A SELF-CONSISTENT CORE-PARTICLE COUPLING MODEL FOR THE ODD-MASS NICKEL ISOTOPES

by

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ABSTRACT

A self-consistent core-particle (core-hole) coupling model is used to calculate the energy levels of the odd-mass nickel isotopes. The cores considered are the ground 0^+ and the first excited 2^+ states of adjacent even-mass nuclei, and the single particle states are $2p_{1/2}$, $2p_{3/2}$ and $1f_{5/2}$ for the neutrons outside the completely filled neutron and proton shells.

The residual interaction between the shell model particles is represented by the pairing-plus-quadrupole force, and a number-nonconserving approximation is made. A generalized Hartree-Fock formalism is used to obtain a set of equations for the coefficients of fractional parentage (cfp) connecting the even and odd nuclei. The eigenstates of the odd nuclei are then obtained as linear combinations of the core-particle and core-hole coupled states.

The energy spectra obtained are in fairly good agreement with the experimental ones in the mid-shell range where the number-nonconserving approximation is expected to be good. The electric quadrupole transition rates B (E2; 0^+ 2^+) for the even-mass nuclei calculated from the cfp also have a reasonable magnitude showing the collective nature of the 2^+ state.

Some suggestions are made for a further improvement of the model.

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CHAPTER 1

INTRODUCTION

As is well known, the nuclear structure problem is a many-body problem. Even if the exact character of the nuclear force were known, it would still not be possible to solve the resulting nuclear many-body problem exactly, since in general, only two-body problems are soluble. In such cases, a useful method of overcoming this difficulty is to construct a model which approximates the actual system as closely as possible and reduces the insoluble problem to a soluble one.

Several types of nuclear models have been developed since the discovery of the neutron in 1932. The shell model is one of the most successful nuclear models in correlating a large number of diverse nuclear data (Elliott and Lane,1957). The shell model, discussed in more detail in Chapter 2, assumes that each nucleon in a nucleus is moving independently in a spherically symmetric potential well with a strong spin-orbit interaction. It achieved a great success in explaining the nuclear magic numbers as well as spins and parities of ground states of many nuclei. A further improvement has been acheived by introducing suitable residual (effective) two-body interactions between the shell model particles and rediagonalizing the Hamiltonian. Such an improved shell model has been shown to explain most of the observed properties of ground and low excited states of medium and heavy nuclei.

Among many phenomenological residual interactions suggested, the so called pairing-plus-quadrupole force model has been widely used in systematic calculations (Kisslinger et al. 1960 and 1963; Baranger and Kumar, 1965 and 1968). The model consists of the one-body shell-model potential plus the pairing and quadrupole-quadrupole forces as residual two-body interactions.

The pairing force tends to couple a pair of like nucleons into a state of zero angular momentum. It was introduced following a suggestion by Bohr, Mottelson and Pines (1958) in order to explain the energy gap in even-even nuclei and the odd-even mass difference. The observed energy spectra for even-even nuclei showed a large gap (Approx. 1 MeV) between the ground and the first excited state (Bohr et al. 1958), which is indicative of a state similar to the superconducting state in solids.

The quadrupole force, on the other hand, was introduced because it was observed that many even-even nuclei have an extraordinarily large (many times a single particle value) electric quadrupole transition probability from the ground state to the first excited 2^+ state. This indicates a collective quadrupole-type correlated motion in this 2^+ state. Besides, in some regions of the nuclear chart, many nuclei exhibit a rotational spectrum, showing a deformation with a considerable static quadrupole moment (Elliott and Lane,1957). Thus the quadrupole force was considered as a source creating such quadrupole vibration and deformation. While the pairing force is essentially a short-range

force, the quadrupole force is a long-range interaction and capable of producing a collective motion of the nucleus.

Although the pairing-plus-quadrupole force has not been explained fully from the basic nucleon-nucleon force, it is undoubtedly an important part of the residual interaction. This residual interaction, which plays a major role in determining the ground and low excited states of nuclei, will be discussed in section 2.3 .

Having the residual interaction specified, it is still difficult to calculate the properties of nuclear states because of the large number of particles involved and numerous configurations which have to be considered. Many further approximations have been suggested since 1953, the successful ones being: the Bardeen, Cooper, Schrieffer approximation (BCS) (Bardeen et al. 1957), the Tam-Dancoff Approximation (TDA) (Dyson,1953 and references suggested in that paper) and its extension to include the ground state correlations, the Random Phase Approximation (RPA) (Anderson, 1958). Many calculations of medium and heavy nuclei have been carried out by using these approximations. A qualitative discussion of these methods is given in Chapter 2 (see also Lane,1964).

Recent experimental and theoretical developments show that certain limitations still exist in these approximations. The BCS approximation can only be applied to the ground state of

even-even nuclei. The RPA treats all vibrations as harmonic and thus has the disadvantage that anharmonicities already apparent in the data cannot be easily treated. Also the diagonal matrix elements of the density operator in the ground state and in the lowest one-phonon state (the first 2^+ state) are assumed to be approximately equal in the RPA. This results in a very small electric quadrupole moment for the first 2^+ state, in disagreement with recent experimental results (deBoer et al. 1965). An improved RPA method is the Quasi-Particle Random Phase Approximation (QRPA), in which quasi-particles, discussed in Chapter 2, are introduced into the Hamiltonian and then the method of RPA is applied. By using the QRPA, Kisslinger and Sorensen (1963) have done a systematic calculation of low-lying excited states of nuclei with some success.

To overcome some of the deficiencies mentioned, a self-consistent core-particle (hole) coupling model (CPCM) has been developed by Klein and his coworkers (Do Dang et al. 1966,1967 and 1968; Dreizler et al. 1967). Their approach is based on the equations of motion for the coefficients of fractional parentage (cfp) (Elliott and Lane,1957) connecting states of even nuclei with A and A-2 nucleons and states of the intervening odd nuclei. In a restricted calculation with a 2^+ core only, they showed that the observed large electric quadrupole moment of the first 2^+ state of Cd^{114} could be obtained from such a model.

In the present work, the self-consistent CPCM method is applied to calculate the energy spectra of low excited states of odd-mass nickel isotopes. The basic configurations of these states are considered to consist of either the ground 0^+ or the first excited 2^+ state of neighboring even-mass isotopes coupled with a particle or a hole. The states of the odd-mass nuclei are calculated in a self-consistent manner in a number-nonconserving approximation similar to the BCS theory. The details of the formalism and approximations will be discussed in Chapter 3.

The calculation of the energy spectra of Ni isotopes has been attempted by several people (Kisslinger et al. 1963; Auerbach, 1967; Hsu and Frence,1965; Cohen et al. 1967) using various approximations and effective forces. Although none of them is completely satisfactory, the results of the present work will be compared in Chapter 4 to those obtained by Auerbach which are considered as the best.

The purpose of this work is twofold; that is, to see whether the self-consistent core-particle (hole) coupling model with the effective pairing-plus-quadrupole force can give an adequate description of the states of these relatively simple nuclei, and to investigate whether such a calculation provides some information regarding the validity and limitation of this self-consistent CPCM approximation.

Although an exact calculation within a truncated space of nuclear states is still manageable in the mass region around the Ni isotopes once the interactions are specified, there are regions where the number of configurations is so large that an exact calculation becomes practically impossible even with the modern computer. The present CPCM method is expected to provide a powerful tool for solving problems in such cases.

CHAPTER 2

THE RESIDUAL INTERACTION AND RELATED APPROXIMATIONS

2.1 The nuclear shell model

The basic idea of the shell model is that each nucleon in the nucleus is moving independently in an average potential field which is spherically symmetric. This potential well represents the average interaction field between each nucleon and all the others in the nucleus. Therefore, as the first approximation, the single-particle states and energy levels are obtained by solving the Schrödinger equation with an assumed potential well. The potential is usually taken as a harmonic well, a square well or a Woods-Saxon well. The first two wells are idealized wells and have analytic solutions. The Wood-Saxon well is more realistic but the calculation is laborious. The ground state of the nucleus is obtained by filling successively the single-particle levels of the average potential well with nucleons and by forming a Slater determinant from all occupied states, as discussed in the following section.

The single-particle model is a special version of the shell model. It assumes that in the ground state all nucleons except the last one (for an even-even nucleus, there is no such unpaired one) are coupled pairwise to a state of zero angular momentum and therefore they do not contribute to the angular momentum and parity of the nucleus. In this model, the spin and

parity of an odd-mass nucleus are determined by the last unpaired nucleon.

The general version of the shell model is the individual particle model, in which all the particles are taken into account. One works with the wave function which is a Slater determinant formed by single-particle wave functions and takes into account all two-body interactions between the nucleons in the nucleus. In this thesis, we work on this general version. However, in an actual calculation, it is a general pratice to consider explicit two-body interactions for only those particles outside certain closed shells, leaving the inner part as an innert core.

Experimental data (Elliott et al. 1957) indicate the presence of a strong spin-orbit force which can be expressed as follows:

$$M = \sum_i \zeta(r_i)\, \vec{s}_i \cdot \vec{\ell}_i \quad . \tag{2.1.1}$$

This force couples the intrinsic spin $\vec{s}_i$ with the orbital angular momentum $\vec{\ell}_i$ of each particle. The spin-orbit force splits the energy level corresponding to each ℓ into two levels with different values of the total single-particle angular momentum

$$\vec{j} = \vec{\ell} + \vec{s} \tag{2.1.2}$$

Since $\vec{s}\cdot\vec{\ell}$ is a single particle operator and is a scalar, the j valur of each particle of an N-nucleon system as well as the total angular momentum J are good quantum numbers. As a result of this coupling, the level with a larger j-value always lies

below the one with smaller j. The splitting is about an order of magnitude larger than that in the atomic spectra. The total angular momentum J is obtained as

$$\vec{J} = \sum_{i=1}^{A} \vec{j}_i \quad , \tag{2.1.3}$$

where A is the mass number and i labels individual nucleons. This type of coupling scheme is called j-j coupling. In shell model calculations, the single-particle potential well is usually represented by an assumed external well with spin-orbit force.

2.2 The Hartree-Fock Approximation

In the Hartree-Fock approximation, the nuclear wave function of the ground state is assumed to be an antisymmetric combination of products of single-particle wave functions of N-occupied states, i.e.

$$\Psi = (N!)^{-\frac{1}{2}} \begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) & \cdots & \varphi_1(x_N) \\ \varphi_2(x_1) & \varphi_2(x_2) & \cdots & \varphi_2(x_N) \\ \cdot & & & \\ \varphi_N(x_1) & \varphi_N(x_2) & \cdots & \varphi_N(x_N) \end{vmatrix} . \tag{2.2.1}$$

The single-particle wave functions $\varphi_\alpha(x_i)$ are to be determined by solving the resulting Hartree-Fock equations, so as to give the lowest nuclear energy for the nucleus.

In the second quantization notation, equation (2.2.1) can

be written in the form

$$|HF\rangle = |\Psi\rangle = a_1^\dagger a_2^\dagger a_3^\dagger \cdots |0\rangle \quad , \qquad (2.2.2)$$

where $a^\dagger$ is a creation operator which creates a particle when it operates on the vacuum $|0\rangle$. The state given by equation (2.2.2) is called the Hartree-Fock ground state for the N-nucleon system. The Hamiltonian of the nuclear system is

$$H = \sum_{\alpha\beta} \langle\alpha|T|\beta\rangle a_\alpha^\dagger a_\beta + \frac{1}{4} \sum \langle\alpha\beta|V|\delta\gamma\rangle a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \quad , (2.2.3)$$

where T is the kinetic energy operator $-\frac{\hbar^2}{2m}\nabla^2$ and V is the two-body interaction between the nucleons. The $a_\alpha^\dagger$ and a_α satisfy the fermion anticommutation rule as follows:

$$\{a_\alpha^\dagger, a_\beta^\dagger\} = 0 = \{a_\alpha, a_\beta\} \quad ,$$

$$\{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta} \quad . \qquad (2.2.4)$$

The minimization of the ground state energy $\langle HF|H|HF\rangle$ leads to the following equations of motion (see Brown, 1967):

$$T\varphi_i(x) + V(x)\varphi_i(x) - \int U(x, x_1)\varphi_i(x_1) d^3x_1 = \varepsilon_i \varphi_i(x) \quad , \qquad (2.2.5)$$

where

$$V(x) = \sum_{j=1}^{N} \int \varphi_j^*(x_1) V(x_1, x) \varphi_j(x) d^3x_1 \quad ,$$

$$U(x, x_1) = \sum_{j=1}^{N} \varphi_j^*(x_1) V(x_1, x) \varphi_j(x) \quad .$$

These are the Hartree-Fock equations. They show that the ith particle is moving in a self-consistent field which is a result

of averaging the effects of all the individual two-body interactions. The solution for single-particle energies ε_λ and single-particle wave functions $\varphi_\lambda(x)$ can be obtained by an iteration process.

In equation (2.2.5), the first sum is called the direct term, and the second sum is the exchange term. The exchange term shows that the self-consistent field contains a non-local potential. For the spherical nucleus, the self-consistent potential can be approximated by a spherically symmetric potential, such as a harmonic well, a square well, or a Woods-Saxon well. For the non-spherical nucleus, each nucleon, instead of moving independently in the spherically symmetric potential, moves independently in a non-spherical potential. In the shell model calculation, it is assumed that the main part of the interactions between the nucleons is represented by an external potential well and the remaining part can be considered as the residual (or effective) interaction between the shell-model particles. The residual interaction may also come from an indirect interaction through a core excitation (Brown,1967).

