

$$+ \tilde{g}_{\pi\Delta^*} \frac{1}{1 - \tilde{\Sigma}^A_{\Delta^*\Delta^*} - \tilde{g}^+_{\Delta^*\pi} G_\pi Q_0 \tilde{g}_{\pi\Delta^*}} \tilde{g}^+_{\Delta^*\pi}$$

$$+ g_{\pi\Delta} \frac{1}{G^{-1}_\Delta - \Sigma^A_{\Delta\Delta} - g^+_{\Delta\pi} G_\pi Q_0 g_{\pi\Delta}} g^+_{\Delta\pi} \Big\} P_0 \qquad \text{(V-26)}$$

In spite of all the simplifications considered so far equation (V-26) gives a potential which is hard to use in actual calculations. The hope in this case is the standard one, i.e., the first order effect can be calculated almost exactly and higher order terms, where many-body effects are present, can be studied in a semi-phenomenological way. In consequence it is important to have an adequate description of the first order term in order to do meaningful phenomenology with higher order terms. The pion absorption process is given in terms of the form $\sum^A_{ij}$ and the lowest order diagram related to them is given in fig. (V-IV). The contribution of this diagram is hard to evaluate and there is no successful attempt to date. The wiggled lines indicate our ignorance about the relevant exchanges to be considered. A

possible approach to this problem is the introduction of Δ , N^* and Δ^* spreading potentials as it is done in references (3), (4) and (5). The essential idea is to replace the process depicted in fig. (V-V,a) and higher order contributions, by an effective interaction represented in fig. (V-V,b). Then the "bubble" of fig. (V-IV) can be replaced by the "tadpole" of fig. (V-V,c). The result is the density dependent spreading potential given by

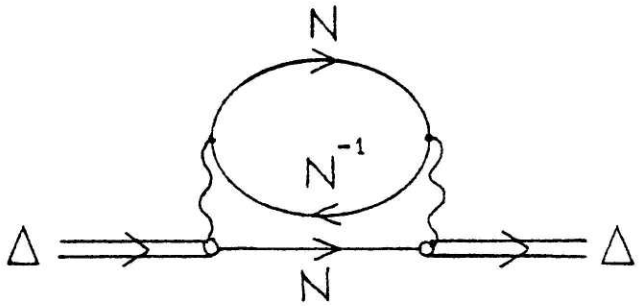

Fig. (V-IV)

$$W_\Delta(E,r) = \frac{W_o(E)}{\rho_o}\,\rho(r) \qquad \text{(V-27)}$$

The strength $W_o(E)$ incorporates the many-body reactive content of the π -nuclear T-matrix through a complex quantity given by

$$W_o \simeq (20 - i\,40)\ \text{MeV} \qquad \text{(V-28)}$$

This value has been tested for pion energies between

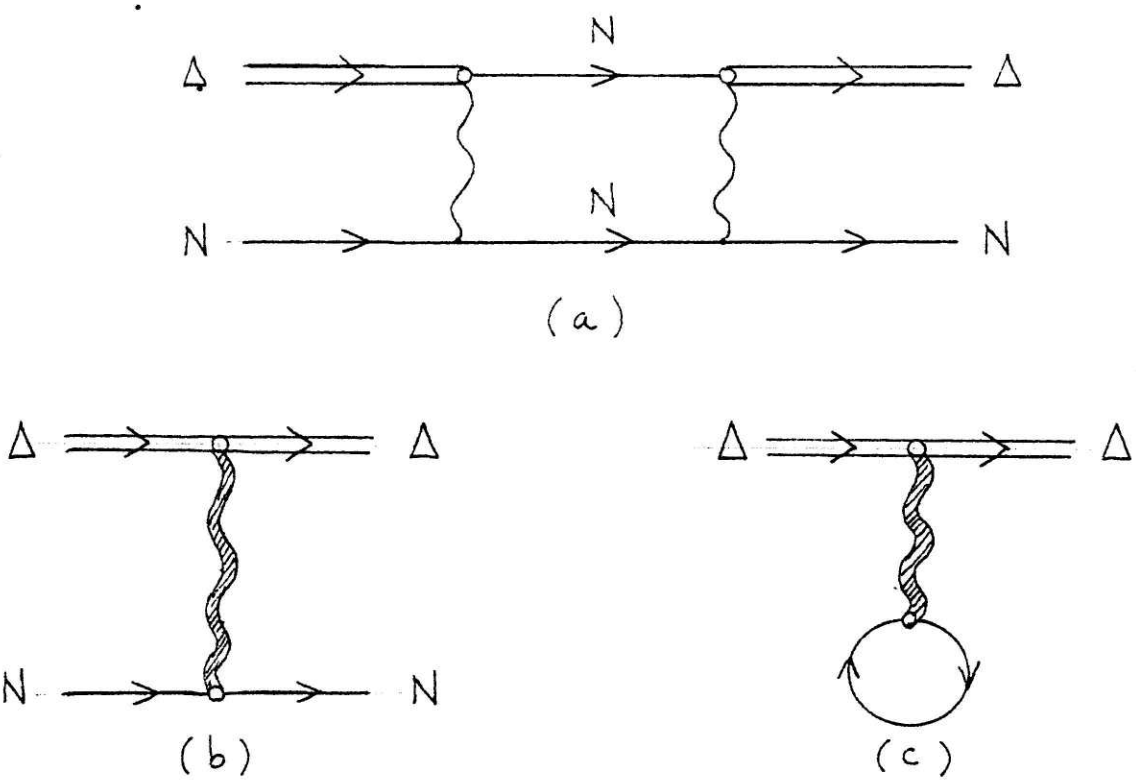

Fig. (V-V)

100 MeV and 250 MeV and it is almost independent of the energy. This strength for the spreading potential is consistent with the widths obtained from the p-wave interaction contribution in the pion-nucleus optical potential in pionic atoms. In the latest version a spin-orbit part has to be included[5]

$$W_\Delta^{so}(r) = 2\,\vec{\ell}_\Delta \cdot \vec{\Sigma}_\Delta\, V_{LS}(r) \qquad \text{(V-29)}$$

where $\vec{\ell}_\Delta$ and $\vec{\Sigma}_\Delta$ are the orbital angular momentum and the spin 3/2 of the propagating $\Delta(1232)$. Non-localities enter through this term and the following functional

form was used:

$$V_{LS}(r) = V_{LS}^{o}\, \mu r^2 e^{-\mu r^2} \qquad \text{(V-30)}$$

by the authors of reference (5) and for $^{16}0$ and ^{12}C the parameters are essentially the same[5]:

$$\mu = 0.3\ fm^{-2} \qquad \text{(V-31)}$$

$$V_{LS}^{o} = (-10 - i4)\ MeV \qquad \text{(V-32)}$$

These parameters independent of the pion energy. The inclusion of the spin-orbit part is necessary to improve in a considerable way the pion - $^{16}0$ differential cross sections at pion energies of 114 MeV and 240 MeV.[5] In the absence of the spin orbit term, the strength of the central term for the spreading potential is strongly energy dependent and in pion - $^{16}0$ scattering case, it was found that W_o = (2 - i55) MeV at 114 MeV and W_o = (-12-i35) MeV at 240 Mev.[5]

In this chapter we are going to consider a "spreading potential" for the S-wave interaction in the same way that it is done for the p-wave i.e., a parametrization of higher order effects through a mean field for the center of mass of the interacting pion-nucleon system. This potential has the form given in equation

(V-27). The strengths of these potentials can be obtained from fits to the energy shifts and widths in pionic atoms and details of this fitting will be studied in the next section. The spin-orbit contribution to the spreading potential will not be taken into account in this work for the S-wave interaction case.

Now we can examine the problem of the construction of the pion-nucleus optical potential, using the Doorway State Approach. For a particular channel in equation (V-26) we can write:

$$\mathcal{U}(\vec{q},\vec{q}') = \sum_{i,j=1}^{A} \langle \vec{q}, o | g_i \frac{1}{\hat{\xi}(\varepsilon) - \sum_{k,\ell} g_k^{\dagger} G_{\pi} Q_o g_\ell} g_j^{\dagger} | \vec{q}', o \rangle \qquad \text{(V-33)}$$

where:

(for the S_{11} and S_{31} channels)

$$\hat{\xi}(\varepsilon) \equiv \begin{cases} 1 - \frac{W_o}{\Delta m^*} \hat{\rho} \\ \\ \varepsilon - H_\Delta - W_\Delta \hat{\rho} - \hat{W}_{so} \end{cases} \qquad \text{(V-34)}$$

(for the P_{33} channel)

being Q_o a projector that projects out the nuclear ground state and $\hat{\rho}$ the nuclear density operator, normalized to 1 in the origin. In the coordinate representation this density operator gives a function of the center of mass of the interacting pair, i.e., pion-nucleon center of mass. The indices i and j label the nucleons. The

parameter W_o gives the strength of the spreading potential in the N^* and Δ^* cases and W_Δ does the same in the Δ particle case. The mass difference ΔM^* is defined as

$$\Delta M^* \equiv M_N + M_\pi - M^* \qquad \text{(V-35)}$$

where M^* represents the Δ^* and N^* bare mass and the ratio in equation (V-34) is a consequence of the renormalization procedure outlined in section (1). The natural starting vectors in the Doorway basis are given by

$$N_o^{-1} |D_o(\vec{q}')\rangle = \tilde{N}_o^{-1} |\tilde{D}_o(\vec{q}')\rangle \equiv \sum_j g_j^\dagger |\vec{q}', o\rangle \qquad \text{(V-36)}$$

The rescattering operators for the S and p-wave are given by

$$\hat{W}_s \equiv \frac{W_o}{\Delta M^*} \hat{\rho} + \sum_{k,\ell} g_k^\dagger G_\pi Q_o g_\ell \qquad \text{(V-37)}$$

$$\hat{W}_p \equiv \frac{1}{\tilde{E} + \Delta M_\Delta} \left\{ T_\Delta + V_\Delta + W_\Delta \hat{\rho} + \hat{W}_{so} + H_{A-1} \right.$$

$$\left. + \sum_{k,\ell} g_k^\dagger G_\pi Q_o g_\ell \right\} \qquad \text{(V-38)}$$

where $\tilde{E}$ is the total energy without the relevant

masses, which are given in ΔM_Δ . The last term of equations (V-37) and (V-38) includes the Pauli-Blocking and nucleon binding effects. For a given channel the contribution to the optical potential can be written as:

$$\mathcal{U}(\vec{q},\vec{q}') = \mathcal{U}_o \sum_{i,j=1}^{A} \langle \vec{q}, o | g_i \frac{1}{1-\hat{W}} g_j^\dagger | \vec{q}', o \rangle \qquad \text{(V-39)}$$

where

$$\mathcal{U}_o \equiv \begin{cases} 1 & \text{in the s-wave case} \\ \dfrac{1}{\bar{\mathcal{E}} + \Delta M_\Delta} & \text{in the p-wave case} \end{cases} \qquad \text{(V-40)}$$

Treating the momenta $\vec{q}$, $\vec{q}'$ as parameters, a doorway basis can be constructed for both waves using the rescattering operators $\hat{W}_s$ and $\hat{W}_p$. Making the insertion of a complete set of doorway states between g_i and $(1-\hat{W})^{-1}$, we obtain:

$$\mathcal{U}(\vec{q},\vec{q}') = \mathcal{U}_o N_o^{-1}(\vec{q}') \sum_{i,n} \langle \vec{q}, o | g_i | \mathcal{D}_n(\vec{q}') \rangle \sigma_{no}(\vec{q}') \qquad \text{(V-41)}$$

If $\wedge_n(\vec{q},\vec{q}')$ is the n-th doorway momentum space range function defined by:

$$\Lambda_n(\vec{q},\vec{q}') \equiv N_o^{-1}(\vec{q}') \sum_i \langle \vec{q}, o | q_i | \mathcal{D}_n(\vec{q}') \rangle \qquad \text{(V-42)}$$

At the first doorway truncation the optical potential is given by

$$\mathcal{U}(\vec{q},\vec{q}') = \mathcal{U}_o \Lambda_o(\vec{q},\vec{q}') \, G_{oo}(\vec{q}') \qquad \text{(V-43)}$$

where

$$G_{oo}(\vec{q}') = \frac{1}{1 - W_{oo}(\vec{q}')} \qquad \text{(V-44)}$$

If we are interested in a coordinate representation for the pion-nucleus optical potential the construction procedure is identical and the starting vectors of equation (V-36) are replaced by

$$N_o^{-1} | \mathcal{D}_o(\vec{r}') \rangle = \tilde{N}_o^{-1} | \tilde{\mathcal{D}}_o(\vec{r}') \rangle \equiv \sum_j q_j^\dagger | \vec{r}', o \rangle \qquad \text{(V-45)}$$

In this case the range function

$$\Lambda_n(\vec{r},\vec{r}') \equiv N_o^{-1}(\vec{r}') \sum_i \langle \vec{r}, o | q_i | \mathcal{D}_n(\vec{r}') \rangle \qquad \text{(V-46)}$$

has a direct physical meaning associated with the range of the effective interaction in the n-th doorway, i.e.,

after n rescatterings.

