ABSTRACT

The approximate projection method of Das Gupta and Van Ginneken is extended to include the calculation of the decoupling parameter for $K=-\frac{1}{2}$ band. The method is tested on the first positive and negative parity bands of F^{19} and is found to give good results even when the strong coupling model seems to fail. The validity of the formula for the decoupling parameter given by the strong coupling model is explored.

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La méthode de projection approximative de Das Gupta et de Van Ginneken est généralisée afin de permettre le calcul du paramètre de découplage des bandes rotationelles avec $K=\frac{1}{2}$. L'application de cette methode aux premières bandes rotationelles de parité positive et négative du noyau F^{19} donne des résultats en bon accord avec les résultats expérimentaux même quand le modèle de Bohr et Mottelson est en erreur. La validité de la formule de Bohr et Mottelson pour le paramètre de découplage est étudiée.

DECOUPLING PARAMETER FOR LIGHT NUCLEI

by

KRISHAN L. BHATIA

Submitted in partial fulfillment of the requirements
for the degree of Master of Science from the Institute
of Theoretical Physics, McGill University, Montreal, Quebec

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TABLE OF CONTENTS

INTRODUCTION

It is well known that the intrinsic state of a nucleus can be approximated by considering SU(3)[1], Nilsson[2], or deformed Hartree-Fock[3,4,5] model (H.F).

The deformation in nuclei is usually interpretted as the effect of long-range correlations among the nucleons. In SU(3) model of the nucleus one takes a long-range specialised quadrupole-quadrupole two-body interaction between the nucleons. On the other hand, in Nilsson model a more phenomenological point of view is adopted. It is assumed that nuclear deformations can be explained by taking a non-spherical single-body potential along with a spin orbit term. A partial justification of such a potential comes from the fact that the long-range two-body forces can be supposed to average out to a deformed potential field in which mutually non-interacting particles move.

A more general way of generating an intrinsic state of a deformed nucleus is to use deformed H. F. model which takes into account both single and two-body forces in its scheme through a self-consistent procedure. This method has been discussed by Kelson[4] and will be followed in the present work.

The total angular momentum J of the intrinsic wave function ϕ_K is not a good quantum number. Because of the assumed axial symmetry, only the z- projection of J (denoted here by K) is a good quantum number. Since the actual

states are those of a definite angular momentum, the wave functions ϕ_K are not physical. The physical states are obtained by projecting (by exact projection or approximate projection technique) out of ϕ_K the states of good angular momentum and normalising them. Corresponding energies are the expectation values of the Hamiltonian with these projected states.

It may be remarked that the method of shell model[6] becomes unduly complex as the number of particles outside a closed shell increases. For example, in Ne^{20}, the number of J=2 states is 56.

The exact projection from the intrinsic state[7] becomes complicated as the number of particles increases. Das gupta and Van Ginneken[8] have developed an approximate method for calculating the energies of states in a rotational band. The method assumes a rotational structure, but departures from J(J+1) rule were also studied and, in particular, the possibility of decoupling in $K=\frac{1}{2}$ bands was included in the formalism. In this case the decoupling parameter was calculated using Bohr-Mottelson Prescription[9].

The purpose of the present work is to fully incorporate the calculation of the decoupling parameter into the formalism of the method of approximate projection. The nucleus that has been treated is F^{19}. The positive parity states correspond to three particles outside (p)shell and negative parity states are obtained by assuming a hole in (p) shell and Four particles outside it. It is found that the decoupling parameter for the negative parity states

agrees with that obtained from Bohr-Mottelson strong coupling formula (eqn. 4.1) but no such agreement is attained for the positive parity states. A possible explanation is given in Chapter IV.

The next three chapters deal with a brief description of deformed H. F. model, exact projection and approximate projection methods.