2.3 The residual interaction between shell-model particles

In general, a spin-independent two-body residual interaction can be expressed as

$$V_{12}(r) = \sum_\ell f_\ell(r_1, r_2)\, P_\ell(\cos\theta_{12}) \,, \qquad (2.3.1)$$

where r_1 and r_2 are the radial distances of particle 1 and 2 from

the center of the nucleus, $\theta_{12}=0$ in angular distance $\approx 1/\ell$. Thus terms with high values of ℓ correspond to the short-range forces and terms with low values of ℓ correspond to the long-range forces. It can be shown (Brown,1967) that the state with total angular momentum J=0 for a pair of particles has a large amplitude at $\theta_{12}=0$. If one compares this characteristic to that of V_{12} as shown above, one sees that a short-range interaction affects this state (J=0) most and its effect diminishes rapidly as the total angular momentum J of the pair increases. Therefore, the pairing force which tends to couple two particles to a state of zero angular momentum is an important part of the short-range force in the two-body residual interaction and comes from terms with high values of ℓ in the expansion (2.3.1). One can define (see Lane,1964 for more discussions) the pairing force in the j-j representation as follows:

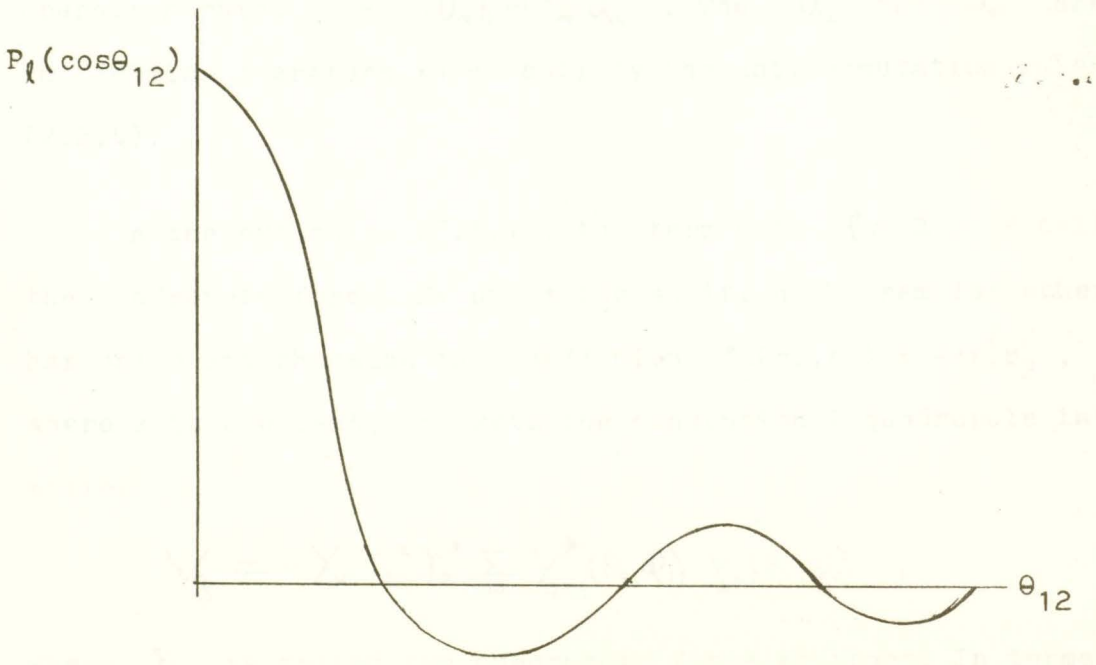

Figure 2.3.1 Plot of $P_\ell(\cos\theta_{12})$ versus θ_{12}.

$$\langle \alpha \alpha'_t | V_p | \beta \beta'_t \rangle = -G \delta_{\alpha\alpha'} \delta_{\beta\beta'} \quad , \qquad (2.3.2)$$

where α stands for all the quantum numbers of the nucleon , i.e. $\alpha = (n, l_a, j_a, m_a)$, G is the pairing force constant and $\alpha'_t = (n', l'_a, j'_a, \bar{m}'_a)$ is the time-reversed state of α' .

The pairing force will act only on states of total angular momentum J=0, in which each term is of the type (j m, j -m) . One can write the pairing Hamiltonian as follows:

$$H_p = \sum_{\alpha\alpha'\beta\beta'>0} \langle \alpha \alpha'_t | V_p | \beta \beta'_t \rangle_{A.S.} (S_\alpha a^+_\alpha a^+_{\bar{\alpha}'}) (S_\beta a_{\bar{\beta}} a_{\beta'})$$

$$= -\tfrac{1}{4} G \sum_{\alpha\beta} (S_\alpha a^+_\alpha a^+_{\bar{\alpha}}) (S_\beta a_{\bar{\beta}} a_\beta) \quad , \qquad (2.3.3)$$

where the matrix elements $\langle \alpha \alpha'_t | V_p | \beta \beta'_t \rangle_{A.S.}$ are taken between the antisymmetrized states. $S_\alpha = (-)^{j_a - m_a}$ comes from the time-reversal operation which gives $(a^+_\alpha)_t = S_\alpha a^+_\alpha$. The a^+_α and a_α are the fermion operators which satisfy the anticommutation rule (2.2.4).

In the expansion (2.3.1), the term with $l = 2$ is called the quadrupole force. By using the addition theorem for spherical harmonics and choosing the coefficient $f_2(r_1, r_2) = -k r_1^2 r_2^2$, where k is constant, one gets the conventional quadrupole interaction

$$V_q = -\chi r_1^2 r_2^2 \sum_m Y^*_{2m}(\theta_1, \varphi_1) Y_{2m}(\theta_2, \varphi_2) \quad ,$$

where χ is called the quadrupole force constant. In terms of

creation and annihilation operators, the Hamiltonian of the quadrupole force has the form

$$H_q = -\tfrac{1}{2}\chi \sum_{\alpha\beta\gamma\delta\, m} \langle\alpha|r^2 Y_{2m}|\delta\rangle\langle\gamma|r^2 Y_{2m}|\beta\rangle a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \ . \quad (2.3.4)$$

The H_q is a long-range force in contrast to the short-range pairing force. Much experimental evidence (such as the large E2 transition rate from 0^+ to first 2^+ excited state) shows that this force is needed in order to explain the observed collective vibrations and rotations of nuclei discussed in section 2.5 .

By taking the pairing force and the quadrupole force, one has included the most important part of both the short-range and long-range effective nucleon-nucleon interaction.

In a shell model calculation, the matrix element of the two-body interaction between two nucleons is small compared with the shell spacing. Hence the residual interaction will not greatly influence the particles in the filled shells. Particles outside the closed shell are of overriding importance in determining the properties of a nucleus. Only the particles in the incomplete shell, in which the residual interaction is important, are treated explicitly in most calculations.

2.4 The BCS theory

The pairing interaction Hamiltonian can be written in the second quantization form as

$$H_p = -\tfrac{G}{4} \sum_{\mu\nu} (s_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger)(s_\nu a_{\bar{\nu}} a_\nu) \ . \quad (2.4.1)$$

For N identical particles (all protons or neutrons) moving in a single-particle level of degeneracy 2Ω , the equations of motion with the Hamiltonian (2.4.1) can be solved exactly (Brown, 1967) and the solution can be given by a simple closed form:

$$E_v(N) = -G/4\ (N-v)(2\Omega-N-v+2), \quad v=0,2,4,... \qquad (2.4.2)$$

where v, the seniority, is the number of unpaired particles, and N the total number of particles. The v is even or odd as the number of particles N is even or odd. The energy gap between the first excited and the ground state is always

$$E_{v=2}(N) - E_{v=0}(N) = G\Omega\ , \qquad (2.4.3)$$

which is independent of N. As long as $v<<\Omega$, the spacings between the successive levels are all approximately $G\Omega$.

For the non-degenerate case, the solution of the pairing Hamiltonian becomes very difficult to obtain as the number of levels and the number of particles increase. The Hamiltonian is

$$H=\sum_\nu \epsilon_\nu a_\nu^\dagger a_\nu - G/4 \sum_{\mu\nu} (s_\mu a_\mu^\dagger a_{\bar\mu}^\dagger)(s_\nu a_{\bar\nu} a_\nu)\ , \qquad (2.4.4)$$

where ϵ_ν is the single-particle energy.

One can perform a canonical transformation (Bogolyubov-Valatin transformation) (Bogolyubov,1958 and Valatin,1958) from the operators $a_\nu^\dagger$ to the quasi-particle operators $\alpha_\nu^\dagger$:

$$\alpha_\nu^\dagger = U_\nu a_\nu^\dagger - s_\nu V_\nu a_{\bar\nu}\ ,$$

$$\alpha_\nu = U_\nu a_\nu - s_\nu V_\nu a_{\bar\nu}^\dagger\ , \qquad (2.4.5)$$

where $\bar{\nu} = -\nu = (n, \ell_\nu, j_\nu, -m_\nu)$, $s_\nu = (-)^{j_\nu - m_\nu}$ and U_ν and V_ν are real amplitudes which satisfy

$$U_\nu^2 + V_\nu^2 = 1 \quad . \tag{2.4.6}$$

Since the particle created by $\alpha_\nu^\dagger$ is not a real particle but a superposition of a particle and a hole, it is called the quasi-particle. The only purpose of intrudocing the quasi-particle is to simplify the calculation. The quasi-particle operators satisfy the fermion anticommutation rule (as can be shown from (2.2.4) and (2.4.5)):

$$\left\{\alpha_\mu^\dagger, \alpha_\nu^\dagger\right\} = 0 = \left\{\alpha_\mu, \alpha_\nu\right\} \quad ,$$

$$\left\{\alpha_\mu^\dagger, \alpha_\nu\right\} = \delta_{\mu\nu} \quad . \tag{2.4.7}$$

For a system with an even number of particles, from (2.4.6) and (2.4.7) one can show that the ground state is given by

$$|BCS\rangle = \prod_{\nu>0} (U_\nu + V_\nu s_\nu a_\nu^\dagger a_{\bar{\nu}}^\dagger)|0\rangle \quad , \tag{2.4.8}$$

and

$$\alpha_\nu |BCS\rangle = 0 \quad , \tag{2.4.9}$$

where $|0\rangle$ is the Hartree-Fock ground state. Thus $|BCS\rangle$ represents the vacuum state of the quasi-particles. Since $\langle BCS|BCS\rangle = \prod_{\nu>0} (U_\nu^2 + V_\nu^2)$, the BCS wave function (2.4.8) is normalized to unity. The physical meaning of the amplitudes V_ν and U_ν in equation (2.4.8) is that the squares of their values give the probability of finding a ν-pair occupied and unoccupied

respectively.

Since the BCS state is not an eigenstate of the particle number $n(=a_\nu^\dagger a_\nu)$, one must add to the Hamiltonian a term λn (where λ is the chemical potential) in order to incorporate the condition that the average value of n is equal to the desired number of particles N. Thus one works with the Hamiltonian

$$H' = H - \lambda n = \sum_\nu \varepsilon_\nu a_\nu^\dagger a_\nu - G/4 \sum_{\mu\nu} (s_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger)(s_\nu a_{\bar{\nu}} a_\nu) , \qquad (2.4.10)$$

where $\varepsilon_\nu = \epsilon_\nu - \lambda$, the indices μ and ν include both positive and negative values. One may compute

$$\langle BCS|H'|BCS\rangle = \sum_\nu \varepsilon_\nu V_\nu^2 - G/4 \left(\sum_\nu U_\nu V_\nu\right)^2 . \qquad (2.4.11)$$

Carrying out the variation with respect to V_ν , i.e.

$$\frac{\delta}{\delta V_\nu} \langle BCS|H'|BCS\rangle = 0 ,$$

one finds

$$2\varepsilon_\nu V_\nu - G/2 \left(\sum_\nu U_\nu V_\nu\right)\left(U_\nu - \frac{V_\nu^2}{U_\nu}\right) = 0 . \qquad (2.4.12)$$

The solution to (2.4.12) is given by

$$V_\nu^2 = \tfrac{1}{2}\left(1 - \frac{\varepsilon_\nu}{E_\nu}\right) ,$$

$$U_\nu^2 = 1 - V_\nu^2 , \qquad (2.4.13)$$

where $E_\nu = (\varepsilon_\nu^2 + \Delta^2)^{1/2}$, (2.4.13a)

and $$\Delta = \frac{G}{2}\langle BCS|\sum_\nu a_\nu^\dagger a_\nu|BCS\rangle = \frac{G}{2}\sum_\nu U_\nu V_\nu . \qquad (2.4.14)$$

The Δ is called the gap parameter. Inserting U_ν and V_ν into

the above equation, one obtains the gap parameter equation

$$\sum_\nu 1/E_\nu = 4/G = \sum_\nu 1/(\varepsilon_\nu^2+\Delta^2)^{1/2} \quad . \tag{2.4.15}$$

Since we are treating even-even nuclei, the condition $\sum_\nu V_\nu^2=N$ gives the auxiliary condition

$$N=\tfrac{1}{2}\sum_\nu (1-\varepsilon_\nu/E_\nu) \quad . \tag{2.4.16}$$

If single-particle energies ϵ_ν are given, equations (2.4.15) and (2.4.16) are sufficient to determine λ and Δ, which in turn determine the wave function and energy for the ground state. From equations (2.4.13), one sees that single-particle energy levels with $\epsilon_\nu<\lambda$ are occupied with a probability V^2 of more than one-half. Levels with $\epsilon_\nu>\lambda$ are occupied with a probability of less than one-half, and those levels far above λ are almost empty. The gap parameters Δ measures the energy range over which the occupation probability V_ν^2 varies from approximately zero to approximately 1 . This is shown in Figure 2.4.1 .