In an initial approach to the problem a shell model may represent the nuclear system and the pion-nucleon interaction is described through the models developed in chapter IV, i.e., we use vertex form factors. Then, the Doorway State can be written as:

$$|D_0(\vec{r}')\rangle = N_0 \sum_{ij} \vartheta_{ij}(\vec{r}')\, \Delta_i^+ h_j^+ |0\rangle \qquad \text{(V-47)}$$

where g_j^+ was replaced in equation (V-36) by

$$g_j^+ \equiv \sum_i \hat{\vartheta}_{ij}\, \Delta_i^+ (h_j^+ + p_j) \qquad \text{(V-48)}$$

The notation used is such that Δ represents N^*, Δ^* or the same Δ . Here the quantized language is introduced for convenience. The operators in equation (V-48) are defined in the following way:

$\Delta_i^+ (\Delta_i)$ creates (destroys) a Delta (N^*, Δ^*, Δ) (V-49a)

$p_i^+ (p_i)$ creates (destroys) a particle (V-49b)

$h_i^+ (h_i)$ creates (destroys) a hole (V-49c)

and for all these Fermions we have the following

conmutation relations:

$$\{ f_i, f_j^+ \} = \delta_{ij} \quad \text{and} \quad \{ f_i^+, f_j^+ \} = \{ f_i, f_j \} = 0 \qquad \text{(V-50)}$$

The operator $\hat{\vartheta}_{ij}$ acts on pion states only and in the coordinate representation we can write:

$$\langle \vec{r} | \hat{\vartheta}_{ij} | s \rangle = \vartheta_{ij}(\vec{r}) \langle \vec{r} | s \rangle \qquad \text{(V-51)}$$

being $\vec{r}$ the pion coordinate and

$$\vartheta_{ij}(\vec{r}) \equiv \int \frac{d\vec{p}}{(2\pi)^3} \frac{d\vec{q}}{(2\pi)^3} \langle i | \vec{p} \rangle f(\vec{q} - \beta_1 \vec{p}) \langle \vec{p} - \vec{q} | \bar{j} \rangle \, e^{-i\vec{q}\cdot\vec{r}} \qquad \text{(V-52)}$$

where $f(\vec{q})$ is the interaction form factor and i ($\bar{j}$) labels the delta (hole) states. The parameter β_1 is due to nucleon recoil as it is given by the ratio

$$\beta_1 = \frac{M_\pi}{M_\pi + M_N} \qquad \text{(V-53)}$$

which is the non-relativistic one. The first doorway normalization can be written as:

$$(\tilde{N}_o^* N_o)^{-1}_{\vec{r}'} \equiv \sum_{ij} \vartheta_{ij}^*(\vec{r}') \, \vartheta_{ij}(\vec{r}') \qquad \text{(V-54)}$$

In the S_{11} channel case we have

$$(\tilde{N}_o^{\dagger} N_o)^{-1}_{\vec{r}'} = -\frac{g^2}{6M_\pi}\sum_j \int \psi_j^*(\vec{p})\, F_s(|\vec{p}-\vec{q}|)\psi_j(\vec{q})\, e^{i(\vec{p}-\vec{q})\cdot\vec{r}'} \frac{d\vec{p}}{(2\pi)^3}\frac{d\vec{q}}{(2\pi)^3} \quad \text{(V-55)}$$

where (see appendix V-A)

$$F_s(|\vec{p}-\vec{q}|) = \frac{1}{8\beta_2^3|\vec{p}-\vec{q}|} \otimes \left\{1 - \theta(2\alpha - |\vec{p}-\vec{q}|) + \frac{1}{\pi}\, \mathrm{arc\,tg}\, \frac{4\alpha|\vec{p}-\vec{q}|}{4\alpha^2 - |\vec{p}-\vec{q}|^2}\right\} \quad \text{(V-56)}$$

and

$$\theta(x) \equiv \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases} \quad \text{(V-57)}$$

The range function for the first doorway is given by

$$\Lambda_o^{11}(\vec{r},\vec{r}') = -\frac{g^2}{6M_\pi}\sum_j \int \psi_j^*(\vec{p})\, F_s(|\vec{p}-\vec{q}|)\,\psi_j(\vec{q})\, e^{i(\vec{p}\cdot\vec{r} - \vec{q}\cdot\vec{r}')} \frac{d\vec{q}}{(2\pi)^3}\frac{d\vec{p}}{(2\pi)^3} \quad \text{(V-58)}$$

The sum runs over proton states. In the S_{31} channel the range function separates the contribution from protons and neutrons:

$$\Lambda_o^{31}(\vec{r},\vec{r}')$$

$$= \frac{g^2}{2m_\pi}\left\{\frac{1}{3}\sum_{j\in F_p}\int \psi_j^{p*}(\vec{p})\,F_s(|\vec{p}-\vec{q}|)\,\psi_j^{p}(\vec{q})\,e^{i(\vec{p}\cdot\vec{r}-\vec{q}\cdot\vec{r}')}\frac{d\vec{p}}{(2\pi)^3}\frac{d\vec{q}}{(2\pi)^3}\right.$$

$$\left.+\sum_{j\in F_n}\int \psi_j^{n*}(\vec{p})\,F_s(|\vec{p}-\vec{q}|)\,\psi_j^{n}(\vec{q})\,e^{i(\vec{p}\cdot\vec{r}-\vec{q}\cdot\vec{r}')}\frac{d\vec{q}}{(2\pi)^3}\frac{d\vec{p}}{(2\pi)^3}\right\} \qquad \text{(V-59)}$$

In equations (V-58) and (V-59) the highly non-local character of the effective potential can be appreciated in detail. From the complexity of the expressions already found for the first doorway normalization, it is clear that to obtain analytical expressions even for the first doorway expectation value of the rescattering operator is going to be difficult. For the time being we are going to postpone the analysis of the considered effects, from the optical potential point of view, for a future project and at this time all the efforts will be concentrated in the 1S energy shifts and widths for light nuclei where the Doorway State Approach will be very useful and will open the possibility of numerical applications with highly non-local potentials as the one we considered in this section. Up to now zero-ranged potentials were used in a variety of numerical calculations and the use of non-local potentials with standard methods is rather difficult.

(3) Energy Shifts and Widths in the Doorway State Approach

Using equations (V-20a), (V-20b) and (V-23) the energy shift can be obtained as:

$$\Delta\mathcal{E}_S = \sum_{ij} \langle o,s|g_i \frac{1}{\hat{\xi} - \sum_{k,\ell} g_k^+ G_\pi Q_o g_\ell - \sum g_k^+ G_\pi Q_s P_o g_\ell} g_j^+ |s,o\rangle \quad \text{(V-60)}$$

where $\hat{\xi}$ is defined by equation (V-34) and more specificly the rescattering terms are given by:

$$\hat{\Sigma} \equiv \sum_{k,\ell} g_k^+ G_\pi Q_o g_\ell = \sum_{k,\ell} g_k^+ \frac{Q_o}{\mathcal{E} - T_\pi - H_A} g_\ell \quad \text{(V-61)}$$

$$\hat{R} \equiv \sum_{k,\ell} g_k^+ G_\pi Q_s P_o g_\ell = \sum_{k,\ell} g_k^+ \frac{|o\rangle Q_s \langle o|}{\mathcal{E}_\pi^s - T_\pi - V_c} g_\ell \quad \text{(V-62)}$$

The $\hat{\Sigma}$ term represents pion rescattering while the nucleus is in an excited state and the $\hat{R}$ term gives the contribution of Coulomb forces to the rescattering process while the nucleus is in its ground state. The nuclear polarization effects related to collective excitations of the nucleus are not going to be considered in this initial stage of the problem since in comparison with the phenomena that we already studied, they constitute second order effects. The vertex interaction g_j^+ is

defined by equation (V-48). The starting vectors are given by:

$$N_o^{-1}\,|D_o\rangle = \tilde{N}_o^{-1}\,|\tilde{D}_o\rangle = \sum_j g_j^\dagger\,|S,o\rangle = \sum_{ij} \vartheta_{ij}^S\,\Delta_i^\dagger\,h_j^\dagger\,|o\rangle \qquad \text{(V-63)}$$

and the first doorway normalization is

$$\left(\tilde{N}_o^* N_o\right)^{-1} = \sum_{ij} |\vartheta_{ij}^S|^2 \qquad \text{(V-64)}$$

$$= \sum_{j\in F} \int \langle \vec{j}\,|\vec{P}-\vec{q}\rangle\,\phi_S^*(\vec{q})\,f^\dagger(\vec{q}-\beta_1\vec{P})\,f(\vec{q}'-\beta_1\vec{P})\,\langle \vec{P}-\vec{q}'\,|\vec{j}\rangle\,\phi_S(\vec{q}')\,\frac{d\vec{q}}{(2\pi)^3}\frac{d\vec{q}'}{(2\pi)^3}\frac{d\vec{P}}{(2\pi)^3}$$

For the S-wave case, which is the one that we are going to consider in detail, the total rescattering operator relevant to the construction of the doorway basis is given by:

$$\hat{W} = \frac{W_o}{\Delta M^*}\,\hat{\rho} + \hat{\Sigma} + \hat{R} \qquad \text{(V-65)}$$

where

$$\hat{\rho} \equiv \sum_{k,\ell} \rho_{k\ell}\,\Delta_k^\dagger\,\Delta_\ell \qquad \text{(V-66)}$$

The density given in equation (V-66) is related to the center of mass of the interacting pair as we stated earlier. The application of every piece of the rescattering operator to the first doorway state, gives

the following results:

$$\hat{\Sigma}\,|D_0\rangle = N_0 \sum_{\substack{k,i,j,l,m \\ (k,j\in F)}} \int \frac{\vartheta^*_{im}(\vec{q})\,\vartheta_{lk}(\vec{q})}{\varepsilon_j - \frac{q^2}{2M_\pi} - \varepsilon_m}\,\vartheta^S_{ij}\,\frac{d\vec{q}}{(2\pi)^3}\,\Delta^+_l\,p^+_m\,h^+_k\,h^+_j\,|0\rangle$$
$$+ N_0 \sum_{\substack{i,j,l,k \\ (j\in F,\ k\notin F)}} \int \frac{\vartheta^*_{ik}(\vec{q})\,\vartheta_{lk}(\vec{q})}{\varepsilon_j - \frac{q^2}{2M_\pi} - \varepsilon_k}\,\vartheta^S_{ij}\,\frac{d\vec{q}}{(2\pi)^3}\,\Delta^+_l\,h^+_j\,|0\rangle \qquad \text{(V-67)}$$

$$\hat{R}\,|D_0\rangle = N_0 \sum_{\substack{k,n,j,i,\nu \\ n\neq s}} \frac{\vartheta^n_{\nu k}\,\vartheta^{n*}_{ij}}{\varepsilon^\pi_s - \varepsilon^\pi_n}\,\vartheta^S_{ij}\,\Delta^+_\nu\,h^+_k\,|0\rangle \qquad \text{(V-68)}$$

$$\hat{\rho}\,|D_0\rangle = N_0 \sum_{\substack{j,k,l \\ (j\in F)}} \rho_{kl}\,\vartheta^S_{lj}\,\Delta^+_k\,h^+_j\,|0\rangle \qquad \text{(V-69)}$$

In equation (V-69) we have the linear combination of Δ-hole and Δ-particle-2hole states. So as early as the second doorway state, we obtain contributions from orders in the optical potential higher than the first one. The first doorway expectation value of the same quantities are:

$$\langle \tilde{D}_0\,|\hat{\Sigma}\,|D_0\rangle = \tilde{N}^*_0 N_0 \sum_{\substack{i,l,j,k \\ (j\in F,\ k\notin F)}} \int \vartheta^{S*}_{lj}\,\frac{\vartheta^*_{ik}(\vec{q})\,\vartheta_{lk}(\vec{q})}{\varepsilon_j - \varepsilon_k - \frac{q^2}{2M_\pi}}\,\vartheta^S_{ij}\,\frac{d\vec{q}}{(2\pi)^3} \qquad \text{(V-70)}$$

$$\langle \tilde{D}_o | \hat{R} | D_o \rangle = \tilde{N}_o^* N_o \sum_{\substack{k,n,j,i,\nu \\ n\neq s \\ (k\in F,\, j\in F)}} \frac{\vartheta_{\nu k}^{*s}\, \vartheta_{\nu k}^{n}\, \vartheta_{ij}^{n*}\, \vartheta_{ij}^{s}}{\mathcal{E}_s^{\pi} - \mathcal{E}_n^{\pi}} \qquad \text{(V-71)}$$

$$\langle \tilde{D}_o | \hat{\rho} | D_o \rangle = \tilde{N}_o^* N_o \sum_{\substack{j,k,l \\ (j\in F)}} \vartheta_{kj}^{s*}\, \rho_{kl}\, \vartheta_{lj}^{s} \qquad \text{(V-72)}$$

with the normalization $\tilde{N}_o^* N_o$ given by equation (V-64).

The ground state energy for the nucleus is taken as a reference, so $\mathcal{E}_o^A \equiv o$. Regrouping factors in equation (V-70) we obtain:

$$\langle \tilde{D}_o | \hat{\Sigma} | D_o \rangle = \frac{1}{\Delta \mathcal{E}_{FOPT}} \sum_{j\in F} \int \frac{d\vec{P}}{(2\pi)^3} \frac{d\vec{Q}}{(2\pi)^3} \frac{d\vec{q}}{(2\pi)^3}\, \phi_s^*(\vec{q})\, \langle \vec{j} | \vec{P} - \vec{q} \rangle$$

$$\otimes\, f^+(\vec{q} - \beta_1 \vec{P}) \tilde{\Sigma}_j^{\cdot}(\vec{P}, \vec{Q})\, f(\vec{q}\,' - \beta_1 \vec{Q}) \langle \vec{Q} - \vec{q}\,' | \vec{j} \rangle \phi_s(\vec{q}\,') \frac{d\vec{q}\,'}{(2\pi)^3} \qquad \text{(V-73)}$$

where the self-energy $\tilde{\Sigma}_j^{\cdot}$ is given by:

$$\tilde{\Sigma}_j^{\cdot}(\vec{P}, \vec{Q}) \equiv \int \frac{d\vec{q}}{(2\pi)^3}\, f(\vec{q} - \beta_1 \vec{P}) \langle \vec{P} | \frac{Q_F}{\mathcal{E}_s^{\pi} + \mathcal{E}_j - \frac{q^2}{2M_\pi} - \frac{(\vec{Q}-\vec{q})^2}{2M_N} - \hat{\vartheta}_N} | \vec{Q} \rangle$$

$$\otimes\, f^+(\vec{q} - \beta_1 \vec{Q}) \qquad \text{(V-74)}$$

The operator Q_F, projects out the Fermi Sea states

and ϑ_N is the mean-field which confines the nucleons. In equation (V-73) Pauli-Blocking and nucleon binding effects are taken into account in this way. Since our interest lies in light and closed shell nuclei and spin-orbit effects are not going to be taken into account, then a choice of a local potential for ϑ_N is a reasonable one. The energy $-\mathcal{E}_j$ is associated to the hole state $|\vec{j}>$ and the operator $\hat{\Sigma}$ can be redefined such that:

$$<\vec{P}|\hat{\Sigma}_s|\vec{Q}> \qquad \text{(V-75)}$$

$$\equiv \sum_{k \neq F} \int \frac{d\vec{q}}{(2\pi)^3} f(\vec{q}-\beta_1\vec{P}) \frac{<\vec{P}-\vec{q}|k><k|\vec{Q}-\vec{q}>}{\mathcal{E}-\hat{H}_{A-1}-\frac{q^2}{2m_\pi}-\mathcal{E}_k} f^+(\vec{q}-\beta_1\vec{Q})$$

where $\hat{H}_{A-1}$ is the Hamiltonian for a (A-1) nucleons. If the self-energy operator of equation (V-71) replaces the full $\hat{\Sigma}$ given by equation (V-61), we are keeping just the contribution of Δ -hole states and neglecting any contribution that is coming from Δ -particle - 2hole states and more complicated combinations. The general assumption (based on our studies of the convergence of this method in Chapter II) is that with a first doorway truncation will suffice to obtain all the essential physics of the pionic atom problem. At the first doorway level there are no contributions from higher excitations like Δ -particle-2hole states as it was shown in equations (V-67), (V-68), (V-69) and specially (V-70).

