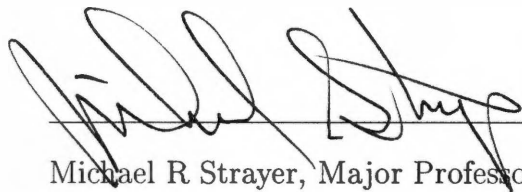
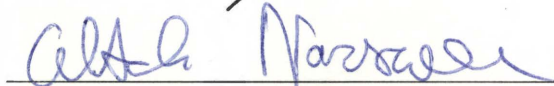


To the Graduate Council:

I am submitting herewith a thesis written by William G Newton entitled Giant Resonances of Argon Isotopes. I have examined the final paper copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Physics.

 25 July 2002
Michael R. Strayer, Major Professor

We have read this thesis
and recommend its acceptance:

 25 July 2002


Accepted for the Council:


Vice Provost
and Dean of Graduate Studies

Giant Resonances in Argon Isotopes

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Abstract

The isoscalar monopole and quadrupole and isovector dipole giant resonance modes for the nuclei of even-even Argon isotopes ^{34}Ar through ^{46}Ar are calculated. The ground state properties of the nuclei are calculated in the Hartree-Fock approximation with BCS pairing added in a deformed oscillator basis. Then the single particle states are evolved in time using the time dependent Hartree-Fock equations. A time dependant perturbation of the appropriate multi-polarity is added and the strength function of the vibrations is calculated. The form and validity of the resulting giant resonances is discussed.

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Chapter 1

Introduction

1.1 Nuclear Structure

The study of nuclear structure started with Rutherford's famous scattering experiment in 1911 [1], which demonstrated the existence of a very small nucleus at the center of atoms, less than 10^{-13}m in diameter, in which all the positive charge of an atom is concentrated. Rutherford again showed strong evidence that nuclei contained protons [2] by bombarding heavy nuclei with energetic α -particles and observing the emission of hydrogen nuclei. The observation that there exist nuclei from the same atom (characterized by the atomic number Z , the number of electrons orbiting the nucleus) but with different masses led to the postulate that there exists a second type of particle in the nucleus, with a similar mass to that of a proton, but electrically neutral. Such a particle, the neutron, was discovered in 1932 by Chadwick [3] and Curie and Joliot [4].

Since these discoveries, an enormous number of phenomena of the nucleus have been observed: the size, shape and mass of the nucleus; the rich spectra of excited states with excitation energies which may be well defined or broad resonances; a variety of radioactive phenomena; cross sections and lifetimes in nuclear reactions; and exotic phenomena such as neutron and proton skins. Each new phenomenon observed challenges us to devise and revise theoretical models of the nucleus, and in turn our models predict phenomena that must be tested by experiment. Through this interplay of theory and experiment, we build up a picture of the structure of the nucleus.

The nucleus of even a light atom is an extremely complicated system. To describe the force between just two nucleons at the most fundamental level, one must describe the interactions between the constituent quarks and gluons - an enormously complicated task in itself. Such calculations are called *ab initio* cal-

culations, and much progress has been made on them recently. However, due to the complexity of these calculations, only a few of the lightest nuclei have been examined at present.

The usual way to treat the nuclear system is to use a model that is in some part phenomenological - that is, contains parameters that can be set to make the model fit experimental data.

There are many theoretical models of the nucleus, but they can be broadly categorized in two ways: as collective and microscopic models. Collective models attempt to describe the nucleus in terms of global properties, such as its shape and total binding energy. Microscopic models describe the nucleus in terms of the degrees of freedom of its microscopic constituents - the nucleons. Some of the important models that we will need to consider in this thesis are as follows:

1) The Liquid Drop Model: A Geometric Collective Model. This model was historically the first to be proposed as an explanation for properties of the nucleus. This model takes as its starting point the assumption that the nucleus behaves like a charged drop of liquid - that it is made up of a continuous nuclear matter which, in the simplest case, is assumed to be incompressible. It is essentially classical model of the nucleus (although more advanced versions quantize its motion to reproduce nuclear properties more accurately).

The model was later refined by taking into account interactions between valence nucleons and core nucleons, which successfully explained deviations in the nuclear charge distribution from spherical symmetry, as well as vibrational and rotational effects of the nuclear surface. This model is called the Bohr-Mottelson model [5].

Although the assumptions of these models neglect some important properties of the nuclear system (such as the Pauli exclusion principle making nucleon-nucleon scattering events extremely rare as compared to scattering events in a classical liquid), they prove very useful in describing bulk properties of the nucleus and in introducing concepts such as collective motion and nuclear deformations in a simple way. The liquid drop model also gives us the semi-empirical mass formula for the binding energy of the nucleus.

2) The Interacting Boson Model (IBM): An Algebraic Collective Model. The IBM takes into account internal nuclear structure. As described in Appendix B, it is observed experimentally that nucleons tend to couple together to a total angular momentum of zero or two (corresponding to a monopole or quadrupole coupling interaction in the IBM), forming pairs. These pairs can be said to approximately act like bosons. The IBM treats collective low lying states of even-even nuclei as the collective motion of such bosons. It has simple solutions

that correspond to the shape vibration solutions of the liquid drop model. Indeed, the Bohr-Mottelson model can be shown to correspond to a classical limit of the IBM [6], [7], [8]

3) The Shell Model: A Microscopic Model The shell model takes its cue from the similar model of the atom, motivated experimentally by the observation of so called magic numbers of nuclei at proton and neutron numbers of 2,8,20,28, and so on, which exhibit shell closure effects like those observed in atomic physics.

The Shell model assumes that all the particles in the nucleus move independently of each other in an average potential. This assumption is reasonable given that the Pauli exclusion principle prevents nucleons from often approaching close to each other in normal (low energy) circumstances. Solving the Schrödinger equation for the system in the average potential then gives the energy levels and angular momentum shells within each level the nucleons occupy.

There are two ways to obtain this average potential. The simplest way is just to assume the form of the potential and calculate the structure by directly solving the Schrödinger equation. The simplest potential to reproduce basic features of nuclear structure is the Nilsson potential: a flat bottomed harmonic oscillator potential with a spin-orbit interaction.

Another way, and the one which is used in this thesis, is to derive the average potential from a phenomenological microscopic interaction between nucleons. The interaction is assumed to be a two body one for simplicity, though three body interactions and higher may be included. To solve the Schrödinger equation for this interaction, operating on all nucleons, is unfeasible, so we must introduce an approximation. The approximation we use, and indeed the most common approximation in many-body physics, is called the Hartree-Fock approximation. This, as explained in more detail in Appendix A, involves restricting the many body wave function to a specific form called a Slater determinant, and minimizing the energy expectation value with respect to this wave function to obtain the ground state energy and one body Hartree-Fock potential. This model is a relatively simple approximation of the exact many body solution and by no means describes all aspects of nuclear structure. However, it serves as a good base on which to build more elaborate, realistic theories.

1.2 Nuclear Reactions

Nuclear structure is examined by probing nuclei with particle beams of some kind in a scattering experiment. Different types of probes will interact with the nucleus through different forces (e.g. α -particles probe with the strong force, photons and electrons probe through the electro-weak interaction), and will be useful in studying different phenomena. We will consider inelastic scattering experiments,

in which beam's particles impart some energy to the nucleus and excite various states.

The most important quantity measured in such scattering experiments is the cross-section: the probability of detecting a scattered particle at an angle θ and energy E . This in turn allows the determination of the nuclear response (or strength) function, which gives the strength of the nuclear response to the probes at different energies - and thus shows up the excited states and resonances. This quantity can then be compared with a theoretically calculated strength function.

To illustrate how we compare experimental results to theory, consider the derivation of the total cross section for the absorption of dipole radiation (see [31]). Theoretically, this is derived from quantum field theory using a hamiltonian that describes the interaction between the external field and the nucleus:

$$H_{int} = - \int j_{\mu} A^{\mu} d^3r \quad (1.1)$$

The initial state $|i\rangle$ of the system is given by the product of the initial nuclear state $|\Psi_i\rangle$ and the initial EM field state, an eigenfunction of the field Hamiltonian H_{field} , given in the occupation number representation as $|\dots n_{\lambda k J m} \dots\rangle$. Here λ labels the type of photon (magnetic or electric), k the energy and J and m the angular momentum. The final state $|f\rangle$ of the system is given by a similar product, this time of the final nuclear ground state $|\Psi_f\rangle$ and the final field state $|\dots n_{\lambda k J m} - 1 \dots\rangle$.

First order perturbation theory gives the transition probability between these two states as

$$T_{fi} = \frac{2\pi}{\hbar} |\langle f | H_{int} | i \rangle|^2 g(E_f) \quad (1.2)$$

where $g(E_f)$ is the number of final states per unit of energy. The cross section of this transition is then

$$\sigma_f(E) = \frac{2\pi}{\hbar} (2\pi)^3 |\langle f | H_{int} | i \rangle|^2 \delta(E - E_f + E_0) \quad (1.3)$$

where E_0 is the initial (in our case ground state) energy of the nucleus. Using the occupation number representation of A^{μ} :

$$\mathbf{A}_r = \sum_{\mu=1}^2 \int \frac{d^3q}{(2\pi)^{3/2}} \frac{\mathbf{e}_{q\mu}}{\sqrt{\hbar\omega_q}} [e^{i\mathbf{q}\cdot\mathbf{r}} a_{q\mu} + \text{h.c.}] \quad (1.4)$$

We take the long wavelength limit (which is good in the case of dipole radiation on the nucleus) and replace all $\mathbf{r}_i$ with $\mathbf{r}_i - \mathbf{R}$. This has no effect on the dipole matrix elements if $|\Psi_i\rangle$ and $|\Psi_f\rangle$ are eigenfunctions of linear momentum since then $\langle \Psi_f | \mathbf{R} | \Psi_i \rangle = 0$. We then finally obtain the cross section

$$\sigma_f(E) = \frac{2\pi e^2}{\hbar} (E_f - E_0) |\langle \Psi_f | D | \Psi_0 \rangle|^2 \delta(E - E_f + E_0) \quad (1.5)$$

where D is the dipole operator

$$D = - \sum_{i=1}^A t_3^i (\mathbf{r}_i - \mathbf{R})_z \quad (1.6)$$

where t_3 is the z component of isospin.

In our case, the initial state $|\Psi_i\rangle$ is the nuclear ground state $|0\rangle$ and the final state $|\Psi_f\rangle$ is an excited nuclear state $|\nu\rangle$ - an eigenstate of the full many body hamiltonian.

The total cross section is given by integrating $\sigma_\nu(E)$ over all possible energies E and summing over all final states $|\nu\rangle$:

$$\sigma_{total} = \sum_{\nu} \int_0^{\infty} \sigma_\nu(E) dE = \frac{2\pi e^2}{\hbar c} \sum_{\nu} (E_\nu - e_0) |\langle \nu | D | 0 \rangle|^2 \quad (1.7)$$

This is proportional to a quantity called the Energy Weighted Sum Rule (EWSR), which in turn depends on the Strength function. This is a model independent quantity that gives very simple properties of the system. It allows one to determine, among other things, the collectivity of a given excitation (the number of nucleons participating in the motion). The ESWR of use here is the first moment of the distribution of excitation strength produced by the dipole operator:

$$\begin{aligned} S_{EWSR} &= \sum_{\nu} (E_\nu - E_0) |\langle \nu | D | 0 \rangle|^2 \\ &= \frac{1}{2} \langle 0 | [D, [H, D]] | 0 \rangle \end{aligned} \quad (1.8)$$

where the last equality is easily shown by expanding out the commutators. We can see the total cross-section is proportional to S_{EWSR} . Assuming the two body potential has no velocity dependence and no exchange mixtures, this can easily be evaluated as

$$\frac{1}{2} \langle 0 | [D, [H, D]] | 0 \rangle = \frac{NZ}{A} \frac{\hbar^2}{m} \quad (1.9)$$

and finally

$$\sigma_{total} \simeq 0.06 \frac{NZ}{A} \quad (1.10)$$

which is known as the Thomas-Reiche-Kuhn sum rule. Here N is the neutron number, Z the proton number and A the sum of the two.

Equation (1.10) gives an estimate of the cross section of an excitation in which all the nucleons participate - in which all the excited states $|\nu\rangle$ are important. Comparison of experimental cross sections with this one will tell us how collective the excitations observed are. For example, in ^{16}O about 3 percent of the dipole sum rule is exhausted by low lying 1^- states below 20MeV, whereas at just beyond 20MeV lies a broad resonant peak (the giant dipole resonance, as we shall see) that contains about 50 percent, reflecting the peak's collective character.

1.3 Giant Resonances

We mention briefly the notation used: it is conventional in nuclear physics to label states which are occupied by particles in the ground state configuration of nuclei as hole (h) states, as when the particles become excited out of this state they leave behind a hole. Similarly, states above the fermi energy are labelled particle (p) states even though they are uninhabited in the ground state, since they are the states that particles jump to when they are excited.

The variety of excited states observed in experiment is not accounted for by simple one particle-one hole ($1p-1h$) excitations in the shell model. For example, in ^{16}O the experimental energy gap between the $1p$ and $2s, 1d$ shells is about 11.5MeV [32]. In the shell model, we would expect to see a number of excited states at this energy, all with roughly the same probability for excitation. Instead, we see a concentration of excitation probability in two states: one near 6MeV (a 3^- state) and two broad resonance states at much higher energies of 22MeV and 25MeV. All other states of negative parity (corresponding to excitations up one oscillator level) are only excited with small probability.

These states are explained if we assume coherent participation by many nucleons takes place - a collective motion. In the liquid drop model, it is easy to visualize the meaning of collective motion - all nucleons move together as though part of some continuous nuclear matter. To understand what it means in a quantum mechanical sense, one must look to theories such as the Random Phase Approximation (RPA), explained in Chapter 2.

In the case of ^{16}O the collective motion leads to the two types of states observed: the low lying (6MeV) state, which in the liquid drop model is seen as multipole vibrations of the sharply defined surface, and the Giant Resonance (GR) (in this case Giant Dipole Resonance, GDR) at 22 and 25MeV. GRs have been observed throughout the periodic table, and are distinguished by their large cross sections that come close to the maximum allowed by the appropriate sum rules. This thesis will be concerned with the calculation of such giant resonances.

1.3.1 Classification of Giant Resonances

Classification by Quantum Numbers

Giant resonances can be classified by their quantum numbers S , T and J^π - spin, isospin, angular momentum and parity. The quantum numbers of a giant resonance are relative to the ground state of the nucleus. If we have a 0^+ ground state, then the quantum numbers are simply those of the resonant state. Also, experimentally, the quantum numbers of a resonant state will be determined by those of the probe used to excite it.

Spin Giant resonances in which there is no overall change in spin between the ground state and the vibration - $\Delta S = 0$ - are termed electric (E) vibrations because they are characteristic of excitation by an electric field (although they may be excited by other means). Physically, the spin up nucleons are oscillating in phase with the spin down nucleons.

When there is an overall change in spin of $\Delta S = 1$, then we have a magnetic (M) vibration, characteristic of excitation by a magnetic field. Now, the spin up nucleons are oscillating against the spin down nucleons.

Isospin We will concern ourselves with excitations in the same nucleus ($\Delta T_z = 0$). In this case we can have a change in total isospin of 0 or 1. When there is no overall change in the isospin of the resonance in relation to the ground state ($\Delta T = 0$), then the vibration is termed isoscalar. The protons and neutrons oscillate in phase with each other. When $\Delta T = 1$, we have an isovector resonance, with the protons oscillating against the neutrons. The isovector modes lie at a higher excitation energy than the isoscalar modes, because of the extra energy needed to separate the protons from the neutrons.

Angular momentum The giant resonances are labelled according to their angular momenta as monopole for $L = 0$, dipole for $L = 1$, quadrupole for $L = 2$, etc. Experimentally, these correspond to the multipolarity of the probe used to excite the resonance.

Parity This is easiest explained with reference to the shell model structure, as follows.

Classification Based on the Shell Model

As explained shortly, the simplest theories of collective vibrations and resonances treat the phenomena as the correlated vibrations of particle - hole pairs in configuration (shell model) space. Since these pairs vibrate between shells and within

shells in the nucleus, it is useful to consider a classification of GRs based on the shell model. Choosing the harmonic oscillator for simplicity, and considering electric resonances for now, we have the following picture:

For a closed shell nucleus, the Fermi surface lies between the closed shell and the next empty shell. Beyond the closed shell, shells exist of alternating parities separated by an energy of the order $\hbar\omega$. We therefore find ph pairs of a $1\hbar\omega$ excitation with negative parity, or a $2\hbar\omega$ excitation with positive parity, or a $3\hbar\omega$ excitation with negative parity, and so on. Using the principle quantum number N , these excitations are denoted $\Delta N = 1, 2, 3$, etc. For nuclei between closed shells, we also find positive parity $0\hbar\omega$ excitations ($\Delta N = 0$).

There are many complications to this picture. For example, when the spin-orbit force is added, the degenerate oscillator shells split and some of the sub-shells of the opposite parity are shifted into a lower shell. However, the basic elements of this picture hold in realistic cases.

Although the collective modes are superpositions of many ph -pairs, and observe large energy shifts due to these correlations, the gross structure is conserved to a large extent.

For high lying states, the energy between major shells varies smoothly over the periodic table as $\hbar\omega \propto A^{-1/3}$, so we expect a similarly smooth A -dependence of the resonance energy for GRs.

Classification in terms of Spatial Degrees of Freedom

A third way to classify giant resonances is by the actual shapes and classically realized motion of the nuclei - vibrations in coordinate space. This is a classification in terms of the Liquid Drop model.

Constant Density Vibrations. We first consider vibrations of the local density $\rho(\vec{r})$ of the nucleus in space. The angular dependance of such vibrations is completely determined by the angular momentum, so we are left to consider only different radial shapes. The simplest vibrations in this case are the surface vibrations of a sphere with a sharply defined surface. In the Liquid Drop model, these vibrations are found to keep the density in the nuclear interior constant.

Breathing Modes We can also imagine radial dependences of the local density in which the density in the nuclear interior changes. These excitations are called Breathing Modes, and the study of them allows for the determination of the nuclear incompressibility [9], [10], [11].

Twist Modes A different type of motion which also involves the spatial degrees of freedom comprises vibrations in the nonlocal part of the density matrix,

$\rho(\vec{r}, \vec{r}')$. An example is the twist mode in which the local density of the nucleus remains unchanged and only the intrinsic velocity distribution oscillates (becomes 'twisted').

1.3.2 Experimental Evidence for Giant Resonances

Here we review the experimentally detected giant resonances:

The Giant Dipole Resonance

This is the most extensively studied giant resonance experimentally. The first evidence for a simple vibratory motion in nuclei came in 1937 in measurements of the radioactivity produced in a variety of targets by a source of 14MeV photons. It was found that several of the targets' photo-absorption cross sections displayed resonant behavior. This was confirmed in 1975 with improved data using bremsstrahlung photon beams from electron accelerators [12].

The resonant energy, about 15MeV, corresponds to photons with wavelengths of about 100fm, which is much larger than the nuclear radius (~ 10 fm). Thus, when a beam of such photons is aimed at the nucleus, the nucleus is exposed to a uniform time dependent electric field. This causes all the protons to move in the same direction. Since the center of mass remains either at rest or in uniform motion in such an experiment, the neutrons must all move in the opposite direction. The strong force between the protons and neutrons acts as a restoring force. This is the Isovector Giant Dipole Resonance (IVGDR).

Over the last couple of decades the IVGDR has been studied extensively using mono-energetic beams of photons. The techniques employed to produce such beams are mainly two: a) positron production followed by annihilation in a secondary target, b) selection of bremsstrahlung radiation produced in the slowing down of electrons by the protons of the target nucleus, leading to particular kinetic energies of the outgoing electrons from which the photon energies are inferred (tagged photon methods). For more information on the second technique, see [15]. For an example of this method used to study the IVGDR in ^{16}O , see [16].

Another method used to excite the IVGDR is Coulomb excitation: heavy ions are fired at the nucleus, and the resonance is excited by Coulomb repulsion between the protons in the respective nuclei [17].

Recently there has been some evidence for the Isoscalar Giant Dipole Resonance (ISGDR) [18]. This resonance is actually a second order effect, since to first order the ISGDR corresponds to a spurious center of mass shift of the whole nucleus. This mode can be visualized as a compression wave analogous to a sound wave oscillating back and forth through the nucleus. It is referred to as the 'squeezing mode.' As an example of an experimental observation of the ISGDR, see [19].

Monopole and Quadrupole Vibrations

Photons are an accurate probe of nuclear structure, but they excite only the giant dipole resonance. This is because even the most energetic of photons we can aim at the nucleus have a long wavelength compared to the radius of the nucleus, and so expose all the nucleons to a roughly constant field. However, to excite monopole and quadrupole vibrations, it is not only necessary to impart a given energy to the nucleus, but to distribute it in such a way that the nucleons are set in motion in different directions. To study these GR modes we must therefore use strong or weak probes rather than EM probes. Such probes include α -particles, protons and neutrons, and electrons.

The first resonance discovered using hadron scattering was the Isoscalar Giant Quadrupole Resonance (ISGQR) [13]. This resonance is an example of a shape vibration. The nucleus is distorted from a spherical shape into an ellipsoidal shape, before moving back through a spherical shape and on to an ellipsoidal shape of a different orientation.

Good examples of the study of GRs using inelastic scattering of α -particles can be found in the experiments of Youngblood et al [20], [21], [22], [23], [24]. Inelastic scattering of protons and neutrons is also often used [25],[26],[27].

Another experimental method used is the coincidence experiment, in which the beam excites resonance and decay of nuclear modes simultaneously - see [29] for an example using electron and proton scattering.

Magnetic (spin flip) resonances of various multi-polarities have also been studied thoroughly in experiments - see [30] for an example using electron scattering.

1.3.3 Theoretical Description of GRs

There are two main ways to describe collective resonances theoretically, and they basically come down to a description of stationary resonant states in configuration space and a description of dynamic resonant states in space and time. They can be shown to be equivalent descriptions.

The first description is given in RPA theory. At the microscopic level, giant resonances are viewed as correlated particle-hole excitations: collections of single particles excited to higher levels in a coordinated way. RPA theory attempts to describe single $p - h$ excitations, and the observed collective behavior is found to emerge naturally.

Linear response theory describes GRs in the second way: the mean field system is evolved in time and a time dependent perturbation of some multipolarity is added, corresponding to some probe on the nucleus. One then can calculate the excitations of the system.

These methods, together with their advantages and disadvantages, are described in Chapter 2.

1.3.4 GRs in Deformed Nuclei

Most nuclei do not possess a purely spherical shape: they are said to be deformed. The Bohr-Mottelson model describes such deformations as excitations of the nuclear surface. The deformations can be parameterized by writing an expression for the radius with an expansion in spherical harmonics:

$$R(\theta, \phi, t) = R_0 \left(1 + \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \alpha_{\lambda\mu}^*(t) Y_{\lambda\mu}(\theta\phi) \right) \quad (1.11)$$

where $R(\theta, \phi, t)$ is the nuclear radius in the direction (θ, ϕ) at time t , and R_0 is the radius of the spherical nucleus. The $\alpha_{\lambda\mu}(t)$ are shape parameters describing the vibration of the surface and thus serve as collective coordinates. Using the model of a charged liquid drop, the energies of surface vibrations can be calculated. When quantized, these vibrations are described in terms of phonons - quanta of vibration. This treatment is given in many textbooks - see for example [31] or [32].

Microscopically, nuclear deformations arise out of the complex interaction of the single particle motion of valence nucleons and the collective multipole vibrations of the surface [34]. As an example of the effects of deformations on nuclei, see [35].

Deformation of nuclei has a significant effect on the strength functions of GRs, and it is part of the aim of this thesis to examine this. If a nucleus becomes deformed, the radius will be different along the three principle axes, and the resonance may split into three peaks, with, in the simplest model, the energy separation of the peaks determined by the axis ratios. If there is axial symmetry, two of these peaks will combine and become one higher peak.

Another interesting effect in nuclei is that of shape mixing - the co-existence of two different deformations in the same nucleus. Experiment and theory suggest [36] that transition strengths of electric giant resonances are particularly strong in such nuclei.

Computationally, calculation of the properties of deformed nuclei is much harder than that of spherical nuclei, and there have been far fewer attempts to calculate GRs in deformed nuclei. This is a large motivation for this thesis.

1.3.5 Proposal to study GRs in Argon Isotopes

Another motivation for this thesis is a proposal to study the giant resonances of argon isotopes experimentally [28]. The goal of the experiment is to determine the photo-absorption cross section as a function of energy for the giant dipole resonance - the GDR strength function - in ^{36}Ar or $^{44,46}\text{Ar}$. In this thesis we will

calculate the isoscalar monopole and quadrupole, and isovector dipole strength functions for the even-even isotopes ^{34}Ar to ^{46}Ar .