Up to now, only the ground states of even-even nuclei have been discussed. For the odd-A nucleus, the lowest state is one of the one-quasi-particle states, i.e.

$$\psi_\nu^{odd} = \alpha_\nu^+ |BCS\rangle \quad . \tag{2.4.17}$$

Since ψ_ν^{odd} is built on the even-A nucleus ground state $|BCS\rangle$,

its energy should be

$$\langle BCS|\alpha_\nu H'\alpha_\nu^\dagger|BCS\rangle - \langle BCS|H'|BCS\rangle$$
$$= (\varepsilon_\nu^2+\Delta^2)^{1/2} = E_\nu^* = \text{quasi-particle energy} . \qquad (2.4.18)$$

This is the same form as equation (2.4.13a). The first excited state of the odd-A nucleus is also a one-quasi-particle state. It has the energy $E_\mu^* = (\varepsilon_\mu^2 + \Delta^2)^{1/2}$, where μ is different from ν. Thus for odd-A nuclei, the difference in energy between the first excited state and the ground state is $\left[(\varepsilon_\nu^2+\Delta^2)^{1/2}-(\varepsilon_\mu^2+\Delta^2)^{1/2}\right] < \Delta$. This shows that in odd-A nuclei, there is no large energy gap in the vicinity of the ground state.

Similary, the first excited state of the even-A nucleus has two unpaired particles. The wave function can be written as follows:

$$\psi_{\mu\nu}^{even} = \alpha_\mu^\dagger \alpha_\nu^\dagger |BCS\rangle \quad . \qquad (2.4.19)$$

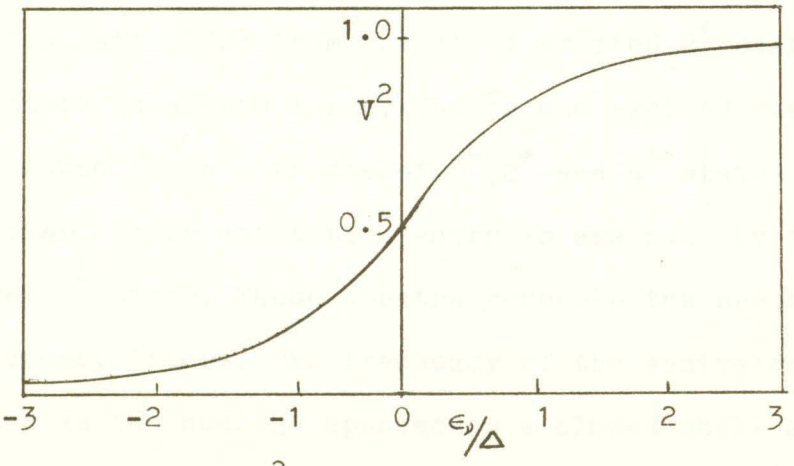

Figure 2.4.1 V_ν^2 as a function of ϵ_ν relative to the Fermi energy.

Thus there are two quasi-particles in the first excited state of even-A nuclei. The difference in energy between the first excited state and the ground state is $(\varepsilon_\nu^2+\Delta^2)^{1/2}+(\varepsilon_\mu^2+\Delta^2)^{1/2} > 2\Delta$. This shows that the minimum excitation energy is approximately 2Δ, that is, the spectrum will have the character of a ground state separated by an energy gap of 2Δ from a group of lowest excited states.

As mentioned before, the $|BCS\rangle$ is not an eigenfunction of N. States that are not eigenstates of N give rise to spurious components in excited states, i.e. components which would not exit if the particle number were fixed.

2.5 Collective vibrational motion of spherical nuclei; Tamm-Dancoff (TD) and Random Phase Approximations (RPA).

Experimental data (Scharff et al. 1955) show that all the even-even, spherical and non-closed shell nuclei have a 0^+ ground state and a 2^+ first excited state. The electric quadrupole transition rate B(E2) from the first excited 2^+ state to the ground state is always large. The second excited states are usually found to be a triplet of $0^+, 2^+$ and 4^+ states in these even-even nuclei. Their excitation energies are roughly twice that of the first 2^+ state. These spectra resemble the spectra of harmonic oscillators. The frequency of the equivalent oscillator increases as the nucleus approaches a closed shell structure and the oscillator-like spectrum disappears at magic numbers. An explanation of the above characteristic of the spectra is that

these excited states with almost equal spacings are due to a surface vibration of the nucleus, and the first and second excited states are refered to as one-phonon and two-phonon states respectively. Since a quadrupole phonon has an energy $\hbar\omega$ and an angular momentum 2, the first excited state should have a corresponding excitation energy and angular momentum. The two-phonon states in this approximation should have an energy of $2\hbar\omega$ and angular momentum of 0,2 and 4. From a microscopic point of view, the vibration is produced by correlated single-particle motions, and therefore the excited states can be represented as a coherent superposition of single-particle excitations.

On the other hand, another group of nuclei, such as O^{16}, C^{12}, Pb^{208} etc., shows vibrational excited states with negative parities. Well-known examples of odd-parity vibrational states are the giant dipole states (at $\approx$ 22.4 and 24.5 MeV for O^{16}) excited by the absorption of dipole gamma rays, and the octupole states seen at much lower energy (at 6.14 MeV for O^{16}) in inelastic proton scattering and other inelastic scattering with various projectiles (see Spicer, 1969). An explanation of these odd-parity vibrations is that the excited state can be obtained by lifting a particle from a closed shell to the next shell at an energy around $\hbar\omega$, where $\hbar\omega$ is the distance between two successive major shells, leaving a hole below the Hartree-Fock Fermi surface. That is, one would produce excited states by particle-hole excitations.

In order to deal with such collective vibrational motion of spherical nuclei, many approximations have been developed, such as the Tamm-Dancoff (TD) approximation and the Random Phase Approximation (RPA). The following is a brief and formal description of the TD and RPA approximations.

In the TD approximation, the Hartree-Fock wave function is accepted as the ground state and then the basis for excited states can be set up by taking all particle-hole configurations. The unperturbed particle-hole state of definite angular momentum J can be written as

$$|mi\rangle = \sum_{m_m m_i} (-)^{j_i - m_i} \langle j_m m_m j_i - m_i | JM \rangle a^{\dagger}_{j_m m_m} a_{j_i m_i} |HF\rangle \quad , \quad (2.5.1)$$

where $\langle j_m m_m j_i - m_i | JM \rangle$ are Clebsch-Gordan coefficients, the phase factor $(-)^{j_i - m_i}$ effectively converts a hole into a particle for the purpose of a proper transformation under rotation, and $|HF\rangle$ is the Hartree-Fock ground state. In this section, m and n label particle states, i and j label hole states.

By diagonalizing the Hamiltonian (2.2.3) between particle-hole states (2.5.1), the eigenvalues and eigenstates can be obtained. Each eigenstate thus obtained is a superposition of the basis particle-hole states, i.e.

$$|\hbar\omega\rangle = \sum_{mi} X_{mi} a^{\dagger}_m a_i |HF\rangle \quad , \quad (2.5.2)$$

in which the excitation energy is $\hbar\omega$. Indices m and i stand for all the quantum numbers of the particle- and hole- states

respectively.

The eigenstate (2.5.2) can be obtained by solving the set of equations

$$(\varepsilon_m - \varepsilon_i) X_{mi} + \sum_{nj} [\langle jm|V|ni\rangle - \langle jm|V|in\rangle] X_{nj} = \omega X_{mi} \quad , \quad (2.5.3)$$

where ε_m and ε_i are Hartree-Fock single-particle energies.

On the other hand, the multipole transition amplitude between the Hartree-Fock ground state and the excited eigenstate is given by the matrix element

$$\langle \hbar\omega | \delta H | HF \rangle = \sum_{mi} X_{mi} D_{mi} \quad , \quad (2.5.4)$$

where δH is the multipole interaction and $D_{mi} = \langle m|\delta H|i\rangle$.

The TD approximation works well in calculating the odd-parity states of O^{16} (Elliott et al. 1957). Fits to the experimental energies and lifetimes are good. The major deficiency in the case of O^{16} is that the predicted transition probability of the octupole 3^- state is still a factor of 3 to 6 below the experimental one. This indicates that the TD description does not give sufficient collectiveness to the 3^- state and that a further development is necessary.

In the TD approximation, the basic idea is that the ground state can be a pure Hartree-Fock ground state and the excited state is a superposition of particle-hole excitations. The RPA assumes instead that if there are particle-hole pairs in the ground states of nuclei, then the excited state can be obtained

either by creating a particle-hole pair or by annihilating a particle-hole pair. The latter would correspond to one of the particles dropping down to one of the holes in the process of absorbing the radiation. Thus the physical ground state is not a Hartree-Fock ground state but has some correlation built into it.

In order to see how the collective vibration arises out of the formalism, one looks for operators $O_\mu^\dagger$ with the following property

$$[H, O_\mu^\dagger] = \omega_\mu O_\mu^\dagger \quad . \tag{2.5.5}$$

Let the ground state of the nucleus be $|0\rangle$. With the property (2.5.5), one has

$$[H, O_\mu^\dagger]|0\rangle = H O_\mu^\dagger |0\rangle = \omega_\mu O_\mu^\dagger |0\rangle \quad , \tag{2.5.6}$$

where one chooses the ground state energy $E_0 = 0$, i.e. $H|0\rangle = 0$. The $O_\mu^\dagger|0\rangle$ is, therefore, the one-phonon excited state with energy ω_μ and $O_\mu^\dagger O_\nu^\dagger|0\rangle$ would correspond to a two-phonon excited state. From the equation (2.5.5) and (2.5.6), one sees that the operator $O_\mu^\dagger$ generates a harmonic spectrum.

With correlated particle-hole pairs in ground state, the operator $O_\mu^\dagger$ in RPA is assumed to be of the form

$$O^\dagger = \sum_{mi} (X_{mi} a_m^\dagger a_i - Y_{mi} a_i^\dagger a_m) \quad . \tag{2.5.7}$$

Whereas $a_m^\dagger a_i$ creates a particle-hole pair, $a_i^\dagger a_m$ annihilates

one, so that the excited state can be reached in two ways. The ground state $|0\rangle$ is defined by requiring $Q_\mu|0\rangle = 0$ for all μ .

The Hamiltonian of the nuclear system as given by equation (2.2.3) is

$$H = \sum_{\alpha\beta} \langle\alpha|T|\beta\rangle a_\alpha^\dagger a_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|V|\delta\gamma\rangle a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \quad . \quad (2.5.8)$$

Substituting equation (2.5.8) into the commutator $[H, a_i^\dagger a_m]$ and expanding it, one obtains terms with 2 operators and 4 operators, a form of $C_{1234}a_1^\dagger a_2^\dagger a_3 a_4$. In order to linearize the expansion of the commutator, term $C_{1234}a_1^\dagger a_2^\dagger a_3 a_4$ with 4 operators is replaced by the following combination,

$$C_{1234}\left\{\langle a_2^\dagger a_3\rangle a_1^\dagger a_4 - \langle a_1^\dagger a_3\rangle a_2^\dagger a_4 - \langle a_2^\dagger a_4\rangle a_1^\dagger a_3 + \langle a_1^\dagger a_4\rangle a_2^\dagger a_3\right\} ,$$

where the expectation values $\langle\ \rangle$ are taken with respect to the Hartree-Fock ground state. Thus the expansion of (2.5.5) contains only particle-hole terms, such as $a_n^\dagger a_j$ and $a_j^\dagger a_n$.

After rearranging various terms, one has the following commutator

$$[H, a_m^\dagger a_i] = (\varepsilon_m - \varepsilon_i)a_m^\dagger a_i + \sum_{nj}\left[\langle ni|V|jm\rangle - \langle in|V|jm\rangle\right]a_n^\dagger a_j$$
$$+ \sum_{nj}\left[\langle ij|V|mn\rangle - \langle ji|V|mn\rangle\right]a_j^\dagger a_n \quad , \quad (2.5.9)$$

where ε_m and ε_i are the Hartree-Fock single-particle energies.

By taking the matrix element of (2.5.9) between the one-phonon state and $|0\rangle$, and making a further approximation that

the particle-hole operators $A^{+}_{mi}=a^{+}_{m}a_{i}$ satisfy the Boson commutation rule:

$$[A^{\dagger}_{mi}, A^{\dagger}_{nj}] = 0 = [A_{mi}, A_{nj}] \quad ,$$

$$[A^{\dagger}_{mi}, A_{nj}] = \delta_{mn}\delta_{ij} \quad , \qquad (2.5.10)$$

one obtains

$$(\varepsilon_m-\varepsilon_i)X_{mi} + \sum_{nj}[\langle jm|v|ni\rangle - \langle jm|v|in\rangle]X_{nj}$$

$$+ \sum_{nj}[\langle mn|v|ij\rangle - \langle mn|v|ji\rangle]Y_{nj} = \omega X_{mi} \quad . \qquad (2.5.11)$$

Similarly, the matrix element of the commutator $[H, a^{\dagger}_{i}a_{m}]$ leads to

$$(\varepsilon_m-\varepsilon_i)Y_{mi} + \sum_{nj}[\langle ni|v|jm\rangle - \langle in|v|jm\rangle]Y_{nj}$$

$$+ \sum_{nj}[\langle ij|v|mn\rangle - \langle ji|v|mn\rangle]X_{nj} = -\omega Y_{mi} \quad . \qquad (2.5.12)$$

Obviously, if there were no correlation built into the Hartree-Fock ground state, we would have $Y_{nj}=0$, and the equation (2.5.11) would be reduced to the TD equation (2.5.3).

The transition amplitude can be obtained in the form

$$D = \langle \hbar\omega|\delta H|0\rangle = \sum_{mi} D_{mi}(X_{mi}+Y_{mi}) \quad . \qquad (2.5.13)$$

One sees that the equation (2.5.13) is defferent from the TD result (2.5.4). The presence of the ground state correlation increases the transition amplitude if the Y_{mi}'s have the same phase as the X_{mi}'s.