Then the suggested replacement will not change the first order physics in which we are interested in. All the published work in pion-nucleus interactions that make use of Δ -hole models and the Doorway State Approach for the scattering case reach the same kind of conclusion about the first doorway truncation role. Usually the treatment of the Pauli-Blocking effect in equations like (V-71) is rather cumbersome due to the number of states that could be involvedif the system is appreciable large. To make the calculation of terms related to equation (V-71) possible, a complement of the Heavyside function like the one given in equation (V-57) is inserted in equation (V-71) to give:

$$\langle \vec{P} | \hat{\Sigma}_s | \vec{Q} \rangle = \sum_k \int \frac{d\vec{q}}{(2\pi)^3} f(\vec{q} - \beta_1 \vec{P}) \frac{\langle \vec{P} - \vec{q} | k \rangle \langle k | \vec{Q} - \vec{q} \rangle}{\mathcal{E} - \frac{q^2}{2m_\pi} - \hat{H}_{A-1} - \mathcal{E}_k} f^+(\vec{q} - \beta_1 \vec{Q}) \, \theta_c(\mathcal{E}_k - \mathcal{E}_F) \tag{V-76}$$

The complement of the Heavyside function in equation (V-76) eliminates any contribution from the states in the Fermi Sea, since $\mathcal{E}_F$ is the Fermi Energy. The complement of the Heavyside function is given by

$$\theta_c(x) \equiv \begin{cases} 1 & x < 0 \\ 0 & x \geq 0 \end{cases} \tag{V-77}$$

Equation (V-70) can be rewritten as:

$$\langle \vec{P}|\hat{\Sigma}_s|\vec{Q}\rangle = \int \frac{d\vec{q}}{(2\pi)^3} f(\vec{q}-\beta_1\vec{P}) \langle \vec{P}| \frac{1}{\varepsilon - \hat{H}_{A-1} - \frac{q^2}{2M_\pi} - \frac{(\hat{\vec{p}}-\vec{q})^2}{2M_N} - \hat{\vartheta}_N}$$

$$\otimes \theta_c \left[\frac{(\hat{\vec{p}}-\vec{q})^2}{2M_N} + \hat{\vartheta}_N - \varepsilon_F \right] |\vec{Q}\rangle f^+(\vec{q}-\beta_1\vec{Q}) \qquad \text{(V-78)}$$

where

$$\langle \vec{P}|\hat{\vec{p}}|\vec{Q}\rangle = (2\pi)^3 \vec{P}\,\delta(\vec{P}-\vec{Q}) \qquad \text{(V-79)}$$

and now the complement of the Heavyside function works as an operator. This operator can be written in terms of the Heavyside function as:

$$\theta_c \left[\frac{(\hat{\vec{p}}-\vec{q})^2}{2M_N} + \hat{\vartheta}_N - \varepsilon_F \right] = \hat{I} - \theta \left[\varepsilon_F - \frac{(\hat{\vec{p}}-\vec{q})^2}{2M_N} - \hat{\vartheta}_N \right] \qquad \text{(V-80)}$$

The second term of equation (V-80) accounts for the Pauli-Blocking effect. We note that:

$$\frac{q^2}{2M_\pi} + \frac{(\hat{\vec{p}}-\vec{q})^2}{2M_N} = \frac{1}{2\mu}(\vec{q}-\beta_1\hat{\vec{P}})^2 + \frac{\hat{\vec{P}}^2}{2M} \qquad \text{(V-81)}$$

In non-relativistic terms equation (V-81) is making a transformation from the pion-nucleon set of coordinates in the left-hand side to the relative-center-of-mass coordinates in the right hand side. The masses μ and M are respectively the reduced and total mass. Aside this

we also note that ϑ_N is a local potential and then:

$$\langle \vec{P}-\vec{q} \,|\, \hat{\vartheta}_N \,|\, \vec{Q}-\vec{q} \rangle = \vartheta_N (\vec{P}-\vec{Q}) \qquad \text{(V-82)}$$

The interaction ϑ_N will act on the center of mass of the interacting pair. With equations (V-81) and (V-82) the self-energy is given now by

$$\langle \vec{P} \,|\, \hat{\Sigma}_s \,|\, \vec{Q} \rangle = \int \frac{d\vec{q}}{(2\pi)^3} f(\vec{q}-\beta_1 \vec{P}) \langle \vec{P} \,| \frac{1}{\mathcal{E} - \hat{H}_{A-1} - \frac{1}{2\mu}(\vec{q}-\beta_1\hat{\theta})^2 - \frac{\hat{P}^2}{2M} - \hat{\vartheta}_N} \qquad \text{(V-83)}$$

$$\otimes \theta_c \left[\frac{1}{2\mu}(\vec{q}-\beta_1\hat{\theta})^2 + \frac{\hat{P}^2}{2M} + \hat{\vartheta}_N - \mathcal{E}_F - \frac{q^2}{2M_\pi} \right] | \vec{Q} \rangle f^\dagger(\vec{q}-\beta_1\vec{Q})$$

Equation (V-83) can now be expanded in the recoil parameter β_1. The zero order term is given by:

$$\langle \vec{P} \,|\, \hat{\Sigma}_s^{(o)} \,|\, \vec{Q} \rangle = \int \frac{d\vec{q}}{(2\pi)^3} G(q^2) \frac{1}{\mathcal{E} - \hat{H}_{A-1} - \frac{q^2}{2\mu} - \hat{h}_\Delta} \theta_c \left[\frac{q^2}{2M_N} + \hat{h}_\Delta - \mathcal{E}_F \right] \qquad \text{(V-84a)}$$

and

$$G(q^2) \equiv f(\vec{q}) f^\dagger(\vec{q}) \qquad \text{(V-84b)}$$

where again Δ represents (N^*, Δ^*, Δ) and in the particular case of the Δ we can make the standard

association:

$$\hat{h}_{CM} \longrightarrow \hat{h}_{\Delta} \qquad \text{(V-85)}$$

being $\hat{h}_{\Delta}$ the Hamiltonian:

$$\hat{h}_{\Delta} \equiv T_{\Delta} + V_{\Delta} \qquad \text{(V-86)}$$

and V_{Δ} is a confining mean-field which is taken to be proportional to the nuclear mean-field. In the recoil parameter expansion the first order term cancels exactly and the next non-zero term is in the second order in β_1. The contribution of this last term is exceedingly small and in the calculations to be presented in the next section, it will be neglected. To see how the cancellation of the first order occurs we use equation (V-80) and the following representation of the Heavyside function:

$$\theta(x-y) \equiv \lim_{\epsilon \to 0} \frac{\epsilon}{\pi} \int_{-\infty}^{x} \frac{dt}{\epsilon^2 + (t-y)^2} \qquad \text{(V-87)}$$

Defining:

$$\hat{A} \equiv \frac{1}{2\mu} (\vec{q} - \beta_1 \vec{P})^2 + \frac{\hat{\theta}^2}{2M} + \hat{v}_N - \frac{q^2}{2M_{\pi}} \qquad \text{(V-88)}$$

From Equation (V-80) we can obtain:

$$\frac{\partial}{\partial\beta_1}\theta_c\left[\hat{A}-\varepsilon_F\right] = -\frac{\partial}{\partial\beta_1}\theta\left[\varepsilon_F-\hat{A}\right] \tag{V-89}$$

$$= -\lim_{\epsilon\to 0}\frac{\epsilon}{\pi}\int_{-\infty}^{\varepsilon_F}\frac{dt}{\epsilon^2+(t-\hat{A}(\beta_1))^2}\frac{\partial}{\partial\beta_1}(t-\hat{A}(\beta_1))^2\frac{1}{\epsilon^2+(t-\hat{A}(\beta_1))^2} \tag{V-90}$$

and then:

$$\frac{\partial}{\partial\beta_1}\theta\left[\hat{A}-\varepsilon_F\right]\Big|_{\beta_1=0} = -\lim_{\epsilon\to 0}\frac{\epsilon}{\mu\pi}\int_{-\infty}^{\varepsilon_F}\frac{dt}{\epsilon^2+(t-\hat{A}(0))^2}\vec{q}\cdot\hat{\theta}\left[t-\frac{q^2}{2M_N}-\hat{h}_\Delta\right] \tag{V-91}$$

$$\otimes\frac{1}{\epsilon^2+(t-\hat{A}(0))^2}$$

When equation (V-91) is inserted in an integral which contains even powers q^2, the total result cancels due to the presence of the $\vec{q}\cdot\hat{\theta}$ factor. Then the self-energy operator can be written as:

$$\hat{\Sigma}_S(\beta_1) = \hat{\Sigma}_S^{(0)} + \vartheta(\beta_1^2) \tag{V-92}$$

The first term of equation (V-86) is diagonal in Δ-hole states:

$$\langle\Delta h|\hat{\Sigma}_S^{(0)}|\Delta' h'\rangle = \int\frac{d\vec{q}}{(2\pi)^3}G(q^2)\frac{1}{\varepsilon_S^{II}-\varepsilon_h-\varepsilon_\Delta-\frac{q^2}{2\mu}}\theta_c\left[\frac{q^2}{2M_N}+\xi_\Delta-\varepsilon_F\right] \tag{V-93}$$

$$\otimes\,\delta_{\Delta\Delta'}\delta_{hh'}$$

It is clear that, in general, higher order terms are not going to exhibit this property. Below threshold this quantity should be naturally real (by "naturally" we mean that the expansion is not going to alter this real character of the self-energy below threshold). Expansions of the self-energy in the absence of the Pauli-Blocking effect may have terms with imaginary contributions that should cancel when they are summed up. It can be shown that the self-energy given by equation (V-93) has no imaginary contribution since the denominator in the integrand of(V-93) never cancels, i.e., does not have poles. The denominator in question is given by:

$$\Delta(q^2) \equiv \varepsilon_s^{II} - \varepsilon_h - \varepsilon_\Delta - \frac{q^2}{2\mu}$$

$$= \varepsilon_s^{II} + (-\varepsilon_h - \varepsilon_F) + (\varepsilon_F - \varepsilon_\Delta - \frac{q^2}{2M_N}) + \left(\frac{q^2}{2M_N} - \frac{q^2}{2\mu}\right) \quad \text{(V-94)}$$

Since ε_h is a hole state energy, the corresponding particle energy is given by $-\varepsilon_h$ and

$$-\varepsilon_h - \varepsilon_F < 0 \quad \text{(V-95a)}$$

by just looking at the argument of the function θ_c in equation (V-93), there are non-vanishing contributions when

$$\mathcal{E}_F - \mathcal{E}_\Delta - \frac{q^2}{2M_N} < 0 \qquad \text{(V-95b)}$$

We note that:

$$\frac{q^2}{2M_N} - \frac{q^2}{2\mu} = -\frac{q^2}{2M_\pi} < 0 \qquad \text{(V-95c)}$$

and finally, since the pion is bound

$$\mathcal{E}_S^{\pi} < 0 \qquad \text{(V-95d)}$$

Equations (V-95) lead to the conclusion that $\Delta(q^2) < 0$ for every value of q^2 and the integrand in equation (V-93) does not have poles. In this way the artifical appearance of imaginary parts is avoided. We can rewrite equation (V-93) as:

$$\langle \Delta h | \hat{\Sigma}_S^{(0)} | \Delta' h' \rangle = \frac{1}{2\pi^2} \int_{q_0}^{\infty} q^2 dq \, \frac{G(q^2)}{\mathcal{E}_S^{\pi} - \mathcal{E}_h - \mathcal{E}_\Delta - \frac{q^2}{2\mu}} \, \delta_{\Delta\Delta'} \delta_{hh'} \qquad \text{(V-96)}$$

where

$$q_0 \equiv \sqrt{2M_N(\mathcal{E}_F - \mathcal{E}_\Delta)} \; \theta(\mathcal{E}_F - \mathcal{E}_\Delta) \qquad \text{(V-97)}$$

and in the S-wave case, using the form factors of

chapter IV we get:

$$G(q^2) \equiv \frac{\lambda g^2}{2M_\pi} \frac{1}{(\alpha^2 + q^2)^2} \qquad \text{(V-98)}$$

where $\lambda = \pm 1$ depending on the channel. In order to check that the procedure outlined here is actually taking into account that Pauli-Blocking effect in the next section a specific calculation will be done with ^{4}He.

The matrix elements of the $\hat{R}$ operator can be rewritten as:

$$\langle \vec{P} | \hat{R}_s | \vec{Q} \rangle \equiv \sum_{k,j \in F} \int \frac{d\vec{q}}{(2\pi)^3} \frac{d\vec{q}'}{(2\pi)^3} f(\vec{q} - \beta_1 \vec{P}) \langle \vec{P} - \vec{q} | k \rangle \vartheta_s(\vec{q}, \vec{q}')$$

$$\otimes \langle j | \vec{Q} - \vec{q} \rangle f^+(\vec{q} - \beta_1 \vec{Q}) \qquad \text{(V-99)}$$

where $\vartheta_s(q,q')$ is the Reduced Green's Function in the momentum representation for the pionic state labeled by S. This Reduced Green's Function is an object described in detail in chapter III and for the Coulomb case in chapter IV also. Equation (V-99) gives the Coulomb contribution to the rescattering process. The methods shown in chapter III are used to calculate the Reduced Green's Function and for the 1S level, which is the one that is going to be studied in the next section, the Reduced Green's Function is given in appendix (IV-A).