CHAPTER I

HARTREE-FOCK THEORY FOR DEFORMED NUCLEI

We can write the Hamiltonian H of the nucleus as

$$H = \sum \langle \alpha | T | \beta \rangle \, c_\alpha^+ c_\beta + \frac{1}{4} \sum \langle \alpha \beta | V | \gamma \delta \rangle \, c_\alpha^+ c_\beta^+ c_\delta c_\gamma \qquad (1.1)$$

Here T is the single-body part of the force which includes kinetic energy of all particles and their average interaction with all the other nucleons in closed shells. $\langle \alpha \beta | V | \gamma \delta \rangle$ is the antisymmetrised matrix element of V. $| \alpha \rangle$, $| \beta \rangle$, etc. is a complete set of orthonormal wave functions. For example, we can choose single particle shell model wave functions in the $| jm \rangle$ basis to be the desired representation.

The intrinsic nuclear wave function ϕ is assumed to have the form of a determinant of single particle orbitals , $| i_1 \rangle$, $| i_2 \rangle$, ... $| i_A \rangle$. In the second quantised notation

$$| \phi \rangle = b_{i_1}^+ b_{i_2}^+ \cdots\cdots\cdots b_{i_A}^+ | 0 \rangle \qquad (1.2)$$

where $| 0 \rangle$ is the vacuum. One can define O^{16} core to be the vacuum. Thus F^{19} (+parity) states can be written as

$$| \phi \rangle = b_{i_1}^+ b_{i_2}^+ b_{i_3}^+ | 0 \rangle \qquad (1.2a)$$

$| i \rangle$ can be expanded in the known single particle basis $| \alpha \rangle$, $| \beta \rangle$, ...

$$|i\rangle = \sum_{\lambda=\alpha,\beta\cdots} C_{i\lambda} |\lambda\rangle \qquad (1.3)$$

the choice of coefficients $C_{i\lambda}$ being determined by minimisation of H. F. energy. It is easy to see that

$$E_{HF} = \langle\phi|H|\phi\rangle = \sum_{i}\langle i|T|i\rangle + \frac{1}{2}\sum_{i,j}\langle ij|V|ij\rangle \qquad (1.4)$$

The summation runs over all occupied orbits occuring in eqn.(1.2). Define e_i as the Lagrange Multiplier associated with fixed solution. Condition of minimisation is

$$\frac{\partial}{\partial C_{i\lambda}^*}\left(E_{HF} - e_j\left(\sum_{j}|C_{j\lambda}|^2-1\right)\right) = 0 \qquad (1.5)$$

Using eqns.(1.3) and (1.4), we get

$$\sum_{\mu}\left[\langle\lambda|T|\mu\rangle + \sum_{i}\langle\lambda i|V|\mu i\rangle\right]C_{i\mu} = e_i C_{i\lambda} \qquad (1.6)$$

This is equivalent to an eigenvalue problem:

$$h|i\rangle = e_i|i\rangle \qquad (1.7)$$

$$\langle\lambda|h|\mu\rangle = \langle\lambda|T|\mu\rangle + \sum_{i}\langle\lambda i|V|\mu i\rangle \qquad (1.8)$$

In our case, the summation in eqn.(1.3) is limited only to the (2s-1d) shell in case of particles and to (1p) shell in case of holes. Further, assuming axial symmetry of H. F. field, summation will be over j's and not m's.

To give an example,

$$|m=\tfrac{1}{2}\rangle \equiv |\tfrac{1}{2}\rangle = C_{\frac{1}{2}\frac{5}{2}}|d_{\frac{5}{2}\frac{1}{2}}\rangle + C_{\frac{1}{2}\frac{3}{2}}|d_{\frac{3}{2}\frac{1}{2}}\rangle + C_{\frac{1}{2}\frac{1}{2}}|s_{\frac{1}{2}\frac{1}{2}}\rangle$$

An iteration method is employed to determine these coefficients and the corresponding energies.

(a) Take H.F. orbitals $|i^{o}\rangle$ to be some starting wave functions and use these to calculate matrix elements of h, eqn.(1.8)

(b) Diagonalise this matrix to obtain orbits $|i^{(1)}\rangle$ and energies $e_i^{(1)}$.

(c) With these wave functions, calculate again matrix elements of h; diagonalise these to get $|i^{(2)}\rangle$, $e_i^{(2)}$.