The thesis is arranged as follows: Chapter 2 deals with the theory of collective motion - RPA and linear response - the connection between the two, and discusses their physical meaning. Chapter 3 describes the program we used to simulate the resonances, and tests used to confirm the validity of the results. Then chapter 4 describes the tests used to confirm the validity of the our method and gives the results and analysis.

Chapter 2

The Theory of Collective Motion

There are two commonly used ways of calculating the properties of collective vibrations and giant resonances theoretically, as mentioned in the introduction: using a configuration space basis (Tamm-Dancoff and RPA theory) and using a space-time basis (linear response). RPA and linear response have been shown to be equivalent, and in this thesis we use the method of linear response. However, we will start by giving a quick synopsis of RPA as it is useful to see what assumptions are made and how it is equivalent to linear response. We follow similar derivations in [31] and [32].

First, we must define the ground state upon which we build these theories. It is a solution to the Hartree-Fock (HF) equations derived in Appendix A, and has the form of a Slater determinant - a product of single particle states with energies up to the Fermi energy. Particles in such states move in the HF mean field.

2.1 Tamm-Dancoff theory

In this theory we seek stationary excited states in configuration space presuming that the only important excitations of the nucleus are $1p - 1h$ excitations. Throughout we use the particle-hole notation of second quantization, in which indices i, j denote hole states, m, n denote particle states and k, l denote arbitrary states. The Hartree-Fock ground state $|HF\rangle$ is treated as the vacuum state in which we create and destroy $1p - 1h$ excitations.

Tamm-Dancoff theory assumes that the excited states are represented by $1p - 1h$ states written

$$|mi\rangle = \hat{a}_m^\dagger \hat{a}_i |HF\rangle \quad (2.1)$$

We represent the excited state wave functions as

$$|\Phi\rangle = \sum_{mi} c_{mi} |mi\rangle \quad (2.2)$$

Just as in Hartree-Fock theory, we use a variational principle to find the optimum $1p - 1h$ excited state:

$$\delta \left(\langle \Phi | \hat{H} | \Phi \rangle - E \langle \Phi | \Phi \rangle \right) = 0 \quad (2.3)$$

Where we have added the constraint that the wave functions be normalized, with the associated Lagrange multiplier E .

The general two body hamiltonian is given by

$$\hat{H} = \sum_{k_1 k_2} t_{k_1 k_2} \hat{a}_{k_1}^\dagger \hat{a}_{k_2} + \frac{1}{2} \sum_{k_1 k_2 k_3 k_4} v_{k_1 k_2 k_3 k_4} \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_4} \hat{a}_{k_3} - \langle HF | \hat{H} | HF \rangle \quad (2.4)$$

where we have subtracted the Hartree-Fock ground state energy as we are only interested in the excitation energies.

Performing the variation with respect to c_{mi}^* :

$$\sum_{minj} \delta c_{mi}^* c_{nj} \langle mi | \hat{H} | nj \rangle - E \sum_{minj} \delta c_{mi}^* c_{nj} \langle mi | nj \rangle = 0 \quad (2.5)$$

This must hold true for any δc_{mi}^* , and we obtain

$$\sum_{nj} c_{nj} (\langle HF | \hat{a}_i^\dagger \hat{a}_m \hat{H} \hat{a}_n^\dagger \hat{a}_j | HF \rangle - E \langle HF | \hat{a}_i^\dagger \hat{a}_m \hat{a}_n^\dagger \hat{a}_j | HF \rangle) = 0 \quad (2.6)$$

The matrix elements may be evaluated:

$$\langle mi | \hat{H} | mi \rangle = t_{mm} - t_{ii} + \sum_j (\langle mj | \bar{v} | mj \rangle - \langle ij | \bar{v} | ij \rangle) + \langle mi | \bar{v} | mi \rangle \quad (2.7)$$

$$= \epsilon_m - \epsilon_i + \langle mi | \bar{v} | im \rangle$$

$$\langle mi | \bar{v} | nj \rangle = \langle mj | \bar{v} | in \rangle \quad (2.8)$$

$$\langle mi | jn \rangle = \delta_{ij} \delta_{mn} \quad (2.9)$$

where the ϵ_i 's are the single particle energies and $\langle mj | \bar{v} | in \rangle = \bar{v}_{mj in} = v_{mj in} - v_{mj ni}$.

Inserting these into equation (2.6) yields the *Tamm-Dancoff* equations.

$$\sum_{jn} [(\epsilon_m - \epsilon_i) \delta_{mn} \delta_{ij} + \langle mj | \bar{v} | in \rangle] c_{nj}^\nu = E_\nu c_{mi}^\nu \quad (2.10)$$

where ν labels the eigenstates of the Hamiltonian and $E_\nu = E - E_{HF}$ are the excitation energies above the ground state. Solving these equations gives the excited states and their energies.

Now, to illustrate the appearance of collective motion in this theory, we consider a simplification called the schematic model. Here we assume the two body interaction is separable in the particle-hole direction:

$$\langle mj|\bar{v}|in\rangle \sim \lambda D_{mi} D_{nj} \quad (2.11)$$

λ is a strength parameter and the D_{mi} are one particle matrix elements of a multipole operator. The multipolarity represents the angular momentum to which the particle-hole pair is coupled.

A potential problem with this is this representation of $\langle mj|\bar{V}|in\rangle$ is not antisymmetric. It is assumed that the anti-symmetrizing exchange term is small, which turns out to be a good approximation.

With this approximation, the Tamm-Dancoff equations become

$$(E_\nu - \epsilon_m + \epsilon_i) c_{mi}^\nu = \lambda D_{mi} \sum_{nj} D_{nj} c_{nj}^\nu \quad (2.12)$$

The sum on the right hand side is just a constant, so we can solve for c_{mi}^ν :

$$c_{mi}^\nu = \frac{D_{mi}}{E_\nu - \epsilon_m + \epsilon_i} \lambda \sum_{nj} D_{nj} c_{nj}^\nu \quad (2.13)$$

multiplying by D_{mi}^* and summing over m, i yields an equation for the energies

$$\sum_{mi} \frac{|D_{mi}^2|}{E_\nu - \epsilon_m + \epsilon_i} = \frac{1}{\lambda} \quad (2.14)$$

To simplify matters further, let us assume all the $p-h$ pair energies are equal, $\epsilon_m - \epsilon_i = \epsilon$. Then all eigenenergies E_ν are the same ($E_\nu = \epsilon$) except one state which is shifted up to a energy

$$E = \epsilon + \lambda \sum_{mi} D_{mi}^2 \quad (2.15)$$

The coefficients of this state are given by

$$c_{mi} = \frac{D_{mi}}{\sqrt{\sum_{nj} D_{nj}^2}} \quad (2.16)$$

This demonstrates that the state is formed by a coherent superposition of all matrix elements of the separable two body interaction. (By coherent we mean

that all the matrix elements contribute with the same sign). It is a collective state, and if λ is positive it has an energy that is much higher than those of the single $p - h$ states, and for λ negative the energy is shifted lower.

2.2 RPA

The Tamm-Dancoff theory assumes that the ground state is the HF ground state, which is not a good approximation: a more realistic ground state would include some $p - h$ states. Then as well as $p - h$ states being created with operators such as $\hat{a}_m^\dagger \hat{a}_i$, excited states can be created which take $p - h$ excitations out of the ground state with operators of the form $\hat{a}_i^\dagger \hat{a}_m$. The resulting theory goes under the name of the *Random Phase Approximation (RPA)* which comes from an approximation made in the original derivation as seen in [14].

We define an operator for generating excitations:

$$\hat{Q}_\nu^\dagger = \sum_{mi} x_{mi}^\nu \hat{a}_m^\dagger \hat{a}_i - \sum_{mi} y_{mi}^\nu \hat{a}_i^\dagger \hat{a}_m \quad (2.17)$$

This operator should fulfil the conditions

$$\hat{Q}_\nu |RPA\rangle = 0 \quad (2.18)$$

$$\hat{Q}_\nu^\dagger |RPA\rangle = |\nu\rangle \quad (2.19)$$

where $|\nu\rangle$ is an excited state.

As in the Tamm-Dancoff method, we employ the variational principle with respect to the excited states:

$$\begin{aligned} 0 &= \delta \langle \nu | \hat{H} | \nu \rangle - E \langle \nu | \nu \rangle \\ &= \delta \langle RPA | \hat{Q}_\nu \hat{H} \hat{Q}_\nu^\dagger | RPA \rangle - E_\nu \langle RPA | \hat{Q}_\nu \hat{Q}_\nu^\dagger | RPA \rangle \end{aligned} \quad (2.20)$$

Where the hamiltonian is the same one we used in the previous section. We can vary over both the x_{mi} and y_{mi} , which leads to two equations:

$$\langle RPA | [\hat{a}_i^\dagger \hat{a}_m, [\hat{H}, \hat{Q}_\nu^\dagger]] | RPA \rangle = (E_\nu - E_0) \langle RPA | [\hat{a}_i^\dagger \hat{a}_m, \hat{Q}_\nu^\dagger] | RPA \rangle \quad (2.21)$$

$$\langle RPA | [\hat{a}_m^\dagger \hat{a}_i, [\hat{H}, \hat{Q}_\nu^\dagger]] | RPA \rangle = (E_\nu - E_0) \langle RPA | [\hat{a}_m^\dagger \hat{a}_i, \hat{Q}_\nu^\dagger] | RPA \rangle \quad (2.22)$$

The commutators on the RHS of these equations can be evaluated:

$$[\hat{a}_i^\dagger \hat{a}_m, \hat{a}_n^\dagger \hat{a}_j] = \delta_{mn} \delta_{ij} - \delta_{mn} \hat{a}_j \hat{a}_i^\dagger - \delta_{ij} \hat{a}_n^\dagger \hat{a}_m \quad (2.23)$$

Now we make an approximation in the matrix elements of this commutator: The last term should be small as the number of particles above the fermi energy is small. In the same way, the second term should be small, being produced by the small presence of holes in the $|RPA\rangle$ state. Thus our approximation is

$$\langle RPA | [\hat{a}_i^\dagger \hat{a}_m, \hat{a}_n^\dagger \hat{a}_j] | RPA \rangle \sim \delta_{ij} \delta_{mn} = \langle HF | [\hat{a}_i^\dagger \hat{a}_m, \hat{a}_n^\dagger \hat{a}_j] | HF \rangle \quad (2.24)$$

We can now see clearly that this approximation implies that the $|RPA\rangle$ state does not differ much from the $|HF\rangle$ state.

Now, defining abbreviations for the matrix elements:

$$A_{mi,nj} = \langle HF | [\hat{a}_i^\dagger \hat{a}_m, [\hat{H}, \hat{a}_n^\dagger \hat{a}_j]] | HF \rangle = (\epsilon_m - \epsilon_i) \delta_{mn} \delta_{ij} + \bar{V}_{mj in} \quad (2.25)$$

$$B_{mi,nj} = -\langle HF | [\hat{a}_i^\dagger \hat{a}_m, [\hat{H}, \hat{a}_j^\dagger \hat{a}_n]] | HF \rangle = \bar{V}_{mn ij} \quad (2.26)$$

We obtain the RPA equations

$$\sum_{nj} (A_{mi,nj} x_{nj}^\nu + B_{mi,nj} y_{nj}^\nu) = E_\nu x_{mi}^\nu \quad (2.27)$$

$$\sum_{nj} (B_{mi,nj}^* x_{nj}^\nu + A_{mi,nj}^* y_{nj}^\nu) = -E_\nu y_{mi}^\nu \quad (2.28)$$

which may be written in matrix notation as

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = E_\nu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} \quad (2.29)$$

The amplitudes x_{mi}^ν and y_{mi}^ν have a direct meaning: their absolute squares give the probability of finding the states $\hat{a}_m^\dagger \hat{a}_i | HF \rangle$ and $\hat{a}_i^\dagger \hat{a}_m | HF \rangle$ in the excited state $|\nu\rangle$. Overall normalization of the excited states requires

$$\sum_{mi} (|x_{mi}^\nu|^2 - |y_{mi}^\nu|^2) = 1 \quad (2.30)$$

There are several things to note:

- We retrieve the TDA equations by putting $y_{mi}^\nu = 0$.
- The schematic model can also be used here to simplify the equations [32].

- We approximated the commutation relations for the $p - h$ pair operators to

$$[\hat{a}_i^\dagger \hat{a}_m, \hat{a}_n^\dagger \hat{a}_j] = \delta_{ij} \delta_{mn} \quad (2.31)$$

which is a commutation relation for bosons. RPA is thus also known as the *Quasi-Boson Approximation*. As a consequence, the Pauli principle is violated for $p - h$ excitations.

- Following on from the Quasi-boson approximation we define can define boson operators

$$\begin{aligned} \hat{B}_{mi}^\dagger &= \hat{a}_m^\dagger \hat{a}_i \\ \hat{B}_{mi} &= \hat{a}_i^\dagger \hat{a}_m \end{aligned} \quad (2.32)$$

and

$$\hat{Q}_\nu^\dagger = \sum_{mi} (x_{mi}^\nu \hat{B}_{mi}^\dagger - y_{mi}^\nu \hat{B}_{mi}) \quad (2.33)$$

Using this we can express the Hamiltonian, keeping up to quadratic terms in $\hat{B}$, as

$$\hat{H}_B = E_{RPA} + \sum_\nu E_\nu \hat{Q}_\nu^\dagger \hat{Q}_\nu \quad (2.34)$$

where E_{RPA} is the energy of the ground state $|RPA\rangle$. This is an harmonic oscillator Hamiltonian, and because of this the RPA is also called the harmonic approximation.

2.3 Linear Response

An alternative way to obtain the response of the nuclear system is to evolve the wave functions in time under an external perturbation H_{ex} . From this, we obtain the strength, or response function which gives the frequencies at which the system resonates and the strengths of those resonances.

2.3.1 Linear Response from the Schrödinger Equation

As a demonstration of the method used, we look at linear response using the exact Schrödinger equation [33], which gives the exact many body wave function as follows:

$$\hat{H}|\Psi_s(0)\rangle = E|\Psi_s(0)\rangle \quad (2.35)$$

where the subscript s refers to the Schrödinger picture.

We now add a time dependent perturbing function to the static Hamiltonian:

$$\hat{H}_{tot} = \hat{H} + \hat{H}_{ex}(t) \quad (2.36)$$

where we define the external piece to be

$$\begin{aligned} \hat{H}_{ex}(t) &= \hat{F} f(t) \\ &= \left[\int d^3x \hat{\rho}(x, t) F(x) \right] f(t) \end{aligned} \quad (2.37)$$

where $F(x)$ corresponds to some particular collective mode. x labels coordinates - spatial, spin and isospin. Physically, the operator $\hat{F}$ simulates the action on the nucleus of some probe of the appropriate multipolarity, distributed over the whole nucleus. This is then multiplied by a function $f(t)$ which determines how the perturbation varies over time. The exact forms of $F(x)$ and $f(t)$ will be chosen later.

$\hat{\rho}(x, t)$ is the number density operator:

$$\langle \Psi_s(t) | \hat{\rho}(x, t) | \Psi_s(t) \rangle = \rho(x, t) \quad (2.38)$$

We can write the number density $\rho(x, t)$ in terms of the single particle wave functions $\phi_i(x, t)$

$$\rho(x, t) = \sum_i |\phi_i(x, t)|^2 \quad (2.39)$$

and from the initial normalization of these states,

$$\int d^3x \rho(x, 0) = A \quad (2.40)$$

where A is the total number of nucleons.

At the time $t = 0$ the external piece of the Hamiltonian is turned on. We now seek a solution to the time dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} |\bar{\Psi}_s(t)\rangle = [\hat{H} + \hat{H}_{ex}(t)] |\bar{\Psi}_s(t)\rangle \quad (2.41)$$

of the form

$$|\bar{\Psi}_s(t)\rangle = e^{-i\hat{H}t/\hbar} \hat{A}(t) |\Psi_s(0)\rangle \quad (2.42)$$

where $\hat{A}(t) = 1$ for $t \leq 0$. Inserting equation (2.42) into equation (2.41) yields

$$\begin{aligned} i\hbar e^{-i\hat{H}t/\hbar} \frac{\partial}{\partial t} \hat{A}(t) |\Psi_s(0)\rangle &= \hat{H}_{ex}(t) e^{-i\hat{H}t/\hbar} \hat{A}(t) |\Psi_s(0)\rangle \\ \Rightarrow i\hbar \frac{\partial}{\partial t} \hat{A}(t) |\Psi_s(0)\rangle &= e^{i\hat{H}t/\hbar} \hat{H}_{ex}(t) e^{-i\hat{H}t/\hbar} \hat{A}(t) |\Psi_s(0)\rangle \\ &= \hat{H}_{ex}^H(t) \hat{A}(t) |\Psi_s(0)\rangle \end{aligned} \quad (2.43)$$

where 'H' refers to the fact that we have written the perturbing Hamiltonian in the Heisenberg picture, evolved in time using the operator $e^{i\hat{H}t/\hbar}$. This must hold for all $|\Psi_s(0)\rangle$, so

$$i\hbar \frac{\partial}{\partial t} \hat{A}(t) = \hat{H}_{ex}^H(t) \hat{A}(t) \quad (2.44)$$

Finally, from this we can write the operator $\hat{A}(t)$ as

$$\hat{A}(t) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}_{ex}^H(t') + \dots \quad (2.45)$$

Inserting this into equation (2.42):

$$|\bar{\Psi}_s(t)\rangle = e^{-i\hat{H}t/\hbar} \left[1 - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}_{ex}^H(t') + \dots \right] |\Psi_s(0)\rangle \quad (2.46)$$

This equation determines how the exact many body wave functions evolve in time. The operators $\hat{A}(t)$ and $e^{-i\hat{H}t/\hbar}$ are unitary, and thus preserve the norm of the wave functions (and thus equation (2.40) is valid for all t). Note also that these operators are equivalent to the operators $U_0(t)$ and $U_I(t)$ of the interaction picture: the operator $\hat{A}(t)$ evolves the wave functions in time and corresponds to $U_I(t)$, and $e^{-i\hat{H}t/\hbar} = U_0(t)$ evolves operators in time and corresponds to $U_I(t)$.

From equation (2.46), we can immediately define linear response approximation: *If we make the perturbation small enough, we only need to keep the first*

order - linear - term in $\hat{A}(t)$. This leads us to linear response.

The expectation value of any operator $\hat{O}(t)$ in this approximation is equal to

$$\begin{aligned}
\langle \bar{\Psi}_s(t) | \hat{O}(t) | \bar{\Psi}_s(t) \rangle &= \langle \Psi_s(0) | \left[1 - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}_{ex}^H(t') + \dots \right] e^{i\hat{H}t/\hbar} \hat{O}(0) e^{-i\hat{H}t/\hbar} \\
&\quad \times \left[1 - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}_{ex}^H(t') + \dots \right] | \Psi_s(0) \rangle + \dots \\
&= \langle \Psi_s(0) | e^{i\hat{H}t/\hbar} \hat{O}(0) e^{-i\hat{H}t/\hbar} | \Psi_s(0) \rangle \\
&\quad + \langle \Psi_s(0) | \left[\frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}_{ex}^H(t') \right] e^{i\hat{H}t/\hbar} \hat{O}(0) e^{-i\hat{H}t/\hbar} | \Psi_s(0) \rangle \\
&\quad - \langle \Psi_s(0) | e^{i\hat{H}t/\hbar} \hat{O}(0) e^{-i\hat{H}t/\hbar} \left[\frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}_{ex}^H(t') \right] | \Psi_s(0) \rangle \quad (2.47)
\end{aligned}$$

keeping only linear terms in $\hat{H}_{ex}$. For the first term we choose the Schrödinger picture: the operator $\hat{O}(0) \rightarrow \hat{O}_S(t)$ does not evolve in time. The operators can only be evolved with the operator $e^{i\hat{H}_{tot}t/\hbar}$, so here the two exponentials cancel. For the next terms we choose the interaction picture: $\hat{O}(0)$ is evolved in time by $\hat{U}_0(t)$ such that $U_0^\dagger(t)\hat{O}(0)\hat{U}_0(t) = \hat{O}_I(t)$. Then we get

$$\begin{aligned}
\langle \bar{\Psi}_s(t) | \hat{O}(t) | \bar{\Psi}_s(t) \rangle &= \langle \Psi_s(0) | \hat{O}(t) | \Psi_s(0) \rangle \\
&\quad + \langle \bar{\Psi}_s(t) | \frac{i}{\hbar} \int_{t_0}^t dt' [\hat{H}_{ex}(t'), \hat{O}_I(t)] | \bar{\Psi}_s(t) \rangle + \dots \quad (2.48)
\end{aligned}$$

We now choose the operator $\hat{O}(t)$ to be the density operator $\hat{\rho}(x, t)$. We can calculate the fluctuation in the density, which is given by

$$\begin{aligned}
\delta < \hat{\rho}(x, t) > &= \langle \bar{\Psi}_s(t) | \hat{\rho}_S(x, t) | \bar{\Psi}_s(t) \rangle - \langle \Psi_s(0) | \hat{\rho}_S(x, t) | \Psi_s(0) \rangle \\
&= \langle \Psi_s(0) | \frac{i}{\hbar} \int_0^t dt' \int d^3x' F(x') f(t') [\hat{\rho}_I(x', t'), \hat{\rho}_I(x, t)] | \Psi_s(0) \rangle \quad (2.49)
\end{aligned}$$

using equation (2.37).

$$\delta < \hat{\rho}(x, t) > = \frac{1}{\hbar} \int_{-\infty}^{\infty} dt' \int d^3x' D^R(x, t; x', t') F(x') f(t') \quad (2.50)$$

where

$$iD^R(x, t; x', t') = \Theta(t - t') \frac{\langle \Psi_0 | [\hat{\rho}_I(x, t), \hat{\rho}_I(x', t')] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad (2.51)$$

is the retarded density correlation function.

Now, the expectation value of the perturbation operator $\hat{F}$ is given by

$$\begin{aligned} \langle \hat{F} \rangle(t) &= \int d^3x \langle F(x) \hat{\rho}(x, t) \rangle \\ &= \int d^3x F(x) \langle \hat{\rho}(x, t) \rangle \end{aligned} \quad (2.52)$$

and the fluctuation in this operator is given by

$$\delta \langle \hat{F} \rangle(t) = \int d^3x F(x) \delta \langle \hat{\rho}(x, t) \rangle \quad (2.53)$$

This equation gives the response of the system to the perturbation. We define the linear response strength function $\bar{S}(\omega)$ as the Fourier transform of this:

$$f(\omega) \bar{S}(\omega) = \int d^3x F(x) \delta \langle n(x, \omega) \rangle \quad (2.54)$$

where we have factored out the function $f(\omega)$, the Fourier transform of $f(t)$.

The strength function gives the frequencies at which the system responds to the perturbation, and the strengths of those responses.

2.3.2 Linear Response in the Hartree-Fock Approximation

The Time Dependant Hartree-Fock approximation restricts the form of the wave functions to Slater determinants $|\Phi\rangle$ at every instant in time. The system will still evolve by the time dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Phi(t)\rangle = \hat{H}_{tot} |\Phi(t)\rangle \quad (2.55)$$

but now the wave function is not an eigenfunction of the total many body Hamiltonian. We see in Appendix A that in the TDHF approximation the individual single particle wave functions evolve in time by

$$i\hbar \frac{\partial}{\partial t} |\phi_i(t)\rangle = \hat{h}^{tot} |\phi_i(t)\rangle \quad (2.56)$$

Where $\hat{h}^{tot}$ is the total single particle hamiltonian, which in our case consists of the Hartree-Fock hamiltonian plus a single particle perturbing hamiltonian:

$$\hat{h}^{tot} = \hat{h}^{HF} + \hat{h}^{ex} \quad (2.57)$$

$\hat{h}^{ex}$ is calculated from H_{ex} , given in equation (2.37), according to the variational principle that was used in Appendix A to calculate h^{HF} : the matrix element of H_{ex} with respect to the Slater determinant is

$$\begin{aligned} \hat{H}_{ex}(t) &= \langle \Phi | \hat{F} f(t) | \Phi \rangle \\ &= \left[\int d^3x \langle \Phi | \hat{\rho}(x, t) | \Phi \rangle F(x) \right] f(t) \\ &= \left[\int d^3x \int d\mathbf{r} \sum_{i=1}^A \phi_i^*(\mathbf{r}) \hat{n}_i(x, t) \phi_i(\mathbf{r}) F(x) \right] f(t) \\ &= \sum_{i=1}^A \int dx F(x) f(t) \phi_i^*(x) \phi_i(x) \end{aligned} \quad (2.58)$$

using the form for the density operator $\hat{\rho}(x) = \sum_{i=1}^A \hat{\rho}_i = \sum_{i=1}^A \delta(x - r_i)$. Then from the variational principle,

$$\begin{aligned} \hat{h}^{ex} \phi_i(x) &= \frac{\delta}{\delta \phi_j^*(x')} \sum_{i=1}^A \int dx F(x) f(t) \phi_i^*(x) \phi_i(x) \\ &= F(x) f(t) \phi_i(x) \end{aligned} \quad (2.59)$$

The road to calculating the strength function used in the last section is much more complicated here, since instead of one many body wave function being evolved in time we have many single particle wave functions, all being evolved in time with different, non-orthogonal frequencies

$$\phi_i(t) = e^{i \int_0^t dt \hat{h}^{tot}} \phi_i(0) \quad (2.60)$$

related to the many body wave function by

$$\Phi(t) = \sum_P (-1)^P \phi_{P_1}(r_1) \dots \phi_{P_A}(r_A) \quad (2.61)$$

Different treatments of this problem can be found in the literature. For example, the problem becomes much simpler if, instead of evolving the spatial wave functions in time, one evolves the configuration space density matrix in time [31], [32]. In this case the linear response approximation amounts to keeping only linear terms in the particle-hole operators.