(4) Energy Shifts and Widths for the 1S pionic state in ^{4}He and ^{16}O

The specific forms of the starting vectors in the S-wave channels are given by

$$N_o^{-1} |D_o\rangle = \tilde{N}_o^{-1} |\tilde{D}_o\rangle \equiv \sum_{N^*h} \vartheta^S_{N^*h} |N^*h\rangle \qquad \text{(V-100a)}$$

for the S_{11} channel and

$$N_o^{-1} |D_o\rangle = \tilde{N}_o^{-1} |\tilde{D}_o\rangle \equiv \sum_{\Delta^*h} \vartheta^S_{\Delta^*h} |\Delta^*h\rangle \qquad \text{(V-100b)}$$

for the S_{31} channel, where

$$|N^*h\rangle \equiv \Delta^\dagger_{N^*} h^\dagger_h |o\rangle \qquad \text{(V-101a)}$$

$$|\Delta^*h\rangle \equiv \Delta^\dagger_{\Delta^*} h^\dagger_h |o\rangle \qquad \text{(V-101b)}$$

For the particular models that we are using the coefficients $\vartheta^S_{N^*h}$ are given by (see appendix V-B)

$$\vartheta^S_{N^*h} \equiv -\sqrt{\frac{2}{3}}\, G\, \delta_{m_\tau,\frac{1}{2}}\, \delta_{M_T,-\frac{1}{2}}\, F_S(*hS) \qquad \text{(V-102a)}$$

$$\vartheta^S_{\Delta^*h} \equiv -\frac{G}{\sqrt{2(1+m_\tau)}}\, \delta_{M_T,m_\tau-1}\, F_S(*hS) \qquad \text{(V-102b)}$$

with

$$G^{+}G = \frac{\lambda g^2}{2M_{\pi}} \qquad \text{(V-103)}$$

and where

$$F_s(*hs) \equiv \frac{(-1)}{4\pi^{5/2}}^{\lambda+\frac{1}{2}+L+m+J^*-M^*} [\ ][\lambda][\ell][J^*]$$

$$\otimes \begin{pmatrix} L & \lambda & \ell \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} J^* & \lambda & j \\ -M^* & \mu & -m \end{pmatrix} \begin{Bmatrix} J^* & j & \lambda \\ \ell & L & \frac{1}{2} \end{Bmatrix}$$

$$\otimes \int_0^{\infty} F_{21}(NLL|\alpha\Lambda^*|x)\, x^2 \psi^h_{n\ell}(x)\, \psi^{\pi}_{\nu\lambda}(x)\, dx \qquad \text{(V-104)}$$

being (N,L,J^*,M^*) the quantum number set for the N^* or Δ^*, (ν,λ,μ) the pion quantum number set and (n,l,j,m) the hole quantum number set. The functions $\psi^h_{n\ell}(x)$ and $\psi^{\pi}_{\nu\lambda}(x)$ are respectively the nucleon and the pion wavefunctions and

$$F_{nm}(NLL'|\alpha\Lambda|x) \equiv \int_0^{\infty} \frac{P^n dP}{(\alpha^2+\beta_1^2P^2)^m}\, \tilde{\psi}_{NL}(P)\, j_L(Px) \qquad \text{(V-105)}$$

with $\psi_{NL}(P) = (-i)^L\ \tilde{\psi}_{NL}(P)$

where $\psi_{NL}(P)$ is the N^* or Δ^* wavefunction in the momentum representation. To obtain (V-99), the original denominator was expanded in the pion momentum and we approximate by just keeping the leading order term which is the one shown in equation (V-105). This approximation is justified on the grounds of the small scale of pion momentum.

The matrix element of the rescattering associated with Coulomb is given by (see appendix V-B)

$$\langle N^* h | \hat{R}_S | N^{*\prime} h' \rangle = \frac{g^2}{3M_\pi} \delta_{m_\tau, \frac{1}{2}} \delta_{m_\tau', \frac{1}{2}} \delta_{M_\tau, -m_\tau} \delta_{M_\tau', -m_\tau'} \otimes g_S(*h, *'h') \qquad \text{(V-106a)}$$

for the S_{11} channel and

$$\langle \Delta^* h | \hat{R}_S | \Delta^{*\prime} h' \rangle = -\frac{g^2}{4M_\pi} \frac{1}{\sqrt{(1+m_\tau)(1+m_\tau')}} \delta_{M_\tau, m_\tau - 1} \delta_{M_\tau', m_\tau' - 1} \otimes g_S(*h, *'h') \qquad \text{(V-106b)}$$

for the S_{31} channel, where

$$g_S(*h,*'h') \equiv \frac{(2\lambda+1)}{16\pi^5}[J^*][j][L][\ell][J^{*\prime}][j'][L'][\ell']$$

$$\otimes \begin{pmatrix} L & \lambda & \ell \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} L' & \lambda & \ell' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} J^{*\prime} & \lambda & j' \\ -M^{*\prime} & \mu & -m' \end{pmatrix}\begin{pmatrix} J^* & \lambda & j \\ -M^* & \mu & -m \end{pmatrix}$$

$$\otimes \begin{Bmatrix} J^* & j & \lambda \\ \ell & L & \frac{1}{2} \end{Bmatrix}\begin{Bmatrix} J^{*\prime} & j' & \lambda \\ \ell' & L' & \frac{1}{2} \end{Bmatrix}(-1)^{L+L'+m+m'+J^*+J^{*\prime}-M^*-M^{*\prime}}$$

$$\otimes \int_0^\infty x^2 dx\, F_{21}(NLL|\alpha\Lambda^*|x)\,\psi^h_{n\ell}(x)\int_0^\infty x'^2 dx'\,\vartheta_{\nu\lambda}(x,x')$$

$$\otimes \psi^h_{n'\ell'}(x')\,F_{21}(N'L'L'|\alpha\Lambda^*|x') \qquad \text{(V-107)}$$

where $\vartheta_{\nu\lambda}(x, x')$ is the Coulomb Reduced Green's Function. The matrix elements for the self-energy $\hat{\Sigma}_s$ are already described by equation (V-96). Finally the matrix elements of the spreading term are simply given by:

$$\langle *h|\hat{W}_{Sp}|*'h'\rangle = \frac{W_o}{\Delta M^*}\delta_{hh'}\delta_{J^*J^{*\prime}}\delta_{M^*M^{*\prime}}\delta_{LL'} \qquad \text{(V-108)}$$

$$\otimes \int_0^\infty x^2 dx\,\psi_{NL}(x)\rho_A(x)\psi_{N'L}(x)$$

With the coefficients and matrix elements already defined we can study the 1S level for two cases: ^{4}He and ^{16}O.

The nuclear model to be used is a shell model with harmonic oscillator wavefunctions. The same kind of

basis is going to be used for N^*-hole and Δ^*-hole states. In the ^{4}He case there are two experimental quantities which are important for the model, the separation energy

$$S(^4He) = -12.516 \text{ MeV} \qquad \text{(V-109)}$$

and Root-Mean-Square radius

$$\sqrt{\langle r^2 \rangle} = 1.63 \text{ fm} \qquad \text{(V-110)}$$

With these parameters and assuming a qaussian density the estimated potential strength is V_o = 85.0 MeV. Other parameters of interest are the oscillator frequency

$$\omega_N = 23.381 \text{ MeV} \qquad \text{(V-111)}$$

and the cut-off parameter

$$\Lambda_N = 0.751 \text{ fm}^{-1} \qquad \text{(V-112)}$$

The oscillator frequency agrees at least with the experimental observation of a first excitation at 20 MeV. The cut-off parameter is extracted from

information coming from form factors obtained through electron scattering, i.e., through the R.M.S. radius. In table (V-I) the relative strengths for the N^*-hole and Δ^*-hole are shown. We see that the state with $N = 0$ and $L = 0$ exhausts almost all the sum rule:

$$S_{n\ell} \equiv \sum_N |A_{Nn\ell}|^2 \qquad \text{(V-113)}$$

where A_{Nn} are the coefficients of the Doorway State expansion in N^*-hole and Δ^*-hole states. Then as a very good approximation we can keep only the contribution from $N = 0$ and $L = 0$ in ^4He . If N is different from n the cancellation is enormous due to the fact that the number of nodes is also different. So in actual calculations we impose the condition $N = n$, in order to keep a particular N^*-hole or Δ^*-hole state. With these rules the number of coefficients to be calculated is completely determined. At this point we can offer a verification for equation (V-96), i.e., the consideration of the Pauli-Blocking effect. This check can be done easily in the ^4He case. A direct calculation of the Pauli-Blocking term gives:

$$\langle m|\Sigma_j^{PB(o)}|m\rangle = -\frac{4G^+G}{\pi^2} M_\pi \left[\frac{\Lambda_c\Lambda_N}{\Lambda_N^2+\Lambda_c^2}\right]^3 \otimes \int_0^\infty \frac{q^2 dq}{(\alpha^2+q^2)^2} \frac{e^{-\frac{q^2}{\Lambda_N^2+\Lambda_c^2}}}{k_j^2+q^2} \qquad \text{(V-114a)}$$

where $\Lambda_N = 0.751\ fm^{-1}$, $\Lambda_c = 0.777\ fm^{-1}$ and

$$K_j^2 = 2M_\pi \left| \mathcal{E}_j + \mathcal{E}_s^\pi \right| \qquad \text{(V-114b)}$$

For comparison we offer the following table:

Channel	$\langle m \vert \sum_j^{(o)} \vert m \rangle$	$\langle m \vert \sum_j^{PB(o)} \vert m \rangle$	Difference	$\langle m \vert \sum_s^{(o)} \vert m \rangle$
S_{11}	0.522387	+0.021105	0.501282	0.499449
S_{31}	-0.382356	-0.0422092	-0.340146	-0.336391

In the first column we have the contribution of the self-energy in the absence of Pauli-Blocking effect, the next column has the Pauli-Blocking contribution described by equation (V-114a) and in the last column we obtain the quantity calculated with equation (V-96). The comparison between this last column and the difference column is a very favorable one. The small observed deviation should be mainly due to the different way in which the expansions are done. Equation (V-114a) is the direct Pauli-Blocking term with $\beta_1 = 0$ just in the vertex functions and the dependence of the nucleon wavefunctions and binding energies, as well as the dependence of the pion kinetic energy on this parameter β_1 is ignored. From the table it is clear that this last contribution

should be a small one.

In table (V-II) the values obtained from the Doorway State Approach calculation are listed. The contribution of the pion-nucleon p-wave interaction to the pionic 1S level should be small and then the experimental values given in table (V-III) are going to be used to find the strenghts for the spreading potential in the S_{11} and S_{31} channels. The expression for the energy shift in this case is given by:

$$\Delta\mathcal{E}_{1S} = \frac{\Delta\mathcal{E}_{1S}(S_{11}, FOPT)}{1 - W_{11} W_{00}^{SP}(S_{11}) - W_{00}^{R}(S_{11})} + \frac{\Delta\mathcal{E}_{1S}(S_{31}, FOPT)}{1 - W_{31} W_{00}^{SP}(S_{31}) - W_{00}^{R}(S_{31})} \quad \text{(V-115)}$$

where W_{OO}^{R} gives all the rescattering contributions, including Coulomb, and W_{OO}^{SP} is the contribution from the spreading potential. If there is no restriction about the proper signs for the contribution of the imaginary part, a direct fit gives the wrong signs. If the proper signs are imposed as a condition, the experimental numbers are not reproduced exactly but the result is remarkable close to the experimental one as it is shown in table (V-III). The contribution from the p-wave interaction is attractive and absorptive so if it were included the result would be a decrease in both real and imag-

inary parts of the already computed energy shifts. This is an indication that we are moving in the right direction since in that case the calculated values will be even closer to the experimental number. Previous fittings of the parameter b_o (as it was commented in Chapter I) for ^{4}He, where b_o is real and Re B_o= o (actually two parameter fit), were not able to provide a number close enough to the experimental value and when the energy shift was perfectly adjusted, the width was off by a rough factor of two. Interestingly enough the ratio $W_o / \Delta M_\Delta$ in the case of the Δ-isobar is 0.14 also. Based on these results a systematic study of the entire periodic table will be considered after this work, using the new optical potential obtained through the N^*, Δ^*, Δ -hole model.

TABLE (V-I)

Relative Strengths ($|A_{Nn\ell}|^2 / S_{n\ell}$) for the Doorway States for the 1S level in pionic ^{4}He. (n=o, = L =o)

	S_{11} channel		S_{31} channel
N	Strengths	N	Strengths
0	0.9981894	0	0.998119
1	0.0001808	1	0.0001878
2	0.0000027	2	0.0000029
3	0.0000000	3	0.0000000

TABLE (V-III)

Extracted Spreading Potential Strengths and experimental values for the energy Shifts and Widths in ^{4}He and ^{16}O.

$\Delta\mathcal{E}_{1S}$ (^{4}He, Experimental) = (75.7±2.0-i22.5±1.0) eV

$\Delta\mathcal{E}_{1S}$ (^{16}O, Experimental) = (15.64±0.1-i3.97±0.15) KeV

Result of the fit:

$W_{11} = -0.45 + i\ 0.14 \quad W_{31} = 0.45 - i\ 0.14$

Recalculated Shifts and Widths values:

$\Delta\mathcal{E}_{1S}$ (^{4}He) = (77.815 - i 22.411) eV

$\Delta\mathcal{E}_{1S}$ (^{16}O) = (18.749 - i 3.01) KeV

TABLE (V-II)

Results of the Doorway State Calculation for ^4He and ^{16}O in the pionic 1S state case.

S_{11} Channel:

$\Delta\mathcal{E}_{1S}$ (^4He, First Order Perturbation Theory) = - 92.707 eV

$\Delta\mathcal{E}_{1S}$ (^{16}O, First Order Perturbation Theory) = - 21.776 KeV

W_{oo} (^4He, Total Rescattering Contribution) = 0.58735

W_{oo} (^{16}O, Total Rescattering Contribution) = 0.54875

W_{oo} (^4He, Spreading Contribution) = 0.37208

W_{oo} (^{16}O, Spreading Contribution) = 0.180075

S_{31} Channel:

$\Delta\mathcal{E}_{1S}$ (^4He, First Order Perturbation Theory) = 356.403 eV

$\Delta\mathcal{E}_{1S}$ (^{16}O, First Order Perturbation Theory) = 83.741 KeV

W_{oo} (^4He, Total Rescattering Contribution) = - 0.67357

W_{oo} (^{16}O, Total Rescattering Contribution) = - 0.48720

W_{oo} (^4He, Spreading Contribution) = 0.37208

W_{oo} (^{16}O, Spreading Contribution) = 0.18075

REFERENCES FOR CHAPTER V

(1) E.J. Moniz and F. Lenz, review article (to be published)

(2) E. Oset, H. Toki and W. Weise, Phys. Reports, vol. 83, p.281, 1982

(3) M. Hirata, F. Lenz and K. Yazaki, Ann. of Phys., vol.108, p.16, 1977

(4) M. Hirata, J. Koch, F. Lenz and E.J. Moniz, Phys. Lett., vol.70B, p.281, 1977. Ann. of Phys., vol. 120, p.205, 1979

(5) Y. Horikawa, M. Thies and F. Lenz, Nucl. Phys., vol. A345, p.386, 1980

CONCLUSIONS

(1) With the Doorway State Approach to Perturbation Theory, a wider range of problems not solved by standard perturbation theory can be treated. In particular it does well with the combination of strong interaction coupling and non-local forces, which is the case in pion-nucleus studies. Other methods fail to offer a solution, even from the numerical point of view. One remarkable feature is that the essential physics of the problem can be obtained within the first doorway truncation due to the strong convergence of the method. This makes the interpretation of the physics easier, because we can read directly in the first doorway expectation value each phenomenon under study.