(d) Repeat the above cycle until convergence is obtained. At this stage the wave functions fed in are the same as come out after diagonalisation procedure.

E_{HF} is given by

$$E_{HF} = \tfrac{1}{2} \sum_i \left[\langle i|T|i \rangle + e_i \right] \tag{1.9}$$

Remarks about Hamiltonian

In the Hamiltonian (1.1), $|\alpha\rangle$ can be taken to be the spherical harmonic oscillator potential wave functions and the energies e_α are determined from the known experimental positions (see TABLE I) of the $1p_{\frac{1}{2}}$, $1p_{\frac{3}{2}}$ hole orbitals $1d_{\frac{5}{2}}$, $2s_{\frac{1}{2}}$ and $1d_{\frac{3}{2}}$ particle orbitals listed in Ref.13.

The potential V can be split into p-p, h-h and p-h parts. It is assumed to be central and therefore

$$V(r) = V_0 \, g(r) \left[W + B P_\sigma + H P_\sigma P_x + M P_x \right] \tag{1.10}$$

g(r) being the radial dependence of the force and V_0 the strength function. P_σ , P_x are spin exchange and space exchange operators respectively. W, B, H, and M represent components of Wigner, Bartlet, Heisenberg and

Majorana type of forces:

$$W + B + H + M = 1 \qquad (1.11)$$

The p-h interaction is calculated using the potential of Gillet and Vinh-Mau[14], while the p-p interaction is taken from the work of Inoue et. al.[15]

The parameters for Gillet and Inoue forces are given in TABLE II.

TABLE I

Level	$0p_{3/2}$	$0p_{1/2}$	$0d_{5/2}$	$1s_{1/2}$	$0d_{3/2}$
Energy in mev	-21.8	-15.65	-4.15	-3.27	0.93

TABLE II

Name	$g(r)$	V_o(Mev)	α in f^{-1}	W	B	H	M
Gillet	$\exp(-\alpha^2 r^2)$	-40.0	0.5682	0.35	-.10	0.40	0.35
Inoue	$\dfrac{\exp(-\alpha r)}{r}$	-35.0	0.6026	0.25	-0.136	0.25	0.636

CHAPTER II

EXACT PROJECTION

It is found that the H.F. wave functions ϕ_K consist of a mixture of angular momentum eigenstates of the ground state rotational band. Definite orientation of the nucleus has been paid by an appropriate uncertainty in angular momentum. Physically meaningful states are obtained by projecting out of ϕ_K the components with angular momentum J.

It can be seen very easily that H.F. wave functions with K≠0 can give projected states with J=K, K+1, K+2,... Of course, higher J components may be negligible. If K=0 however, only even J values are allowed.

A simple proof follows. For a more rigorous treatment of this standard result see Ref. 16.

Consider the ground state (K=0) band in an even-even nucleus.

$$|\phi_0\rangle = \sum_J a_J |J 0\rangle \tag{2.1}$$

$$\exp(-i\pi J_y)|\phi_0\rangle = \sum_{JM} a_J \, d^J_{m0}(\pi)\, |JM\rangle$$

$$= \sum_J a_J \, (-)^J \, |J 0\rangle$$

Now we prove that $|\phi_0\rangle$ should remain unchanged under application of the time reversal operator $\exp(-i\pi J_y)$.

Since $J_y = \sum_{i=1}^{A} (j_y)_i$, $\exp(-i\pi J_y)|\phi_0\rangle$ is itself a determinant. Thus we can write

$$\exp(-i\pi J_y)|\phi_0\rangle = \left(\exp(-i\pi j_y) b_{k_1}^{+}\right)\left(\exp(-i\pi j_y) b_{\tilde{k}_1}^{+}\right)\cdots\cdots|0\rangle$$

$$= b_{\tilde{k}_1}^{+}\cdot(-b_{k_1}^{+})\cdots\cdots\cdots\cdots|0\rangle$$

$$= b_{k_1}^{+}\, b_{\tilde{k}_1}^{+}\cdots\cdots\cdots\cdots|0\rangle$$

$$= |\phi_0\rangle$$

Thus

$$\sum_J a_J (-)^J |J\,0\rangle = \sum_J a_J |J\,0\rangle \tag{2.2}$$

which gives only even J values.