However, in our case we do not need to calculate explicit expressions for equations (2.53) and (2.54) since we may write equation (2.53) as

$$\delta < \hat{F} > (t) = < \hat{F} > (t) - < \hat{F} > (0) \quad (2.62)$$

where $< \hat{F} > (0)$ may be taken as the average of $\hat{F}$ over time. Then to obtain the strength function we just Fourier transform this quantity. Writing

$$\begin{aligned} < \hat{F} > (t) &= \int d^3x F(x) < \hat{\rho}(x, t) > \\ &= \int d^3x F(x) \rho(x, t) \end{aligned} \quad (2.63)$$

we get an expression for the strength function

$$\begin{aligned} f(\omega) \bar{S}(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} [< \hat{F} > (t) - < \hat{F} > (0)] \\ &= \int_{-\infty}^{\infty} dt e^{i\omega t} \int d^3x [\rho(x, t) - \rho(x, 0)] F(x) \end{aligned} \quad (2.64)$$

where we have factored out the Fourier transform of the function $f(t)$ which is given by

$$\begin{aligned} f(\omega) &= \xi \int_{-\infty}^{\infty} dt e^{i\omega t} e^{-(t-t_0)^2/T^2} \\ &= \xi T \sqrt{\pi} e^{\omega^2 T^2/4} e^{i\omega t_0} \end{aligned} \quad (2.65)$$

As a final note, if one lets the perturbation go to zero in the linear response equations, one gets back equations which have the same form as the RPA equations. That these equations can be interpreted in the same way as the RPA equations is not obvious, as is discussed in the following section.

2.4 Discussion of the Theories

Experimentally and theoretically, anharmonic deviations from the predictions of RPA and linear response have been observed [42], [43]. They arise from the approximations used in both theories, which we shall now discuss.

Firstly, the matrix RPA equation involves non-Hermitian matrices, so the eigenfrequencies may be complex. This often happens in deformed nuclei.

Next, the violation of the Pauli principle in the quasi-boson approximation should be cause for concern. However, for very collective states we have many x_{mi}^ν 's of the same order of magnitude. Then each $p - h$ component has only a small probability of being excited, and Pauli principle violation is relatively unimportant. Also, the quasi-boson approximation is equivalent to the approximation that the $|RPA\rangle$ state is close to the $|HF\rangle$ state, which is good if the y_{mi}^ν 's are small compared to the x_{mi}^ν 's.

The quasi boson approximation is not good for $2p - 2h$ states and higher. The operator $\sum_{mi} x_{mi} \hat{a}_m^\dagger \hat{a}_i$ does not exactly represent a boson and application of it twice does not produce two uncoupled bosons since the Pauli principle excludes the occupation of any one level by 2 or more particles or holes.

Finally, the Hamiltonian we have been using includes no interactions of higher order than two body. The higher order terms will couple together different collective modes and couple collective modes to non-collective modes.

Another important aspect arises from symmetry violation of the mean field used in both RPA and linear response. The exact many body Hamiltonian is invariant under a number of symmetry operations - that is, it commutes with the corresponding symmetry operators: $[\hat{H}, \hat{S}] = 0$, where $\hat{S}$ could represent linear momentum $\mathbf{P}$, angular momentum $\mathbf{J}^2, J_z$ or particle number N .

However, the Hartree-Fock Hamiltonian describes a localized mean field, and thus immediately breaks translational invariance. A deformed mean field violates rotational invariance, while the BCS pairing formalism we use (see Appendix B) violates particle number invariance. Thus RPA and linear response start out with wave functions that violate a number of symmetries.

The effect of these symmetry violations on giant resonances is to create spurious modes of resonance: modes that do not correspond to physical vibrations of the nucleus. For example, violation of translational invariance leads to a spurious center of mass motion in the dipole resonances that corresponds to the nucleus as a whole moving back and forth.

To restore the broken symmetries one can use projection methods, which are fully described in [31]. Here, projection operators are defined which project the wave function onto eigenstates of the corresponding symmetry operators. There are two ways to do this.

The simpler method, Variation Before Projection (VBP), involves solving the variational equations for the wave functions and then projecting these solutions onto eigenstates of a good symmetry. This method has the advantage that the variational equations only have to be solved once, but it violates the variational principle. For example, if we project onto states of good angular momentum, we create a rotational spectrum, but because we solved the variational equations before doing this, we do not allow for variations of the mean field within the

rotational bands.

The second way is Variation After Projection (VAP), in which we project the wave functions before solving the variational equations. Although this is better than VBP, it means we must solve the variational equations for each projection operator, and is much more complicated.

In this thesis we will not be worried with carrying out these projections, but must be aware of the consequences of the symmetry violations for our results. The spurious center of mass motion will be our main concern, and corrections to it are discussed in [45].

The theory of linear response produces equations of exactly the same form as those of RPA. But can we interpret them in the same way? Both theories begin with an ansatz for the ground state wave function and use a variational principle to determine the equations of motion in their respective bases. Then they linearize the equation of motions - keeping only terms linear in the $p - h$ creation operators - and end up with an harmonic approximation. The assumption of small amplitude oscillations in linear response is equivalent to the assumption that the RPA ground state does not differ much from the HF ground state. The linear approximation physically corresponds to ignoring modifications to the single particle density by ground state correlations.

Thus we may conclude that the theories of linear response and RPA are entirely equivalent. However, one must still be careful in the interpretation of the two theories. For example, it is unclear what the wave function means physically in linear response. It does not describe a single stationary state of the system, since its constituent single particle wave functions evolve in time at different frequencies. The frequencies are non-orthogonal, so the state cannot be a superposition of stationary states.

Such problems are often attributed to the TDHF theory being semi classical: we follow the wave function Φ and its time derivative $\dot{\Phi}$ as they evolve in a multi dimensional energy surface - the TDHF manifold - which includes all possible configurations representable by Slater determinants. We can identify canonical co-ordinates for this system [41] and the time evolution looks like a classical trajectory.

Also, the TDHF equations are non-linear, which means the principle of superposition no longer works: a linear combination of two Slater determinants is usually not another Slater determinant. As a result of this, the probability distributions do not exhibit quantum mechanical dispersion, so the Slater determinants explore only a tiny part of the full Hilbert space.

Finally, although the time dependant variational principle guarantees the time

derivative will be approximated in the optimum way possible, as it moves on the multi dimensional energy surface there is no guarantee it will not stray far from the true solution after a certain amount of time.

A treatment of these problems through an alternative interpretation of the TDHF theory can be found in [37]. Here, TDHF theory is developed in terms of the classical harmonic oscillator, but expressed entirely in the language of quantum mechanics, with no semi-classical approximation.

In conclusion, we note that the theories of RPA and linear response give a reasonable description of nuclear spectra, especially for collective $p-h$ states, but contain significant approximations of which we must be aware when interpreting the results.

Chapter 3

Computational Implementation

The program we used to carry out the giant resonance calculations was an axially symmetric Hartree-Fock code with the Skyrme force, called *skyax*. With the axial symmetry, the code uses a two dimensional uniform grid with cylindrical co-ordinates r and z on which to calculate the wave functions. The grid size and spacing could be altered. Derivatives are represented by matrices using either a Fourier definition or a finite difference method.

skyax has two parts: the first solves the static Hartree-Fock equations to obtain the single particle wave functions ϕ_i^{HF} and the ground state properties of the nucleus. The second part evolves the single particle wave functions in time with a perturbation added to the Hamiltonian, and outputs the expectation value of the perturbation operator versus time.

3.1 The Static Hartree-Fock Iteration

Appendix A derives the Hartree-Fock equations, which give the one body mean field in which the single particle wave functions move. These equations must be solved self consistently since the wave functions enter into the expression for the mean field (A.49) - (A.53) which in turn determines the wave functions. This suggests an iterative procedure to solve for the wave functions. The iteration in *skyax* consists of three parts:

3.1.1 The Damped Gradient Iteration

The Damped Gradient Step [40] consists of iterating each single particle wave function according to the formula

$$\phi_i^{k+1} = O[\phi_i^k - x_0 D(e_0)(h_{HF}^k - \epsilon_i^k)\phi_i^k] \quad (3.1)$$

where the damping operator in two dimensions is given by

$$\begin{aligned}
D &= \left[1 + \frac{t}{e_0} \right]^{-1} \\
&= \left[1 + \frac{t_r}{e_0} \right]^{-1} \left[1 + \frac{t_z}{e_0} \right]^{-1}
\end{aligned} \tag{3.2}$$

i labels the wave function, t is the kinetic energy operator, x_0 and e_0 are adjustable parameters, and O denotes a Gram-Schmidt orthonormalization of the states.

We need to start with a guess of the wave functions. In *skyax* the initial wave functions are chosen to be deformed cylindrical harmonic oscillator wave functions. The deformation is parameterized by the quadrupole deformation parameter β which is related to the parameters $\alpha_{2\mu}$ given by the Bohr-Mottelson model (equation (1.11)).

3.1.2 The Newton-Raphson Method

The damped gradient iteration achieves convergence in the total energy E_{HF} to machine accuracy ($\log(E_{HF}^{k+1} - E_{HF}^k) = -15$). However, to obtain good results in the time iteration, one must also achieve good convergences of the single particle wave functions. The single particle convergences are given by

$$v_i = |\langle \phi_i^{HF} | h_{HF} | \phi_i^{HF} \rangle^2 - \langle \phi_i^{HF} | h_{HF}^2 | \phi_i^{HF} \rangle| \tag{3.3}$$

The dynamic iteration does not achieve a good convergence in v_i , so we must supplement it with another iteration scheme. The scheme we use is the Newton-Raphson (NR) iteration. In the code there is a switch between this iteration and the Damped gradient step: after a certain number of iterations N_{NR} , or after E_{HF} has been solved to a certain accuracy, we switch to the NR iteration.

The NR iteration solves the wave functions exactly for a given hamiltonian. On its own, this method is not self-consistent, since the hamiltonian itself depends on the wave functions. One must therefore perform several sets of NR iterations, recalculating the hamiltonian from the wave functions at the end of each set. In this way, the hamiltonian (and thus total energy) converges as well as the wave functions.

The method proceeds as follows: We wish to solve the Schrödinger equation $(h - \epsilon)x = 0$ exactly in the wave function x for a given hamiltonian h . We start with a guess wave function x_0 , and write

$$\begin{aligned}
x &= x_0 + \delta x \\
\epsilon &= \epsilon_0 + \delta \epsilon
\end{aligned} \tag{3.4}$$

where $\epsilon_0 = \langle x_0 | h | x_0 \rangle$. Inserting this in the Schrödinger equation, and keeping first order terms, we get

$$(h - \epsilon_0)x_0 + (h - \epsilon_0)\delta x - \delta\epsilon x_0 = 0 \quad (3.5)$$

Now if x_0 has N components then δx has N components and h is an $N \times N$ matrix. $\delta\epsilon$ is also unknown. Thus in equation (3.5) we have N equations but $N+1$ unknowns.

To solve these equations, we keep one component of x constant. In our case, we set $x^\alpha = x_0^\alpha$ where α labels some component. This reduces the number of unknowns to N , and allows us to solve equation (3.5) which we write as the matrix equation:

$$\begin{pmatrix} h^{11} & h^{12} & \dots & h^{1\alpha-1} & -x_0^1 & h^{1\alpha+1} & \dots & h^{1N} \\ h^{21} & & & & & & & \vdots \\ \vdots & & & & & & & \vdots \\ \vdots & & & & & & & \vdots \\ \vdots & & & & & & & \vdots \\ h^{N1} & \dots & \dots & \dots & -x_0^N & \dots & \dots & h_{NN} \end{pmatrix} \begin{pmatrix} \delta x^1 \\ \vdots \\ \delta x^{\alpha-1} \\ \delta\epsilon \\ \delta x^{\alpha+1} \\ \vdots \\ \delta x^N \end{pmatrix} = \begin{pmatrix} [-(h - \epsilon_0)x_0]^1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ [-(h - \epsilon_0)x_0]^N \end{pmatrix}$$

Writing $(h - \epsilon_0)x_0 = -b$, this is written

$$\mathbf{A} \cdot \mathbf{y} = \mathbf{b} \quad (3.6)$$

The component α is chosen to be the one at which the value of the wave function ϕ^α is at its largest. If the wave function is well behaved, this will correspond to a region in where the wave function varies slowly. The only potential problem is if the maximum occurs at a boundary. In order to avoid this, *skya* calculates α as the component at which the value of $\vec{r}^2 \phi^\alpha = (r^2 + z^2) \phi^\alpha$ is a maximum.

3.1.3 BCS iteration

In order to more accurately represent the properties of the nucleus in our code, we include a pairing formalism, added on top of the Hartree-Fock iteration. Appendix B gives the motivation for including a pairing force and derives the equations of the BCS model of pairing.

In many cases the BCS force used causes the pairing energy to depend on the wave functions. Then the HF and BCS equations become one set that must be solved self-consistently. However, this is not the case for the delta function force we use, and the HFBCS equations separate [44]. Then the HF equations

determine the single particle wave functions and the BCS equations determine the occupation probabilities.

We can conveniently express the BCS equations in the co-ordinate space used in the program using an energy functional formalism [45], [46]. Our pairing force in co-ordinate space takes the form of the zero range delta function force:

$$V_q(\mathbf{r}, \mathbf{r}') = V_{0,q} \delta(\mathbf{r} - \mathbf{r}') \quad (3.7)$$

where q represents protons $q = p$ or neutrons $q = n$. Then the pairing-energy functional is written

$$\mathcal{E}_q = \frac{V_{0,q}}{4} \int d\mathbf{r} \chi_q^2(\mathbf{r}) \quad (3.8)$$

where the pairing density $\chi(\mathbf{r})$ is given by

$$\chi_q(\mathbf{r}) = -2 \sum_{k>0} u_k v_k |\phi_k(\mathbf{r})|^2 \quad (3.9)$$

where u_k and v_k are the occupation probabilities.

In principle we must now derive a set of coupled equations for the mean field (Hartree-Fock) plus pairing system by varying the Hartree-Fock energy functional and the pairing-energy functional together with the constraints on the particle number and orthonormalization of the single particle wave functions with respect to the single particle wave functions and the occupation probabilities. This is known as the Hartree-Fock-Bogoliubov method.

Here we make an approximation: the pairing term in the mean field equation obtained in the above method is omitted. The 2 sets of equations become decoupled: one is the Hartree-Fock equation and the other is the pairing equation (B.22). This approximation is fair for nuclei away from the neutron drip line [47].

If we define a local pairing potential

$$\Delta_q(\mathbf{r}) = \frac{\delta \mathcal{E}_q}{\delta \chi_q(\mathbf{r})} = \frac{1}{2} V_{0,q} \chi_q(\mathbf{r}) \quad (3.10)$$

we can express the pairing gap (B.23) as the single particle expectation value of the pairing potential:

$$\Delta_k = \int d\mathbf{r} \phi_k^\dagger(\mathbf{r}) \Delta_q(\mathbf{r}) \phi_k(\mathbf{r}) \quad (3.11)$$

One final matter to consider is as follows: the zero range pairing force we use tends to over-estimate the coupling of the bound states to the continuum

(positive energy) states. Thus our BCS scheme as it is will scatter particles to the continuum. Finite range forces can suppress this effect but are cumbersome to deal with.

To cure this, we add smooth energy dependent cutoff weights that simulate the effect of a finite range force [45], [46]:

$$f_k = \frac{1}{1 + \exp(\epsilon_k^0 - \lambda_q - \Delta E_q)/\mu_q)} \quad (3.12)$$

These are inserted into the expression for the local pair density:

$$\chi_q(\mathbf{r}) = -2 \sum_{k>0} f_k u_k v_k |\phi_k(\mathbf{r})|^2 \quad (3.13)$$

The effect of the weights is to confine the active pairing space to the vicinity of the Fermi surface. To this end the cutoff parameter Δ_q is chosen such that the sum of the cutoff weights is equal to the number of single particle states up to the Fermi level plus one additional shell above [46]

$$\sum_k f_k = N_q + 1.65 N_q^{2/3} \quad (3.14)$$

and the spread $\mu_q = \Delta E_q/10$.

The procedure to solve the BCS equation is now as follows: Equations (3.12) and (3.14) are solved iteratively. Then starting with the input strengths of the pairing force $V_{0,p}$ and $V_{0,n}$, we calculate the pairing potential and gaps according to equations (3.10) and (3.11).

Next we solve iteratively for the Fermi energy λ_q using the particle number condition

$$2 \sum_{k>0} v_k^2 = N \quad (3.15)$$

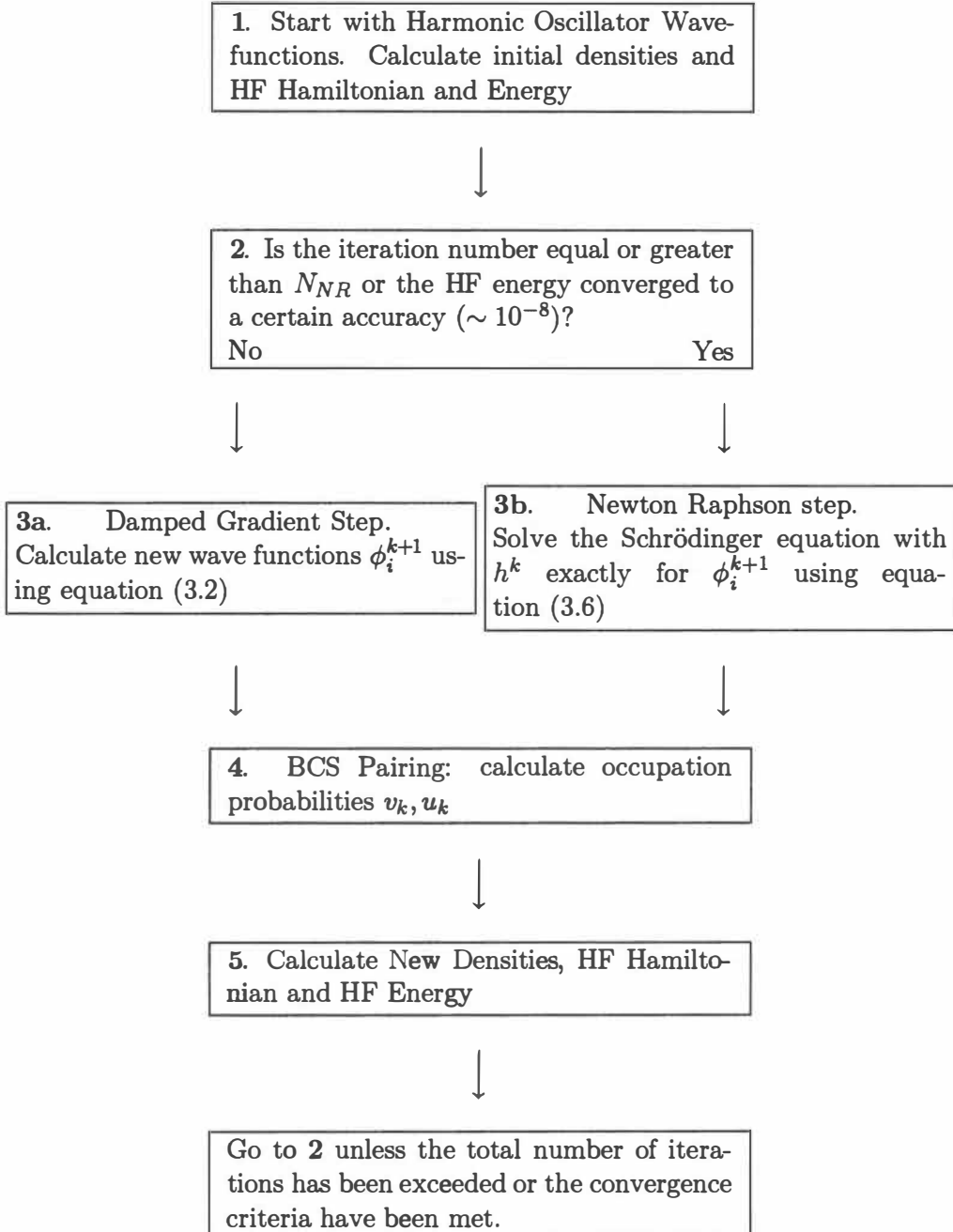
together with the expression for v_k which, from equations (B.24) and (B.25) is given by

$$v_k^2 = \frac{1}{2} \left(1 - \frac{\epsilon_k^0 - \lambda}{\sqrt{(\epsilon_k^0 - \lambda)^2 + \Delta^2}} \right) \quad (3.16)$$

And finally the occupation probabilities v_k and u_k are calculated from (B.25). This procedure is performed after every damped gradient or Newton-Raphson step.

Figure (3.1) shows a basic flow chart for the program.

Figure 3.1: Flowchart for the Static Iteration



3.2 The Dynamic Iteration

First we note that to be rigorous we ought to include a time development of the BCS states. However, to simplify the code we take as an ansatz the BCS states to remain constant in time: they are effectively frozen at time $t = 0$ and only the single particle HF wave functions are evolved in time.

We start with the wave functions ϕ_n^{HF} and hamiltonian h^{HF} from the static iteration. We add the perturbation term

$$h^{tot} = h^{HF} + h^{ex} \quad (3.17)$$

where h^{ex} is given by equation (2.59). Then we need to evolve the wave functions in time according to equations (A.38) and (A.40):

$$i\hbar\dot{\phi}_n(\mathbf{r}, t) = h^{tot}\phi_n(\mathbf{r}, t) \quad (3.18)$$

which can be written

$$\phi_n(\mathbf{r}, t) = e^{ih^{tot}t}\phi_n^{HF}(\mathbf{r}) \quad (3.19)$$

In order to implement this in our program, we must discretize time $t \rightarrow t_i, \Delta t = t_i - t_{i-1}$. Then the method we use is as follows: we evolve the wave functions one time step by

$$\phi'_n(\mathbf{r}, t + \Delta t) = e^{ih^{tot}\Delta t}\phi_n(\mathbf{r}, t) \quad (3.20)$$

Then we calculate the densities at *half time step* as

$$\rho(t_{1/2}) = \frac{\rho(t) + \rho'(t + \Delta t)}{2} \quad (3.21)$$

where the $\rho'(t + \Delta t)$ is calculated from the $\phi'_i(\mathbf{r}, t + \Delta t)$. Then the hamiltonian at half time step is

$$h_{1/2}^{tot} = h^{tot}(\rho_{1/2}) \quad (3.22)$$

Then we take as our actual wave function at time $t + \Delta t$ as

$$\phi_n(\mathbf{r}, t + \Delta t) = e^{ih_{1/2}^{tot}\Delta t}\phi_n(\mathbf{r}, t) \quad (3.23)$$

To calculate the exponential operator, we simply expand it out to enough terms to preserve the normalization of the wave functions:

$$e^{ih_{1/2}^{tot}\Delta t} = \sum_k \frac{1}{k!} [i\Delta t h_{1/2}^{tot}]^k \quad (3.24)$$

We now need to choose the perturbation functions $F(x)$ and $f(t)$. We set them to be:

$$F(x) = F_{\lambda L}(\mathbf{r}) = e^{-(r^2+z^2)/a^2} \cdot I(\lambda) \cdot Q_L(\mathbf{r}) \quad (3.25)$$

$$f(t) = \xi e^{-(t-t_0)^2/T^2} \quad (3.26)$$

where

$$I(\lambda) = \begin{cases} 1, & \lambda = 0 \\ (-1)^\tau, & \lambda = 1 \end{cases} \quad (3.27)$$

$Q_L(\mathbf{r})$ is a multipole moment, angular momentum L . τ labels the isospin of the state being acted on: 1 for protons and 0 for neutrons. The factor I gives the phase difference between the vibrations protons and neutrons: when $\lambda = 0$ the nucleons oscillate in phase (the isoscalar mode) and when $\lambda = 1$ the protons oscillate out of phase with the neutrons (the isovector phase). T, a, ξ and t_0 are parameters. ξ gives the strength of the perturbation and should be small enough that the linear approximation is good, yet large enough that any noise effects are drowned out. $f(t)$ is given a gaussian form, and causes the perturbation to peak in time at $t = t_0$.