(2) Nuclear structure effects can not explain the anomaly observed in ^{110}Pd Dynamical Nuclear Polarization. The standard pion-nucleus optical potentials also fail in explaining the widths of the 3d levels in heavy elements and this problem remains without explanation.

(3) The $[\Delta(A-1), N^*(A-1), \Delta^*(A-1)]$ model is used to determine a new optical potential. This potential is characterized by a phenomenology of higher orders different from the standard forms used to date. Effects like Pauli-Blocking, nucleon recoil, nucleon binding and

finite range of the interactions are included in order to make a correct description of the first order term and the physical interpretation of the higher order terms becomes easier. There is a "spreading potential" for the S-wave contribution to the optical potential which is related directly to the pion absorption problem. In this way the absorption process is treated phenomenologically in a first step and our intention is to pursue a detailed microscopic description of this process in the future using the parametrization developed in this work as a reference. In this way the energy shifts and widths of ^{4}He and ^{16}O can be explained in a simultaneous way for the first time, according to the discussion of Chapter I in regards to the ^{4}He case. The "strengths" for the spreading potential are

$$W_{11} = - 0.45 + i\ 0.14$$

$$W_{31} = 0.45 - i\ 0.14$$

which is the result of the best fitting if the condition for the signs in the imaginary parts is imposed to produce the absorption effect. At the same time the recalculated shifts and widths are consistent with the experimental observations. The absolute value of imaginary part of these strengths is given by:

$$\left|\frac{W_o}{\Delta M^*}\right| = 0.14$$

Interestingly enough for the Δ-isobar this ratio is the same

$$\left| \frac{W_0}{\Delta M_\Delta} \right| = 0.14$$

APPENDIX (II-A)

REDUCED TRANSITION PROBABILITIES AND QUADRUPOLE MOMENTS IN THE THREE SURFON MODEL.

(a) Quadrupole Matrix Elements:

In order to calculate the quadrupole moment, we have to work with the operator:

$$\hat{Q}_{20} = A\,\hat{q}^{+}_{f20} - \sqrt{\frac{10}{7}}\,B \sum_{m} \begin{pmatrix} 2 & 2 & 2 \\ -m & 0 & m \end{pmatrix} \hat{q}_{f2,-m}\,\hat{q}_{f2m} \qquad \text{(II-A-1)}$$

where

$$A \equiv e\,a_p \int_0^{\infty} dr\; r^4 \cdot \frac{\partial \rho_p}{\partial a_p} \qquad \text{(II-A-2a)}$$

$$B \equiv \frac{e}{2}\sqrt{\frac{5}{4\pi}}\; a_p^2 \int_0^{\infty} dr\; r^4\, \frac{\partial^2 \rho_p}{\partial a_p^2} \qquad \text{(II-A-2b)}$$

and

$$\hat{q}_{\ell m} \equiv \chi_{\ell}\left[a_{\ell m} + (-1)^m\, a^{+}_{\ell,-m}\right] \qquad \text{(II-A-3)}$$

with

$$\left[a_{\ell m},\, a_{\ell' m'}\right] = \left[a^{+}_{\ell m},\, a^{+}_{\ell' m'}\right] = 0 \qquad \text{(II-A-4a)}$$

$$\left[a_{\ell m},\, a^{+}_{\ell' m'}\right] = \delta_{\ell\ell'}\,\delta_{m m'} \qquad \text{(II-A-4b)}$$

In equations (II-A-2) ρ_p is the proton density and

is the proton radius, Now we consider the product:

$$\hat{q}_{2,-m}\, q_{2m} = \chi_2^2 \left\{ a_{2,-m}\, a_{2m} + a_{2m}^{\dagger}\, a_{2,-m}^{\dagger} \right.$$

$$\left. + (-1)^m \left[1 + a_{2,-m}^{\dagger}\, a_{2,-m} + a_{2m}^{\dagger}\, a_{2m} \right] \right. \qquad \text{(II-A-5)}$$

but

$$\sum_m (-1)^m \begin{pmatrix} 2 & 2 & 2 \\ -m & 0 & m \end{pmatrix} = 0 \qquad \text{(II-A-6)}$$

Then, we have:

$$\hat{Q}_{20} = A\, \hat{q}_{20}^{\dagger} - \sqrt{\frac{10}{7}}\, \beta \chi_2^2 \sum_m \begin{pmatrix} 2 & 2 & 2 \\ -m & 0 & m \end{pmatrix} \left\{ a_{2,-m}\, a_{2m} \right.$$

$$\left. + a_{2m}^{\dagger}\, a_{2,-m}^{\dagger} + (-1)^m \left[a_{2,-m}^{\dagger}\, a_{2,-m} + a_{2m}^{\dagger}\, a_{2m} \right] \right\} \qquad \text{(II-A-7)}$$

We define the coupling in each term of equation (II-A-7) as:

$$\left[a_2\, a_2 \right]_{20} \equiv \sum_m \begin{pmatrix} 2 & 2 & 2 \\ -m & 0 & m \end{pmatrix} a_{2,-m}\, a_{2m}$$

$$= \sum_m \begin{pmatrix} 2 & 2 & 2 \\ -m & +m & 0 \end{pmatrix} a_{2,-m}\, a_{2m} \qquad \text{(II-A-8a)}$$

$$\left[a_2^{\dagger}\, a_2^{\dagger} \right]_{20} \equiv \sum_m \begin{pmatrix} 2 & 2 & 2 \\ -m & 0 & m \end{pmatrix} a_{2m}^{\dagger}\, a_{2,-m}^{\dagger}$$

$$= \sum_m \begin{pmatrix} 2 & 2 & 2 \\ m & -m & 0 \end{pmatrix} a_{2m}^{\dagger}\, a_{2,-m}^{\dagger} \qquad \text{(II-A-8b)}$$

$$[a_2^\dagger a_{\bar{2}}]_{20} \equiv \sum_m (-1)^m \begin{pmatrix} 2 & 2 & 2 \\ -m & 0 & m \end{pmatrix} a^\dagger_{2,-m}\ a_{\bar{2}m}$$

$$= \frac{1}{\sqrt{5}} \sum_m \begin{pmatrix} 2 & 2 & 2 \\ -m & m & 0 \end{pmatrix} a^\dagger_{2,-m}\ a_{\bar{2}m} \qquad \text{(II-A-8c)}$$

The equation (II-A-8c) applies also to the last term of equation (II-A-7). Now we apply the Wigner-Eckard Theorem to equations (II-A-8) to obtain:

$$\langle I_n' \| [a_2 a_2]_2 \| I_n \rangle = (-1)^{I_n' + I_n} \sum_{I''} \begin{Bmatrix} 2 & 2 & 2 \\ I_n & I_n' & I'' \end{Bmatrix}$$

$$\otimes \langle I_n' \| a_2 \| I'' \rangle \langle I'' \| a_2 \| I_n \rangle \qquad \text{(II-A-9a)}$$

$$\langle I_n' \| [a_2^\dagger a_2^\dagger]_2 \| I_n \rangle = (-1)^{I_n' + I_n} \sum_{I''} \begin{Bmatrix} 2 & 2 & 2 \\ I_n & I_n' & I'' \end{Bmatrix}$$

$$\otimes \langle I_n' \| a_2^\dagger \| I'' \rangle \langle I'' \| a_2^\dagger \| I_n \rangle \qquad \text{(II-A-9b)}$$

$$\langle I_n' \| [a_2^\dagger a_{\bar{2}}]_2 \| I_n \rangle = (-1)^{I_n' - I_n} \sum_{I''} (-1)^{I''} \begin{Bmatrix} 2 & 2 & 2 \\ I_n & I_n' & I'' \end{Bmatrix}$$

$$\otimes \langle I_n' \| a_2^\dagger \| I'' \rangle \langle I_n \| a_2^\dagger \| I'' \rangle \qquad \text{(II-A-9c)}$$

where I labels the nuclear spin. Equation (II-A-7) can be written as:

$$\hat{Q}_{20} = A \hat{q}_{20}^\dagger - \sqrt{\frac{10}{7}}\, B \chi_2^2 \left\{ [a_2 a_2]_{20} + [a_2^\dagger a_2^\dagger]_{20} + \right.$$

$$\left. + 2 [a_2^\dagger a_{\bar{2}}]_{20} \right\} \qquad \text{(II-A-10)}$$

Using the following notation for one, two and three surfon states:

$$|1\rangle \equiv |1,22\rangle \qquad \text{(II-A-11a)}$$

$$|2\rangle \equiv |2,22\rangle \qquad \text{(II-A-11b)}$$

$$|3\rangle \equiv |3,22\rangle \qquad \text{(II-A-11c)}$$

We obtain:

$$\langle 1|\hat{Q}_{20}|1\rangle = -\sqrt{\frac{10}{7}}\, 2\beta\chi_2^2 \langle 1|[a_2^\dagger a_{\bar{2}}]_{20}|1\rangle$$

$$= -2\sqrt{\frac{10}{7}}\,\beta\chi_2^2 \begin{pmatrix} 2 & 2 & 2 \\ -2 & 0 & 2 \end{pmatrix} \begin{Bmatrix} 2 & 2 & 2 \\ 2 & 2 & 0 \end{Bmatrix} \left(\langle 2_1 \| a_2^\dagger \| 0\rangle\right)^2 \qquad \text{(II-A-12)}$$

and $\langle 2_1 \| a_2^\dagger \| 0\rangle = \sqrt{5}$, then:

$$\langle 1|\hat{Q}_{20}|1\rangle = -\frac{4}{7}\beta\chi_2^2 \qquad \text{(II-A-13)}$$

Now:

$$\langle 1|\hat{Q}_{20}|2\rangle = A\langle 1|\hat{q}_{20}^\dagger|2\rangle = A\chi_2\langle 1|a_{20}|2\rangle$$

$$= A\chi_2 \begin{pmatrix} 2 & 2 & 2 \\ -2 & 0 & 2 \end{pmatrix} \langle 2_1 \| a_2 \| 2_2\rangle \qquad \text{(II-A-14)}$$

But $\langle I_2 \| a_\lambda^\dagger \| I_1 = \lambda\rangle = [2(2I_2+1)]^{1/2}$, so:

$$\langle 1 | \hat{Q}_{20} | 2 \rangle = \langle 2 | \hat{Q}_{20} | 1 \rangle = \frac{2}{\sqrt{7}} A X_2 \qquad \text{(II-A-15)}$$

$$\langle 1 | \hat{Q}_{20} | 3 \rangle = -\sqrt{\frac{10}{7}} B X_2^2 \begin{pmatrix} 2 & 2 & 2 \\ -2 & 0 & 2 \end{pmatrix} \langle 2_1 \| [a_2 a_2]_2 \| 2_3 \rangle$$

$$= -\frac{2}{7} B X_2^2 \begin{Bmatrix} 2 & 2 & 2 \\ 2 & 2 & 2 \end{Bmatrix} \langle 2_1 \| a_2 \| 2_2 \rangle \langle 2_2 \| a_2 \| 2_3 \rangle$$

$$= \frac{6}{49}\sqrt{\frac{2}{7}} B X_2^2 = \langle 3 | \hat{Q}_{20} | 1 \rangle \qquad \text{(II-A-16)}$$

$$\langle 2 | \hat{Q}_{20} | 2 \rangle = \frac{12}{49} B X_2^2 \qquad \text{(II-A-16a)}$$

$$\langle 2 | \hat{Q}_{20} | 3 \rangle = A \langle 2 | \hat{q}^{\dagger}_{20} | 3 \rangle = \sqrt{\frac{2}{35}} A X_2 \langle 2_2 \| a_2 \| 2_3 \rangle$$

$$= \frac{2\sqrt{2}}{7} A X_2 = \langle 3 | \hat{Q}_{20} | 2 \rangle \qquad \text{(II-A-17)}$$

and finally:

$$\langle 3 | \hat{Q}_{20} | \; \rangle = -\frac{4}{49} B X_2^2 \langle 2_3 \| [a_2^{\dagger} a_2^{-}]_2 \| 2_3 \rangle = \frac{24}{343} B X_2^2 \qquad \text{(II-A-18)}$$

where the following table was used:

I_3 \ I_2	0	2	4
0		$3^{1/2}$	
2	$7^{1/2}$	$(20/7)^{1/2}$	$(36/7)^{1/2}$
3		$15^{1/2}$	$-6^{1/2}$
4		$(99/7)^{1/2}$	$(90/7)^{1/2}$
6			$39^{1/2}$

This table was taken from A. Bohr and B. Mottelson, vol. II, p. 691, 1975.

Other important matrix elements are:

$$\langle o \| Q_2 \| 2_1 \rangle = \sqrt{5}\, A X_2 \qquad \text{(II-A-19a)}$$

and

$$\langle o \| Q_2 \| 2_2 \rangle = -\sqrt{\frac{10}{7}}\, B X_2^2 \, \langle o \| [a_2 a_2]_2 \| 2_2 \rangle$$

$$= \frac{3}{2}\sqrt{\frac{5}{7}}\, B X_2^2 \qquad \text{(II-A-19b)}$$

since

$$\langle o \| [a_2 a_2]_2 \| 2_2 \rangle = \begin{Bmatrix} 2 & 2 & 2 \\ 2 & 2 & 2 \end{Bmatrix} \langle o \| a_2 \| 2_1 \rangle \otimes \langle 2_2 \| a_2 \| a_2 \rangle \qquad \text{(II-A-19c)}$$

With the matrix elements given in this section, we are going to find expressions for the relevant reduced transition probabilities and quadrupole moments in the next section of this appendix.