For non-zero K values, the H.F. wave function is not unchanged by the time-reversal operator and there is no reason why odd J values should not be allowed.

Define P_J^M to be the angular momentum projection operator.

$$P_M^J = \sum_{JM} |JM\rangle\langle JM| \tag{2.3a}$$

$$\left(P_M^J\right)^2 = P_M^J \tag{2.3b}$$

where $|JM\rangle$ are a complete set of orthonormal eigen-states of J^2 and J_z.

To project states of good J out of ϕ_k, note

$$|\phi\rangle = \sum_{JM} P_M^J |\phi\rangle = \sum_{JM} a_{JM} |JM\rangle \qquad (2.4)$$

Assuming $|JM\rangle$ to be normalised,

$$|JM\rangle = \frac{P_M^J |\phi\rangle}{\sqrt{\langle\phi| P_M^J |\phi\rangle}} \qquad (2.5)$$

$$E_J = \langle JM|H|JM\rangle = \frac{\langle\phi| H P_M^J |\phi\rangle}{\langle\phi| P_M^J |\phi\rangle} \qquad (2.6)$$

When $|\phi\rangle$ has axial symmetry it can be shown that

$$\langle\phi| P_M^J |\phi\rangle = (J+\tfrac{1}{2})\int_0^\pi \sin\theta\, d\theta\; d_{MM}^J(\theta) \langle\phi| e^{-i\theta J_y} |\phi\rangle \qquad (2.7)$$

$$\langle\phi|H P_M^J |\phi\rangle = (J+\tfrac{1}{2})\int_0^\pi \sin\theta\, d\theta\; d_{MM}^J(\theta) \langle\phi|H e^{-i\theta J_y} |\phi\rangle \qquad (2.8)$$

where $d_{MM}^J(\theta)$ is the reduced rotation matrix

$$\langle JM | \exp(-i\theta J_y) | JM\rangle$$

The integrals (2.7) and (2.8) can be solved numerically. There are other methods of writing (2.7) and (2.8)(See Ref.10) and each is suited to a specific purpose.

The defect of this method lies in its increasing complexity as the number of particles increases.

A few features of this method are listed below:

(1) Energy levels are determined by occupied orbits only.

(2) Absolute value of the energy is obtained and it does not depend on the calculation of the moment of inertia for which a model has to be introduced.

(3) Deviations from a pure $J(J+1)$ spectrum may be obtained. In particular, decoupling of $K=\frac{1}{2}$ band is contained in the expression (2.6).

CHAPTER III

APPROXIMATE PROJECTION

The chief disadvantage of the exact projection described earlier is that it becomes very complex as the number of particles increases. If it is known a priori that the nucleus under consideration has rotational spectra, approximate projection technique proves very helpful. The present work is an extention (to $K=\frac{1}{2}$ band) of the work done by Das Gupta and Van Ginneken[8].

To start with, let us assume that for $K=\frac{1}{2}$ band, the energy E_J for a state of total angular momentum J is given by

$$E_J \equiv \langle J\tfrac{1}{2}|H|J\tfrac{1}{2}\rangle = E_0 + AJ(J+1) + Aa\,(-)^{J+\frac{1}{2}}\,(J+\tfrac{1}{2}) \quad (3.1)$$

$$|\phi\rangle = \sum_J a_J\,|J\tfrac{1}{2}\rangle \quad\quad\quad (3.2)$$

Here E_0 is the band head, $A=\frac{\hbar^2}{2\mathcal{J}}$ where $\mathcal{J}$ is moment of inertia and 'a' is the decoupling parameter. To determine these three parameters E_0, A, and 'a', let us define a pseudo-hamiltonian:

$$\mathcal{H} = E_0 + A\vec{J}^2 + Aa\,J_+T \quad\quad\quad (3.3)$$

which is required to have the same intra-band matrix elements as the true Hamiltonian H. In eqn.(3.3), J is angular momentum operator with components J_+, J_-, J_z

and $T = e^{-i\pi J_y}$ is essentially the time-reversal operator. Following conditions can be imposed now.