The Q_L for $L=0, 1$ and 2 are given in our cylindrical coordinates as

$$\begin{aligned} Q_0(r, z) &= r^2 + z^2 \\ Q_1(r, z) &= z \\ Q_2(r, z) &= 2z^2 - r^2 \end{aligned} \quad (3.28)$$

The function $e^{-(r^2+z^2)/a^2}$ is a screening function designed to remove effects of the box: as r or z approach the edge of the box, this factor becomes very small.

With this perturbation we evolve the system in time as previously outlined. We output to screen the expectation value of the perturbation operator $\langle \hat{F} \rangle (t)$ every 20 time steps and from this data set we can calculate the average value $\langle \hat{F} \rangle (0)$:

$$\langle \hat{F} \rangle (0) = \frac{1}{n} \sum_{i=1}^n \langle \hat{F} \rangle (t_i) \quad (3.29)$$

where n is the number of times we output $\langle \hat{F} \rangle (t)$. Then we Fourier transform to obtain our strength function

$$S_{\lambda L}(\omega) = f(\omega)\bar{S}_{\lambda L}(\omega) = \sum_{\tau} \int_{-\infty}^{\infty} dt e^{i\omega t} \int d\mathbf{r} [\rho_{\tau}(\mathbf{r}, t) - \rho_{\tau}(\mathbf{r}, 0)] F_{\lambda L}(\mathbf{r}) \quad (3.30)$$

In our calculations we use the function $S_{\lambda L}(\omega)$ rather than $\bar{S}_{\lambda L}(\omega)$.

Chapter 4

Results

We begin with a few notes on the running of the code and the way we analyze the results.

The grid size we use in all our runs is 15 by 15, spacing 0.9fm, resulting in a box size of 13.5fm.

The parameters for the perturbation given in table (4.1) were used in all runs of the code, both in the testing and the collection of the main data. Here Δt is the time step used in the dynamic iteration.

The program outputs the average of the multipole moment used $\langle F_{\lambda L}(t) \rangle$ every 1fm/c (20 time steps). This forms the raw data. After the run, a simple program calculates the mean of this data set $\langle F_{\lambda L}(0) \rangle$ and subtracts it to form $\langle F_{\lambda L}(t) \rangle - \langle F_{\lambda L}(0) \rangle$.

This data is then imported into a data analysis program and graphs of this response of the multipole moments to the perturbations are formed. Then a Fast Fourier Transform (FFT) is taken to give the Strength function $S(E)$ as a function of energy.

We must be careful when interpreting the strength functions produced. There are two important factors to bear in mind:

In experiment we do not obtain resolution of resonance peaks less than widths

Table 4.1: Parameters for the dynamic iteration

Parameter	Value
a (fm)	1
T (fm/c)	3
t ₀ (fm/c)	7.5
Δt (fm/c)	0.05

of about 5MeV. Thus the fine structure seen in the raw FFTs is not useful. This is why we choose to treat the data with some kind of smoothing. At the same time, we do not wish to wash out all detail. We have therefore used the simplest kind of smoothing, based on an averaging procedure. 3 point averaging takes every point on the plot and replaces it with the average itself and the point either side. 5 point averaging takes 2 points either side. Generally this is sufficient to smooth out all the fine detail.

A second aspect to consider about these results is that our code conducts linear response that corresponds to discrete RPA rather than continuum RPA. This is because we are conducting the calculation in a finite box. The giant resonances we study are excitations of particles into continuum states. The density of these states depends on the size of the box, so the resonances will depend on the box's size too. The boundary conditions are that the wave functions go to zero at the edges of the box - so we get standing waves, with discrete energies. The density of states goes as $b^{3/2}$, where b is the box size. As the box size increases, there are more available continuum states with energies that are closer together. Eventually we tend towards continuum RPA, in which the box size is effectively infinite and the energies are continuous. This would most closely represent experimental data.

How does this affect our results for giant resonances? A study [52] shows that the discreteness of the energies for a finite box translates into a discrete spectrum for the giant resonances. For small box sizes, only a single mode may be present. More and more modes appear as the box size is increased, with the modes finally converging to a spectrum that resembles the experimental spectrum of a giant resonance, with a broad width. However, the average energy remains more or less constant - fully converged - regardless of box size.

So when studying the following results, we must be aware that since we are using a relatively small box, the structures we observe may not be fully converged in their widths. However, we can assume that their average energies are good.

4.1 Tests of the Program

In order to validate our method we conducted some tests of the program. We took as our test nucleus the doubly magic, spherical ^{16}O whose resonances have been widely studied. First we used the Skyrme force called SkM* [49], whose parameters are given in table (4.2) together with the pairing force parameters $V_{0,p}, V_{0,n}$. In the static part of the code, the single particle variances converged to values of $\sim 10^{-7}$. The dynamic iteration was carried out to a time of $t = 8,000\text{fm}/c$ (160,000 time steps) for the isoscalar monopole and quadrupole forces with a perturbation strength of $\xi = 1$.

Figures (4.1) and (4.2) give the raw data obtained $\langle F_{\lambda L}(t) \rangle - \langle F_{\lambda L}(0) \rangle$

Table 4.2: SkM* parameters

Parameter	Value	Parameter	Value
t_0 (MeV fm ³)	-2645.0	x_0	0.09
t_1 (MeV fm ⁵)	410.0	x_1	0.0
t_2 (MeV fm ⁵)	-135.0	x_2	0.0
t_3 (MeV fm ⁶)	15595.0	x_3	0.0
$V_{0,p}$ (MeV fm ³)	279.082	x_4	32.5
$V_{0,n}$ (MeV fm ³)	258.962		

for the isoscalar monopole and quadrupole moments, and Figures (4.3) and (4.4) show the strength functions, both raw and smoothed with 5 point averaging.

The average energies of the two resonances are 25.1 MeV for the monopole and 20.4 MeV for the quadrupole. The Widths are 5.1 MeV and 1.6 MeV respectively. Also in evidence is low lying activity, demonstrating that not only giant resonances show up in our calculations. These low energy peaks are probably caused by single $p - h$ excitations. One would expect these to be weak in ¹⁶O since it is a doubly magic nucleus. Any $p - h$ excitations would have to be from the filled proton and neutron $1p_{1/2}$ shells up to the vacant $1d_{5/2}$ shell.

An alternative calculation of the strength function of the isoscalar quadrupole resonance is given in [50]. Our strength function is in excellent agreement with it. For the high energy giant resonance peak, the alternative calculation obtains an average energy of 20.7MeV compared to our 20.4MeV. The low energy activity is also generated in this paper.

Our isoscalar monopole strength function may be compared to one calculated in [51]. This paper obtains an average energy of 24.5MeV, as compared to our 25.1MeV.

Table 4.3: SkO* Parameters

Parameter	Value	Parameter	Value
t_0 (MeV fm ³)	-2103.653	x_0	-0.210701
t_1 (MeV fm ⁵)	303.352	x_1	-2.810752
t_2 (MeV fm ⁵)	791.674	x_2	-1.461595
t_3 (MeV fm ⁶)	13553.252	x_3	-0.429881
$V_{0,p}$ (MeV fm ³)	253.771	x_4	88.289
$V_{0,n}$ (MeV fm ³)	269.942		

Figure 4.1: Response of the O^{16} isoscalar monopole moment $\langle F_{00}(t) \rangle$ to the perturbation with time for the SkM* force

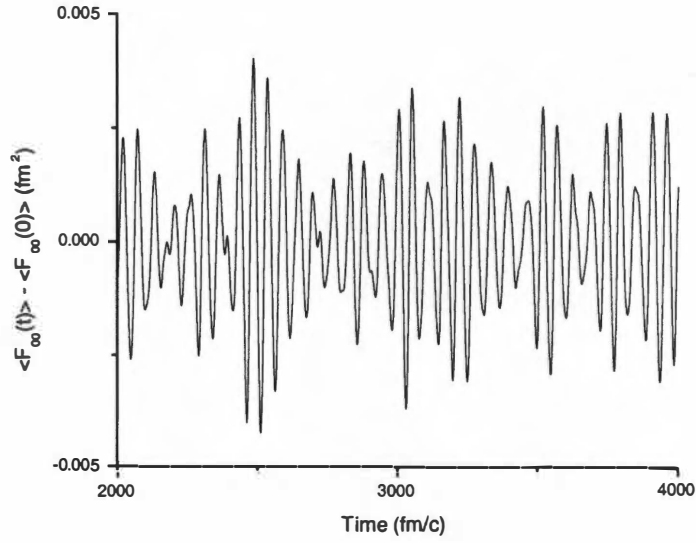


Figure 4.2: Response of the O^{16} isoscalar quadrupole moment $\langle F_{20}(t) \rangle$ to the perturbation with time for the SkM* force

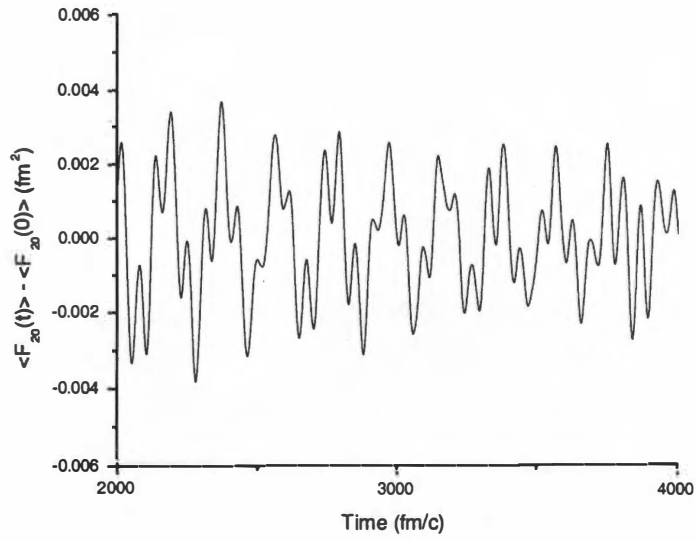


Figure 4.3: Top: raw FFT for the isoscalar monopole response of O^{16} with the SkM* force. Bottom: smoothed version.

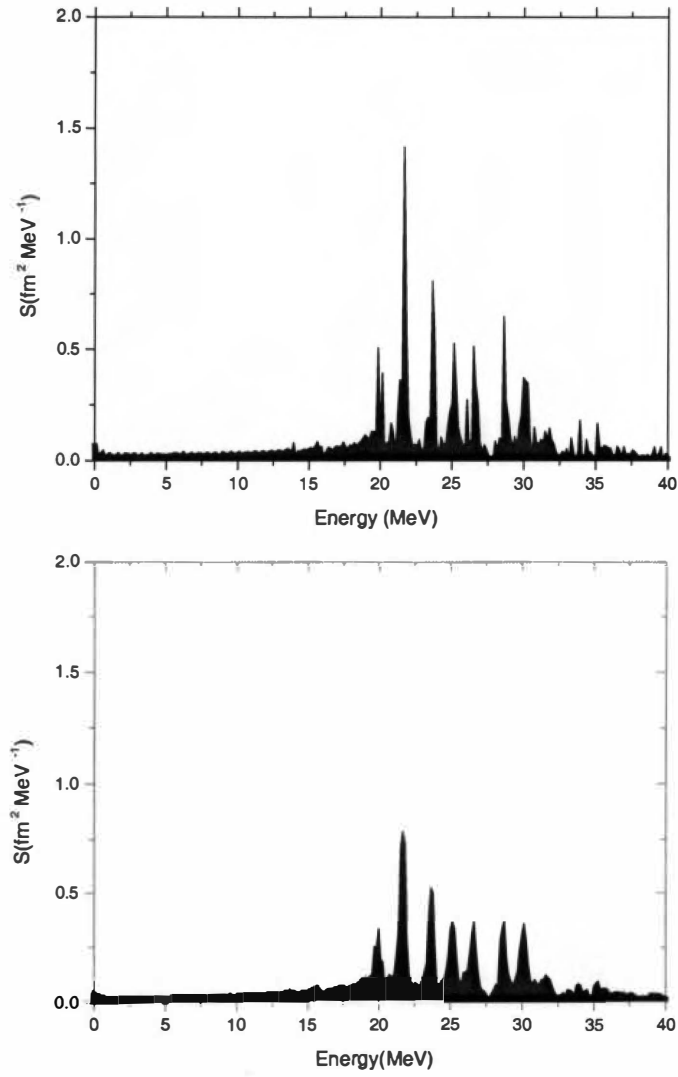


Figure 4.4: Top: raw FFT of the isoscalar quadrupole Response of O^{16} with the SkM* force. Bottom: smoothed version.

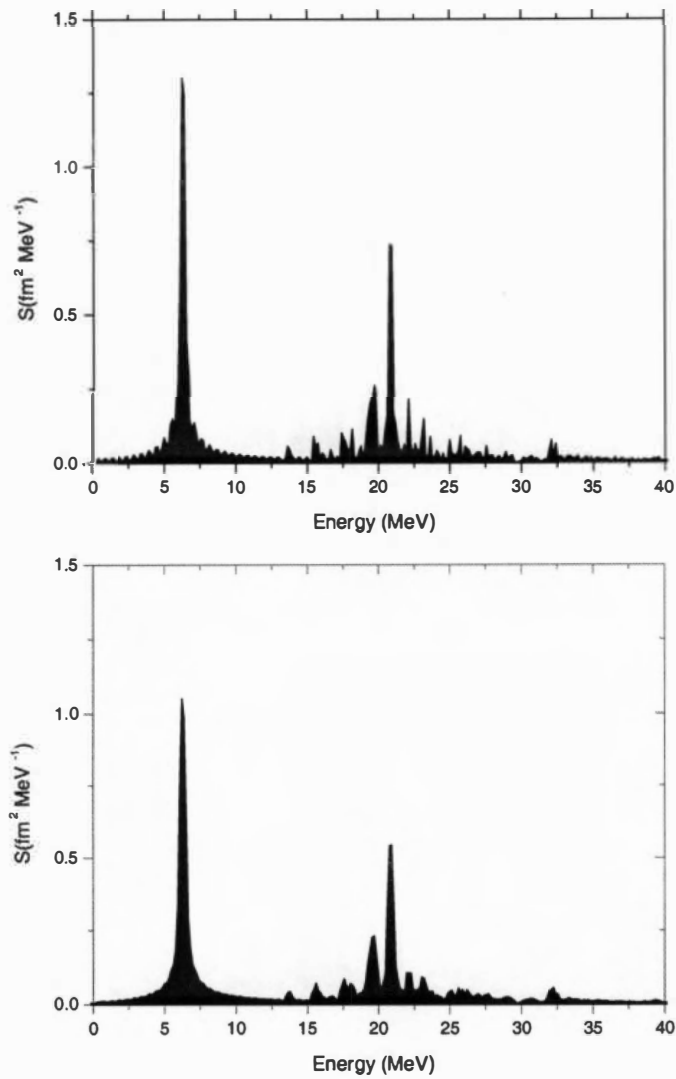
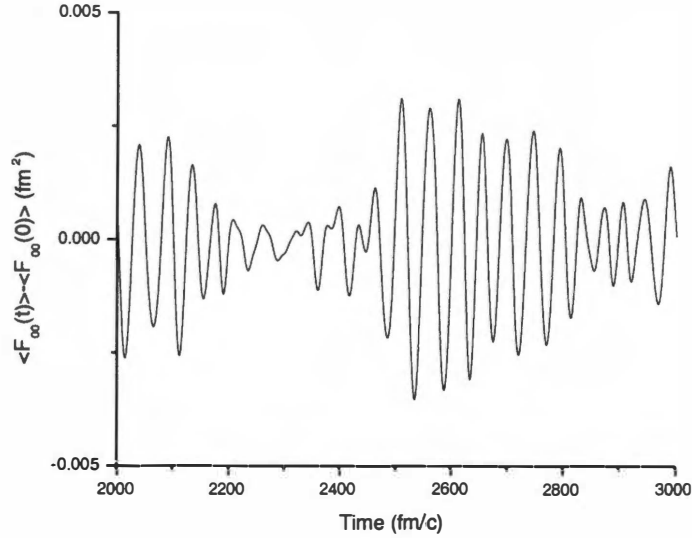


Figure 4.5: Response of the O^{16} isoscalar monopole moment $\langle F(t)_{00} \rangle$ to the perturbation with time for the SkO* force



Our results are in good agreement with these, so we are confident the method we used and its implementation are valid.

We will use a Skyrme force called SkO* [48] in our calculations of argon resonances. Its parameters are given in table (4.3). To test any dependance of our results on the force used, we calculate the above oxygen strength functions using the SkO* force.

Figures (4.5) and (4.6) show the raw data, and figures (4.7) and (4.8) show the strength functions, raw and smoothed with 5 point averaging. The mean energy of the isoscalar monopole resonance is now 25.1 MeV and the width 6.0 MeV. The isoscalar quadrupole results show a giant resonance at an average energy of 20.1 MeV and width of 2.6 MeV, and a low lying peak at the energy of around 6 MeV and the width 2 MeV

These results show no strong force dependance for the resonances calculated: although the amplitudes of the strength functions are slightly smaller for the SkO* calculations, the structure of the strength functions are very similar. However, that is not to say there is no force dependance. In fact many calculations show strong dependance of the giant resonances on the force used [53].

Finally, we checked that the perturbation strength ($\xi = 1$) left us in the linear response regime. If we are, the amplitude of the resonances should scale linearly with ξ . When we ran the isoscalar monopole with strength $\xi = 0.5$, we found the amplitude of the resonance was approximately 0.6 of what it was before.

Figure 4.6: Response of the O^{16} isoscalar quadrupole moment $\langle F(t)_{20} \rangle$ to the perturbation with time for the SkO* force

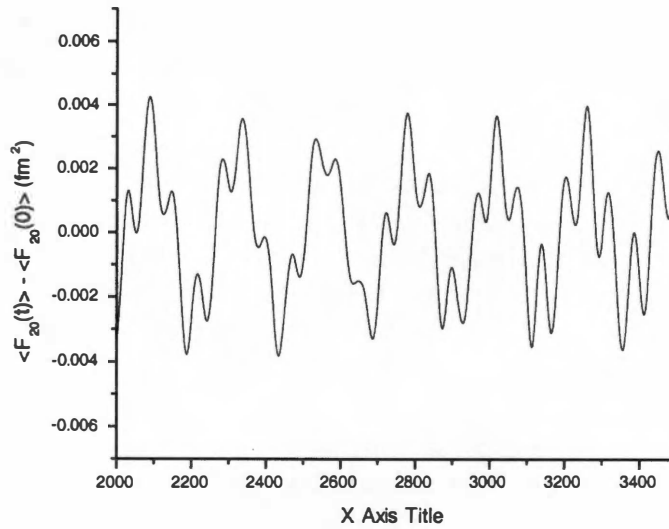


Figure 4.7: Top: raw FFT for the isoscalar monopole response of O^{16} with the SkO* force. Bottom: smoothed version.

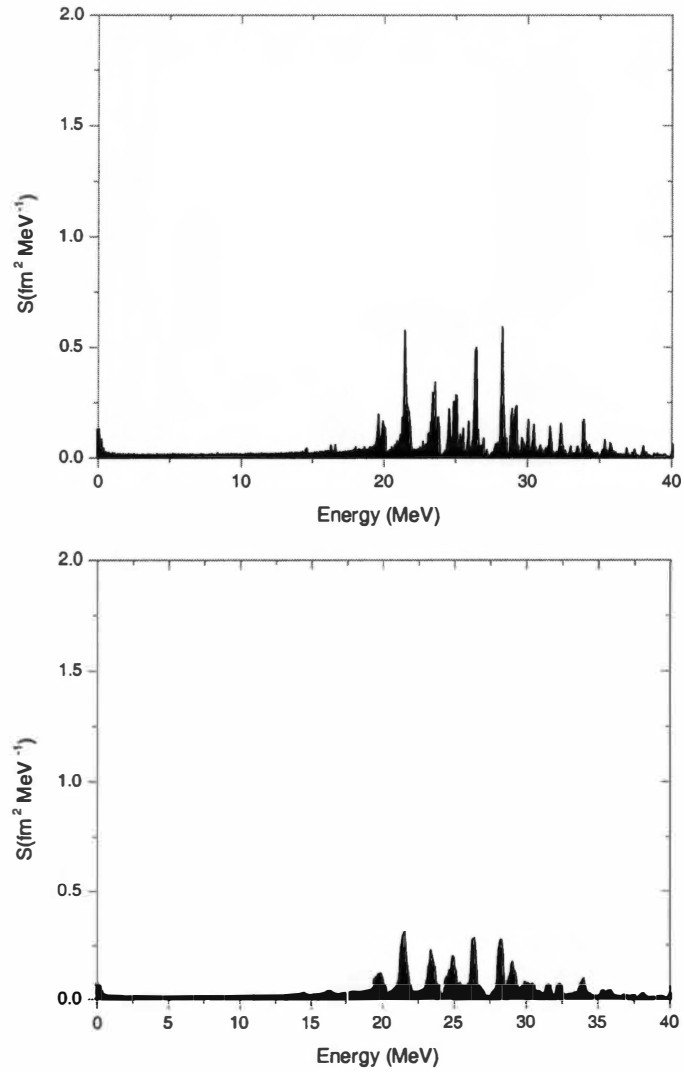


Figure 4.8: Top: raw FFT for the isoscalar quadrupole response of O^{16} with the SkO* force. Bottom: smoothed version.

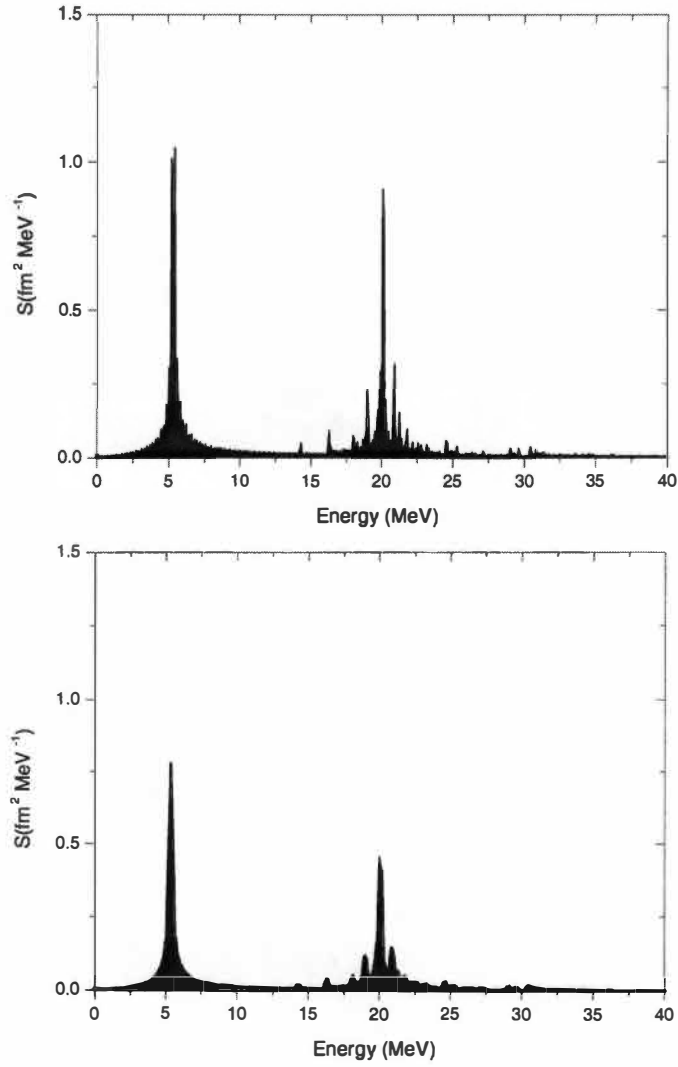


Table 4.4: Binding energies and quadrupole deformations β for the argon isotopes

Isotope	Total Energy (MeV)	Binding Energy Per Nucleon (MeV)	β
34	-288.0	-8.47	-0.003
36	-341.1	-8.73	-0.001
38	-338.0	-8.89	0.000
40	-354.7	-8.87	0.005
42	-369.4	-8.80	-0.089
44	-382.9	-8.70	-0.163
46	-395.0	-8.59	-0.200

4.2 Results for Argon Isotopes

Our results for argon consist of the response of the isotopes 34, 36, 38, 40, 42, 44, and 46 to isoscalar monopole and quadrupole and isovector dipole perturbations.

To obtain our results for argon we used the SkO* given before. Again we used a perturbation strength $\xi = 1$.