(b) Reduced Transition Probabilities and Quadrupole Moments related to the problem:

The state 2_1^+ with energy 373.8 KeV above the ground state level can be written in our model as:

$$|\psi_{374}\rangle \equiv \alpha_1 |1\rangle + \alpha_2 |2\rangle + \alpha_3 |3\rangle \qquad \text{(II-A-20)}$$

and then the quadrupole moment is given by:

$$Q_{374} = \sqrt{\frac{16\pi}{5}} \left\{ -\frac{4}{7} BX_2^2 \alpha_1^2 + \frac{12}{49} BX_2^2 \alpha_2^2 + \frac{24}{343} BX_2^2 \alpha_3^2 \right.$$

$$\left. + \frac{4}{\sqrt{7}} AX_2 \alpha_1 \alpha_2 + \frac{12}{49}\sqrt{\frac{2}{7}} BX_2^2 \alpha_1 \alpha_3 + \frac{4\sqrt{2}}{7} AX_2 \alpha_2 \alpha_3 \right\} \quad \text{(II-A-21)}$$

The reduced transition probabilities are given by:

$$B(EL; I_1 \to I_2) = \frac{1}{2I_1 + 1} \left| \langle I_2 \| Q_L \| I_1 \rangle \right|^2 \quad \text{(II-A-22)}$$

and in the 2_1^+ state case, we have:

$$\langle 0 \| Q_2 \| 374 \rangle = \sqrt{5} AX_2 \alpha_1 + \frac{3}{7}\sqrt{\frac{5}{7}} BX_2^2 \alpha_2 \quad \text{(II-A-23)}$$

and for the 2_2^+ state, a similar expression can be found with the results:

$$B(E2; 374 \to 0) = \frac{1}{5} \left[\sqrt{5} AX_2 \alpha_1 + \frac{3}{7}\sqrt{\frac{5}{7}} BX_2^2 \alpha_2 \right]^2 \quad \text{(II-A-24a)}$$

$$B(E2; 814 \to 0) = \frac{1}{5} \left[\sqrt{5} AX_2 \beta_1 + \frac{3}{7}\sqrt{\frac{5}{7}} BX_2^2 \beta_2 \right]^2 \quad \text{(II-A-24b)}$$

and with the matrix elements calculated previously, we also have:

$$B(E2; 814 \to 374) = \frac{1}{5} \left| \langle 374 \| Q_2 \| 814 \rangle \right|^2 \quad \text{(II-A-25)}$$

and

$$\langle 374 \| Q_2 \| 814 \rangle = -\frac{4}{7}\sqrt{\frac{35}{2}}\, BX_2^2 \alpha_1\beta_1 + \frac{2}{\sqrt{7}}\sqrt{\frac{35}{2}}\, AX_2 \alpha_1\beta_2$$

$$+ \frac{6}{49}\sqrt{5}\, BX_2^2 \alpha_1\beta_3 + \frac{12}{49}\sqrt{\frac{35}{2}}\, BX_2^2 \alpha_2\beta_2$$

$$+ \sqrt{10}\, AX_2 \alpha_2\beta_1 + 2\sqrt{5}\, AX_2 \alpha_2\beta_3$$

$$+ \frac{6}{49}\sqrt{5}\, BX_2^2 \alpha_3\beta_1 + 2\sqrt{5}\, AX_2 \alpha_3\beta_2$$

$$+ \frac{24}{343}\sqrt{\frac{35}{2}}\, BX_2^2 \alpha_3\beta_3 \qquad \text{(II-A-26)}$$

APPENDIX (II-B)

MATRIX ELEMENTS RELATED TO THE NUCLEAR POLARIZATION PROBLEM.

In actual calculations we used square densities of the form

$$\rho(r) = \rho_0\, \theta(a-r) \qquad \text{(II-B-1)}$$

to simplify the calculations and based on the low sensitivity of the results on the detailed form of the nuclear density in previous work. Powers of the density will have the same form. In such conditions, the contribution of the electromagnetic part is given by:

$$\begin{aligned} &\langle \tilde{n}\ell\, I\, J \mid \Delta H^{\pi}_{em} \mid n'\ell' I' J \rangle \\ &= -\sqrt{\frac{4\pi}{5}}\, e\, (-1)^{J+\ell'+\ell+I}\, (2\ell+1)(2I+1) \left[\frac{2\ell'+1}{2J+1}\right]^{1/2} \\ &\otimes \left[B(E2, I\to I')\right]^{1/2} \begin{pmatrix} \ell & 2 & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \ell & \ell' & 2 \\ I' & I & J \end{Bmatrix} \\ &\otimes \int_0^{\infty} \frac{1}{r} R_{n\ell}\, R_{n'\ell'}\, dr \end{aligned} \qquad \text{(II-B-2)}$$

where the overlap integral is calculated numerically using radial wavefunctions of the pion, generated by the computer code PIATOM, and from the s-wave interaction contribution to the optical potential:

$$\langle \tilde{n}\ell\, I\, J \mid \Delta H^{\pi}_{s} \mid n'\ell' I' J \rangle = \frac{\sqrt{20\pi}}{3} (-1)^{J+\ell'+\ell+I} (2\ell+1) \left[\frac{(2\ell'+1)}{2J+1}\right]^{1/2}$$

$$\otimes (2I+1)\,\frac{a_0 V_S}{Ze}\begin{pmatrix} \ell & 2 & \ell' \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} \ell & \ell' & 2 \\ I' & I & J \end{Bmatrix} R_{n\ell}\, R_{n'\ell'}\Big|_{r=a_0}$$

$$\otimes \left[B(E2, I \to I') \right]^{1/2} \qquad \text{(II-B-3)}$$

The proton and neutron radius is taken to be the same, a_0, and the essential form of this potential is given by

$$\hat{V}_S^{\Pi} = \left(V_S^{(0)} + V_S^{(1)}\right)\theta(a-r) \equiv V_S\,\theta(a-r) \qquad \text{(II-B-4)}$$

where $V_S^{(0)}$ includes the isoscalar amplitude and $V_S^{(1)}$ contains the absorption coefficients and it is proportional to the square of the density in the interior of the nucleus. In the p-wave interaction case the optical potential is given by

$$\hat{V}_p^{\Pi} = V_p\,\vec{\nabla}\cdot\theta(a-r)\,\vec{\nabla} \qquad \text{(II-B-5)}$$

within the square density approximation, and

$$\frac{\partial \hat{V}_p^{\Pi}}{\partial a} = V_p\left\{-\frac{\partial}{\partial a}\delta(a-r)\frac{\partial}{\partial r} + \delta(a-r)\right.$$

$$\left.\otimes\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\ell(\ell+1)}{r^2}\right]\right\} \qquad \text{(II-B-6)}$$

and then, the corresponding matrix element is given by

$$\langle \tilde{n}\ell\, I J \,|\, \Delta H_p^{\parallel} \,|\, n'\ell' I' J' \rangle = \frac{\sqrt{2\pi}}{3} (-1)^{J+\ell'+\ell+I} (2\ell+1) \left[\frac{(2\ell'+1)}{2J+1}\right]^{1/2}$$

$$\otimes (2I+1) \frac{a_0 V_p}{Ze} \begin{pmatrix} \ell & 2 & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \ell & \ell' & 2 \\ I' & I & J \end{Bmatrix} \left[B(E2, I \to I')\right]^{1/2}$$

$$\otimes \left\{ \left[-\frac{\partial}{\partial a} \left(R_{n\ell} \frac{\partial}{\partial r} R_{n'\ell'} \right)_{r=a} \right]_{a=a_0} \right. \qquad \text{(II-B-7)}$$

$$\left. + \left[\frac{R_{n\ell}}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} R_{n'\ell'} \right) - \frac{\ell(\ell+1)}{r^2} R_{n\ell} R_{n'\ell'} \right]_{r=a_0} \right\}$$

APPENDIX (III-A)

FINITE SQUARE WELL REDUCED GREENS FUNCTION FOR THE GROUND STATE.

In this appendix we are going to use the differential representation of the Reduced Green's Function to treat the finite square well case. The first step is to find the radial part of the Green's Function given by

$$\tilde{g}_\ell(r,r') \equiv rr' G_\ell(r,r') \qquad \text{(III-A-1)}$$

where $G_\ell(r,r')$ is the full radial Green's Function for a given partial wave. To the differential equation problem:

$$\left\{ \mathcal{E}_{n\ell} + \frac{1}{2\mu}\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{2\mu r^2} - V(r) \right\} \tilde{g}_\ell(r,r') = \delta(r-r') \qquad \text{(III-A-2)}$$

we add the boundary conditions:

$$\tilde{g}(0,r') = \tilde{g}(\infty,r') = 0 \qquad \text{(III-A-3a)}$$

$$\tilde{g}(r,r')\Big|_{r=r'+} = \tilde{g}(r,r')\Big|_{r=r'-} \qquad \text{(III-A-3b)}$$

$$\frac{d}{dr}\tilde{g}(r,r')\Big|_{r=r'+} - \frac{d}{dr}\tilde{g}(r,r')\Big|_{r=r'-} = 2\mu \qquad \text{(III-A-3c)}$$

and the potential in this case can be written as:

$$V(r) = -V_c\,\theta(a-r) \qquad \text{(III-A-4)}$$

The solution for l=0 is given by:

$$\tilde{g}(r,r') = \begin{cases} -\frac{2\mu}{W_+} e^{-K(r'-a)} \sin kr & r<a \\ -\frac{\mu}{k}\left\{\frac{W_1}{W_+} e^{-K(r+r'-2a)} + e^{-K(r_>-r_<)}\right\} & r,r'>a \end{cases} \quad \text{(III-A-5a)}$$

and

$$\tilde{g}(r,r') = \begin{cases} -\frac{2\mu}{k}\left\{\cos kr_> \sin kr_< + \frac{W_-}{W_+} \sin kr \sin kr'\right\} & r,r'<a \\ -\frac{2\mu}{W_+} e^{-K(r-a)} \sin kr' & r>a \end{cases} \quad \text{(III-A-5b)}$$

where

$$k^2 \equiv 2\mu(V_c - |E|) \quad \text{(III-A-6a)}$$

$$K^2 \equiv 2\mu|E| \quad \text{(III-A-6b)}$$

and

$$W_+(k,K) \equiv k\cos ka + K \sin ka \quad \text{(III-A-7a)}$$

$$W_-(k,K) \equiv k \sin ka - K\cos ka \quad \text{(III-A-7b)}$$

$$W_1(k,K) \equiv K \sin ka - k \cos ka \qquad \text{(III-A-7c)}$$

We note that

$$W_+(k,K) = 0 \qquad \text{(III-A-8)}$$

is the eigenvalue equation for l=0,

The next step is the direct application of the differential formula:

$$\tilde{\vartheta}(r,r') = \lim_{\varepsilon \to \varepsilon_0} \frac{d}{d\varepsilon} \left\{ (\varepsilon - \varepsilon_0) \tilde{g}(r,r') \right\} \qquad \text{(III-A-9)}$$

where ε_0 is the ground state energy for l=0, which will be the studied case in Chapter III. The momenta k and K are functions of the energy and equation (III-A-8) is satisfied for = , i. e., has a pole there. It is convenient then to consider the expansion:

$$W_+(k,K) = \tilde{a}(\varepsilon - \varepsilon_0) + \tilde{b}(\varepsilon - \varepsilon_0)^2 + \vartheta[(\varepsilon - \varepsilon)^3] \qquad \text{(III-A-10)}$$

There is no order zeroth term in equation (III-A-10) since

$$W_+(\varepsilon_0) = 0 \qquad \text{(III-A-11)}$$

due to the eigenvalue condition. Next, we are going to consider the limit process of equation (III-A-9) for all the

sensitive terms of equations (III-A-5a) and (III-A-5b). Then, the first term to be treated is:

$$\lim_{\varepsilon\to\varepsilon_0}\frac{d}{d\varepsilon}\left\{(\varepsilon-\varepsilon_0)\frac{W_-}{kW_+}\sin kr\sin kr'\right\}$$

$$=\lim_{\varepsilon\to\varepsilon_0}\frac{d}{d\varepsilon}\left\{\frac{W_-\sin kr\sin kr'}{k\left[\tilde{a}+\tilde{b}(\varepsilon-\varepsilon_0)+\delta[(\varepsilon-\varepsilon_0)^2]\right]}\right\}$$

$$=\frac{1}{\tilde{a}}\frac{d}{d\varepsilon}\left\{\frac{W_-}{k}\sin kr\sin kr'\right\}_{\varepsilon=\varepsilon_0}-\frac{\tilde{b}}{\tilde{a}^2}\left\{\frac{W_-}{k}\sin kr\sin kr'\right\}_{\varepsilon=\varepsilon_0} \qquad \text{(III-A-12)}$$

where

$$\tilde{a}\equiv\left.\frac{\partial W_+}{\partial\varepsilon}\right|_{\varepsilon=\varepsilon_0}=-\mu\sin k_0a\left\{\frac{1}{K}+\frac{1}{k}\left[ka+\frac{K}{k}(1+Ka)\right]\right\} \qquad \text{(III-A-13a)}$$

$$\tilde{b}\equiv\frac{1}{2!}\left.\frac{\partial^2W_+}{\partial\varepsilon^2}\right|_{\varepsilon=\varepsilon_0}=-\frac{\mu}{2k_0^2}\left\{\tilde{a}+\frac{\mu}{K_0}\sin k_0a\right\}$$

$$-\frac{\mu^2a}{2k_0^2}\left\{(2+K_0a)\sin k_0a+k_0a\cos k_0a\right\}-\frac{\mu^2a}{k_0K_0}\cos k_0a$$

$$-\frac{\mu^2}{2K_0^3}\sin k_0a \qquad \text{(III-A-13b)}$$

and

$$\left.\frac{dW_-}{d\varepsilon}\right|_{\varepsilon=\varepsilon_0}=\frac{\mu}{k_0}\left[(1+K_0a)\sin k_0a+k_0a\cos k_0a\right]+\frac{\mu}{K_0}\cos k_0a \qquad \text{(III-A-14)}$$

the rest of the derivatives are elementary. The second sensitive term is given by:

$$\lim_{\varepsilon \to \varepsilon_0} \frac{d}{d\varepsilon} \left\{ \frac{e^{-K(r-a)}}{W_+} \sin kr' \; (\varepsilon - \varepsilon_0) \right\}$$

$$= \frac{1}{\tilde{a}} \frac{d}{d\varepsilon} \left\{ e^{-K(r-a)} \sin kr' \right\}_{\varepsilon=\varepsilon_0} - \frac{\tilde{b}}{\tilde{a}^2} \left\{ e^{-K(r-a)} \sin kr' \right\}_{\varepsilon=\varepsilon_0} \qquad \text{(III-A-15)}$$