CHAPTER 3

SELF-CONSISTENT CORE-PARTICLE COUPLING MODEL FOR ODD-MASS NUCLEI

3.1 Equations of motion (Generalized Hartree-Fock Approximation)

The generalized Hartree-Fock formalism used in this calculation originates from the work of Kerman and Klein (1963), in which a general discussion of the method can be found. A formalism slightly modified from the original form so as to facilitate the application on spherical nuclei is presented in the following.

The Hamiltonian which represents the interactions between the shell model particles with the pairing-plus-quadrupole force can be written (see preceding Chapter) in the second quantization form:

$$H=\sum_{\alpha i}\epsilon_{\alpha i}a^{\dagger}_{\alpha i}a_{\alpha i}-\frac{1}{4}\sum_{\alpha\beta i}G_i\left(s_\alpha a^{\dagger}_{\alpha i}a^{\dagger}_{\bar{\alpha} i}\right)\left(s_\beta a_{\bar{\beta} i}a_{\beta i}\right)$$

$$-\frac{1}{2}\sum_{ij}\chi_{ij}\sum_{\alpha\beta\gamma\delta}\langle\alpha i|r^2Y_{2q}|\delta i\rangle\langle\gamma j|r^2Y_{2q}|\beta j\rangle a^{\dagger}_{\alpha i}a^{\dagger}_{\gamma j}a_{\delta j}a_{\delta i}\ , \qquad (3.1.1)$$

where i and j label both protons and neutrons, $\alpha=(n,l_a,j_a,m_\alpha)$, $\bar{\alpha}=-\alpha=(n,l_a,j_a,-m_\alpha)$, $\bar{\beta}=-\beta$, $s_\alpha=(-)^{j_a-m_\alpha}$. G_i and χ_{ij} are the pairing and quadrupole force constants of neucleons respectively. $\epsilon_{\alpha i}$ is the single particle energy.

For the harmonic oscillator wave functions, the following definitions can be made,

$$\langle \alpha_i | r^2 Y_{2q} | \beta_i \rangle = S_\beta \langle j_a j_b m_\alpha \bar{m}_\beta | 2 q \rangle \langle \alpha_i \| r^2 Y_2 \| \beta_i \rangle / \sqrt{5}$$
$$= S_\beta \langle j_a j_b m_\alpha \bar{m}_\beta | 2 q \rangle \nu_i (5/4\pi)^{1/2} F_i(ab) ,$$

$$\text{i.e.} \quad F_i(ab) = \nu_i^{-1} (5/4\pi)^{-1/2} \langle \alpha_i \| r^2 Y_2 \| \beta_i \rangle / \sqrt{5} , \qquad (3.1.2)$$
$$\nu_i = (N_i + 3/2) \hbar / M\omega_0 ,$$

where ω_0 is the harmonic-oscillator frequency, $\hbar\omega_0 \simeq 41/A^{1/3}$ MeV (Bes and Sorensen, 1969), M is the nucleon mass and N is the principal quantum number of the shell considered. Then the quadrupole operator can be written in the form,

$$Q_q^{i\dagger} = \sum_{\alpha\beta} \nu_i^{-1} \left(\frac{4\pi}{5}\right)^{1/2} \langle \alpha_i | r^2 Y_{2q} | \beta_i \rangle a^\dagger_{\alpha i} a_{\beta i}$$
$$= \sum_{\alpha\beta} F_i(ab) S_\beta \langle j_a j_b m_\alpha \bar{m}_\beta | 2 q \rangle a^\dagger_{\alpha i} a_{\beta i} . \qquad (3.1.3)$$

By using the previous definitions (3.1.2), the fermion anticommutation rule (2.2.4) of the creation and annihilation operators $a^\dagger_\alpha$ and a_α, the Wigner Eckart Theorem and the properties of the Clebsch-Gordon and Racah coefficients (Appendix), the Heisenberg equations of motion can be obtained from (3.1.1). They can be simplified to the following useful form:

$$[a_{\alpha i}, H] = (\epsilon_{\alpha i} + 2F_{ai}) a_{\alpha i} - \tfrac{1}{2} G_i S_\alpha a_{\bar{\alpha} i} \left(\sum_\beta S_\beta a_{\beta i} a_{\bar{\beta} i}\right)$$
$$- \chi_i \sum_{\beta q} F_i(ab) S_\beta \langle j_a j_b m_\alpha \bar{m}_\beta | 2 q \rangle a_{\beta i} \Lambda^i_q , \qquad (3.1.4)$$

$$[a^\dagger_{\bar{\alpha} i}, H] = -(\epsilon_{\bar{\alpha} i} - G_i) a^\dagger_{\bar{\alpha} i} - \tfrac{1}{2} G_i S_\alpha a_{\alpha i} \left(\sum_\beta S_\beta a^\dagger_{\beta i} a^\dagger_{\bar{\beta} i}\right)$$
$$+ \chi_i \sum_{\beta q} F_i(ab) S_\alpha \langle j_a j_b m_\alpha \bar{m}_\beta | 2 q \rangle a^\dagger_{\beta i} \Lambda^i_q , \qquad (3.1.5)$$

where
$$F_{ai} = \tfrac{1}{2} \chi_i \sum_\beta 5 F_i^2(ab) / 2\Omega_a ,$$
$$2\Omega_a = 2 j_a + 1 ,$$

$$\Lambda^{i}_{q} = Q^{i}_{q} + X^{i}_{np}\, Q^{i'}_{q} \quad , \quad i \neq i' \quad ,$$

$$X^{i}_{np} = X_{np} / X_{i} \quad ,$$

$$X_{ij} = (5/4\pi)\, v_i v_j \chi_{ij} \quad . \qquad (3.1.6)$$

In order to find the eigenvalues and eigenvectors of the Hamiltonian, i.e. the energy levels and state vectors of the nucleus, we must express the Hamiltonian in a matrix representation and diagonalize it. The major endeavor is to extract information from the selected matrix elements of (3.1.4) and (3.1.5) and from the associated normalization and consistency conditions.

The matrix elements of (3.1.4) between the states $|IMS(A)\rangle$ of the even nucleus with A particles and those $|J\bar{\mu}\nu(A-1)\rangle$ of the intervening odd nucleus with (A-1) particles are:

$$\langle J\bar{\mu}\nu(A-1)|[a_{\alpha i}, H]|IMS(A)\rangle = [W_{IS}(A) - W_{J\nu}(A-1)]\langle J\bar{\mu}\nu(A-1)|a_{\alpha i}|IMS(A)\rangle$$

$$= h_{\alpha i} + 2F_{ai}\langle J\bar{\mu}\nu(A-1)|a_{\alpha i}|IMS(A)\rangle - \tfrac{1}{2}G_i S_\alpha \times$$

$$\sum_n \langle J\bar{\mu}\nu(A-1)|a^{+}_{\alpha i}|n(A-2)\rangle\langle n(A-2)|\sum_\beta S_\beta a_{\beta i}\, a_{\bar{\beta} i}|IMS(A)\rangle$$

$$- X_i \sum_{\beta q} F_i(ab) S_\beta \langle j_a j_b m_\alpha \bar{m}_\beta | 2q\rangle \sum_n \langle J\bar{\mu}\nu(A-1)|a_{\beta i}|n(A)\rangle \times$$

$$\langle n(A)|\Lambda^{i}_{q}|IMS(A)\rangle \quad ,$$

where the closure property $\sum_n |n(A)\rangle\langle n(A)| = 1$ has been used. Generally, the sum over n should cover all contributing intermediate states. In the present case, n is limited by the fact that $\sum_\alpha S_\alpha a_{\bar{\alpha} i}\, a_{\alpha i}$ carries zero angular momentum and the other operator Λ^{i}_{q} carries an angular momentum 2. The W's are the total energies.

After rearrangement, one gets the final form:

$$\left(W_{IS}(A)-W_{IS}(A-1)-h_{\alpha i}-2F_{\alpha i}\right)\langle J\bar{\mu}\nu(A-1)|a_{\alpha i}|IMS(A)\rangle$$
$$=-\tfrac{1}{2}G_i S_\alpha \sum_n \langle J\bar{\mu}\nu(A-1)|a^+_{\bar{\alpha}i}|n(A-2)\rangle\langle n(A-2)|\sum_\beta S_\beta a_{\beta i}a_{\bar{\beta}i}|IMS(A)\rangle$$
$$-X_i\sum_{\beta q}F_i(ab)S_\beta\langle j_a j_b m_\alpha\bar{m}_\beta|2q\rangle\sum_n\langle J\bar{\mu}\nu(A-1)|a_{\beta i}|n(A)\rangle\times$$
$$\langle n(A)|\Lambda^i_q|IMS(A)\rangle\ . \qquad (3.1.7)$$

Similarly, the martix element of (3.1.5) between the state $|IMS(A-2)\rangle$ of the even nucleus and the intervening states $|J\bar{\mu}\nu(A-1)\rangle$ of the odd nucleus is

$$\left(W_{IS}(A-2)-W_{J\nu}(A-1)+h_{\alpha i}-G_T\right)\langle J\bar{\mu}\nu(A-1)|a^+_{\bar{\alpha}i}|IMS(A-2)\rangle$$
$$=-\tfrac{1}{2}G_i S_\alpha\sum_n\langle J\bar{\mu}\nu(A-1)|a_{\alpha i}|n(A)\rangle\langle n(A)|\sum_\beta S_\beta a^+_{\beta i}a^+_{\bar{\beta}i}|IMS(A)\rangle$$
$$+X_i\sum_{\beta q}F_i(ab)\langle j_a j_b m_\alpha\bar{m}_\beta|2q\rangle\sum_n\langle J\bar{\mu}\nu(A-1)|a^+_{\bar{\beta}i}|n(A-2)\rangle\times$$
$$\langle n(A-2)|\Lambda^i_q|IMS(A-2)\rangle\ . \qquad (3.1.8)$$

The derivation of the equations of motion of our core-particle coupling model (CPCM) is based on the definition of the relevant coefficients of fractional parentage (cfp). The cfp of one-body operators are

$$\Psi_{J\mu\nu}(\alpha,IMS)=\langle J\bar{\mu}\nu(A-1)|a_\alpha|IMS(A)\rangle\ , \qquad (3.1.9)$$

$$\Phi^*_{J\mu\nu}(\bar{\alpha},IMS)=\langle J\bar{\mu}\nu(A-1)|a^+_{\bar{\alpha}}|IMS(A-2)\rangle\ , \qquad (3.1.10)$$

which connect the states of the A or (A-2)-nucleon system with those of the intervening (A-1)-nucleon system.

By using these cfp and inserting the states of the intervening even nuclei $|I'M'S'(A)\rangle$ and odd nuclei $|J'\mu'\nu'(A-1)\rangle$ into (3.1.7) and (3.1.8), and using the closure properties $\sum_{I'M'} |I'M'S'\rangle\langle I'M'S'| = 1$ and $\sum_{J'\mu'} |J'\mu'\nu(A-1)\rangle\langle J'\mu'\nu'(A-1)| = 1$, one obtains the form:

$$
\begin{aligned}
&\left[W_{IS}(A-2) - W_{J\nu}(A-1) + h_{\alpha i} - G_i\right] \Phi^{i\,*}_{J\bar{\mu}\nu}(\bar{\alpha}, IMS) \\
&= -\tfrac{1}{2} G_i S_\alpha \sum_{S'} \Big[\sum_{J'\mu'\nu'\beta} \Psi^{i\,*}_{J'\bar{\mu}'\nu'}(\beta, IMS') \, \Phi^{i\,*}_{J'\mu'\nu'}(\bar{\beta}, IMS') \Big] \Psi^{i}_{J\bar{\mu}\nu}(\bar{\alpha}, IMS') \\
&\quad - \sum_{\substack{I'M'S' \\ q\beta}} \Big(\sum_j X_{ij} \sum_{\gamma\delta} F_j(cd) S_\delta \langle j_c j_d m_\gamma \bar{m}_\delta | 2 q \rangle \sum_{J'\mu'\nu'} \Phi^{j}_{J'\mu'\nu'}(\gamma, I'M'S') \\
&\quad \times \Phi^{j\,*}_{J'\mu'\nu'}(\delta, IM) \Big] F_i(ab) S_\alpha \langle j_a j_b m_\alpha \bar{m}_\beta | 2 q \rangle \Phi^{i\,*}_{J\bar{\mu}\nu}(\bar{\beta}, I'M'S') \,,
\end{aligned}
\tag{3.1.11}
$$

$$
\begin{aligned}
&\left[W_{IS}(A) - W_{J\nu}(A-1) - h_{\alpha i} - 2F_{\alpha i}\right] \Psi^{i}_{J\mu\nu}(\alpha, IMS) \\
&= -\tfrac{1}{2} G_i S_\alpha \sum_{S'} \Big[\sum_{J'\mu'\nu'\beta} S_\beta \, \Phi^{i}_{J'\mu'\nu'}(\bar{\beta}, IMS') \Psi^{i}_{J'\mu'\nu'}(\beta, IMS') \Big] \Phi^{i\,*}_{J\mu\nu}(\bar{\alpha}, IMS') \\
&\quad - \sum_{\substack{I'M'S' \\ q\beta}} \Big(\sum_j X_{ij} \sum_{\gamma\delta} F_j(cd) S_\delta \langle j_c j_d m_\gamma \bar{m}_\delta | 2 q \rangle \sum_{J'\mu'\nu'} \Psi^{j\,*}_{J'\mu'\nu'}(\delta, I'M'S') \\
&\quad \times \Psi^{j}_{J'\mu'\nu'}(\gamma, IMS') \Big] F_i(ab) S_\beta \langle j_a j_b m_\alpha \bar{m}_\beta | 2 q \rangle \Psi^{i}_{J\mu\nu}(\beta, I'M'S') \,.
\end{aligned}
\tag{3.1.12}
$$