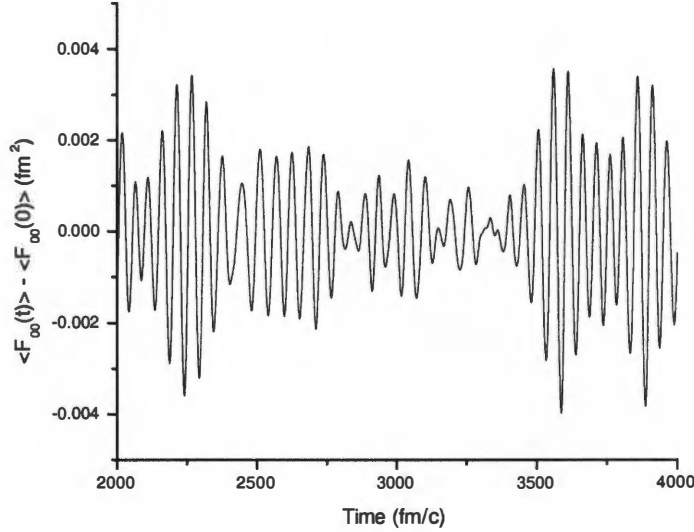
The static part of the code converged to machine accuracy in the total energy and to single particle variances of $\sim 10^{-4}$ and better.

The number of time steps for which we could run the dynamic code depended on the type of response being calculated. For the monopole responses we ran the code to 8,000-10,000fm/c (160,000 - 200,000 time steps) before iteration became unstable. For the dipole and quadrupole responses, we reached 6,000-8,000fm/c (120,000-160,000 time steps). As an example of the raw data obtained, Figures (4.9), (4.10) and (4.11) show the response of ^{38}Ar to the isoscalar monopole and quadrupole and isovector dipole perturbations.

The Strength functions obtained were smoothed using 3 point and 5 point averaging. These results are displayed in Figures (4.12) through (4.20).

In order to analyze the strength functions we obtained, we must first examine the properties of the isotopes as calculated in the static part of the code.

Figure 4.9: Response of the Ar^{38} isoscalar monopole moment $\langle F(t)_{00} \rangle$ to the perturbation with time.



4.2.1 Ground State Properties of the Argon Isotopes

The ground state properties may be compared to similar calculations in [54]

Table (4.4) lists some relevant parameters for the argon isotopes: the total ground state energy, the binding energy per nucleon, and the quadrupole deformation parameter β .

From this table we note that the most negative binding energy per nucleon is for ^{38}Ar , which makes it the most tightly bound of the isotopes. It is also closest to spherical in shape, having a quadrupole deformation of 0.0. The first four isotopes are all close to spherical, with only the last three exhibiting significant deformation.

To account for these observations and gain real insight into the structure of these nuclei, it is useful to look at the single particle energies of both proton and neutron states as calculated by the program. These are the energies of hole states, and are therefore of great interest when examining the giant resonances, which we have assumed to be made up of just $1p - 1h$ excitations. The p states are mostly continuum states - positive energy states. The code gives single particle states, which may be occupied by two nucleons coupled to zero angular momentum (see Appendix B), together with their occupation probabilities. For example an occupation probability of 1.0 means a pair of nucleons occupy the state, while an

Figure 4.10: Response of the Ar^{38} isovector dipole moment $\langle F(t)_{11} \rangle$ to the perturbation with time.

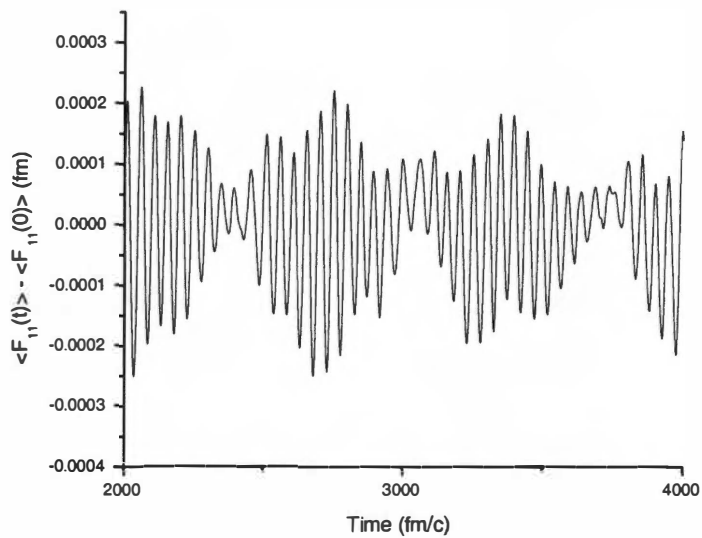


Figure 4.11: Response of the Ar^{38} isoscalar quadrupole moment $\langle F(t)_{20} \rangle$ to the perturbation with time.

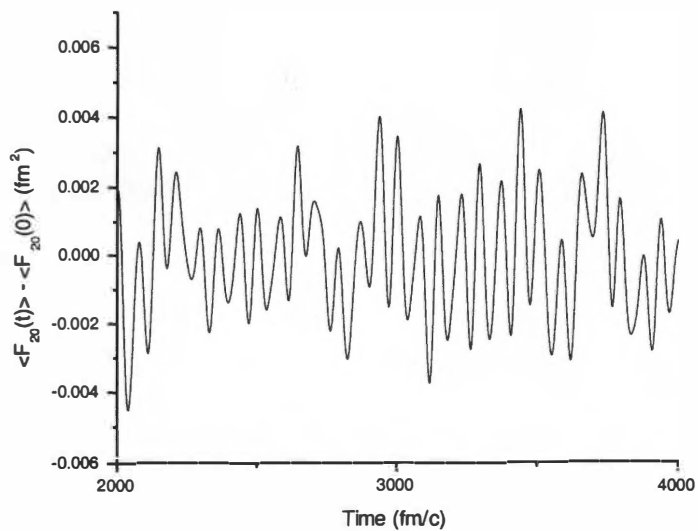


Figure 4.12: Raw FFT for the isoscalar monopole response of the argon isotopes

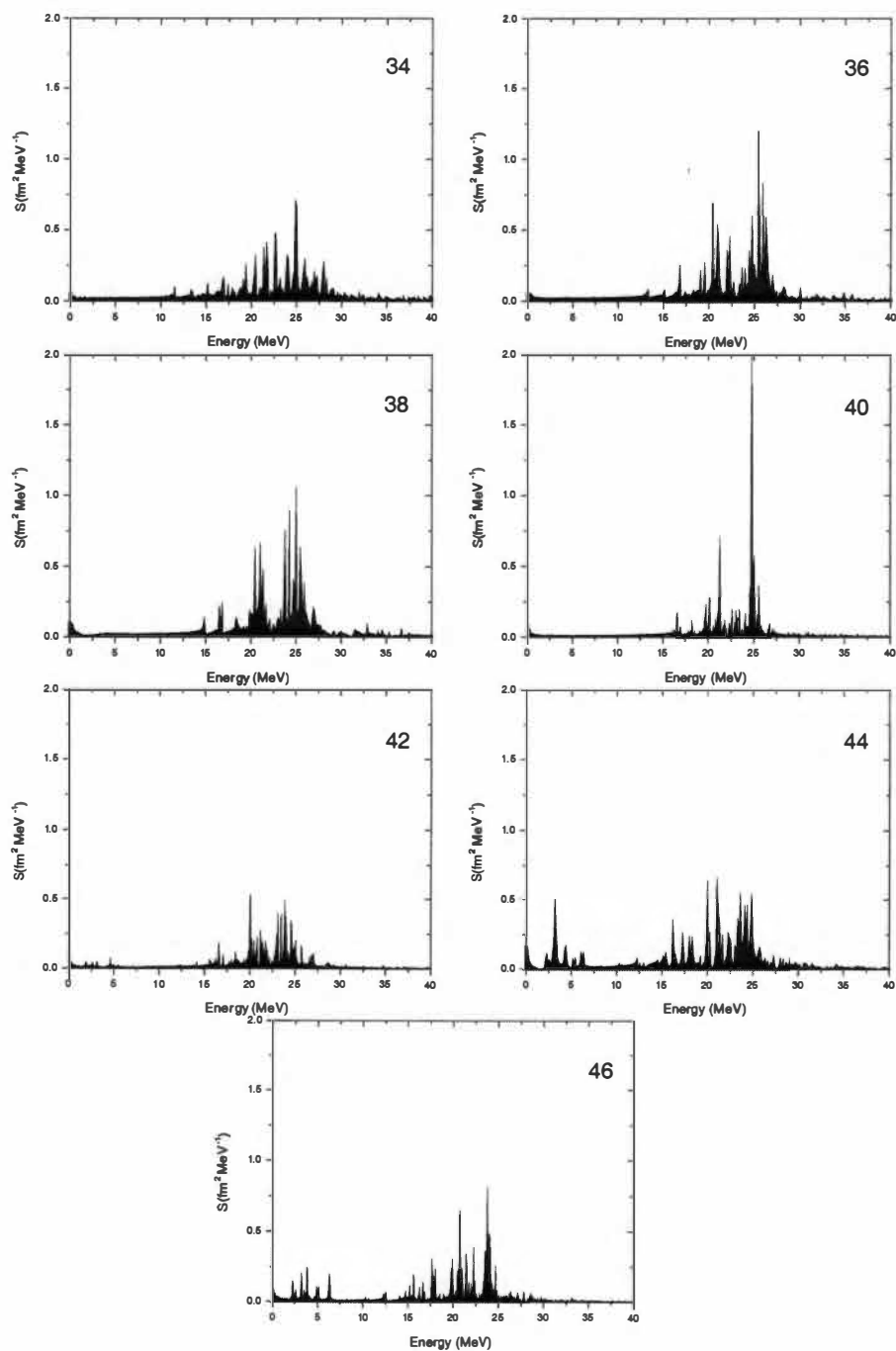


Figure 4.13: Smoothed FFT using 3 point averaging for the isoscalar monopole response of the argon isotopes

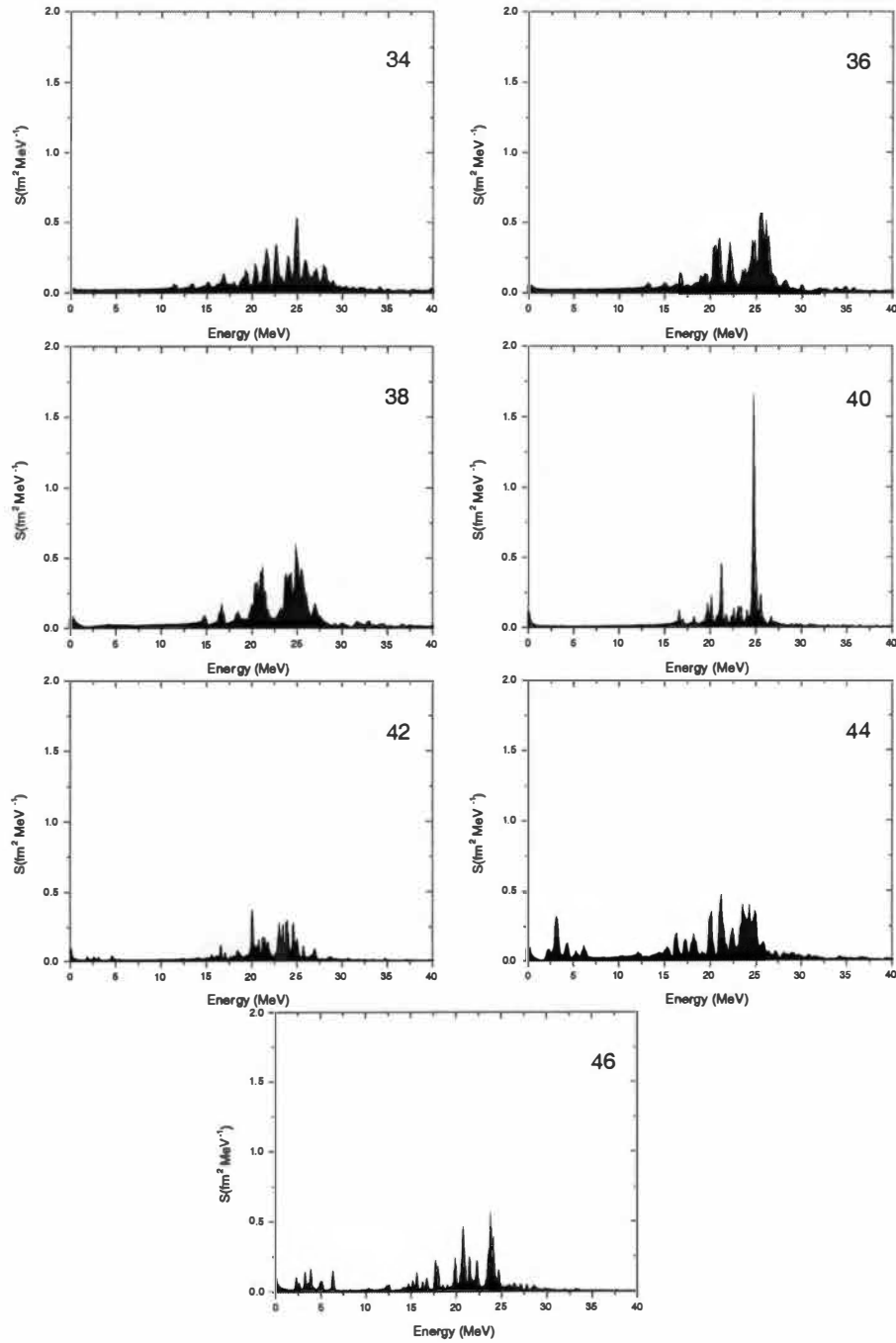


Figure 4.14: Smoothed FFT using 5 point averaging for the isoscalar Monopole response of the argon isotopes

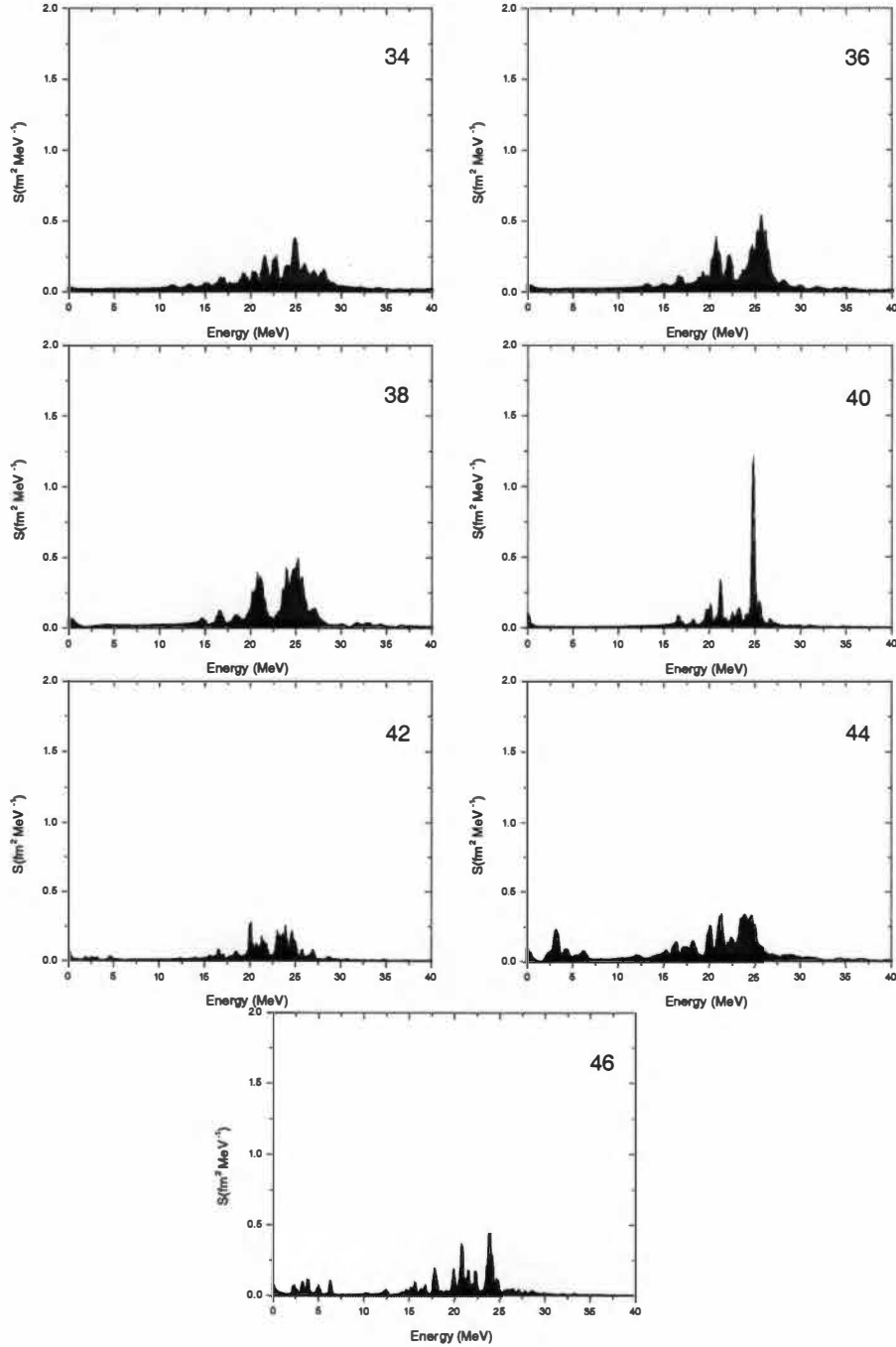


Figure 4.15: Raw FFT for the isovector dipole response of the argon isotopes

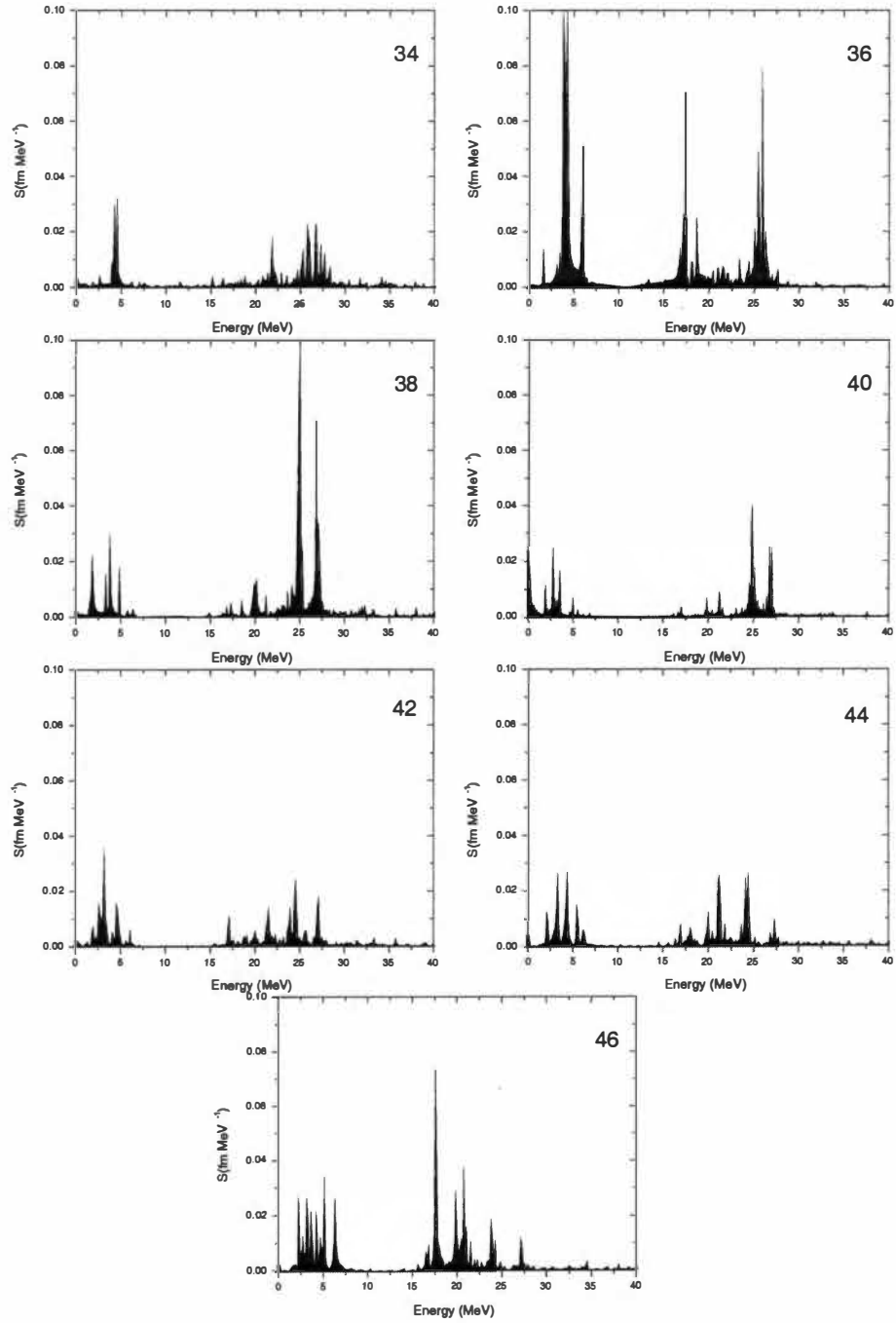


Figure 4.16: Smoothed FFT using 3 point averaging for the isovector dipole response of the argon isotopes

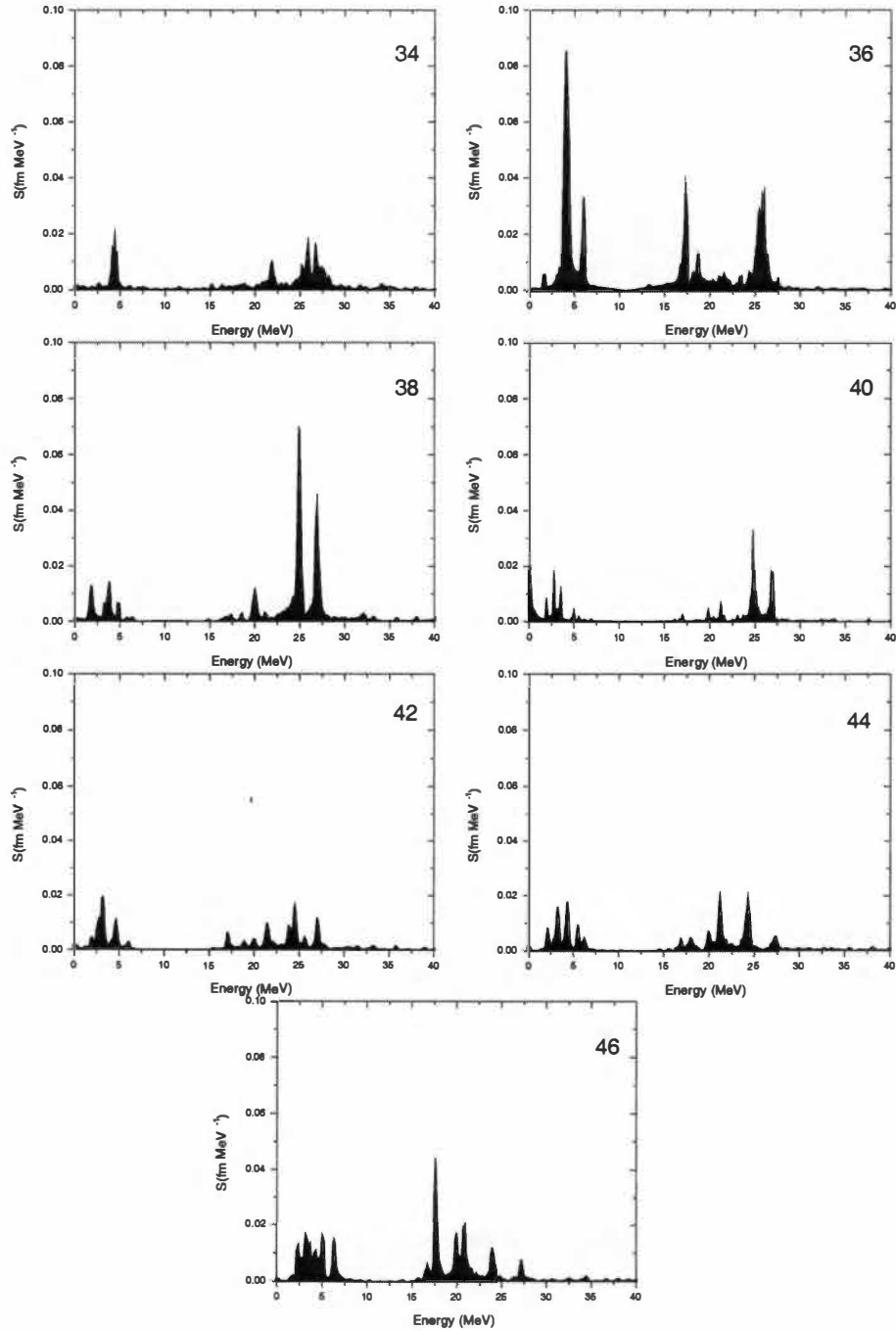


Figure 4.17: Smoothed FFT using 5 point averaging for the isovector dipole response of the argon isotopes