The last sensitive term is written as:

$$\lim_{\varepsilon \to \varepsilon_0} \frac{d}{d\varepsilon} \left\{ (\varepsilon - \varepsilon_0) \frac{W_1}{K W_+} e^{-K(r+r'-2a)} \right\}$$

$$= \frac{1}{\tilde{a}} \frac{d}{d\varepsilon} \left\{ \frac{W_1}{K} e^{-K(r+r'-2a)} \right\}_{\varepsilon=\varepsilon_0} - \frac{\tilde{b}}{\tilde{a}^2} \left\{ \frac{W_1}{K} e^{-K(r+r'-2a)} \right\}_{\varepsilon=\varepsilon_0} \qquad \text{(III-A-16)}$$

with

$$\left. \frac{dW_1}{d\varepsilon} \right|_{\varepsilon=\varepsilon_0} = \frac{\mu}{k_0} \left[(K_0 a - 1) \cos k_0 a + k_0 a \sin k_0 a \right] - \frac{\mu}{k_0} \sin k_0 a \qquad \text{(III-A-17)}$$

If the following definitions are introduced:

$$C_0 \equiv -\frac{\mu}{k_0^2} W_- \Big|_{\varepsilon=\varepsilon_0} + \left. \frac{dW_-}{d\varepsilon} \right|_{\varepsilon=\varepsilon_0} \qquad \text{(III-A-18)}$$

$$C_1 \equiv \frac{\mu}{k_0^2} W_1 \Big|_{\varepsilon=\varepsilon_0} + \left. \frac{dW_1}{d\varepsilon} \right|_{\varepsilon=\varepsilon_0} \qquad \text{(III-A-19)}$$

the result for the radial Reduced Green's Function is given by:

$$\tilde{\theta}(r,r') = \begin{cases} -\frac{2\mu}{k_0}\left\{\cos k_0 r_< \sin k_0 r_> + \tilde{R}_0 \sin k_0 r \sin k_0 r' \right. \\ \left. + \tilde{R}_1 (r \cos k_0 r \sin k_0 r' + r' \sin k_0 r \cos k_0 r')\right\} & r, r' < a \\ -\frac{2\mu}{K_0}\left\{\tilde{R}_2 e^{-K_0 r} r \sin k_0 r' + \tilde{R}_3 r' e^{-K_0 r} \cos k_0 r' \right. \\ \left. + \tilde{R}_4 e^{-K_0 r} \sin k_0 r'\right\} & r > a \end{cases} \quad \text{(III-A-20a)}$$

and

$$\tilde{\theta}(r,r') = \begin{cases} -\frac{2\mu}{K_0}\left\{\tilde{R}_2 e^{-K_0 r'} r' \sin k_0 r + \tilde{R}_3 r e^{-K_0 r'} \cos k_0 r \right. \\ \left. + \tilde{R}_4 e^{-K_0 r'} \sin k_0 r\right\} & r < a \\ -\frac{2\mu}{K_0}\left\{\frac{1}{2} e^{-K_0 (r_> - r_<)} + \tilde{R}_5 e^{-K_0 (r+r')} \right. \\ \left. + \tilde{R}_6 (r+r') e^{-K_0 (r+r')}\right\} & r', r > a \end{cases} \quad \text{(III-A-20b)}$$

where the coefficients $\tilde{R}_i$ are defined as:

$$\tilde{R}_0 \equiv \frac{C_0}{\tilde{a}} - \frac{\tilde{b}}{\tilde{a}^2} W_- \quad \text{(III-A-21a)}$$

$$\tilde{R}_1 \equiv \frac{W_- \mu}{\tilde{a} k_0} \quad \text{(III-A-21b)}$$

$$\tilde{R}_2 \equiv \frac{\mu}{\tilde{a}} e^{K_0 a} \qquad \text{(III-A-21c)}$$

$$\tilde{R}_3 \equiv \frac{\mu K_0}{\tilde{a} k_0} e^{K_0 a} \qquad \text{(III-A-21d)}$$

$$\tilde{R}_4 \equiv -a \tilde{R}_2 - \frac{\tilde{b} K_0}{\tilde{a}^2} e^{K_0 a} \qquad \text{(III-A-21e)}$$

$$\tilde{R}_5 \equiv e^{2K_0 a} \left[\frac{C_1}{2\tilde{a}} - \frac{\mu W_1 a}{\tilde{a} K_0} - \frac{\tilde{b} W_1}{2\tilde{a}^2} \right] \qquad \text{(III-A-21f)}$$

$$\tilde{R}_6 \equiv \frac{\mu W_1}{2\tilde{a} K_0} e^{2K_0 a} \qquad \text{(III-A-21g)}$$

The full radial Reduced Green's Function is

$$\vartheta(r,r') = \frac{\tilde{\vartheta}(r,r')}{rr'} \qquad \text{(III-A-22)}$$

APPENDIX (IV-A)

REDUCED GREENS FUNCTION IN THE COULOMB CASE FOR THE 1S PIONIC STATE.

The Reduced Green's Function in the Coulomb case can be found using equations (III-85), (III-86) and (III-89). The functions $G_A(r,r')$ and $G_B(r,r')$ are defined as:

$$G_A^{n\ell}(r,r') \equiv \int_{r'}^{r} \frac{dy}{y^2 \phi_{n\ell}^2(y)} \int_0^y t^2 \phi_{n\ell}^2(t)\, dt \qquad \text{(IV-A-1)}$$

$$G_B^{n\ell}(r,r') \equiv \int_{r'}^{r} \frac{dy}{y^2 \phi_{n\ell}^2(y)} \int_y^{\infty} t^2 \phi_{n\ell}^2(t)\, dt \qquad \text{(IV-A-2)}$$

In the case of the state 1s, the radial wavefunction is given by

$$\phi_{1S}(r) = C_{1S}\, e^{-K_1 r} \qquad \text{(IV-A-3)}$$

$$K_1 \equiv \mu Z \alpha_{FS} \qquad \text{(IV-A-4)}$$

where μ is the pion-nucleus reduced mass, α_{FS} is the fine structure constant and

$$C_{1S}^2 = 4K_1^3 \qquad \text{(IV-A-5)}$$

The integration in equations (IV-A-1) and (IV-A-2) is almost inmediate and the result is:

$$G_A^{1S}(r,r') = -\frac{1}{4K_1^2}(x-x') + \frac{1}{2K_1^2}\sum_{n=2}^{\infty}\frac{2^{n-1}}{n!\,(n-1)}\left(x^{n+1}-x'^{n+1}\right) \qquad \text{(IV-A-6)}$$

$$G_B^{1S}(r,r') = \frac{1}{2K_1^2}\left\{x-x'+\log\frac{x}{x'}-\frac{1}{2x}+\frac{1}{2x'}\right\} \qquad \text{(IV-A-7)}$$

and we introduce the definition:

$$G_0^1(x) \equiv \sum_{n=1}^{\infty}\frac{2^n x^n}{n(n+1)!} \qquad \text{(IV-A-8)}$$

Then:

$$\mathcal{M}_{1S}^{>}(r,r') = C_0(r') + \frac{\mu}{K_1^2}\left\{x-x'+\log\frac{x}{x'}-\frac{1}{2x}+\frac{1}{2x'}\right\} \qquad \text{(IV-A-9)}$$

$$\mathcal{M}_{1S}^{<}(r,r') = C_0(r') - \frac{\mu}{K_1^2}\left\{x-x'-G_0^1(x)+G_0^1(x')\right\} \qquad \text{(IV-A-10)}$$

With the definitions of equations (IV-A-1) and (IV-A-2) we can write $C_0(r')$ as:

$$C_0(r') = 2\mu\, G_A^{1S}(0,r') - 2\mu\int_0^{\infty} x^2 dx\, \phi_{1S}^2(x)\, G_B(x,r') \qquad \text{(IV-A-11)}$$

Using the tables of I. S. Gradsteyn and I. M. Ryzhik, the integral

$$\int_0^{\infty} x^2 dx\, e^{-x}\log x = 3-2\gamma \qquad \text{(IV-A-12)}$$

which is a particular case of:

$$\int_0^{\infty} x^n e^{-\mu x}\log x\, dx = \frac{n!}{\mu^{n+1}}\left[1+\frac{1}{2}+\ldots+\frac{1}{n}-\gamma-\log\mu\right] \qquad \text{(IV-A-13)}$$

being γ the Mascherioni Constant, and $\mathrm{Re}\,\mu > 0$.

Using equation (IV-A-12) in equation (IV-A-11) we obtain:

$$C_0(r') = \frac{\mu}{k_1^2}\left\{ 2x' + \log 2x' - \frac{1}{2x'} - G_0^1(x') - \frac{5}{2} + \gamma \right\} \qquad \text{(IV-A-14)}$$

Replacing equation (IV-A-14) in equations (IV-A-9) and (IV-A-10) we get:

$$M_{1S}(r,r') = -\frac{\mu}{k_1^2}\left\{ \frac{5}{2} - \gamma - x - x' - \log 2x_> + \frac{1}{2x_>} + G_0^1(x_<) \right\} \qquad \text{(IV-A-15)}$$

and the radial part of the Reduced Green's Function is given by:

$$\begin{aligned} \mathcal{G}_{1S}(r,r') &= \phi_{1S}(r)\, M_{1S}(r,r')\, \phi_{1S}(r') \\ &= -4\mu k_1 e^{-k_1(r+r')} \left\{ \frac{5}{2} - \gamma - k_1(r+r') - \log 2k_1 r_> + \frac{1}{2k_1 r_>} \right. \\ &\left. + G_0^1(k_1 r_<) \right\} \end{aligned} \qquad \text{(IV-A-16)}$$

Equation (IV-A-16) will be used for pionic ^1H, ^4He and ^{16}O calculations. It is interesting to note that equation (IV-A-16) includes contributions from the continuum of states, which is not taken into account in most of the estimates done up to date in perturbation theory.

APPENDIX (V-A)

FORM FACTOR INTEGRAL $F_s(Q)$ FOR THE PION-NUCLEON S-WAVE INTERACTION.

In Chapter V the first doorway normalization for the S_{11} channel and S_{31} channel is given by

$$\left(\tilde{N}_o^* N_o\right)^{-1}$$

$$= G^\dagger G \sum_j \int \frac{d\vec{p}}{(2\pi)^3} \frac{d\vec{q}}{(2\pi)^3} \frac{d\vec{p}}{(2\pi)^3} \psi_j^*(\vec{p}-\vec{p}) \frac{M_j \, e^{-i(\vec{p}-\vec{q})\cdot\vec{r}'}}{\left[\alpha^2+(\vec{p}-\beta_1\vec{p})^2\right]\left[\alpha^2+(\vec{q}-\beta_1\vec{p})^2\right]} \psi_j(\vec{p}-\vec{q}) \quad \text{(V-A-1)}$$

where M_j is an isospin weight factor defined by

$$M_j = 1/3 \qquad (S_{11}) \qquad \text{(V-A-1a)}$$

$$M_j = \begin{cases} 1/3 & (S_{31}) \text{ PROTONS} \qquad \text{(V-A-1b)} \\ 1 & (S_{31}) \text{ NEUTRONS} \qquad \text{(V-A-1c)} \end{cases}$$

since

$$T_+ T_- = 1 \quad \text{for the } S_{11} \text{ channel} \quad \text{(V-A-2a)}$$

and

$$T_+ T_- = \begin{bmatrix} 1/3 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{for the } S_{31} \text{ channel} \quad \text{(V-A-2b)}$$

The form factor integral is defined by:

$$F_s(\vec{p},\vec{q}) \equiv \int \frac{d\vec{P}}{(2\pi)^3} \frac{1}{\left[\alpha^2+(\vec{p}-\beta_2\vec{P})^2\right]\left[\alpha^2+(\vec{q}-\beta_2\vec{P})^2\right]} \qquad \text{(V-A-3)}$$

and it is part of the integrand of equation (V-A-1) if the following shift is done:

$$\vec{p} \rightarrow \vec{p}+\vec{P} \qquad \vec{q} \rightarrow \vec{q}+\vec{P} \qquad \text{(V-A-4)}$$

followed by the inversions

$$\vec{p} \rightarrow -\vec{p} \qquad \vec{q} \rightarrow -\vec{q} \qquad \text{(V-A-5)}$$

with the result:

$$\left(\tilde{N}_o^* N_o\right)^{-1}_{\vec{r}\,'}$$

$$= G^+G \sum_j \int \frac{d\vec{p}}{(2\pi)^3}\frac{d\vec{q}}{(2\pi)^3}\, \psi_j^*(\vec{p})\, M_j\, F_s(\vec{p},\vec{q})\, e^{-i(\vec{q}-\vec{p})\cdot\vec{r}\,'}\, \psi_j(\vec{q}) \qquad \text{(V-A-6)}$$

Defining:

$$\vec{K} \equiv \vec{p}-\vec{q} \qquad \text{(V-A-7)}$$

equation (V-A-3) can be rewritten as:

$$F_s(\vec{p},\vec{q}) = F_s(\vec{K}) = \frac{1}{\beta_2^3}\int \frac{d\vec{P}}{(2\pi)^3} \frac{1}{\left[\alpha^2+(\vec{K}+\vec{P})^2\right]\left[\alpha^2+P^2\right]}$$

$$= 8\pi^2\beta_2^3 K \int_0^\infty \frac{P\,dP}{\alpha^2+P^2} \log\left[\frac{\alpha^2+(K+P)^2}{\alpha^2+(K-P)^2}\right] \qquad \text{(V-A-8)}$$

The fundamental integral to be found is given by

$$I_F \equiv \int_0^\infty \frac{P\,dP}{\alpha^2+P^2} \log\left[\frac{\alpha^2+(K+P)^2}{\alpha^2+(K-P)^2}\right] \qquad \text{(V-A-9)}$$

and using the known results:

$$\int_0^\infty dx\, e^{-px} \sin qx = \frac{q}{p^2+q^2} \qquad \text{(V-A-10)}$$

with $p > 0$, and

$$\int_0^\infty \log\left[\frac{(x+\beta)^2+\gamma^2}{(x-\beta)^2+\gamma^2}\right] \sin bx\, dx = \frac{2\pi}{b} e^{-\gamma b} \sin \beta b \qquad \text{(V-A-11)}$$

with $\mathrm{Re}\,\gamma > 0$, $|\mathrm{Im}\,\beta| \leq \mathrm{Re}\,\gamma$ and $b > 0$, the integral I_F can be found:

$$I_F = \int_0^\infty dx\, e^{-\alpha x} \int_0^\infty dP \sin Px \log\left[\frac{\alpha^2+(K+P)^2}{\alpha^2+(K-P)^2}\right]$$

$$= 2\pi \int_0^\infty \frac{\sin Kx}{x} e^{-2\alpha x}\, dx$$

$$= S\pi^2 + \pi \arctg \frac{4\alpha K}{4\alpha^2 - K^2} \qquad \text{(V-A-12)}$$

where

$$S \equiv \begin{cases} 0 & \alpha^2 \geq \frac{K^2}{4} \\ 1 & \alpha^2 < \frac{K^2}{4} \end{cases} \qquad \text{(V-A-13)}$$

Then $F_s(K)$ can be rewritten as:

$$F_s(K) = \frac{}{8\beta_2^3 K}\left\{1 - \theta(2\alpha - K) + \frac{1}{\pi}\,\text{arc tg}\,\frac{4\alpha K}{4\alpha^2 - K^2}\right\} \quad \text{(V-A-14)}$$

where

$$K \equiv |\vec{p} - \vec{q}| \quad \text{(V-A-15)}$$

APPENDIX (V-B)

MATRIX ELEMENTS FOR THE COULOMB RESCATTERING OPERATOR IN THE N*-HOLE, *-HOLE APPROACH.