$$\langle \phi_{\frac{1}{2}} | H - \mathcal{H} | \phi_{\frac{1}{2}} \rangle = 0 \tag{3.4}$$

$$\langle \phi_{\frac{1}{2}} | (H - \mathcal{H}) J_- J_+ | \phi_{\frac{1}{2}} \rangle = 0 \tag{3.5}$$

$$\langle \phi_{\frac{1}{2}} | (H - \mathcal{H}) J_+ T | \phi_{\frac{1}{2}} \rangle = 0 \tag{3.6}$$

Basically, these equations are the three simplest, differently weighted, sum rules that involve only intra-band matrix elements. The three equations (3.4), (3.5), and (3.6) are then solved for the parameters E_0, A and a. It is easy to see that

$$\langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}} \rangle = E_0 + A \langle \phi_{\frac{1}{2}} | \vec{J}^2 | \phi_{\frac{1}{2}} \rangle + A a \langle \phi_{\frac{1}{2}} | J_+ T | \phi_{\frac{1}{2}} \rangle \tag{3.7}$$

$$\langle \phi_{\frac{1}{2}} | H J_+ T | \phi_{\frac{1}{2}} \rangle = E_0 \langle \phi_{\frac{1}{2}} | J_+ T | \phi_{\frac{1}{2}} \rangle + A \langle \phi_{\frac{1}{2}} | J_+ \vec{J}^2 T | \phi_{\frac{1}{2}} \rangle$$
$$+ A a \langle \phi_{\frac{1}{2}} | J_+ T J_+ T | \phi_{\frac{1}{2}} \rangle \tag{3.8}$$

$$\langle \phi_{\frac{1}{2}} | H J_- J_+ | \phi_{\frac{1}{2}} \rangle = E_0 \langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}} \rangle + A \langle \phi_{\frac{1}{2}} | J_- \vec{J}^2 J_+ | \phi_{\frac{1}{2}} \rangle$$
$$+ A a \langle \phi_{\frac{1}{2}} | J_- J_+ J_+ T | \phi_{\frac{1}{2}} \rangle \tag{3.9}$$

Note that

$$\langle \phi_{\frac{1}{2}} | H J_- J_+ | \phi_{\frac{1}{2}} \rangle = \langle \phi_{\frac{1}{2}} | J_- J_+ H | \phi_{\frac{1}{2}} \rangle$$
$$= \langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}} \rangle \langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}} \rangle$$
$$+ \sum'' \langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}}'' \rangle \langle \phi_{\frac{1}{2}}'' | H | \phi_{\frac{1}{2}} \rangle \tag{3.10}$$

and

$$\langle \phi_{\frac{1}{2}} | H\, J_+ T | \phi_{\frac{1}{2}} \rangle = \langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}} \rangle \langle \phi_{\frac{1}{2}} | J_+ T | \phi_{\frac{1}{2}} \rangle$$

$$+ \sum {}'' \langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}}'' \rangle \langle \phi_{\frac{1}{2}}'' | J_+ T | \phi_{\frac{1}{2}} \rangle \qquad (3.11)$$

In equations (3.10) and (3.11) the summation runs over two particles two holes (2p-2h) only. There is no summation over 1p-1h because of H.F. condition for minimum energy. Let

$$E_{HF} = \langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}} \rangle$$

Following equations ensue by equating (3.9) with (3.10) and (3.8) with (3.11) and making use of (3.7).