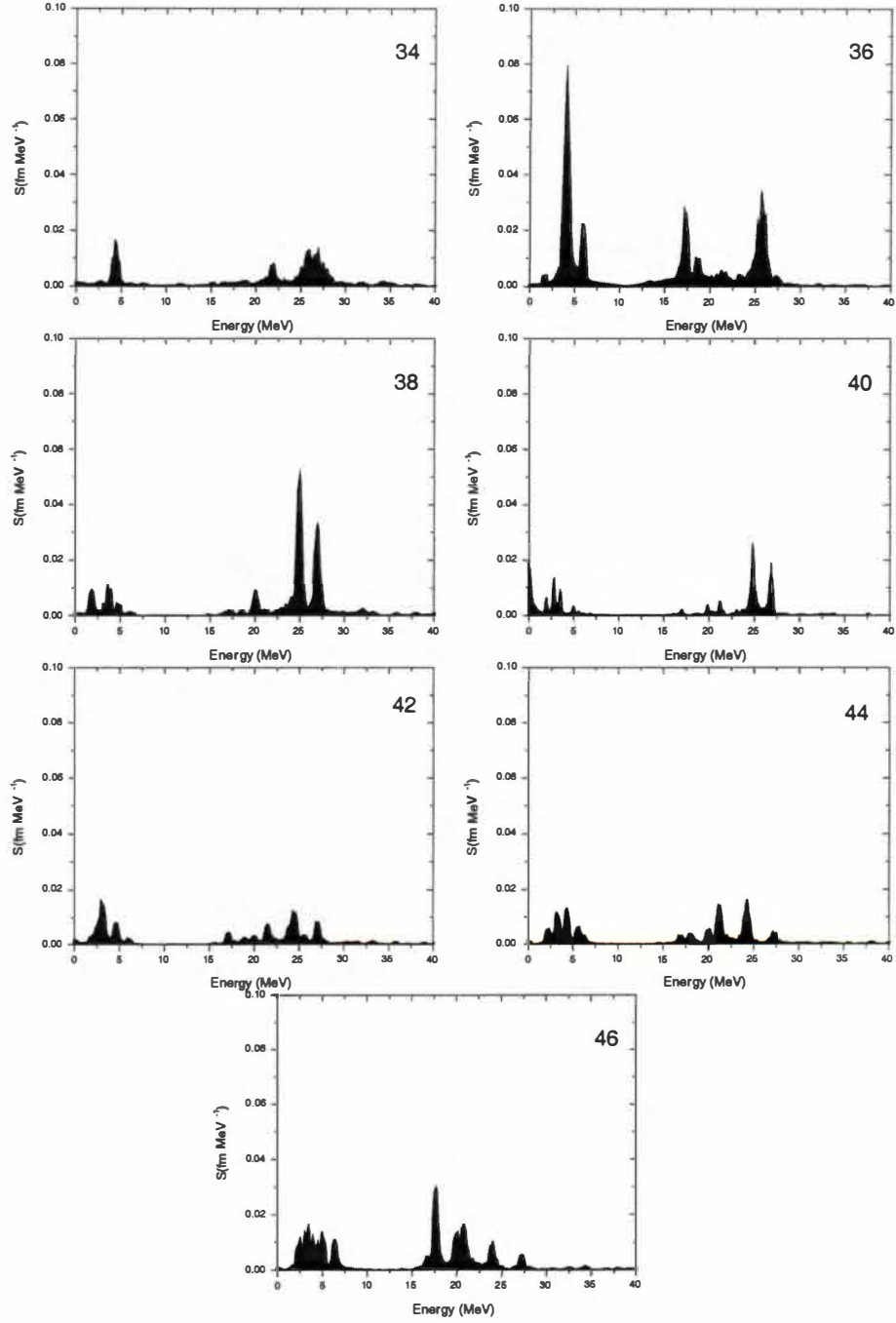


Figure 4.18: Raw FFT for the isoscalar quadrupole response of the argon isotopes

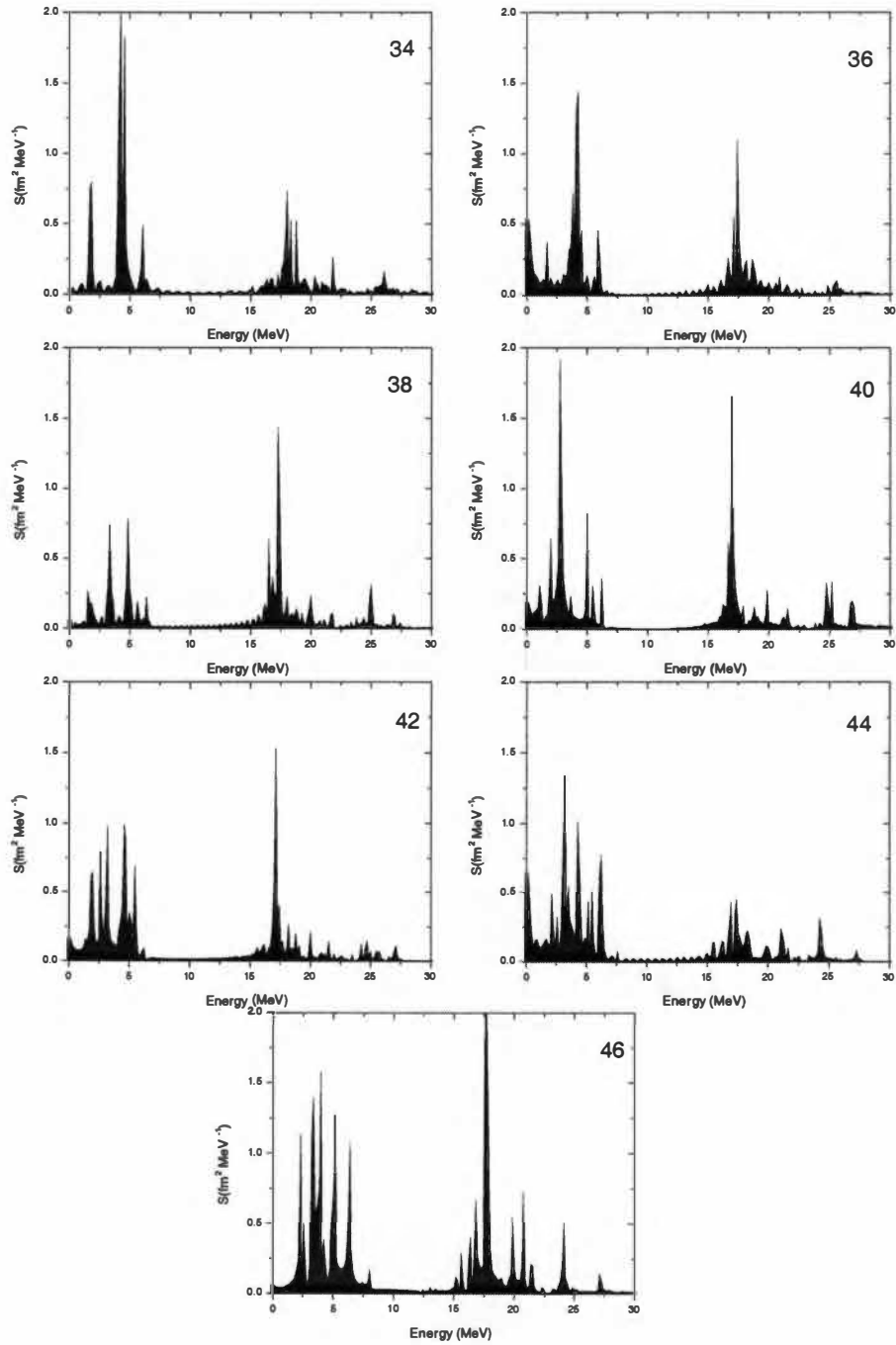


Figure 4.19: Smoothed FFT using 3 point averaging for the isoscalar quadrupole response of the argon isotopes

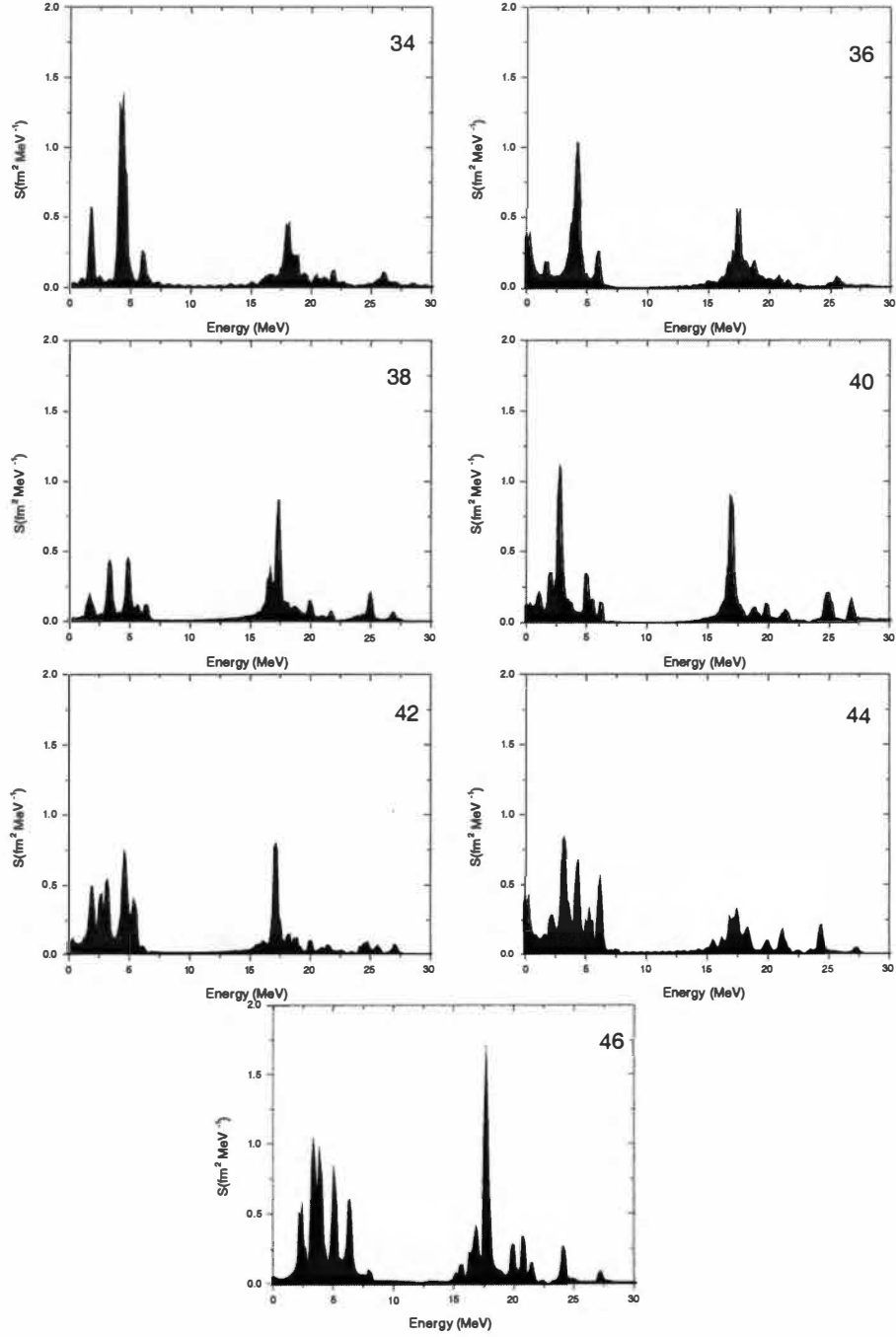


Figure 4.20: Smoothed FFT using 5 point averaging for the isoscalar quadrupole response of the argon isotopes

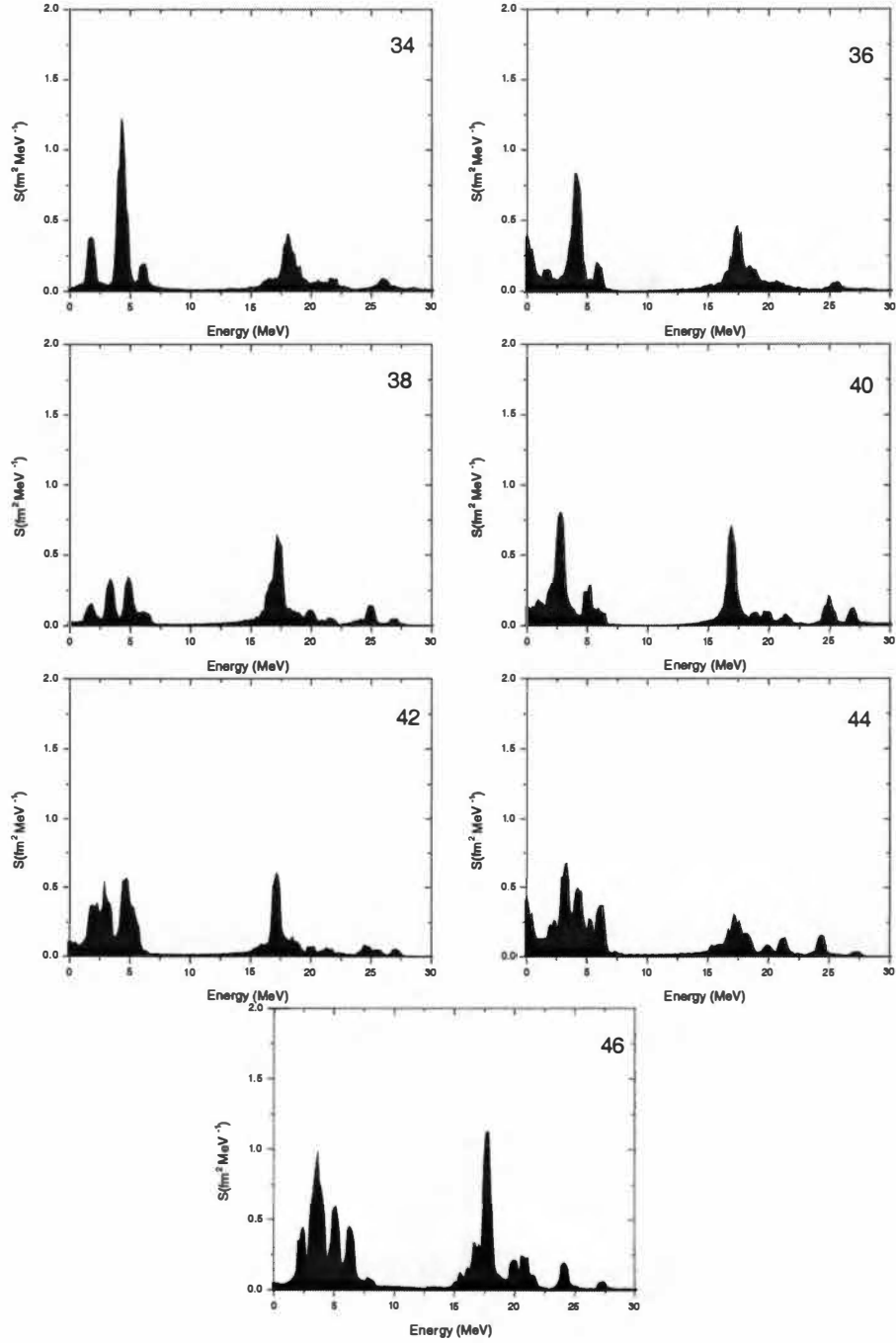


Table 4.5: Energies of the top 4 proton states in MeV

Isotope	$2s$	$1d_{3/2}$ $J_z = 3/2$	$1d_{3/2}$ $J_z = 1/2$	Fermi Energy
34	-6.8	-4.4	-4.4	-4.3
36	-8.6	-6.6	-6.6	-6.5
38	-10.2	-8.6	-8.6	-8.6
40	-12.1	-10.9	-10.8	-10.7
42	-14.1	-13.3	-12.1	-12.6
44	-15.9	-15.4	-13.0	-14.1
46	-17.5	-17.1	-14.0	-15.6

occupation probability of 0.5 means that, on average, the state is occupied by a single unpaired nucleon.

The single particle states reproduce the structure described by the shell model with a Nilsson potential. The shells and sub-shells occupied by the proton and neutron states in argon nuclei, in order of increasing energy, are the first shell ($1s_{1/2}$), the second shell ($1p_{3/2}$ and $1p_{1/2}$ sub-shells), the third shell ($1d_{5/2}$, $2s$ and $1d_{3/2}$ sub-shells) and the lowest sub-shell of the fourth shell, $1f_{7/2}$.

Tables (4.5) and (4.6) give the highest energy occupied proton states in each isotope, together with their energies and occupation probabilities.

The argons have eighteen protons, the first sixteen of which completely fill the first two shells and the $1d_{5/2}$ and $2s$ sub-shells of the third shell. The remaining two occupy positions in the $1d_{3/2}$ sub-shell. As can be seen in table (4.6), in ^{34}Ar to ^{40}Ar the protons are unpaired, on average occupying two different states - one occupying a state with z component of angular momentum $J_z = 3/2$, the other in a $J_z = 1/2$ state. These two levels are almost degenerate in energy, which is

Table 4.6: Occupation probabilities of the top 4 proton states

Isotope	$2s$	$1d_{3/2}$ $J_z = 3/2$	$1d_{3/2}$ $J_z = 1/2$
34	1.0	0.5	0.5
36	1.0	0.5	0.5
38	0.9	0.5	0.5
40	0.9	0.5	0.6
42	0.9	0.8	0.3
44	1.0	1.0	0.1
46	1.0	1.0	0.0

Table 4.7: Energies of the top neutron states in MeV

Isotope	2s	$1d_{3/2}$ $J_z = 3/2$	$1d_{3/2}$ $J_z = 1/2$	$1f_{7/2}$ $J_z = 7/2$	$1f_{7/2}$ $J_z = 5/2$	$1f_{7/2}$ $J_z = 3/2$	$1f_{7/2}$ $J_z = 1/2$	Fermi Energy
34	-15.1	-13.0	-13.0					-14.2
36	-15.0	-13.1	-13.1					-13.0
38	-15.0	-13.1	-13.1					-10.5
40	-15.0	-13.0	-13.0	-7.6	-7.6	-7.6	-7.5	-8.3
42	-14.8	-13.2	-12.3	-8.1	-7.6	-7.3	-7.1	-7.5
44	-14.5	-13.4	-11.5	-8.6	-7.7	-7.3	-7.1	-6.9
46	-14.2	-13.4	-11.1	-8.9	-7.7	-7.4	-7.0	-5.8

consistent with the fact that these particular isotopes are nearly spherical. In ^{42}Ar , the first deformed isotope, these levels start to split in energy, and it is more probable that the two protons occupy the lower energy state $J_z = 3/2$. Finally, in ^{44}Ar and ^{46}Ar , we see that the two protons are fully paired up and occupy the lower energy state $J_z = 3/2$.

The root mean square (rms) radius of the protons remains more or less constant at $3.3fm$.

We now move on to the neutron states. Our starting point is ^{34}Ar , with sixteen neutrons. We add two neutrons each time. Tables (4.7) and (4.8) show the energies and occupation probabilities of the highest energy neutron states, on top of a central core of fourteen neutrons which fill the first and second shell and the $1d_{5/2}$ sub-shell.

^{34}Ar fills the 2s level, though there is some slight filling of the two $1d_{3/2}$ states above it. These states are filled up in ^{36}Ar and ^{38}Ar , completing the Third shell. The extra stability gained from the filling of the shell in ^{38}Ar is consistent with

Table 4.8: Occupation probabilities of top neutron states

Isotope	2s	$1d_{3/2}$ $J_z = 3/2$	$1d_{3/2}$ $J_z = 1/2$	$1f_{7/2}$ $J_z = 7/2$	$1f_{7/2}$ $J_z = 5/2$	$1f_{7/2}$ $J_z = 3/2$	$1f_{7/2}$ $J_z = 1/2$
34	0.8	0.1	0.1				
36	1.0	0.5	0.5				
38	1.0	1.0	1.0				
40	1.0	1.0	1.0	0.27	0.27	0.26	0.25
42	1.0	1.0	1.0	0.7	0.5	0.4	0.3
44	1.0	1.0	1.0	0.9	0.8	0.7	0.6
46	1.0	1.0	1.0	1.0	1.0	1.0	1.0

the fact that it has the most negative binding energy per nucleon and has no deformation.

^{40}Ar to ^{46}Ar fill up the shell $1f_{7/2}$, with the most probable states being the lowest lying, highest angular momentum states.

The rms radius of the neutrons increases as we would expect, starting at 3.1fm for ^{34}Ar and increasing uniformly to 3.7fm for ^{46}Ar .

We must check that our BCS pairing scheme does not scatter particles to the continuum - that our pairing space is confined to the vicinity of the Fermi surface. Tables (4.5) and (4.7) show the Fermi energies. The occupation numbers of levels below those shown in the tables are 1.0 and the occupation numbers of the states above those shown are 0.0. Thus the desired effect of our cutoff distribution (3.12) is realized.

4.2.2 Analysis of Results

Isoscalar Monopole Resonance

Throughout this discussion we refer to Figure (4.14).

All the isotopes exhibit a giant resonance. In calculating their average energies and widths, we have presumed that in each case the resonance is a single structure - that where two peaks are visible in the high energy range, the discreteness of the continuum states is responsible.

Table 4.9 shows the average energies and the widths of the resonances, together with the window in which the calculations were performed. We see that the resonance energy varies slowly up from about 22MeV for ^{36}Ar to about 23MeV for ^{40}Ar , then drops slightly for ^{42}Ar , ^{44}Ar and ^{46}Ar . The strength of the resonance increases steadily over the first 4 isotopes before dropping at ^{42}Ar and rising slowly again. We can account for these observations by supposing the significant deformations in the last 3 isotopes suppress the resonance strength since it is spread over more than one symmetry axis.

Since the results are not fully converged we cannot read too much into the differences in widths.

In ^{44}Ar and ^{46}Ar we see a small amount of low lying strength at around 4MeV. It cannot be caused by collective motion at this low energy, so it must be a results of single $p - h$ excitations. The obvious cause are the neutrons occupying the $1d_{5/2}$ sub shell being excited to the nearby $2s$ shell (written $2s(1d_{5/2})^{-1}$).

Isovector Dipole Resonance

We reference Figure (4.15) for the dipole results. These results are somewhat harder to interpret than the monopole and quadrupole results since the structure

Table 4.9: Average energies $\langle E \rangle$ and widths σ for the isoscalar giant monopole resonances

Isotope	Energy Window (MeV)	$\langle E \rangle$ (MeV)	σ
34	10 - 30	22.1	4.6
36	12 - 29	22.6	3.7
38	13 - 29	22.5	3.5
40	15 - 28	22.9	2.8
42	14 - 28	21.9	4.3
44	12 - 28	21.3	3.5
46	12 - 28	21.1	3.2

of the strength function has some ambiguous features. For example, are there are two separate peaks observed throughout the isotopes or are they part of the same structure and their discreteness is a result of the discrete spectrum of continuum energies? We simply do not have enough information to know.

Table (4.10) shows the average energies and widths obtained assuming that there is a single giant resonance peak.

Two main features appear in the giant resonance region: a peak around 17-18MeV appears prominently in ^{36}Ar and ^{46} , but is extremely weak elsewhere. A second structure at around 24-26MeV appears in all the isotopes. It starts off weak in ^{34}Ar and increases significantly up to the singly closed shell nucleus ^{38}Ar , before dropping in strength in ^{40}Ar . The deformed nuclei once again show significantly suppressed strength for this resonance. This structure itself shows some ambiguities, splitting into two peaks from ^{38}Ar onwards.

In addition to these giant resonances, some low lying activity around 4MeV is observed. The strength of this activity is generally small, apart from in ^{36}Ar , which has an anomalously high strength.

Table 4.10: Average energies $\langle E \rangle$ and widths σ for the low lying and giant isoscalar dipole resonances

Isotope	Low Lying			Giant		
	Energy Window (MeV)	$\langle E \rangle$ (MeV)	σ	Energy Window (MeV)	$\langle E \rangle$ (MeV)	σ
34	1 - 8	4.3	1.6	12 - 32	24.3	4.0
36	1 - 8	4.3	1.2	12 - 32	21.7	4.3
38	1 - 8	3.4	1.3	12 - 32	24.8	3.0
40	1 - 8	3.4	1.4	12 - 32	24.0	3.6
42	1 - 8	3.6	1.2	12 - 32	23.3	4.0
44	1 - 8	4.1	1.3	12 - 32	22.4	3.7
46	1 - 8	4.3	1.5	12 - 32	20.5	3.5

Table 4.11: Dipole Energy Weighted Sum Rule

Isotope	% of theoretical value
34	69
36	136
38	122
40	102
42	54
44	58
46	84

These low energy structures may be explained by $p - h$ excitations of the highest energy neutrons, which are stated in the next section. However, another possibility exists: that some spurious motion as explained in chapter 2 is responsible. This motion would shift the energies of the peaks up in energy about 4 - 5MeV. Then these low lying resonances would actually be at 0MeV, and would just be numerical effects. In addition, the 24MeV giant resonance would be shifted down to around 19MeV, in agreement with previous calculations (see the next section). To examine this possibility one should carry out momentum and angular momentum projections as previously outlined. Such an operation is beyond the scope of this thesis, but should be kept in mind for future calculations.