From the fermion anticommutation rule $\{a^{\dagger}_{\alpha i}, a_{\beta i}\} = \delta_{\alpha\beta}$, one obtains the exact normalization condition:

$$\begin{aligned}
&\langle I'M'S'(A)|\{a^{\dagger}_{\alpha i}, a_{\beta i}\}|IMS(A)\rangle \\
&= \sum_{J\mu\nu}\left[\psi^{i\,*}_{J\mu\nu}(\alpha, I'M'S')\,\psi^{i}_{J\mu\nu}(\beta, IMS) + \varphi^{i}_{J\mu\nu}(\beta, I'M'S')\,\varphi^{i\,*}_{J\mu\nu}(\alpha, IMS)\right] \\
&= \delta_{\alpha\beta}\,\delta_{II'}\,\delta_{MM'}\,\delta_{SS'} \quad ,
\end{aligned} \tag{3.1.13}$$

where $\varphi^{i\,*}_{J\mu\nu}(\alpha, IMS) = \langle J\bar{\mu}\nu(A+1)|a^{\dagger}_{\alpha i}|IMS(A)\rangle$ are the cfp connecting the A-nucleon state with the (A+1)-nucleon state. In the number non-conserving approximation, we assume that

$$\langle J\bar{\mu}\nu(A+1)|a^{\dagger}_{\alpha i}|IMS(A)\rangle \cong \langle J\bar{\mu}\nu(A-1)|a^{\dagger}_{\alpha i}|IMS(A-2)\rangle \quad , \tag{3.1.14}$$

and one reduces (3.1.14) to the following form

$$\begin{aligned}
&\sum_{J\mu\nu}\left[\psi^{i\,*}_{J\mu\nu}(\alpha, I'M'S')\,\psi^{i}_{J\mu\nu}(\beta, IMS) + \phi^{i}_{J\mu\nu}(\beta, I'M'S')\,\phi^{i\,*}_{J\mu\nu}(\alpha, IMS)\right] \\
&\cong \delta_{\alpha\beta}\,\delta_{II'}\,\delta_{MM'}\,\delta_{SS'} \quad .
\end{aligned} \tag{3.1.15}$$

Equation (3.1.15) can be used to normalize the ψ's and ϕ's in the equations of motion.

The matrix element of the number operator $N = \sum_{\alpha} a^{\dagger}_{\alpha i} a_{\alpha i}$ is

$$\langle IMS(A)|\sum_{\alpha} a^{\dagger}_{\alpha i} a_{\alpha i}|IMS(A)\rangle = \sum_{J\mu\nu}|\psi^{i}_{J\mu\nu}(\alpha, IMS)|^2 = A_i \quad , \tag{3.1.16}$$

where A_i is the number of extra core particles.

Up to now, the **only** approximation is equation (3.1.14).. Equations (3.1.11) and (3.1.12) constitute a set of nonlinear equations for the amplitudes ψ and ϕ and the energies

W(A-1). The equation (3.1.15) serves as a normalization condition and (3.1.16) as a condition to determine λ_i which shall be explained later.

The equations (3.1.11) and (3.1.12) can be reduced to rotatationally invariant forms by introducing the reduced cfp u and v as follows:

$$\Psi^{i}_{J\mu\nu}(\alpha, IMS) = S_{\alpha} \langle I\, j_a\, M\, \bar{m}_{\alpha} | J\mu \rangle V^{i}_{J\nu}(j_a, IS), \qquad (3.1.17)$$

$$\Phi^{i\,*}_{J\mu\nu}(\bar{\alpha}, IMS) = \langle I\, j_a\, M\, \bar{m}_{\alpha} | J\mu \rangle U^{i}_{J\nu}(j_a, IS), \qquad (3.1.18)$$

where u^{i}_{J} and v^{i}_{J} are independent of the projection quantum numbers m and M, that is, they are rotational invariants.

With the following definitions, a set of simple non-linear equations of motion of the reduced cfp can be obtained:

$$\begin{aligned}
e_{J\nu} &= W_0(A) - W_{J\nu}(A-1) \ , \\
E_{J\nu i} &= -e_{J\nu} + \lambda^{i}_{1} \ , \\
\omega_I(A) &= W_I(A) - W_0(A) \ , \\
2\lambda(A) &= W_0(A) - W_0(A-2) \ , \\
2\lambda^{i}_{1}(A) &= 2\lambda(A) + G_i \ , \\
\epsilon_{\alpha i} &= h_{\alpha i} + F_{\alpha i} - \lambda^{i}_{1} \ , \qquad (3.1.19)
\end{aligned}$$

where $\omega_I(A) = W_I(A) - W_0(A)$ is the excitation energy of state I

λ_1^i is the chemical potential and $h_{\alpha i}$ is the single particle energy. Thus (3.1.11) and (3.1.12) are reduced to the simple form:

$$E^i_{J\nu} V^i_{J\nu}(aIS) = (\omega_I(A) + \lambda_1^i - 2F_{\alpha i} - h_{\alpha i}) V^i_{J\nu}(aIS) - \sum_{I'bS'} \Lambda^i_J(aIS, bI'S') V^i_{J\nu}(bI'S') + \sum_{S'} \Delta^i(IS, I'S') U^i_{J\nu}(aIS) \quad , \qquad (3.1.20)$$

$$E^i_{J\nu} U^i_{J\nu}(aIS) = (\omega_I(A-2) - \lambda_1^i + h_{\alpha i}) U^i_{J\nu}(aIS) + \sum_{bI'S'} \Lambda^i_J(aIS, bI'S') U^i_{J\nu}(bI'S') + \sum_{S'} \Delta^i(IS, I'S') V^i_{J\nu}(aIS') \quad , \qquad (3.1.21)$$

where

$$\Delta^i(IS, I'S') = G/2 \sum_{J'\nu'} \left(\frac{2J'+1}{2I+1}\right) U^{i\,*}_{J'\nu'}(bIS) V^i_{J'\nu'}(bIS) \, ,$$

$$\Lambda^i_J(aIS, bI'S') = -5 \sum_j X_{ij} \Gamma_j(IS, I'S') F_i(ab) (-)^{J-b} W(II'ab; 2J) \, ,$$

$$\Gamma_j(IS, I'S') = \sum_{J'\nu' cd} (-)^{J'-d} (2J'+1) W(II'cd; 2J') \times F_j(cd) V^{j\,*}_{J'\nu'}(cIS) V^j_{J'\nu'}(dIS') \, ,$$

W(II′ab;2J) and W(II′cd; 2J′) are the Racah coefficients (see Appendix). (3.1.22)

The normalization condition (3.1.15) and the matrix element of the number operator can be written in the following forms:

$$\sum_{\nu} V^{i}_{J\nu}(aI'S')\, V^{i}_{J\nu}(bIS) - \sum_{J'\nu'} (2J'+1) W(IabI'; J'J) \times U^{i}_{J'\nu'}(bI'S')\, U^{i}_{J'\nu'}(aIS) \cong \delta_{ab}\,\delta_{II'}\,\delta_{SS'} \quad , \tag{3.1.23}$$

$$\sum_{J\nu a} \left(\frac{2J+1}{2I+1}\right) V^{i}_{J\nu}(aIS)\, V^{i}_{J\nu}(aIS) = A_i(I) \quad . \tag{3.1.24}$$

If we replace $\omega_{Is}(A-2)$ in equation (3.1.21) by $\omega_{Is}(A)$ then the equations (3.1.20) through (3.1.22) determine the eigenvalues $E^{i}_{J\nu}$ and the cfp $U^{i}_{J\nu}(aIS)$, $V^{i}_{J\nu}(aIS)$ up to normalization factors.

3.2 E2 transition probability from the ground state to the first excited 2^+ state

Recall that the quadrupole operator is defined as (3.1.3)

$$Q^{i\dagger}_{q} = \sum_{\alpha\beta} \nu_i^{-1} \left(\frac{4\pi}{5}\right)^{1/2} \langle \alpha_i | r^2 Y_{2q} | \beta_i \rangle\, a^{\dagger}_{\alpha i} a_{\beta i}$$

$$= \sum_{\alpha\beta} F_i(ab)\, \delta_{\beta} \langle j_a j_b m_\alpha \bar{m}_\beta | 2q \rangle\, a^{\dagger}_{\alpha i} a_{\beta i} \quad . \tag{3.1.3}$$

The ordinary shell-model definition of the E2 transition probability is

$$B(E2; I \to I') = (2I+1)^{-1} \sum_{iMM'q} \left| \langle I'M'S'(A) | e_i \sum_{\alpha\beta} \langle \alpha_i | r^2 Y_{2q} | \beta_i \rangle\, a^{\dagger}_{\alpha i} a_{\beta i} | IMS(A) \rangle \right|^2 \tag{3.2.1}$$

where e_i is the effective charge (more details in section 4.3) of

the nucleon that takes part in the transition. From (3.1.3), we have

$$B(E2;I\to I') = (2I+1)^{-1}\sum_{M'Mq i} e_i^2 \nu_i^2 \left(\frac{5}{4\pi}\right)|\langle I'M'S'|Q_q^{i\dagger}|IMS\rangle|^2 \quad . \quad (3.2.2)$$

Inserting the states $|J'\mu'\nu'\rangle$ of the intervening odd nucleus, and using the reduced cfp as defined in equations (3.1.17) and (3.1.18), one finds

$$\begin{aligned}
&\langle I'M'S'(A)|Q_q^{i\dagger}|IMS(A)\rangle \\
&= \sum_{\alpha\beta i} \nu_i^{-1}(4\pi/5)^{1/2}\langle\alpha i|r^2 Y_{2q}|\beta i\rangle \sum_{J\mu\nu}\langle I'M'S'(A)|a_{\alpha i}^{+}|J\bar{\mu}\nu(A-1)\rangle \\
&\quad\times\langle J\mu\nu(A-1)|a_{\beta i}|IMS(A)\rangle \\
&= (-)^{q-I}\sqrt{5}/(2I+1)^{1/2}\,\Gamma_i(IS,I'S')\langle I'2M'\bar{q}|IM\rangle \quad , \quad (3.2.3)
\end{aligned}$$

where the self-consistent $\Gamma_i(IS,I'S')$ is given by (3.1.22). Equation (3.2.1) can be written:

$$B(E2;I\to I') = 5/(2I+1)\sum_i \Gamma_i^2 e_i \sum_{MM'q}\langle I'2M\bar{q}|IM\rangle^2 \nu_i^2 \frac{5}{4\pi} \ ,$$

$$\therefore \quad B(E2;0^+\to 2^+) = \frac{25}{4\pi}\sum_i e_i^2 \nu_i^2 \Gamma_i^2 \quad . \quad (3.2.4)$$

The equation (3.1.20) through (3.1.24) and (3.2.4) are the main formulas used in Chapter 4.

3.3 The self-consistent core-particle (core-hole) coupling model

A useful model to describe the low-lying states of odd-mass nuclei of mass number A+1 is to consider the state formed by coupling a particle to the core of an even-even nucleus of mass

number A. Thus the ground state of the odd nucleus will be obtained by putting the odd nucleon in the lowest allowed orbit of the average potential created by the ground state core of the even-even nucleus. Excited states of the odd nucleus will be obtained either by lifting the odd nucleon to a higher single-particle orbit or by exciting the core, or both. The core excitation may produce an excited state lower than that produced by the particle excitation if the next single-particle state is high compared with the core excitation energy, which is often the case if the core has a collective mode of excitation. The validity of such core-particle coupling model has been demonstrated by several previous work (Lawson et al. 1957; deShalit,1960).

Although the simple version of the core-particle coupling model described above is useful in a weak coupling limit, as the interaction between the odd particle and the core becomes stronger, it may become necessary to consider a mixing of several core-particle configurations due to the interaction. The intermediate core-particle coupling model based on such idea is used by Kisslinger and Sorensen (1963) to calculate the odd nuclear states of spherical nuclei, in which the ground, one-phonon and two-phonon states obtained from the RPA are considered as the cores.

The self-consistent core-particle coupling model used in this calculation emerges in a natural way when one looks at the equations of motion described in section 3.1. The cfp, $\langle J\mu\nu(A-1)|a^{\dagger}_{\alpha}|IMS(A-2)\rangle\left(\langle J\mu\nu(A-1)|a_{\alpha}|IMS(A)\rangle\right)$ describes the amplitude in

the state $|J\mu\nu(A-1)\rangle$ of the configuration of the core $|I_1M_1S(A-2)\rangle$ ($|I_1M_1S(A)\rangle$) coupled with a particle (hole) in a state α . The solution of the equations of motion gives $|J\mu\nu(A-1)\rangle$ as a superposition of these core-particle (core-hole) coupled states. However, unlike the conventional core-particle coupling model which assumes a fixed configuration for the core, the structure of the core is determined through the self-consistent calculation in our formalism. Thus the core in our model may be quite different from the one obtained in RPA as was demonstrated in a previous work (Dreizler et al. 1967). The first excited 2^+ state of a spherical nuclei appears to possess a large electric quadrupole moment in contrast with the almost zero value obtained in the RPA.