$$E_0 = E_{HF} - \left[\frac{3}{4} + \langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}} \rangle + a \langle \phi_{\frac{1}{2}} | J_+ T | \phi_{\frac{1}{2}} \rangle \right] A$$

$$A = \frac{C_4}{C_5 + a\, C_1}$$

$$a = \frac{C_4 C_1 - C_3 C_5}{C_3 C_1 - C_4 C_2}$$

where

$$C_1 = \sum {}' \langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}}' \rangle \langle \phi_{\frac{1}{2}}' | J_+ T | \phi_{\frac{1}{2}} \rangle + \sum {}'' \langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}}'' \rangle \langle \phi_{\frac{1}{2}}'' | J_+ T | \phi_{\frac{1}{2}} \rangle$$

$$C_2 = \sum {}' \langle \phi_{\frac{1}{2}} | J_+ T | \phi_{\frac{1}{2}}' \rangle^2 + \sum {}'' \langle \phi_{\frac{1}{2}} | J_+ T | \phi_{\frac{1}{2}}'' \rangle^2$$

$$C_3 = \sum {}'' \langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}}'' \rangle \langle \phi_{\frac{1}{2}}'' | J_+ T | \phi_{\frac{1}{2}} \rangle$$

$$C_4 = \sum{}'' \langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}}'' \rangle \langle \phi_{\frac{1}{2}}'' | J_- J_+ | \phi_{\frac{1}{2}} \rangle$$

$$C_5 = \sum{}' \langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}}' \rangle^2 + \sum{}'' \langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}}'' \rangle^2$$

Thus the problem reduces to calculation of matrix elements $\langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}}' \rangle$, $\langle \phi_{\frac{1}{2}} | J_- J_+ | \phi_{\frac{1}{2}}'' \rangle$, etc. For this, refer to APPENDIX I

CHAPTER IV

APPLICATION OF APPROXIMATE PROJECTION METHOD

The method of approximate projection can be tested on the three particle (3p) $K=\frac{1}{2}^{+}$ band and the four particle one hole (4p-1h) $K=\frac{1}{2}^{-}$ band of F^{19} which are known to have a good rotational structure[17].

The values of E_{o}, A and 'a' obtained from the calculation are shown in TABLE III and the resulting spectrum is compared to the experimental spectrum[17, 18] in Fig. 1. The agreement with experiment is satisfactory.

The intrinsic states which give rise to the $K=\frac{1}{2}^{-}$ and $K=\frac{1}{2}^{+}$ bands of F^{19} are very well approximated by removing a proton from the last occupied $K=\frac{1}{2}^{-}$ and $K=\frac{1}{2}^{+}$ orbitals of Ne^{20}.

The strong coupling model (S.C. M.)[19] predicts that the decoupling parameter be given by

$$a = -\sum_{j} (-)^{j+\frac{1}{2}} (j+\tfrac{1}{2}) \left| C_{j\frac{1}{2}} \right|^{2}$$

where $C_{j\frac{1}{2}}$ are the expansion coefficients of the deformed $K=\frac{1}{2}$ orbital in spherical shell model states. The values of 'a' obtained from eqn. (4.1) are listed in TABLE III along with the experimental values of 'a', A, E_{o}, which are obtained by least square fit on the experimental energies given in Fig. I. Although for $K=\frac{1}{2}^{-}$ band the strong coupling model formula (eqn. 4.1) is reasonably accurate, this is not the case for the $K=\frac{1}{2}^{+}$ band.