An additional check we can perform is the energy weighted sum rule: we sum up the strength function over the giant resonance region and compare to the predicted value given in equation (1.10). These provide a test of convergence: if the ESWR is close to 100% the predicted value then the resonance is near full convergence.

The results are shown in table (4.11). These seem to indicate that isotopes 34,42,44,46 are not fully converged.

Isoscalar Quadrupole Resonance

Here we refer to Figure (4.20). We note two main features of the strength function: A giant resonance and some low lying excitations can be seen in all the isotopes. The average energy and widths of these structures are given in Table (4.12).

The giant resonance energy remains fairly stable around 18 MeV. Its strength increases slowly from ^{34}Ar to ^{40}Ar , before dipping slightly at ^{42}Ar . We should expect that the deformations of isotopes ^{42}Ar onwards suppress the strength, but that it continues to increase slowly. However, the strength all but disappears in ^{44}Ar before returning strongly in ^{46}Ar . The ^{44}Ar result is anomalous.

There are low lying states observed too, much like the ones in the dipole results except with much larger strengths. These may be explained by single $p-h$ excitations. In ^{34}Ar and ^{36}Ar , the most probable excitations are $1d_{3/2}(2s)^{-1}$. ^{38}Ar has a completely filled neutron shell, so should have very little low lying strength. What there is may be caused by $1d_{3/2}(2s)^{-1}$ proton excitations. ^{40}Ar to ^{46}Ar have likely $2p_{3/2}(1f_{7/2})^{-1}$ excitations causing the broad low lying features seen.

4.3 Comparison of Results

There exists a previous study of the resonances in the argon isotopes [55].

This earlier paper calculates the resonances using the RPA method with finite rank separable interaction (a $p-h$ interaction which is a sum of N separable terms, where N is much smaller than the dimension of the $p-h$ space). It assumes spherical symmetry for the HF ground states, so is not equipped to deal with deformations. The isovector dipole and isoscalar quadrupole strength functions are studied.

The dipole results show a giant resonance that starts at about 18MeV in ^{34}Ar , and increases slowly in strength and decreases slowly in energy to about 17MeV in ^{40}Ar . The strength then decreases slowly as does the energy, ending up at around 16MeV in ^{46}Ar . No low lying states are observed.

This appears to be at odds with our results, though it is hard to be certain due to the ambiguity of our dipole results.

The quadrupole results closely match ours. In [55], the giant resonance states are fairly stable at around 17MeV, compared with our stable resonances at about 18MeV. The small strength in ^{44}Ar does not show up. Since the code used in [55] assumes spherical Hartree Fock ground states, the results in that paper do not

Table 4.12: Average energies $\langle E \rangle$ and widths σ for the low lying and giant isoscalar quadrupole resonances

Isotope	Low Lying			Giant		
	Energy Window (MeV)	$\langle E \rangle$ (MeV)	σ	Energy Window (MeV)	$\langle E \rangle$ (MeV)	σ
34	1 - 8	4.0	1.3	15 - 23	18.7	1.7
36	1 - 8	4.0	1.2	14 - 23	18.0	1.7
38	1 - 8	4.0	1.5	14 - 23	18.4	2.4
40	1 - 8	3.3	1.4	14 - 23	17.7	1.7
42	1 - 8	3.7	1.4	14 - 23	17.7	1.6
44	1 - 8	4.0	1.5	14 - 23	18.0	2.0
46	1 - 8	4.2	1.5	14 - 23	18.1	1.6

show the reduced strength in the deformed nuclei ^{42}Ar to ^{46}Ar . The paper [55] also shows the low lying states at around 4MeV.

4.4 Summary

We have calculated the isoscalar monopole and quadrupole and isovector dipole responses of even-even argon nuclei for $N = 34$ to $N = 46$. To the best of our knowledge, our calculation is the first fully deformed calculation of these responses.

The quadrupole results were similar to those of a previous calculation, and in addition exhibited effects caused by deformation such as the suppression of resonance strength. The dipole results were somewhat ambiguous, and might benefit from calculating them again using different forces and box sizes. The monopole results are the first of their kind, and demonstrated a stable giant resonance at around 22MeV.

Bibliography

Bibliography

- [1] E. Rutherford, *Phil. Mag.* **21**, 669 (1911)
- [2] E. Rutherford, *Phil. Mag.* **37**, 537 (1919)
- [3] J. Chadwick, *Nature* **129**, 312 and *Proc. Roy. Soc. (London)* **A136**, 692, (1932)
- [4] M. Curie and F. Joliot, *C.R. Acad. Sci.*, **194**, 273, 708, 876, 2208, (1932)
- [5] A. Bohr and B.Mottelson *Nuclear Structure* Benjamin, Reading, MA, 1975
- [6] A.E.L.Dieperink, O.Scholton and F.Iachello *Phys. Rev. Lett.* **44**, 26, 1747, (1980)
- [7] A. Bohr and B.R.Mottelson *Physica Scripta* **22**, 468, (1980)
- [8] J.N.Ginocchio and M.W. Kirson *Nucl. Phys.* **A350**, 31, (1980)
- [9] D.H.Youngblood, H.L.Clark, and Y.-W.Lui *Nucl. Phys.* **A649**, 49c, (1999)
- [10] J.-P. Blaizot *Nucl. Phys.* **A649**, 61c, (1999)
- [11] Zhong-yu Ma et al *Nucl. Phys* **A686**, 173, (2001)
- [12] Berman, B.L. and Fultz, S.C., *Rev.Mod.Phys.*, **47**, 713, (1975)
- [13] Bertrand F.E. *Ann.Rev.Nucl.Sci* **26**, 457, (1976)
- [14] A.M.Lane *Nuclear Physics* W.A.Benjamin, New York, 1964
- [15] D.I.Sober et al *Nucl. Inst. and Meth. in Phys.Res.* **A440**, 263, (2000)
- [16] S.F.LeBrun, A.M. Nathan and S.D.Hoblit *Phys. Rev. C* **35**, 2005, (1987)
- [17] D. Galetti et al *Phys Rev* **C48**, 3131, (1993)
- [18] U. Garg *Nucl.Phys.* **A649**, 66c, (1999)
- [19] H.L.Clark et al *Nucl.Phys.* **A649**, 57c, (1999)

- [20] D.H. Youngblood, Y.-W.Lui and H.L.Clark *Phys.Rev.C* **63**, 067301, (2001)
- [21] D.H. Youngblood, Y.-W.Lui and H.L.Clark *Phys.Rev.C* **64**, 064308, (2001)
- [22] D.H. Youngblood, Y.-W.Lui and H.L.Clark *Phys.Rev.C* **60**, 014304, (1999)
- [23] D.H. Youngblood, Y.-W.Lui and H.L.Clark *Phys.Rev.C* **57**, 1134 (1997)
- [24] D.H. Youngblood, Y.-W.Lui, U.Garg and R.J.Peterson *Phys.Rev.C* **45**, 2172, (1991)
- [25] J. Lisantti et al *Phys.Rev.C* **40**, 1, 211, (1989)
- [26] M. Buenerd, P.Martin, P. de Saintignon and J.M.Loiseaux *Phys.Rev.C* **14**, 4, 1316, (1976)
- [27] J.P. Delaroche et al *Phys.Rev.C* **27**, 5, 2385, (1981)
- [28] Proposal to the National Superconducting Cyclotron Laboratory, Michigan State University Spokesperson Robert Varner May, 2001
- [29] S.Stauch *Nucl.Phys. A***649**, 85c, (1999)
- [30] P.von Neumann-Cosel *Nucl. Phys. A***649**, 77c, (1999)
- [31] Peter Ring and Peter Schuck *The Nuclear Many Body Problem*
- [32] Greiner and Maruhn *Nuclear Models*
- [33] Alexander Fetter and John Walecka *Quantum Theory of Many Particle Systems*
- [34] W. Nazarewicz *Nucl. Phys A***574**, 27c, 1994
- [35] D.Hirata et al *Nucl. Phys A***609**, 131, 1996
- [36] J.L.Wood, E.F.Zganjar, C. De Coster, K.Heyde *Nucl. Phys A***651**, 323, 1999
- [37] D.J.Rowe *Nucl. Phys* **80**, 209, 1966
- [38] J.-S.Wu, M.R.Strayer and M.Baranger *Phys.Rev C***60**, 60, 04403, 1999
- [39] J.Friedrich and P.-G. Reinhard *Phys.Rev. C***33**, 1, 335, 1986
- [40] A.S.Umar, M.R.Strayer, R.Y.Cusson, P.-G.Reinhard and D.A.Bromley *Phys. Rev. C***32**, 172, (1985)
- [41] A.K.Kerman and S.E.Koonin *Ann. Phys* **100**, 332-358 (1976)

- [42] V.Yu.Ponomarev, P.F.Bortignon, R.A.Brogia and V.V.Voronov *Phys. Rev. Let.* **85**, 7, 1400, (2000)
- [43] Ikuko Hamamoto *Phys. Rev.* **C60**, (1999)
- [44] N. Tajima, P.Bonche, H.Flocard, P.-H.Heenen, M.S.Weiss *Nucl. Phys* **A551**, 434, (1993)
- [45] M.Bender, K.Rutz, P.-G.Reinhard and J.A.Maruhn *Eur. Phys. J.A.* **A7**, 467, (2000)
- [46] M.Bender, P.-G.Reinhard, K.Rutz, and J.A.Maruhn, Private communication
- [47] J.Dobaczewski, W.Nazarewicz, T.R.Werner, J.F.Berger, C.R.Chinn and J.Decharge *Phys. Rev.* **C53**, 2809, (1996)
- [48] P.-G.Reinhard, D.J.Dean, W.Nazarewicz, J.Dobaczewski, J.A.Mahrn and M.R.Strayer, *Phys. Rev.* **C60**, 014316, (1999)
- [49] J.Bartel, P.Quentin, M.Brack, C.Guet and H.-B.Hakansson *Nucl.Phys.* **A386**, 79, (1982)
- [50] C.R.Chinn, A.S.Umar, M.Vallieres and M.R.Strayer *Phys. Rep.* **264**, 107, (1983)
- [51] J.M.Pacheco, E.Maglione and R.A.Brogia *Phys Rev* **C37**, 5, 2257, (1988)
- [52] P.D.Stevenson, M.R.Strayer, J.Wu *Abstract*
- [53] P.-G.Reinhard *Nucl. Phys.* **A649**, 305c, (1999)
- [54] T.R.Werner et al *Nucl. Phys.* **A597**, 327, (1996)
- [55] Nguyen Van Giai, Ch. Stoyanov, V.V.Voronov *Phys Rev* **C57**, 4, 1204, (1997)
- [56] Bardeen, Cooper, Schreiffer *Phys. Rev.* **108**, 1175, (1957)

Appendix

Appendix A

Hartree Fock Theory

A.1 The Hartree-Fock Approximation

The set of wave functions that exactly describe all possible states of a nucleus are given by the solutions to the many body Schroödinger equation

$$\hat{H}\Psi = \left(\sum_{i=1}^A \hat{t}(\mathbf{r}_i) + \sum_{i<j}^A \hat{v}(\mathbf{r}_i, \mathbf{r}_j) \right) \Psi = E\Psi \quad (\text{A.1})$$

where A is the number of nucleons and $(\mathbf{r}_i) = (\vec{r}_i, s_i, t_i)$ represents all coordinates of the i th nucleon - spatial, spin and isospin. We have included one and two body interactions in the many body Hamiltonian, and may include higher orders. The many body wave function solutions are in general given by a sum over states which are a product of single particle wave functions occupying the available states in all possible combinations. Since we are dealing with fermions, only one single particle wave function can occupy each state, and each product of the single particle wave functions must be anti-symmetrized to obey the Pauli principle. Such a product is called a Slater Determinant, written

$$\Phi_{k_1 \dots k_A}(\mathbf{r}_1, \dots, \mathbf{r}_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{k_1}(\mathbf{r}_1) & \dots & \phi_{k_1}(\mathbf{r}_A) \\ \vdots & & \vdots \\ \phi_{k_A}(\mathbf{r}_1) & \dots & \phi_{k_A}(\mathbf{r}_A) \end{vmatrix} \quad (\text{A.2})$$

$\phi_k(\mathbf{r}_i)$ is the single particle wave function of the i th nucleon in state k . The labels $k_1 \dots k_A$ represent the states that the nucleons occupy, selected from the infinite available states.

Then the solution to equation (A.1) is given by the sum of all possible Slater determinants:

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_A) = \sum_{k_1 \dots k_A} c_{k_1 \dots k_A} \Phi_{k_1 \dots k_A}(\mathbf{r}_1, \dots, \mathbf{r}_A) \quad (\text{A.3})$$

The states k provide an orthogonal basis for an occupation number representation in the framework of second quantization. In other words, we define creation and annihilation operators $a_k^\dagger, a_k$ which create or annihilate particles with a wave function ϕ_k . Now the Pauli principle, which was encoded in the antisymmetrization of the Slater determinant, is encoded by the anti-commutation of the creation and annihilation operators. The Slater determinant now assumes the simpler form

$$|\Phi_{k_1 \dots k_A}\rangle = \hat{a}_{k_1}^\dagger \dots \hat{a}_{k_A}^\dagger |0\rangle \quad (\text{A.4})$$

where $|0\rangle$ is the vacuum state, and the solution (A.4) is written

$$|\Psi\rangle = \sum_{k_1 \dots k_A} c_{k_1 \dots k_A} |\Phi_{k_1 \dots k_A}\rangle \quad (\text{A.5})$$

In the notation of second quantization, the many body Hamiltonian is written

$$\hat{H} = \sum_{i,j=1}^A t_{ij} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{i,j,k,l=1}^A v_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k \quad (\text{A.6})$$

where now t_{ij} and v_{ijkl} are one and two body matrix elements.

The number of states in the sum of (A.5) is enormous, and the problem is generally intractable. To solve it, some approximation must be made.

In the shell model, the assumption is made that the interaction term in the Hamiltonian can be treated as a one body interaction - an average potential in which the nucleons move independently of each other: then

$$\hat{H}_0 \Psi = \sum_{i=1}^A \left(\hat{t}(\mathbf{r}_i) + \hat{v}(\mathbf{r}_i) \right) \Psi = \left(\sum_{i=1}^A \hat{h}(\mathbf{r}_i) \right) \Psi = E \Psi \quad (\text{A.7})$$

Writing this in second quantized form,

$$\hat{H}_0 = \sum_{i,j=1}^A t'_{ij} \hat{a}_i^\dagger \hat{a}_j \quad (\text{A.8})$$

The eigenfunctions of this Hamiltonian are the Slater determinants, $|\Phi_{k_1 \dots k_A}\rangle$, with eigenvalues

$$E_{k_1 \dots k_A} = \sum_{i=1}^A t'_{k_i, k_i} = \sum_{i=1}^A \epsilon_i \quad (\text{A.9})$$

where ϵ_i is the energy of a particle in the state i .

The success of the shell model in describing properties of the nucleus justifies the assumption of an average potential that operates on single particles only. We thus look for an approximation to the many body problem that allows us to extract a one body potential from the the two (or more) body potential.

The form of the wave functions in the shell model suggests an approximation. The eigenfunctions are Slater determinants, so the ground state of the shell model is given by a Slater determinant:

$$\hat{H}|\Phi_{k_1\dots k_A,0}\rangle = E_0|\Phi_{k_1\dots k_A,0}\rangle \quad (\text{A.10})$$

whereas the exact solution of the ground state of the many body problem is a linear combination of all possible Slater determinants.

We then formulate the Hartree-Fock approximation as follows: *we restrict the form of the ground state wave function of the nucleus to a Slater determinant.* To determine the exact form of this wavefunction and the ground state energy, we must use a variational principle.

The ground state Slater determinant that we take as our ansatz is

$$|\Phi_{k_1\dots k_A,0}\rangle = \sum_{k_1\dots k_A < \epsilon_f} \hat{a}_{k_1}^\dagger \dots \hat{a}_{k_A}^\dagger |0\rangle \quad (\text{A.11})$$

i.e. the nucleons occupy all the available states up to the fermi energy.

A.2 The Variational Principle

As an example of the use of the variational principle, we show that the exact Schrödinger equation may be written as a variational equation

$$\delta E[\Psi] = 0 \quad (\text{A.12})$$

where the energy expectation value in Ψ is given by

$$E[\Psi] = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad (\text{A.13})$$

Carrying out the variation:

$$\begin{aligned} \delta \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} &= \frac{\langle \delta \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} + \frac{\langle \Psi | H | \delta \Psi \rangle}{\langle \Psi | \Psi \rangle} - \langle \delta \Psi | \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle^2} - \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle^2} | \delta \Psi \rangle = 0 \\ &\quad \langle \delta \Psi | H - E | \Psi \rangle + \langle \Psi | H - E | \delta \Psi \rangle = 0 \end{aligned} \quad (\text{A.14})$$

In general, $|\Psi\rangle$ is a complex function, and we carry out the variation over the real and imaginary parts separately. To obtain the variation over the imaginary parts, replace $|\Psi\rangle$ with $i|\Psi\rangle$ in (A.14):

$$-i\langle\delta\Psi|H - E|\Psi\rangle + i\langle\Psi|H - E|\delta\Psi\rangle = 0 \quad (\text{A.15})$$

Multiplying equation (A.14) by i and combining it with (A.15) yields

$$\langle\delta\Psi|H - E|\Psi\rangle = 0 \quad (\text{A.16})$$

together with its complex conjugate. Since $|\delta\Psi\rangle$ is arbitrary, we can write

$$H|\Psi\rangle = E|\Psi\rangle \quad (\text{A.17})$$

which is the Schrödinger equation. We have obtained it by minimizing the energy expectation value with respect to the wave functions.

In the Hartree-Fock approximation, we wish to restrict the form of the many body wave functions, which means they will no longer be exact eigenvalues of the many body Hamiltonian, and $|\delta\Psi\rangle$ is no longer arbitrary. To examine this further, consider the Schrödinger equation for the exact many body problem $H\Psi_i = E\Psi_i$, where i labels the different eigenfunctions. Since this equation is exact, the eigenfunctions span the entire Hilbert space.

We seek a solution in the form of a wave function Φ that is restricted in form, so that all possible Φ s span only a subset of Hilbert space. Whatever the form of Φ , it can be expanded in the Ψ_i s:

$$\Phi = \sum_i c_i \Psi_i \quad (\text{A.18})$$

with the condition $\sum_i |c_i|^2 = 1$. The indices i are ordered in increasing energy of the eigenvalues, such that $i = 0$ denotes the ground state of the Hamiltonian. The expectation value of the Hamiltonian in Φ will then be

$$\begin{aligned} E[\Phi] &= \langle\Phi|\hat{H}|\Phi\rangle = \sum_i |c_i|^2 E_i = |c_0|^2 E_0 + \sum_{i>0} |c_i|^2 E_i \\ &= (1 - \sum_{i>0} |c_i|^2) E_0 + \sum_{i>0} |c_i|^2 E_i \\ &= E_0 + \sum_{i>0} |c_i|^2 (E_i - E_0) \geq E_0 \end{aligned} \quad (\text{A.19})$$

This equals E_0 only if $c_0 = 1$ and $c_i = 0$ for all $i > 0$, i.e. if $\Phi = \Psi_0$. This is of course not possible if we restrict the form of the wave function. Thus we must instead minimize the extra terms. The variational principle then states that *The*

best approximation to the ground state for the Hamiltonian $\hat{H}$ is obtained for that wave function Φ whose energy expectation value is minimal. Mathematically, we write

$$\delta E[\Phi] = \delta \langle \Phi | \hat{H} | \Phi \rangle = 0 \quad (\text{A.20})$$

This way, we expect to obtain a one body hamiltonian that describes the mean field in which the nucleons move in the shell model.

A.3 Matrix Elements

In order to proceed further we must be able to calculate matrix elements of the general one and two body operators $u(\mathbf{r}_i)$ and $v(\mathbf{r}_i, \mathbf{r}_j)$ with respect to the Slater determinants. Here we calculate $\langle \Phi | \sum_i u(\mathbf{r}_i) | \Phi \rangle$ and $\langle \Phi | \sum_{i,j} v(\mathbf{r}_i, \mathbf{r}_j) | \Phi \rangle$.

To start with, we write the Slater determinant (A.2) in a more convenient form:

$$\Phi_{k_1 \dots k_A}(\mathbf{r}_1 \dots \mathbf{r}_A) = \frac{1}{\sqrt{A}} \sum_P (-1)^P \phi_{P_1}(\mathbf{r}_1) \dots \phi_{P_A}(\mathbf{r}_A) \quad (\text{A.21})$$

where P stands for a certain permutation of the particles among the available states and P_i is a certain number within that permutation. For example, a two particle Slater determinant would be written as $1/\sqrt{2}$ times

$$\begin{aligned} \phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) & \quad (P = 0, P_1 = 1, P_2 = 2) \\ -\phi_2(\mathbf{r}_1)\phi_1(\mathbf{r}_2) & \quad (P = 1, P_1 = 2, P_2 = 1) \end{aligned} \quad (\text{A.22})$$

Let us first calculate the expectation value of a single body operator:

$$\langle \Phi | \sum_{i=1}^A t_i | \Phi \rangle = \frac{1}{A!} \int d\mathbf{r}_1 \dots d\mathbf{r}_A \sum_{P, P'} (-1)^{(P+P')} \phi_{P_1}^*(\mathbf{r}_1) \dots \phi_{P_A}^*(\mathbf{r}_A) \left(\sum_i u(\mathbf{r}_i) \right) \phi_{P'_1}(\mathbf{r}_1) \dots \phi_{P'_A}(\mathbf{r}_A) \quad (\text{A.23})$$

Now $u(\mathbf{r}_1)$ operates on the wave function $\phi_{P'_1}(\mathbf{r}_1)$ and all other wave functions move behind. Using

$$\int d\mathbf{r}_i \phi_{P_j}^*(\mathbf{r}_i) \phi_{P'_j}(\mathbf{r}_i) = \delta_{P_j P'_j} \quad (\text{A.24})$$

We get

$$\frac{1}{A!} \int d\mathbf{r}_1 \sum_{P,P'} (-1)^{(P+P')} \delta_{P_2 P'_2} \dots \delta_{P_A P'_A} \phi_{P_1}^*(\mathbf{r}_1) u(\mathbf{r}_1) \phi_{P'_1}(\mathbf{r}_1) \quad (\text{A.25})$$

Since $A - 1$ of the indices are the same, so must the A th be, thus $P_1 = P'_1$ and $P = P'$, and we get

$$\frac{1}{A!} \int d\mathbf{r}_1 \phi_{P_1}^*(\mathbf{r}_1) u(\mathbf{r}_1) \phi_{P'_1}(\mathbf{r}_1) \quad (\text{A.26})$$

Repeating this procedure for all $u(\mathbf{r}_i)$ gives the result

$$\langle \Phi | \sum_{i < \epsilon_f} u(\mathbf{r}_i) | \Phi \rangle = \frac{1}{A!} \sum_{i=1}^A \int d\mathbf{r}_i \phi_{P_i}^*(\mathbf{r}_i) u(\mathbf{r}_i) \phi_{P_i}(\mathbf{r}_i) \quad (\text{A.27})$$

and relabelling the dummy indices

$$\langle \Phi | \sum_{i < \epsilon_f} u(\mathbf{r}_i) | \Phi \rangle = \frac{1}{A!} \sum_{i=1}^A \int d\mathbf{r}_i \phi_i^*(\mathbf{r}_i) u(\mathbf{r}_i) \phi_i(\mathbf{r}_i) \quad (\text{A.28})$$

For the two body force $\sum_{i,j < \epsilon_f} v(\mathbf{r}_i, \mathbf{r}_j)$, we proceed as above. The $v(\mathbf{r}_1, \mathbf{r}_2)$ matrix element is

$$\frac{1}{A!} \int d\mathbf{r}_1 d\mathbf{r}_2 \sum_{P,P'} (-1)^{(P+P')} \delta_{P_3 P'_3} \dots \delta_{P_A P'_A} \phi_{P_1}^*(\mathbf{r}_1) \phi_{P_2}^*(\mathbf{r}_2) v(\mathbf{r}_1, \mathbf{r}_2) \phi_{P'_1}(\mathbf{r}_1) \phi_{P'_2}(\mathbf{r}_2) \quad (\text{A.29})$$

Only two of the permutation indices remain undetermined, and there are two possibilities, resulting in

$$\frac{1}{A!} \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_1^*(\mathbf{r}_1) \phi_2^*(\mathbf{r}_2) v(\mathbf{r}_1, \mathbf{r}_2) [\phi_1(\mathbf{r}_1) \phi_2(\mathbf{r}_2) - \phi_2(\mathbf{r}_1) \phi_1(\mathbf{r}_2)] \quad (\text{A.30})$$

Then the matrix elements of a two body force is

$$\langle \Phi | \sum_{i,j < \epsilon_f} v(\mathbf{r}_i, \mathbf{r}_j) | \Phi \rangle = \frac{1}{2A!} \sum_{i,j=1}^A \int d\mathbf{r}_i d\mathbf{r}_j \phi_i^*(\mathbf{r}_i) \phi_j^*(\mathbf{r}_j) v(\mathbf{r}_i, \mathbf{r}_j) [\phi_i(\mathbf{r}_i) \phi_j(\mathbf{r}_j) - \phi_j(\mathbf{r}_i) \phi_i(\mathbf{r}_j)] \quad (\text{A.31})$$

Where the extra factor of one half comes in because the matrix element of $v(\mathbf{r}_i, \mathbf{r}_j)$ gives the same result as the matrix element of $v(\mathbf{r}_j, \mathbf{r}_i)$.