In the equations of motion, we have the intermediate sum $\sum_{I'M'S'} |I'M'S'\rangle\langle I'M'S'| = 1$ which in principle should include a complete set of even nuclear states. However, such formalism would not have any practical value unless we can approximate this sum by including only a few states. Fortunately, such approximation is possible for the low-lying states of spherical nuclei. As discussed in section 2.5, the experimental data show a large electric quadrupole transition rate between the ground and the one-phonon state, while the transition between the ground and the two-phonon states is neglible. From the preceding derivation (e.g. equation 3.2.3) one sees that both the quadrupole transition rate and the quadrupole moment are given by the self-consistent kernel $\Gamma(IS,I'S')$.

Therefore, in taking the intermediate sum over the even nuclear states, we may include only those states which are expected to yield a large self-consistent kernel $\Gamma(IS, I'S')$. For example, if the $|IMS\rangle$ is the ground 0^+ state of even nuclei, the first 2^+ state is the only important state in the intermediate sum. Similarly, if $|IMS\rangle$ is the first 2^+ state of even nuclei, the ground 0^+, the first 2^+ and the two-phonon triplet states $0^+, 2^+, 4^+$ are possibly important. However, it is reasonable to assume that the amplitudes $\langle J\mu\nu|a_\alpha^+|IMS\rangle$ between the low-lying states $|J\mu\nu(A-1)\rangle$ of odd nuclei, which are normally considered as one-quasi-particle states, and the two-phonon states $|IMS\rangle$ of even nuclei are small compared with others. Thus the omission of the two-phonon core states in the configuration would not affect much in the calculation of the low-lying states of odd nuclei. In such an approximation, the low-lying states of odd nuclei can be considered as a mixture of the ground state core and the 2^+ core of the adjacent even nuclei coupled with a particle or a hole. Of course, if one is interested in the higher excited states of odd nuclei, such as one-quasi-particle plus one-phonon states, the two-phonon states should be included as important cores, and future studies should be conducted along this direction.

Although the type of core-particle mixing considered in this calculation is similar to the one considered by Kisslinger and Sorensen (1963), the additional self-consistent feature of our

formalism should give a beter description of the nuclear states of spherical nuclei. It is worthwhile to point out that the Kisslinger and Sorensen's calculation fails to produce good agreement with the experiment for the odd-mass nickel isotopes.

CHAPTER 4

CALCULATION OF THE ODD MASS NICKEL ISOTOPES

The self-consistent core-particle (core-hole) coupling formalism described in Chapter 3 was used to calculate the ground and low excited states of the nickel isotopes. There are two reasons for choosing the nickel isotopes in this calculation. First, protons in the nickel isotopes form closed shells and therefore the calculation involves only those neutrons outside the closed shells. Second, several detailed calculations (Auerbach, 1967; Hsu and French,1965; Cohen et al. 1967) have been carried out on these isotopes, and it is possible to compare the results of this calculation with previous results to determine the validity of this approximation before applying this model to more complex nuclei.

In this calculation, only the two lowest states of even nuclei, 0^+ and 2^+, are included as the cores contributing to the low-energy states of odd nuclei. The single particle states included are $2p_{1/2}$, $2p_{3/2}$ and $1f_{5/2}$ for the neutrons. The $1g_{9/2}$ state which is known to lie in the same shell is not included because of its relatively high energy compared with the other three states, and also because of its different parity.

The choice of the cores and of the single-particle states mentioned above puts a limitation on the solution, so that only the three lowest levels of odd nuclei which are normally called

one-quasi-particle states can be well-represented by the solution of this calculation. The higher excited states of the odd nuclei may have considerable cfp linked to the higher excited states, particularly the two-phonon states, of even nuclei. Since these states are not included in this calculation, the solutions of this calculation corresponding to these higher excited states are not as reliable as the lower ones. These states may also be affected by the omission of the $1g_{9/2}$ single-particle state. However, if this method works well for the lower states at this stage of approximation, we would be able to obtain better results on the higher excited states by simply adding a few more cores, particularly the three so-called two-phonon states, or even adding the $1g_{9/2}$ state.

The details of the calculation are discussed presently.

4.1 Procedure of calculation

The procedure of the self-consistent calculation can be outlined as follows:

1) The two cores are the ground 0^+ and the one phonon 2^+ states. The single particle orbits are $2p_{1/2}$, $2p_{3/2}$ and $1f_{5/2}$. After having specified the single-particle states and the corresponding energy ϵ_α, one shooses an initial set of parameters Δ, Γ and chemical potential λ.

2) Solve the equations of motion (3.1.20) and (3.1.21) for the energy $E_{J\nu}$ and the reduced cfp $u_{J\nu}$ and $v_{J\nu}$.

3) The solutions of the equations of motion have a redundancy, and only a half of these solutions obtained are real physical ones. The physical solutions are chosen by the following criteria:

$$(E_{J\nu} - \omega_I)_{\text{physical}} > (E_{J\nu} - \omega_I)_{\text{unphysical}}$$

4) From the physical cfp obtained in step 3, recalculate Δ and Γ .

5) Using the new set of Δ and Γ , return to step 2.

6) Repeat the cycle described above until the nth solution differs only by a prescribed amount from the (n-1)th solution.

7) The number of particles A(I), equation (3.1.24), is calculated in order to check whether the value of the chemical potential λ has been properly taken in step 1. If A(I) is not close to the extra core particle number of each Ni isotope , the λ is adjusted until the correct value is obtained for A(I).

The normalization condition (3.1.23) is not used in this calculation and instead the "machine normalization", i.e. $\sum_{\nu}(u_{\nu}^2+v_{\nu}^2)=1$ is used. For nickel isotopes, the result of the calculation is not expected to be affected much by the normalization condition (3.1.23). This fact has been examined in the final calculation. A further discussion will be given in section 4.2 and Chapter 5.

In this calculation, the pairing force constant $G_i=26/A$, where A=mass number, is taken from Kisslinger and Sorensen (1963). The quadrupole force constant is adjusted according to the

relation $X=54.2A^{-3/2}$ (Kisslinger and Sorensen,1963), where A=mass number. Single particle energies h_α and the excitation energies $\omega_2(A)$ are taken from experiments (Way et al. 1967 and 1968). They are listed in Table 4.1.1 and Table 4.1.2 .

Isotopes	G	X	λ	$\omega_2(A)$
Ni^{58}	0.4483	0.1227	0.120	1.4500
Ni^{60}	0.4333	0.1166	0.945	1.3330
Ni^{62}	0.4194	0.1110	1.335	1.1717
Ni^{64}	0.4063	0.1059	1.900	1.3480

Table 4.1.1 G, X, λ and $\omega_2(A)$ for nickel isotopes used in this calculation.

j	h_α	F_α/X_i
$2p_{3/2}$	0.00	4.6499
$1f_{5/2}$	0.78	4.1143
$2p_{1/2}$	1.08	8.2499

Table 4.1.2 Single particle energies h_α and F_α .

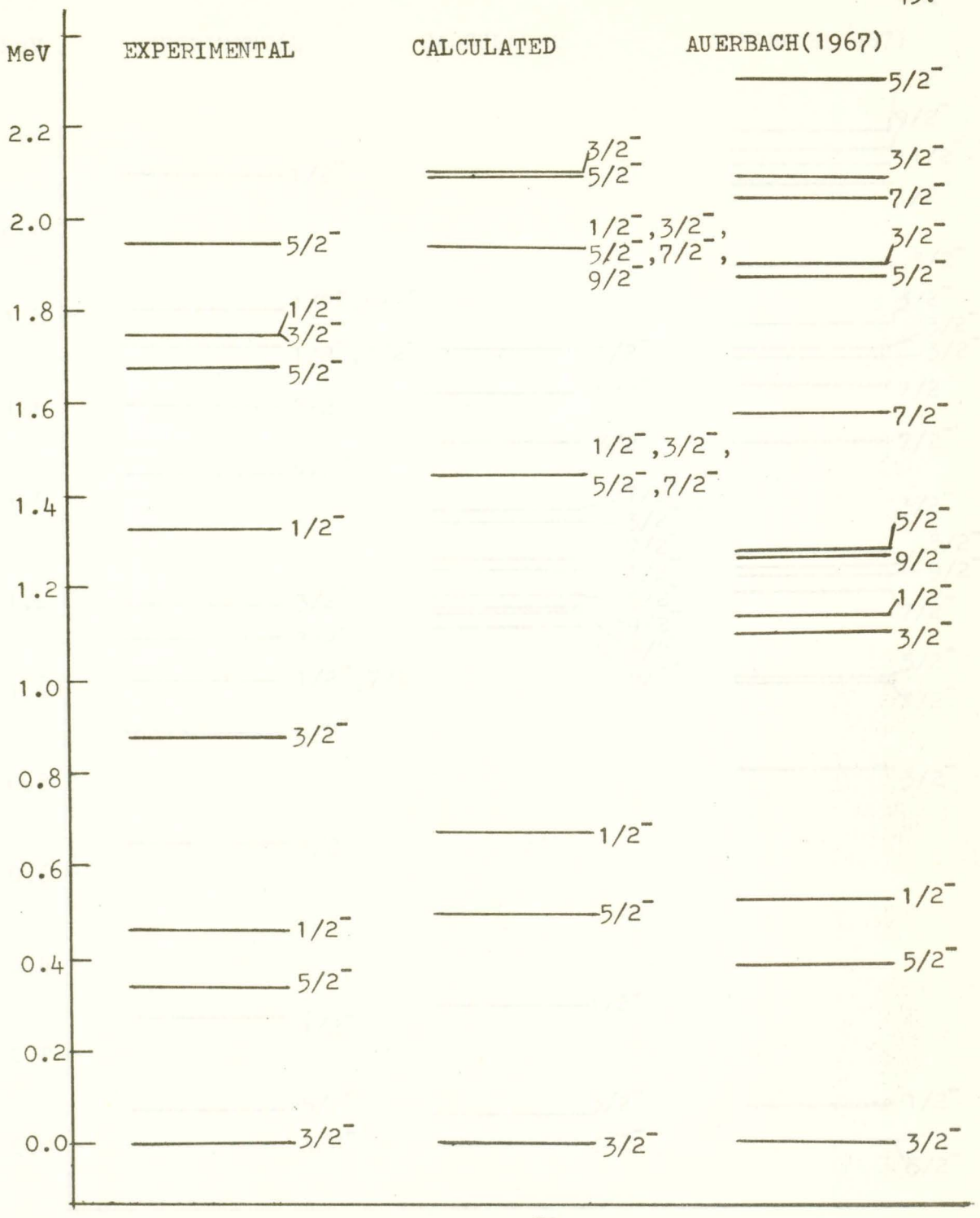

FIGURE 4.2.1 Energy levels of Ni^{59} . The experimental levels are taken from "Nuclear Data Sheet" (Way et al. 1968) .

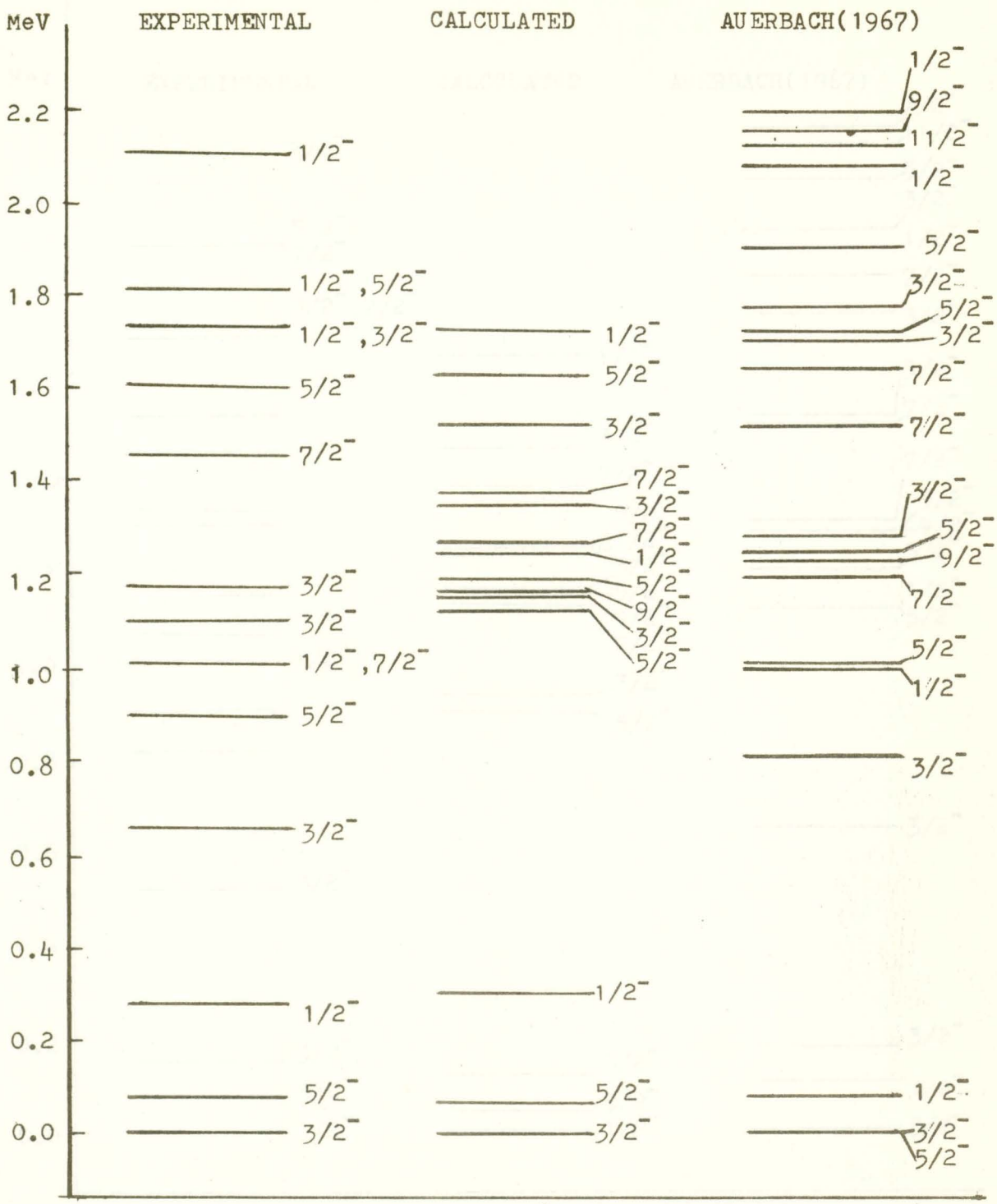

FIGURE 4.2.2 Energy levels of Ni^{61} . The experimental levels are taken from "Nuclear Data Sheet" (Way et al. 1968).