The vertex function for the S_{11} channel is given by:

$$f^{\dagger}(\vec{q}) = \frac{G}{\sqrt{3}} \frac{\vec{\tau}}{\alpha^2 + q^2} \qquad \text{(V-B-1)}$$

where

$$G^{\dagger}G = -\frac{g^2}{2M_{\pi}} \qquad \text{(V-B-2)}$$

The Coulomb Rescattring matrix element reads:

$$\langle N^* h | \hat{R}_S | N^{*\prime} h' \rangle = \int \frac{d\vec{q}}{(2\pi)^3} \frac{d\vec{q}'}{(2\pi)^3} \frac{d\vec{Q}}{(2\pi)^3} \frac{d\vec{P}}{(2\pi)^3} \langle N^* | \vec{P} \rangle f(\vec{q} - \beta_1 \vec{P})$$

$$\otimes \langle \vec{P} - \vec{q} | h \rangle \vartheta_S(\vec{q}, \vec{q}') \langle h' | \vec{Q} - \vec{q}' \rangle f^{\dagger}(\vec{q}' - \beta_1 \vec{Q}) \langle \vec{Q} | N^{*\prime} \rangle \qquad \text{(V-B-3)}$$

Before any further development of this matrix element, we consider the coefficient of the Doorway State in a N*-hole basis:

$$\vartheta(N^* h S) \equiv \int \frac{d\vec{q}}{(2\pi)^3} \frac{d\vec{P}}{(2\pi)^3} \langle N^* | \vec{P} \rangle \frac{G}{\sqrt{3}} \frac{\vec{\tau}_-}{\alpha^2 + (\vec{q} - \beta_1 \vec{P})^2} \langle \vec{P} - \vec{q} | h \rangle \psi_{\nu\lambda}(\vec{q})$$

$$\equiv \sqrt{\frac{2}{3}}\, G\, \delta_{m_T, \frac{1}{2}}\, \delta_{m_T, -\frac{1}{2}}\, \tilde{\vartheta}(\tilde{N}^* \tilde{h} S) \qquad \text{(V-B-4)}$$

where we used

$$\tau_- \left|\tfrac{1}{2} m_\tau\right\rangle = \frac{1}{\sqrt{2}}\left(1+2m_\tau\right)\left|\tfrac{1}{2}, -m_\tau\right\rangle \qquad \text{(V-B-5)}$$

We define the different set of quantum numbers related to the problem as:

$$\tilde{N}^* \equiv \left(N L \tfrac{1}{2} J^* M^*\right) \qquad \text{(V-B-6a)}$$

$$\tau_h \equiv \left(n \ell \tfrac{1}{2} j, -m\right) \qquad \text{(V-B-6b)}$$

$$S \equiv \left(\nu \lambda \mu\right) \qquad \text{(V-B-6c)}$$

Then we can write:

$$\tilde{\vartheta}\left(\tilde{N}^* \tau_h S\right) \equiv \int \frac{d\vec{q}}{(2\pi)^3} \frac{d\vec{P}}{(2\pi)^3} \left\langle N^* \middle| \vec{P} \right\rangle \frac{\psi_{\nu\lambda\mu}(\vec{q})}{\alpha^2 + \left(\vec{q} - \beta_1 \vec{P}\right)^2} \left\langle \vec{P} - \vec{q} \middle| \tau_h \right\rangle$$

$$= (-1)^{j+m} \left\langle N L \tfrac{1}{2} J^* M^* \middle| V_{\nu\lambda\mu} \middle| n \ell \tfrac{1}{2} j, -m \right\rangle \qquad \text{(V-B-7)}$$

Using the Wigner-Eckart Theorem:

$$\left\langle N L \tfrac{1}{2} J^* M^* \middle| V_{\nu\lambda\mu} \middle| n \ell \tfrac{1}{2} j, -m \right\rangle = (-1)^{J^* - M^*} \left[J^*\right] \otimes \begin{pmatrix} J^* & \lambda & j \\ -M^* & \mu & -m \end{pmatrix} \left\langle N L \tfrac{1}{2} J^* \middle\| \vartheta_{\nu\lambda} \middle\| n \ell \tfrac{1}{2} j \right\rangle \qquad \text{(V-B-8)}$$

where $\left[J^*\right] \equiv \sqrt{2J^* + 1}$, and

$$\left\langle N L \tfrac{1}{2} J^* \middle\| V_{\nu\lambda} \middle\| n \ell \tfrac{1}{2} j \right\rangle = (-1)^{\lambda + \frac{1}{2} + j + L} \left[j\right]\left[L\right] \otimes \begin{Bmatrix} J^* & j & \lambda \\ \ell & L & \frac{1}{2} \end{Bmatrix} \left\langle N L \middle\| V_{\nu\lambda} \middle\| n \ell \right\rangle \qquad \text{(V-B-9)}$$

Using the Wigner-Eckard Theorem again, we find:

$$(-1)^{L}[L]\begin{pmatrix} L & \lambda & \ell \\ 0 & 0 & 0 \end{pmatrix}\langle NL\|V_{\nu\lambda}\|n\ell\rangle$$

$$=\int \frac{d\vec{p}}{(2\pi)^3}\frac{d\vec{q}}{(2\pi)^3}\,\phi^{*}_{NL0}(\vec{p})\,\frac{\psi_{\nu\lambda}(q^2)}{\alpha^2+(\vec{q}-\beta_1\vec{p})^2}\,\phi_{n\ell 0}(\vec{p}-\vec{q}) \qquad \text{(V-B-10)}$$

The scale of $\vec{q}$ is fixed by $\psi_{\nu\lambda}(q^2)$ and in the pionic atom case it is a very small quantity. So, if the following expansion is considered:

$$\frac{1}{\alpha^2+(\vec{q}-\beta_1\vec{p})^2}=\frac{1}{\alpha^2+\beta_1^2p^2}+\frac{2\beta_1\vec{q}\cdot\vec{p}}{(\alpha^2+\beta_1^2p^2)^2}+\vartheta(q^2) \qquad \text{(V-B-11)}$$

The approximation of keeping just the first term of equation (V-B-11) is more than justified since the second term is 10^{-3} times smaller than the leading one. If this approximation is done, the reduced matrix element is given by:

$$\langle NL\|V_{\nu\lambda}\|n\ell\rangle=\frac{1}{2\pi^{5/2}}[\lambda][\ell]\begin{pmatrix} L & \lambda & \ell \\ 0 & 0 & 0 \end{pmatrix}$$

$$\otimes\int_0^\infty \frac{p^2dp}{\alpha^2+\beta_1^2p^2}\,\tilde{\psi}_{NL}(p)\int_0^\infty x^2dx\,j_L(px)\,\psi^{h}_{n\ell}(x)\,\psi^{\Pi}_{\nu\lambda}(x) \qquad \text{(V-B-12)}$$

Introducing the definition:

$$F_{nm}(NL'|\alpha\lambda|x)\equiv\int_0^\infty\frac{p^n\,dp}{(\alpha^2+\beta_1^2p^2)^m}\,\tilde{\psi}_{NL}(p)\,j_L(px) \qquad \text{(V-B-13)}$$

we can write the matrix element given by equation (V-B-9) as:

$$\langle NL\tfrac{1}{2}J^*\|\vartheta_{\nu\lambda}\|n\ell\tfrac{1}{2}j\rangle = \frac{(-1)^{\lambda+\frac{1}{2}+j+L}}{4\pi^{5/2}}[j][L][\lambda][\ell]$$

$$\otimes\begin{pmatrix} L & \lambda & \ell \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} J^* & j & \lambda \\ \ell & L & \frac{1}{2}\end{Bmatrix}\int_0^\infty x^2dx\ F_{21}(NLL|\alpha\Lambda^*|x)$$

$$\otimes\ \psi^h_{n\ell}(x)\,\psi^{\tilde{\pi}}_{\nu\lambda}(x) \qquad \text{(V-B-14)}$$

Then, we define:

$$F(*hs) \equiv (-1)^{\lambda+\frac{1}{2}+L+m+J^*-M^*}[j][L][\lambda][\ell][J^*]$$

$$\otimes\begin{pmatrix} L & \lambda & \ell \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} J^* & \lambda & j \\ -M^* & \mu & -m\end{pmatrix}\begin{Bmatrix} J^* & j & \lambda \\ \ell & L & \frac{1}{2}\end{Bmatrix}$$

$$\otimes\int_0^\infty F_{21}(NLL|\alpha\Lambda^*|x)\,x^2\,\psi^h_{n\ell}(x)\psi^{\pi}_{\nu\lambda}(x)\,dx \qquad \text{(V-b-15)}$$

and the full coefficient is given by:

$$\vartheta(N^*hs) \equiv -\sqrt{\frac{2}{3}}\,G\,\delta_{m_T,\frac{1}{2}}\,\delta_{M_T,-\frac{1}{2}}\ F(*hs) \qquad \text{(V-B-16)}$$

In equation (V-b-13) the function $\tilde{\psi}_{NL}(p)$ is related to the N* wavefunction in momentum space through

$$\psi_{NL}(p) = (-i)^L\tilde{\psi}_{NL}(p) \qquad \text{(V-B-17)}$$

Once the coefficients $\vartheta(N^*hs)$ are found the calculation of the matrix element given by equation (V-B-3) is immediate if we make the replacement:

$$\psi_{\nu\lambda}(q) \longrightarrow \vartheta_{\nu\lambda}(q,q') \qquad \text{(V-B-18)}$$

The result is:

$$\langle N^* h \,|\, \hat{R}_s \,|\, N^{*\prime} h' \rangle \equiv \frac{g^2}{3M_\pi} \delta_{m_\tau,\frac{1}{2}} \delta_{m_{\tau'},\frac{1}{2}} \delta_{M_\tau, m_\tau} \delta_{M_{\tau'}, m_{\tau'}}$$

$$\otimes\ g_s(^*h, ^{*\prime}h') \qquad \text{(V-B-19)}$$

where:

$$g_s(^*h, ^{*\prime}h') \equiv \frac{(2\lambda+1)}{16\pi^5} [J^*][j][L][\ell][J^{*\prime}][j'][L'][\ell']$$

$$\otimes \begin{pmatrix} L & \lambda & \ell \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L' & \lambda & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} J^{*\prime} & \lambda & j' \\ -M^{*\prime} & \mu & -m' \end{pmatrix} \begin{pmatrix} J^* & \lambda & j \\ -M^* & \mu & -m \end{pmatrix}$$

$$\otimes \begin{Bmatrix} J^* & j & \lambda \\ \ell & L & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} J^{*\prime} & j' & \lambda \\ \ell' & L' & \frac{1}{2} \end{Bmatrix} (-1)^{L+L'+m+m'+J^*_+ J^{*\prime}_- M^*_- M^{*\prime}}$$

$$\otimes \int_0^\infty x^2\, dx\, F_{21}(NLL\,|\alpha\Lambda^*|\,x)\, \psi^h_{n\ell}(x) \int_0^\infty \vartheta_{\nu\lambda}(x,x')\, \psi^h_{n'\ell'}(x)$$

$$\otimes\ F_{21}(N'L'L'\,|\alpha\Lambda^*|\,x')\ x'^2 dx' \qquad \text{(V-B-20)}$$

The vertex function for the S_{31} channel is given by:

$$f^+(\vec{q}) = G\,\frac{\widetilde{T}}{\alpha^2+q^2} \qquad \text{(V-B-21)}$$

where

$$G^+G = \frac{g^2}{2M_\pi} \qquad \text{(V-B-22)}$$

and

$$T_- \left|\tfrac{1}{2}\, m_T\right> = \frac{1}{\sqrt{2\,(1+m_T)}} \left|\tfrac{3}{2}\,, m_T - 1\right> \qquad \text{(V-B-23)}$$

So, formally speaking is not different from the S_{11} channel, aside the isospin factors and we can write down inmediatly

$$\vartheta(\Delta^* h\, s) = -\frac{G}{\sqrt{2(1+m_T)}}\, \delta_{m_T, m_T - 1}\, F_s(* h s) \qquad \text{(V-B-24)}$$

and

$$\left<\Delta^* h \left| \hat{R}_s \right| \Delta^{*\prime} h'\right> = -\frac{g^2}{4m_\pi} \frac{1}{\sqrt{(1+m_T)(1+m_T')}}\, \delta_{m_T, m_T-1}\, \delta_{m_T', m_T'-1}$$

$$\otimes\, g_s(* h, *' h')$$