A.4 The Time Dependant Hartree Fock Approximation

In order to describe the resonant states we are interested in, we need a theory that allows time evolution of the system. The Time Dependant Hartree-Fock approximation is used - a generalization of the time independent approximation which supposes that *The many body wave function at every instant in time is a Slater Determinant*.

We need also to generalize the variational principle. Following the prescription given in [41], we define the Lagrangian of the system as

$$\begin{aligned}\mathcal{L}[\Phi, \Phi^*] &= \langle \Phi | i\hbar \frac{\partial}{\partial t} - H | \Phi \rangle \\ &= \int (dr)^A \Phi^*(r_1, \dots, r_A, t) \left(i\hbar \frac{\partial}{\partial t} - H \right) \Phi(r_1, \dots, r_A, t) \\ &= \int (dr)^A \Phi^*(r_1, \dots, r_A, t) \left(i\hbar \frac{\partial}{\partial t} \right) \Phi(r_1, \dots, r_A, t) + \mathcal{H}[\Phi, \Phi^*]\end{aligned}\quad (\text{A.32})$$

With Φ a Slater determinant, we can work out the matrix elements using the formulas derived above. Noting that $i\hbar \frac{\partial}{\partial t}$ is a one body operator,

$$\mathcal{L}[\Phi, \Phi^*] = \mathcal{L}[\{\phi_n\}, \{\phi_n^*\}] = i\hbar \sum_{i=1}^A \int dr \phi_i^*(r, t) \dot{\phi}_i(r, t) + \mathcal{H}[\{\phi_n\}, \{\phi_n^*\}] \quad (\text{A.33})$$

where, using equations (A.28) and (A.31),

$$\begin{aligned}\mathcal{H}[\{\phi_n\}, \{\phi_n^*\}] &= \sum_{i=1}^A \int dr \phi_i^*(r, t) t(\mathbf{r}_i) \phi_i(r, t) \\ &\quad + \frac{1}{2} \sum_{i,j=1}^A \int dr dr' \phi_i^*(r, t) \phi_j^*(r', t) v(\mathbf{r}_i \mathbf{r}_j) [\phi_i(r, t) \phi_j(r', t) - \phi_j(r, t) \phi_i(r', t)]\end{aligned}\quad (\text{A.34})$$

We then define the action to be

$$S[\{\phi_n\}, \{\phi_n^*\}] = \int_{t_1}^{t_2} dt \mathcal{L}[\{\phi_n\}, \{\phi_n^*\}] \quad (\text{A.35})$$

and the variational principle we use is

$$\frac{\delta S}{\delta \phi_n^*} = 0 \quad \text{or} \quad \frac{\delta S}{\delta \phi_n} = 0 \quad (\text{A.36})$$

using the result from functional calculus

$$\int d\mathbf{r}_i \sum_i \frac{\delta\phi_i^*(\mathbf{r}, t)}{\delta\phi_k^*(\mathbf{r}', t)} = \delta_{ik}\delta(\mathbf{r} - \mathbf{r}') \quad (\text{A.37})$$

we obtain (for the variation over ϕ_n^* or ϕ_n respectively)

$$i\hbar\dot{\phi}_n(\mathbf{r}, t) = \frac{\delta\mathcal{H}}{\delta\phi_n^*} \quad (\text{A.38})$$

$$i\hbar\dot{\phi}_n^*(\mathbf{r}, t) = -\frac{\delta\mathcal{H}}{\delta\phi_n} \quad (\text{A.39})$$

The one body Hartree-Fock Hamiltonian is then defined to be

$$\frac{\delta\mathcal{H}}{\delta\phi_n^*} = h^{HF}\phi_n \quad (\text{A.40})$$

with $h^{\dagger HF} = h^{HF}$

We write the solutions in time as

$$\phi_n(\mathbf{r}, t) = e^{-i\epsilon_n t} \phi_n^{HF}(\mathbf{r}) \quad (\text{A.41})$$

where ϵ_n are the single particle energies. Then equation (A.38) becomes

$$\frac{\delta\mathcal{H}}{\delta\phi_n} - \epsilon_n \phi_n^{HF} = (h^{HF} - \epsilon_n)\phi_n^{HF} = 0 \quad (\text{A.42})$$

These are the static Hartree-Fock equations, with solutions $\phi_n^{HF}(\mathbf{r})$.

A.5 Derivation of the Hartree-Fock Equations

Now we are ready to calculate h^{HF} from equations (A.34) and (A.38). Using equation (A.37) we get

$$\begin{aligned}
0 &= \frac{\delta}{\delta\phi_k^*(\mathbf{r}_n)} \langle \Phi | H | \Phi \rangle = \frac{1}{A!} \frac{\delta}{\delta\phi_k^*(\mathbf{r}_n)} \left(\sum_{i=1}^A \int d\mathbf{r}_i \phi_i^*(\mathbf{r}_i) t(\mathbf{r}_i) \phi_i(\mathbf{r}_i) \right. \\
&\quad + \frac{1}{2} \sum_{i,j=1}^A \int d\mathbf{r}_i d\mathbf{r}_j \phi_i^*(\mathbf{r}_i) \phi_j^*(\mathbf{r}_j) v(\mathbf{r}_i, \mathbf{r}_j) \phi_i(\mathbf{r}_i) \phi_j(\mathbf{r}_j) \\
&\quad \left. - \frac{1}{2} \sum_{i,j=1}^A \int d\mathbf{r}_i d\mathbf{r}_j \phi_i^*(\mathbf{r}_i) \phi_j^*(\mathbf{r}_j) v(\mathbf{r}_i, \mathbf{r}_j) \phi_j(\mathbf{r}_i) \phi_i(\mathbf{r}_j) \right) \\
&= t(\mathbf{r}_i) \phi_i(\mathbf{r}_n) + \sum_{i=1}^A \int d\mathbf{r}_i \phi_i^*(\mathbf{r}_i) \frac{\delta t(\mathbf{r}_i)}{\delta\phi_k^*(\mathbf{r}_n)} \phi_i(\mathbf{r}_i) \\
&\quad + \frac{1}{2} \sum_{j=1}^A \int d\mathbf{r}_j \phi_j^*(\mathbf{r}_j) v(\mathbf{r}_k, \mathbf{r}_j) \phi_k(\mathbf{r}_n) \phi_j(\mathbf{r}_j) \\
&\quad + \frac{1}{2} \sum_{i=1}^A \int d\mathbf{r}_i \phi_i^*(\mathbf{r}_i) v(\mathbf{r}_i, \mathbf{r}_k) \phi_i(\mathbf{r}_i) \phi_k(\mathbf{r}_n) \\
&\quad + \frac{1}{2} \sum_{i,j=1}^A \int d\mathbf{r}_i d\mathbf{r}_j \phi_i^*(\mathbf{r}_i) \phi_j^*(\mathbf{r}_j) \frac{\delta v(\mathbf{r}_i, \mathbf{r}_j)}{\delta\phi_k^*(\mathbf{r}_n)} \phi_i(\mathbf{r}_i) \phi_j(\mathbf{r}_j) \\
&\quad - \frac{1}{2} \sum_{j=1}^A \int d\mathbf{r}_j \phi_j^*(\mathbf{r}_j) v(\mathbf{r}_k, \mathbf{r}_j) \phi_j(\mathbf{r}_n) \phi_k(\mathbf{r}_j) \\
&\quad - \frac{1}{2} \sum_{i=1}^A \int d\mathbf{r}_i \phi_i^*(\mathbf{r}_i) v(\mathbf{r}_i, \mathbf{r}_k) \phi_k(\mathbf{r}_i) \phi_i(\mathbf{r}_n) \\
&\quad - \frac{1}{2} \sum_{i,j=1}^A \int d\mathbf{r}_i d\mathbf{r}_j \phi_i^*(\mathbf{r}_i) \phi_j^*(\mathbf{r}_j) \frac{\delta v(\mathbf{r}_i, \mathbf{r}_j)}{\delta\phi_k^*(\mathbf{r}_n)} \phi_j(\mathbf{r}_i) \phi_i(\mathbf{r}_j)
\end{aligned} \tag{A.43}$$

We can see that, under a simple relabelling of dummy variables, the third and fourth, and the sixth and seventh terms are equal. If we define the one and two particle density matrices as

$$\rho(\mathbf{r}) = \sum_{i=1}^A \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}) \tag{A.44}$$

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{i=1}^A \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}') \tag{A.45}$$

Then equation (A.43) becomes

$$\begin{aligned}\epsilon_i \phi_i(\mathbf{r}) = & \left(u(\mathbf{r}') + \int d\mathbf{r}' \rho(\mathbf{r}) v(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}) \right) - \int d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}') v(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}) \\ & + \int d\mathbf{r} \rho(\mathbf{r}) \frac{\delta t_i}{\delta \phi_k^*(\mathbf{r}_n)} + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \rho(\mathbf{r}) \rho(\mathbf{r}') \frac{\delta v_{ij}}{\delta \phi_k^*(\mathbf{r}_n)} \\ & - \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}, \mathbf{r}') \frac{\delta v_{ij}}{\delta \phi_k^*(\mathbf{r}_n)}\end{aligned}\quad (\text{A.46})$$

The Hartree-Fock potential is defined from the first line of this equation:

$$U_{HF}(\mathbf{r}) \phi_i(\mathbf{r}) = \left(u(\mathbf{r}') + \int d\mathbf{r}' \rho(\mathbf{r}) v(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}) \right) - \int d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}') v(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}) \quad (\text{A.47})$$

The other terms are zero unless the one and two body interactions depend on the wave functions (and consequently the densities).

A.6 The Skyrme Interaction

Now all that remains to be done is choose the form of our two body interaction. In our treatment we use the widely studied Skyrme interaction, an effective force which is zero range and density and momentum dependant, and has the form:

$$\begin{aligned}V_{\text{skyrm}} = & t_0(1 + x_0 P_0) \delta(\vec{r}_i - \vec{r}_j) \\ & + \frac{1}{2} t_1(1 + x_1 P_x) [\vec{p}_{12}^2 \delta(\vec{r}_i - \vec{r}_j) + \delta(\vec{r}_i - \vec{r}_j) \vec{p}_{12}^2] \\ & + t_2(1 + x_2 P_x) \vec{p}_{12} \cdot \delta(\vec{r}_i - \vec{r}_j) \vec{p}_{12} \\ & + \frac{1}{6} t_3(1 + x_3 P_x) \rho^\alpha(\bar{r}) \delta(\vec{r}_i - \vec{r}_j) \\ & + i t_4 \vec{p}_{12} \delta(\vec{r}_i - \vec{r}_j) (\vec{\sigma}_i + \vec{\sigma}_j) \times \vec{p}_{12}\end{aligned}\quad (\text{A.48})$$

where $\vec{p}_{12} = \vec{p}_i - \vec{p}_j$ is the relative momentum, P_x is the space exchange operator $\vec{r}_i \leftrightarrow \vec{r}_j$, $\vec{\sigma}$ is the vector of Pauli spin matrices and $\bar{r} = (\vec{r}_i + \vec{r}_j)/2$. The five parameters t_0, t_1, t_2, t_3 and t_4 are adjusted to fit the experimental binding energies and radii.

Then the Hartree-Fock potential is calculated to be [39]

$$\begin{aligned}
U_{HF} = & t_0(1 + \tfrac{1}{2}x_0)\rho - t_0(\tfrac{1}{2} + x_0)\rho_q \\
& + \frac{1}{12}t_3\rho^\alpha \left[(2 + \alpha)(1 + \tfrac{1}{2}x_3)\rho - 2(\tfrac{1}{2} + x_3)\rho_q - \alpha(\tfrac{1}{2} + x_3)\frac{\rho_{pr}^2 + \rho_{ne}^2}{\rho} \right] \\
& + \frac{1}{4}[t_1(1 + \tfrac{1}{2}x_1) + t_2(1 + \tfrac{1}{2}x_2)]\tau - \frac{1}{4}[t_1(\tfrac{1}{2} + x_1) - t_2(\tfrac{1}{2} + x_2)]\tau_q \\
& - \frac{1}{8}[3t_1(1 + \tfrac{1}{2}x_1) - t_2(1 + \tfrac{1}{2}x_2)]\Delta\rho + \frac{1}{8}[3t_1(\tfrac{1}{2} + x_1) + t_2(\tfrac{1}{2} + x_2)]\Delta\rho_q \\
& - \frac{1}{2}t_4(\nabla\vec{J} + \nabla\vec{J}_q) + U_{coul}
\end{aligned} \tag{A.49}$$

with the following densities and currents:

$$\rho_q(r) = \sum_{i=1}^A w_i \phi_i^*(r) \phi_i(r) \tag{A.50}$$

$$j_q(r) = \frac{i}{2} \sum_{i=1}^A w_i [\nabla \phi_i^*(r) \phi_i(r) - \phi_i^*(r) \nabla \phi_i(r)] \tag{A.51}$$

$$\tau_q(r) = \sum_{i=1}^A w_i \nabla \phi_i^*(r) \cdot \nabla \phi_i(r) \tag{A.52}$$

$$\nabla J_q(r) = -i \sum_{i=1}^A w_i \nabla \phi_i^*(r) \cdot \nabla \times \vec{\sigma} \phi_i(r) \tag{A.53}$$

where q is an isospin label $\in \{ pr, ne \}$, and w_i is the occupation probability of each state (1 or 0 in a pure Hartree Fock basis).

Appendix B

BCS Pairing

It is observed in experiment that for even-even nuclei the ground state always has zero angular momentum, even when they contain a partially filled j shell, indicating that there is some residual interaction which makes it energetically favorable for the nucleons in the unfilled shell to couple to zero angular momentum rather than any other value. The simplest way to model this behavior is to assume an attractive interaction that aligns nucleon spins in the same orbit anti-parallel, forming a pair with zero angular momentum. This behavior is not described by basic Hartree-Fock theory. There are several methods of describing the pairing interaction, and here we present the model used in our code, that of BCS pairing, which was originally introduced in 1957 in the theory of superconductivity [56]

BCS theory introduces correlations between particles into the ground state wave function. We begin with the ansatz that the ground state wave function has the form

$$|BCS\rangle = \prod_{k>0} (u_k + v_k \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger) |0\rangle \quad (\text{B.1})$$

$\{k, \bar{k}\}$ generate the complete single particle space. $k > 0$, $\bar{k} < 0$ and $|k| = |\bar{k}|$. The states $|k\rangle$ and $|\bar{k}\rangle$ correspond to the spherical harmonics $|nljm\rangle$ and $|nlj-m\rangle$ for $m > 0$. The state $|0\rangle$ can be taken to the Hartree-Fock ground state.

In this state each pair of single particle levels $(k, -k)$ is occupied with probability $|u_k|^2$ and remains empty with probability $|v_k|^2$. We assume the parameters u_k and v_k are real, which is still sufficiently general for most problems.

Let us examine the properties of this state:

We gain insight by expressing $|BCS\rangle$ in the following way: dividing equation (B.1) by u_k and expanding out the product yields

$$|BCS\rangle \propto |0\rangle + \sum_{k>0} \frac{v_k}{u_k} \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger + \sum_{k,k'>0} \frac{v_k v_{k'}}{u_k u_{k'}} \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger \hat{a}_{k'}^\dagger \hat{a}_{\bar{k}'}^\dagger + \dots \quad (\text{B.2})$$

which shows that it is the HF ground state plus a sum over all pairs plus a sum over all sets of two pairs, and so on.

The norm of the state is given by

$$\langle BCS|BCS\rangle = \langle 0| \prod_{k>0} (u_k + v_k \hat{a}_{\bar{k}} \hat{a}_k) \prod_{k'>0} (u_{k'} + v_{k'} \hat{a}_{\bar{k}'}^\dagger \hat{a}_{k'}^\dagger) |0\rangle \quad (\text{B.3})$$

All the terms with different values of their indices commute, so we must only calculate

$$(u_k + v_k \hat{a}_{\bar{k}} \hat{a}_k)(u_k + v_k \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger) = u_k^2 + u_k v_k (\hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger + \hat{a}_{\bar{k}} \hat{a}_k) + v_k^2 \hat{a}_{\bar{k}} \hat{a}_k \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger \quad (\text{B.4})$$

From this, we note

$$\langle 0| \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger |0\rangle = \langle 0| \hat{a}_{\bar{k}} \hat{a}_k |0\rangle = 0 \quad (\text{B.5})$$

since both of these matrix elements include annihilation of a pair on the vacuum, and

$$\langle 0| \hat{a}_{\bar{k}} \hat{a}_k \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger |0\rangle = 1 \quad (\text{B.6})$$

Thus we have

$$\langle BCS|BCS\rangle = \prod_{k>0} (u_k^2 + v_k^2) \quad (\text{B.7})$$

and for the normalization requirement $\langle BCS|BCS\rangle$ to be fulfilled,

$$|u_k|^2 + |v_k|^2 = 1 \quad (\text{B.8})$$

We can also calculate the particle number expectation value using the number operator $\hat{N}$

$$\begin{aligned} N &= \langle BCS| \hat{N} |BCS\rangle \\ &= \langle BCS| \sum_{k>0} (\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}}) |BCS\rangle \end{aligned} \quad (\text{B.9})$$

For each value of k , $\hat{N}$ projects out the component proportional to v_k multiplied by its particle number 2:

$$\hat{N}|BCS\rangle = \sum_{k>0} 2v_k \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger |0\rangle \quad (\text{B.10})$$

This also shows that $\hat{N}$ is not a good quantum number. Then from equation (B.9) we get

$$\begin{aligned} N &= \langle 0 | 2v_k^2 \sum_{k,k'>0} \hat{a}_{\bar{k}'} \hat{a}_{k'} \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger | 0 \rangle \\ &= \sum_{k>0} 2v_k^2 \end{aligned} \quad (\text{B.11})$$

This fits the interpretation of v_k^2 as the probability of having the state $(k, \bar{k})$ occupied.

Now let us calculate the particle number uncertainty:

$$(\Delta N)^2 = \langle BCS | \hat{N}^2 | BCS \rangle - \langle BCS | \hat{N} | BCS \rangle^2 \quad (\text{B.12})$$

where

$$\hat{N}^2 = \sum_{k>0} (\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}}) (\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}}) \quad (\text{B.13})$$

Each term produces a factor of $2v_k^2 \times 2v_k^2$, except the $k = k'$ term which gives a factor of $4v_k^2$. Then

$$\begin{aligned} (\Delta N)^2 &= 4 \sum_{k \neq k', k, k'>0} v_k^2 v_{k'}^2 + 4 \sum_{k>0} v_k^2 - 4 \sum_{k, k'>0} v_k^2 v_{k'}^2 \\ &= -4 \sum_{k>0} v_k^4 + 4 \sum_{k>0} v_k^2 \\ &= 4 \sum_{k>0} u_k^2 v_k^2 \end{aligned} \quad (\text{B.14})$$

where the last result comes using $v_k^2 = 1 - u_k^2$. Again, this shows that in general particle number is not conserved in the BCS model.

The program uses the simplest case of BCS pairing. We take the pairing Hamiltonian to be:

$$\hat{H} = \sum_k \epsilon_k^0 \hat{a}_k^\dagger \hat{a}_k + \sum_{k, k'>0} V_{k\bar{k}k'\bar{k}'} \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}'} \hat{a}_{k'} \quad (\text{B.15})$$

which includes a pure (diagonal) single particle part , with ϵ_k^0 the single particle energies, and a residual interaction that operates only on pairs. We take the simplest case of a constant pairing force G :

$$\hat{H} = \sum_k \epsilon_k^0 \hat{a}_k^\dagger \hat{a}_k - G \sum_{k,k'>0} \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}'} \hat{a}_{k'} \quad (\text{B.16})$$

To calculate the matrix elements of this Hamiltonian, we work out the following:

$$\langle BCS | \hat{a}_k^\dagger \hat{a}_k | BCS \rangle = v_k^2 \quad (\text{B.17})$$

and

$$\langle BCS | \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}'} \hat{a}_{k'} | BCS \rangle = v_k^2 \begin{cases} u_k v_k u_{k'} v_{k'}, & \text{for } k \neq k' \\ v_k^2, & \text{for } k = k' \end{cases} \quad (\text{B.18})$$

using arguments already given in calculating N and $(\Delta N)^2$. Then

$$\begin{aligned} \langle BCS | G \sum_{k,k'>0} \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}'} \hat{a}_{k'} | BCS \rangle &= G \sum_{k \neq k', k,k'>0} u_k v_k u_{k'} v_{k'} + G \sum_{k>0} v_k^4 \\ &= G \left(\sum_{k>0} u_k v_k \right)^2 + G \sum_{k>0} v_k^4 \end{aligned} \quad (\text{B.19})$$

So the full matrix element is

$$\langle BCS | \hat{H} - \lambda \hat{N} | BCS \rangle = 2 \sum_{k>0} (\epsilon_k - \lambda) v_k^2 - G \left(\sum_{k>0} u_k v_k \right)^2 + G \sum_{k>0} v_k^4 \quad (\text{B.20})$$

where we have added the constraint that equation (B.11) is satisfied, with the lagrange multiplier λ , called the chemical potential or fermi energy.

To calculate the parameters v_k and u_k we use a variational principle. We vary the matrix element (B.20) with respect to one of those parameters, and set the variation to zero. Since v_k and u_k are related through the normalization condition, differentiating with respect to one of them (say v_k) is given by:

$$\frac{\partial}{\partial v_k} = \frac{\partial}{\partial v_k} \Big|_{u_k} + \frac{\partial u_k}{\partial v_k} \frac{\partial}{\partial u_k} \Big|_{v_k} \quad (\text{B.21})$$

thus differentiating (B.20), using $\partial u_k / \partial v_k = -v_k / u_k$, and setting the result to zero, we get:

$$2\epsilon_k v_k u_k + \Delta(v_k^2 + u_k^2) = 0 \quad (\text{B.22})$$

where

$$\Delta = G \sum_{k>0} u_k v_k \quad (\text{B.23})$$

$$\epsilon_k = \epsilon_k^0 - \lambda - G v_k^2 \quad (\text{B.24})$$

Squaring equation (B.22) and replacing u_k^2 by v_k^2 yields

$$v_k^2 = \frac{1}{2} \left(1 \pm \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2}} \right) \quad (\text{B.25})$$

and inserting this back in (B.22) yields

$$u_k^2 = \frac{1}{2} \left(1 \pm \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2}} \right) \quad (\text{B.26})$$

Now we know that as $\Delta \rightarrow 0$, $v_k \rightarrow 1$ and $u_k \rightarrow 0$ so v_k takes the positive sign and u_k takes the negative sign.

Putting u_k and v_k back into the equation for Δ gives us the *gap equation*:

$$\Delta = \frac{G}{2} \sum_{k>0} \frac{\Delta}{\sqrt{\epsilon_k^2 + \Delta^2}} \quad (\text{B.27})$$

We get λ by simultaneously fulfilling the condition

$$2 \sum_{k>0} v_k^2 = N \quad (\text{B.28})$$

from before. In doing this we ignore the term $-G v_k^2$ from the expression for ϵ_k . This is ok - it corresponds only to a renormalization of the single particle energies.

Finally, we note that the expressions for the gap and fermi energy are isospin independent. Experimentally, it is observed that this is not the case, so we explicitly break isospin symmetry by introducing a separate pairing strength for protons and neutrons: $G \rightarrow G_q$, $\Delta \rightarrow \Delta_q$ and $\lambda \rightarrow \lambda_q$ where $q = p$ for protons, n for neutrons.

Vita

I obtained my first degree, Master of Physics, at the University of Oxford, UK. There I became interested in astrophysics, and worked on a project to calculate the rate at which stars drift out from or into the center of the galaxy.

I came to the University of Tennessee through a connection between Oxford and Oak Ridge National Laboratory. Here I worked with the nuclear theory group on the program which I used to carry out the work in this thesis.

I plan to return to Oxford to get my doctorate. I will be carrying on the work laid out here and also using the program to calculate properties neutron stars.

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