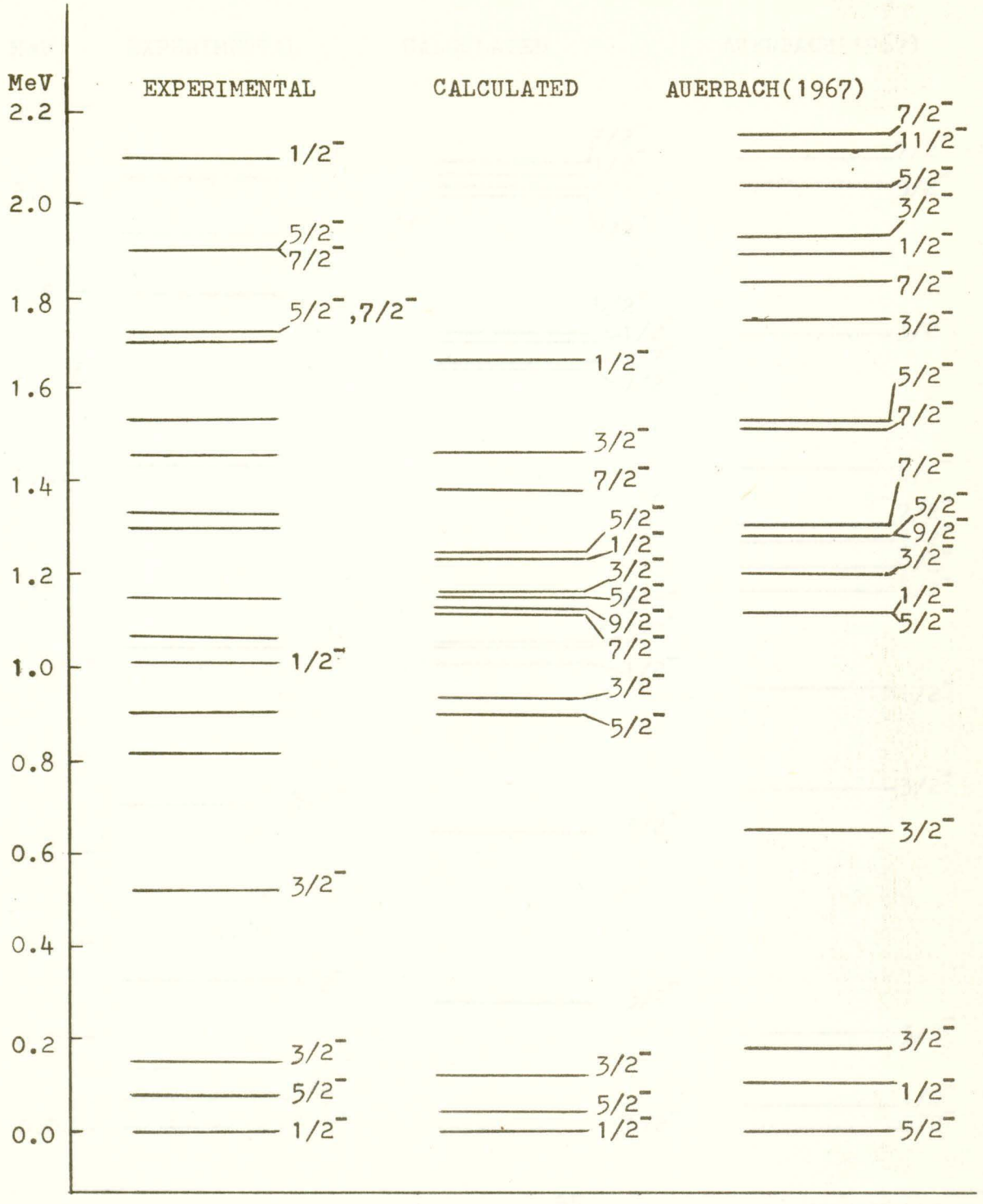

FIGURE 4.2.3 Energy levels of Ni^{63} . The experimental levels are taken from "Nuclear Data Sheet" (Way et al. 1967).

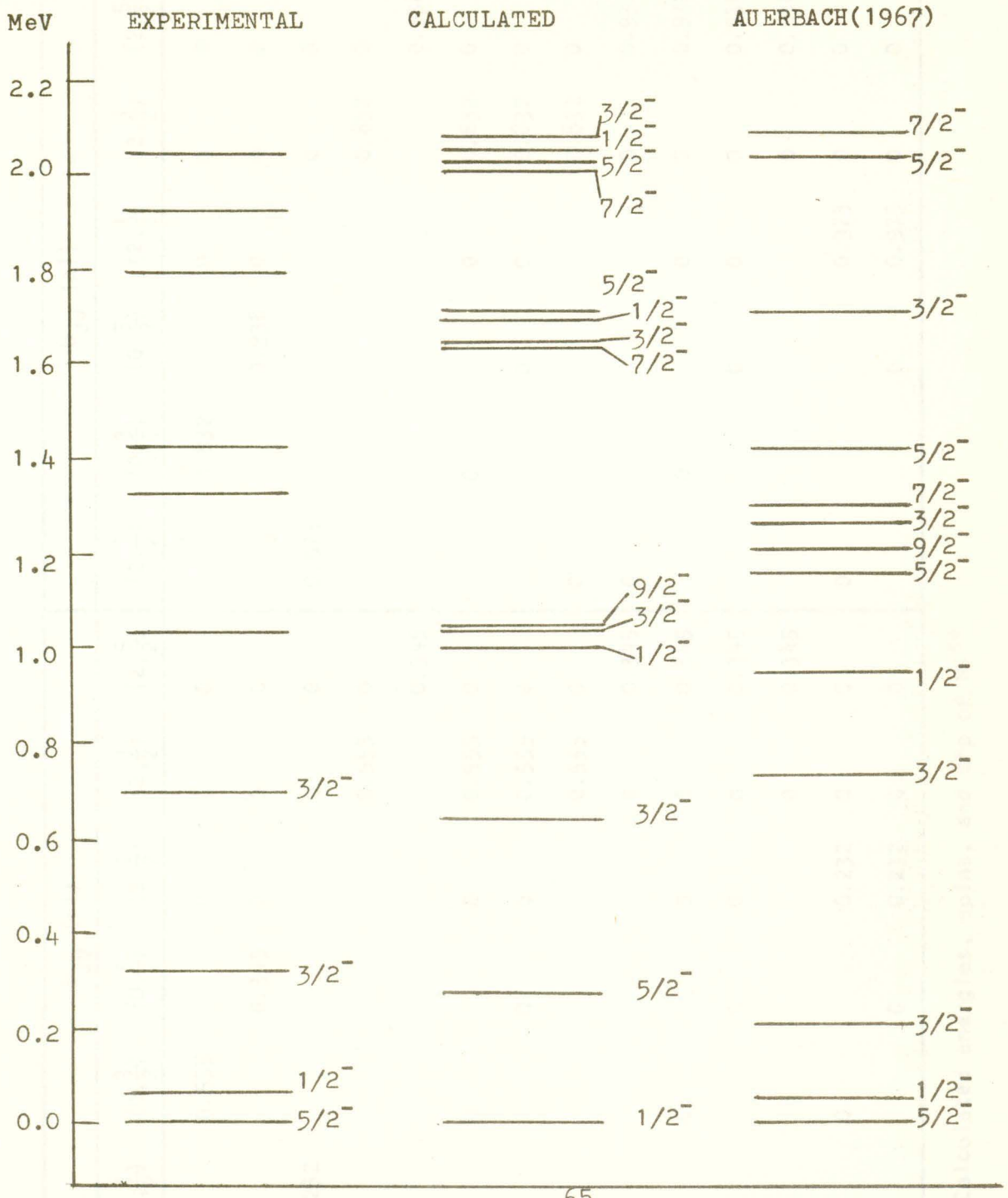

FIGURE 4.2.4 Energy levels of Ni^{65}. The experimental levels are taken from "Nuclear Data Sheet" (Way et al. 1967).

		V_{JV} (al)						U_{JV} (al)					
E_{th}	$J\pi$	$(0,\frac{1}{2})$	$(0,\frac{3}{2})$	$(0,\frac{5}{2})$	$(2,\frac{1}{2})$	$(2,\frac{3}{2})$	$(2,\frac{5}{2})$	$(0.\frac{1}{2})$	$(0,\frac{3}{2})$	$(0,\frac{5}{2})$	$(2,\frac{1}{2})$	$(2,\frac{3}{2})$	$(2,\frac{5}{2})$
0	$\frac{3}{2}-$		0.555		0	0	0		0.832		0	0	0
0.496	$\frac{5}{2}-$			0.345	0	0	0			0.938	0	0	0
0.673	$\frac{1}{2}-$	0.232				0	0	0.973				0	0
1.449	$\frac{7}{2}-$					0.555	0					0.832	0
1.946	$\frac{9}{2}-$						0.345						0.938
1.449	$\frac{3}{2}-$		0		0	0.555	0		0		0	0.832	0
1.449	$\frac{5}{2}-$			0	0	0.555	0			0	0	0.832	0
1.447	$\frac{1}{2}-$	0				0.555	0	0				0.832	0
1.946	$\frac{1}{2}-$	0				0	0.345	0				0	0.938
1.946	$\frac{3}{2}-$		0		0	0	0.345		0		0	0	0.938
1.946	$\frac{5}{2}-$			0	0	0	0.345			0	0	0	0.938
1.946	$\frac{7}{2}-$					0	0.345					0	0.938
2.123	$\frac{3}{2}-$		0		0.232	0	0	0			0.973	0	0
2.123	$\frac{5}{2}-$			0	0.232	0	0			0	0.973	0	0

TABLE 4.2.1. Calculated energies, spins, and cfp of Ni^{59}

		V_{JV} (al)						U_{JV} (al)					
E_{th}	$J\pi$	$(0,\frac{1}{2})$	$(0.\frac{3}{2})$	$(0,\frac{5}{2})$	$(2,\frac{1}{2})$	$(2,\frac{3}{2})$	$(2,\frac{5}{2})$	$(0,\frac{1}{2})$	$(0,\frac{3}{2})$	$(0,\frac{5}{2})$	$(2,\frac{1}{2})$	$(2,\frac{3}{2})$	$(2,\frac{5}{2})$
0	$\frac{3}{2}-$		-0.649		0.131	-0.040	0.190		-0.524		-0.235	0.381	-0.223
0.062	$\frac{5}{2}-$			0.523	0.196	0.074	0.372			0.654	-0.159	-0.214	-0.215
0.300	$\frac{1}{2}-$	0.302				0.084	0.332	0.767				-0.336	-0.301
1.128	$\frac{5}{2}-$			0.104	0.233	0.691	0.124			-0.064	0.244	0.612	-0.061
1.147	$\frac{9}{2}-$						0.692						0.722
1.143	$\frac{3}{2}-$		-0.102		0.243	0.094	0.661		0.081		0.390	0.104	0.562
1.168	$\frac{5}{2}-$			0.075	0.033	-0.130	0.410			-0.183	0.623	-0.301	0.431
1.250	$\frac{1}{2}-$	0.022				-0.434	0.677	-0.129				-0.201	0.543
1.262	$\frac{7}{2}-$					0.865	-0.094					0.493	-0.016
1.355	$\frac{3}{2}-$		0.215		-0.352	0.703	0.142		-0.049		-0.463	0.049	0.189
1.379	$\frac{7}{2}-$					0.014	0.461					0.092	0.883
1.522	$\frac{3}{2}-$		0.099		0.098	0.414	-0.203		0.017		0.633	0.469	-0.383
1.613	$\frac{5}{2}-$			0.037	-0.122	0.102	0.342			-0.059	-0.577	0.149	0.705
1.750	$\frac{1}{2}-$	0.182				0.800	0.406	-0.109				0.319	0.219

TABLE 4.2.2. Calculated energies, spins, and cfp of Ni^{61}

		V_{JV} (al)						U_{JV} (al)					
E_{th}	$J\pi$	$(0,\frac{1}{2})$	$(0,\frac{3}{2})$	$(0,\frac{5}{2})$	$(2,\frac{1}{2})$	$(2,\frac{3}{2})$	$(2,\frac{5}{2})$	$(0,\frac{1}{2})$	$(0,\frac{3}{2})$	$(0,\frac{5}{2})$	$(2,\frac{1}{2})$	$(2,\frac{3}{2})$	$(2,\frac{5}{2})$
0	$\frac{1}{2}-$	0.386				0.057	0.249	0.765				-0.292	-0.337
0.031	$\frac{5}{2}-$			0.653	0.119	-0.014	0.218			0.624	-0.140	-0.135	-0.290
0.122	$\frac{3}{2}-$		0.800		-0.074	-0.102	-0.032		0.447		0.193	-0.250	-.195
0.916	$\frac{5}{2}-$			0.082	0.485	-0.047	0.192			-0.086	0.835	-0.122	-0.001
0.937	$\frac{3}{2}-$		-0.110		0.470	0.055	0.116		0.054		0.844	0.184	-0.038
1.110	$\frac{7}{2}-$					0.081	0.652					0.080	0.749
1.129	$\frac{9}{2}-$						0.780						0.626
1.150	$\frac{5}{2}-$			0.024	-0.055	-0.551	0.486			-0.045	-0.166	-0.332	0.563
1.170	$\frac{3}{2}-$		-0.099		0.024	0.053	0.770		0.005		-0.102	-0.031	0.618
1.246	$\frac{1}{2}-$	0.059				-0.305	0.777	-0.080				-0.137	0.525
1.264	$\frac{5}{2}-$			0.135	0.090	0.652	0.462			-0.042	-0.085	0.373	0.433
1.388	$\frac{7}{2}-$					0.904	-0.101					0.413	-0.054
1.457	$\frac{3}{2}-$		0.233		-0.163	0.870	0.007		0.010		-0.025	0.401	-0.023
1.674	$\frac{1}{2}-$	0.159				0.872	0.287	-0.049				0.332	0.143

TABLE 4.2.3. Calculated energies, spins, and cfp of Ni^{63}

		V_{JV} (a1)						U_{JV} (a1)					
E_{th}	$J\pi$	$(0,\frac{1}{2})$	$(0,\frac{3}{2})$	$(0,\frac{5}{2})$	$(2,\frac{1}{2})$	$(2,\frac{3}{2})$	$(2,\frac{5}{2})$	$(0,\frac{1}{2})$	$(0,\frac{3}{2})$	$(0,\frac{5}{2})$	$(2,\frac{1}{2})$	$(2,\frac{3}{2})$	$(2,\frac{5}{2})$
0	$\frac{1}{2}-$	0.405				0.033	0.261	0.592				-0.285	-0.579
0.277	$\frac{5}{2}-$			0.797	0.118	-0.030	0.020			0.425	-0.213	-0.077	-0.343
0.644	$\frac{3}{2}-$		0.839		0.102	-0.130	0.058		0.269		0.396	-0.135	0.135
1.000	$\frac{5}{2}-$			0.113	0.668	-0.014	-0.058			-0.047	0.732	-0.001	-0.021
1.049	$\frac{3}{2}-$		-0.351		0.655	0.089	-0.073		-0.014		0.656	0.037	-0.052
1.643	$\frac{9}{2}-$						0.895						0.450
1.653	$\frac{7}{2}-$					-0.006	0.897					-0.003	0.441
1.660	$\frac{3}{2}-$		-0.126		0.032	0.088	0.885		-0.003		0.020	0.030	0.436
1.690	$\frac{1}{2}-$	0.110				-0.118	0.880	-0.042				-0.032	0.441
1.706	$\frac{5}{2}-$			0.166	0.033	-0.048	0.887			-0.013	0.025	-0.016	0.427
2.124	$\frac{7}{2}-$					0.961	0.007					0.278	0.002
2.145	$\frac{5}{2}-$			0.068	0.007	0.958	0.037			0.000	0.004	0.274	0.015
2.178	$\frac{1}{2}-$	0.135				0.946	0.098	-0.016				0.273	0.042
2.190	$\frac{3}{2}-$		0.203		-0.029	0.939	-0.062		0.010		-0.013	0.265	-0.022

TABLE 4.2.4. Calculated energies, spins, and cfp of Ni^{65}

4.2 Calculated energy spectra of odd mass isotopes of nickel

Following the procedures of section 4.1, the calculation was done by using IBM 360 44 and the results are shown in Figures 4.2.1, 4.2.2, 4.2.3 and 4.2.4, where the calculated energy levels are plotted together with experimental levels and those calculated by Auerbach (1967). In Figure 4.2.2 (Ni^{61}), the calculated three lowest levels are in very good agreement with the experimental levels while those obtained by Auerbach are not. For Ni^{63} (Figure 4.2.3), both the experimental and our calculated ground states have spin 1/2 while the ground state of Auerbach has spin 5/2. The order of the calculated 5/2- and 3/2- are also in agreement with experiment. Good results for these three lowest levels of Ni^{61} and Ni^{63} are expected within the approximation scheme described in Chapter 3. The number of particles outside the closed shell of Ni^{61} and Ni^{63} is 5 and 7 respectively. The external shell is about half filled for these two nuclei. Therefore the particle-number nonconserving approximation is expected to have little effect on the accuracy of the calculation. In Figure 4.2.1 (Ni^{59}), the order of the three lowest levels is in agreement with both experimental data and those calculated by Auerbach. The higher levels are not in agreement with experimental levels. Since Ni^{59} has only three particles outside the closed shell, it may be sensitive to the particle number nonconserving approximation. In Figure 4.2.4 (Ni^{65}), the calculated ground state is 1/2- while the experimental one

and that calculated by Auerbach are found to be 5/2-. This may be an indication that the neglected $1g_{9/2}$ in the configuration has an important effect for this isotope and/or that the error due to the particle non-conserving approximation is large. In examining the normalization of the cfp that were picked up in the procedure 3 of section 4.2 , one observes that there is a deviation from the cfp of 1/2- level. This shows that the results will improve if the cfp is normalized in the procedure 3.

Tables 4.2.1, 4.2.2, 4.2.3 and 4.2.4 are the wave functions (cfp). From these tables we can see the percentage of the mixing of different configurations, combinations of even nuclear cores $0^+, 2^+$ and the single-particle levels $2p_{1/2}, 2p_{3/2}$ and $1f_{5/2}$. For example, as can be seen in Table 4.2.2, the ground state 3/2- of Ni^{61} has a higher percentage of the coupling between 0^+ and $2p_{3/2}$ than the others, since its amplitude $(u^2 + v^2)$ is higher than the others.

4.3 Ground-state-to-one-phonon-state transition probabilities in the even mass isotopes of nickel

The electric quadrupole transitions (γ decay, Coulomb excitation, etc.) are described by the off diagonal matrix elements of the electric quadrupole (E2) operator (3.1.3). The E2 transition rate from a nuclear state $|IMS\rangle$ to another nuclear state $|I'M'S'\rangle$ is given in equation (3.2.1):

$$B(E2, I \to I') = (2I+1)^{-1} \sum_{MM'_q} \left| \langle I'M'S'(A) | e_i \sum_{\alpha\beta} \langle \alpha | r^2 Y_2 | \beta_i \rangle Q^+_\alpha Q_\beta | IMS(A) \rangle \right|^2 \quad (3.2.1)$$

where e_i is the effective charge. One often refers to it as the sum of the charge of the single nucleon and the polarization charge:

$$e_i = e(1/2 - t_z) + e_{pol} \quad , \qquad (4.3.1)$$

where t_z is the z-component of the isospin of the nucleon and e_{pol} is the polarization charge (The polarization effect can be treated in terms of the coupling between the particles and the collective oscillators associated with deformations of the cores).

Since the z-component of isospin t_z of the neurton is $+1/2$, equation (4.3.1) gives

$$(e_i)_{E2} = (e_{pol})_{E2} \quad .$$

That is, the effective charge of a neutron is not zero, and the value of e_i normally used for the nickel isotopes is one (in unit of e) (Kisslinger and Sorensen,1963).

After the iteration process of section 4.1,the self-consistent kernel Γ is obtained. By substituting this Γ into (3.2.4),

$$B(E2;0^+\rightarrow 2^+) = \frac{25}{4\pi} e_\lambda^2 \nu_\lambda^2 \Gamma_\lambda^2 \qquad (3.2.4)$$

and choosing the effective charge of the neutron to be 0.6e, where e is the electron charge, the $B(E2;0^+ \longrightarrow 2^+)$ of the nickel isotopes are calculated. The calculated values are shown in Table 4.3.1 .

Isotopes	$B(E2)_{th.}$	$B(E2)_{expt.}$
Ni^{60}	0.113	0.0970 ± 0.0080
Ni^{62}	0.077	0.0840 ± 0.0170
Ni^{64}	0.057	0.0870 ± 0.0170

Table 4.3.1 $B(E2;0^+ \longrightarrow 2^+)$ of the even-mass nickel isotopes in unit of $e^2 x 10^{-48}$ cm^{-4}. The experimental values are taken from "Nuclear Data" (Stelson and Gradzins, 1965).

CHAPTER 5

DISCUSSION AND CONCLUSION

As shown in the preceding chapter, our calculated results are in reasonable agreement with experiments for the one quasi-particle states (i.e. the three lowest levels) of the odd nickel isotopes, but the agreement is not so good for the higher excited states. This is understandable because the solutions for the higher excited states are greatly affected by the omission of the two-phonon states---0^+, 2^+ and 4^+ (we would be able to obtain better results for these higher excited states if the two-phonon states are included).

The agreement is particularly food for Ni^{61} and Ni^{63} where approximately half of the external shell is filled and where the effect of the number non-conserving approximation is expected to be small. A better result at the two ends (i.e. the three-particle nucleus Ni^{59} and the three-hole nucleus Ni^{65}) could be obtained if the particle number conservation were taken into account and if the $1g_{9/2}$ single-particle state were included. However the number non-conserving approximation is a useful method for a great number of mid-shell range nuclei where an exact shell model calculation is practically impossible because of too many configurations which have to be considered.

In the final calculation , the physical cfp chosen in procedure 3 (section 4.2) was re-examined for the normalization

condition (3.1.23). It turned out that for Ni^{59}, Ni^{61} and Ni^{63}, the normalization condition was approximately satisfied and in most cases the deviation from it was less than 10%. For Ni^{65}, the cfp of the lowest 1/2 state deviated about 40% from the normalization condition and the rest were within 10%-20% deviation.

The calculated values of $B(E2;0^+ \longrightarrow 2^+)$ are in reasonable agreement with the experimental values, showing a satisfactory collective nature of the calculated 2^+ state.

The agreement between our calculation and the experimental spectra for Ni^{61} and Ni^{63} is particularly encouraging in view of the less accurate results obtained by Kisslinger and Sorensen (1963) for the odd nickel isotopes. They used exactly the same pairing-plus-quadrupole interaction, but the calculation was based on the RPA with mixing of the ground 0^+ and the one phonon 2^+ cores considered. The improvement of this result over theirs can be attributed to the self-consistent formalism of this theory.

The result of this work suggest that the model is fundamentally good and that future studies should be conducted towards the inclusion of a more accurate normalization condition which incorporates particle number conservation for extending the range of validity to near closed-shell nuclei, together with the inclusion of more cores, particularly the 0^+_2, 2^+_2 and 4^+ triplet states, for obtaining good solutions for the higher excited states.

APPENDIX

(1) Wigner Eckart Theorem

$$\langle \alpha j m | T_q^{(k)} | \alpha' j' m' \rangle = (2j+1)^{-1/2} \langle j' k m' q | j m \rangle \langle \alpha j \| T^{(k)} \| \alpha' j' \rangle$$

(2) Racah Coefficient and 6-j symbol

$$W(abcd;ef) = (-)^{a+b+c+d} \begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix}$$

(3) Useful relations of the Clebsch-Gordon and Racah coefficients in deriving the equations of motion (note: $\bar{m}=-m$).

$$\begin{aligned}
\langle j_1 j_2 m_1 m_2 | j_3 m_3 \rangle &= (-)^{j_1+j_2-j_3} \langle j_1 j_2 \bar{m}_1 \bar{m}_2 | j_3 \bar{m}_3 \rangle \\
&= (-)^{j_1+j_2-j_3} \langle j_2 j_1 m_2 m_1 | j_3 m_3 \rangle \\
&= (-)^{j_1-m_1} (2j_3+1/2j_2+1)^{1/2} \langle j_1 j_3 m_1 \bar{m}_3 | j_2 \bar{m}_2 \rangle \\
&= (-)^{j_2+m_2} (2j_3+1/2j_1+1)^{1/2} \langle j_3 j_2 \bar{m}_3 m_2 | j_1 \bar{m}_1 \rangle \\
&= (-)^{j_1-m_1} (2j_3+1/2j_2+1)^{1/2} \langle j_3 j_1 m_3 \bar{m}_1 | j_2 m_2 \rangle \\
&= (-)^{j_2+m_2} (2j_3+1/2j_1+1)^{1/2} \langle j_2 j_3 \bar{m}_2 m_3 | j_1 m_1 \rangle
\end{aligned}$$

$$\langle j_1 j_2 m_1 m_2 | j m \rangle \langle j_3 j_4 m_3 m_4 | j m \rangle$$

$$= (-)^{j_4 - m_4} \left(2j+1 / 2j_3+1 \right)^{1/2} \langle j_1 j_2 m_1 m_2 | j m \rangle \langle j\, j_4\, \bar{m}\, m_4 | j_3 \bar{m}_3 \rangle$$

$$= (-)^{j_4 + m_4 + j + j_4 - j_3} \left(2j+1 / 2j_3+1 \right) \langle j_1 j_2 m_1 m_2 | j m \rangle \langle j\, j_4\, m\, \bar{m}_4 | j_3 m_3 \rangle$$

$$= (-)^{j - j_3 + j_1 - m_4 - m_1} (2j+1) \sum_{j'} W(j_1 j_2 j_3 j_4 ; j j') \langle j_1 j_3 m_1 \bar{m}_3 | j' m_1 - m_3 \rangle$$

$$\times \langle j_2 j_4 m_2 \bar{m}_4 | j' m_2 - m_4 \rangle$$

$$= (-)^{j + j_1 + j_3 - m - m_1 - m_3} (2j+1) \sum_{j'} W(j_1 j_2 j_3 j_4 ; j j') \langle j_1 j_3 m_1 \bar{m}_3 | j' m_1 - m_3 \rangle$$

$$\times \langle j_2 j_4 m_2 \bar{m}_4 | j' m_2 - m_4 \rangle$$

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