TABLE III

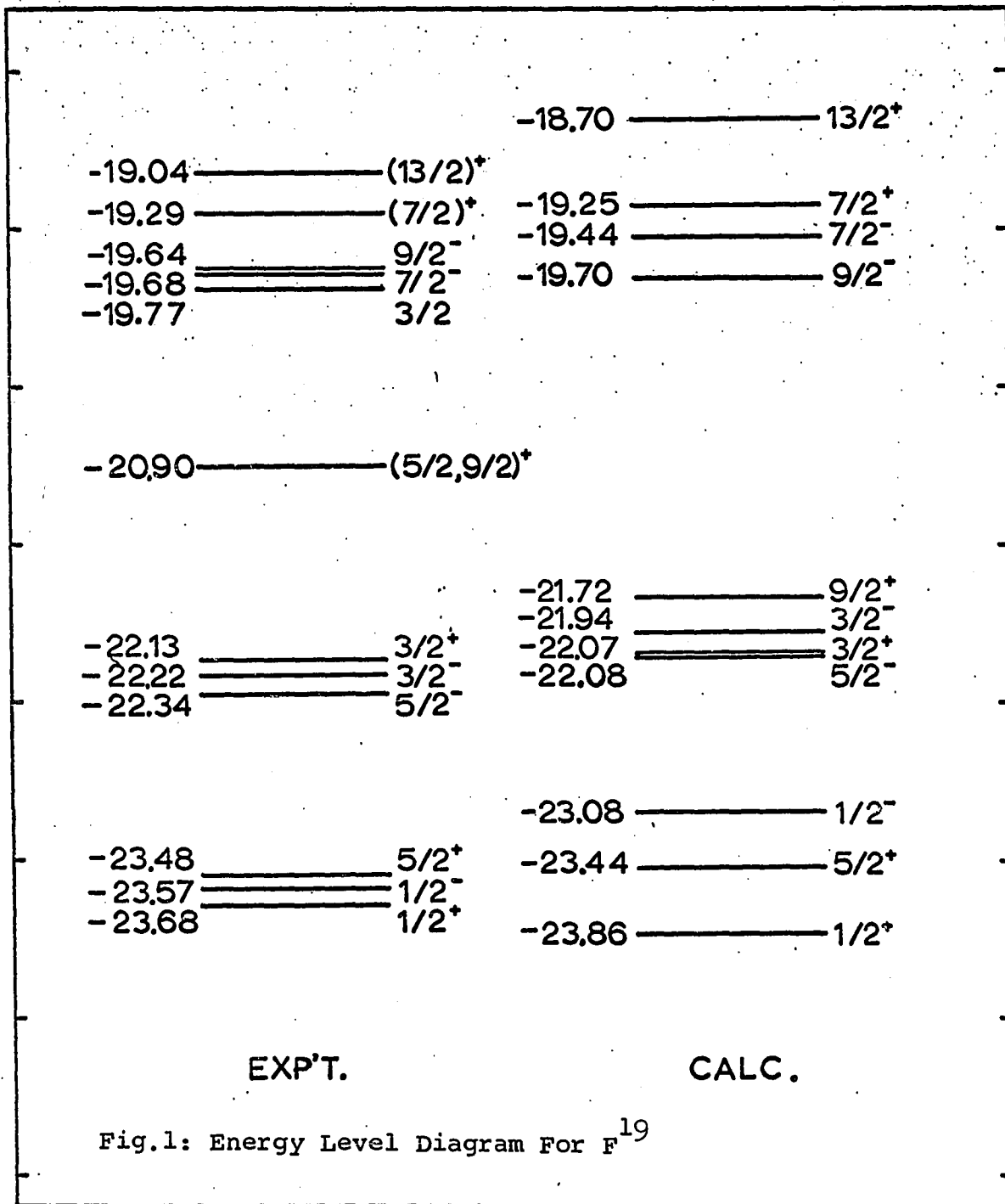|	$K=\frac{1}{2}^+$			$K=\frac{1}{2}^-$		
	E_0	A	a	E_0	A	a
expt.	-23.34	0.151	2.59	-23.44	0.192	1.02
s. c. m	-23.88	0.177	1.58	-23.06	0.177	0.88
Approx. proj.	-23.55	0.162	2.69	-23.00	0.175	1.16

Fig.1: Energy Level Diagram For F^{19}

Validity of the strong coupling formula for the decoupling parameter

Let us now introduce the following assumptions:

(1) The intrinsic state can be written as

$$|\phi_{\frac{1}{2}}\rangle = b_{\frac{1}{2}}^+ |\chi_0\rangle$$

where $|\chi_0\rangle$ is an intrinsic core wave function with K=0 and $b_{\frac{1}{2}}^+$ adds a deformed particle (or a hole) to this core. The operator $b_{\frac{1}{2}}^+$ has the usual expansion in spherical shell model operators with coefficients $c_{j\frac{1}{2}}$ and its H.F. energy is $\epsilon_{\frac{1}{2}}$.

(2) The Hamiltonian can be written as

$$H = H_0 + h = H_0 + h^{(1)} + h^{(2)}$$

where H_0 acts only on the core, and h contains all the terms that involve the extra particle (hole). Clearly, h can be written as a sum of one-body ($h^{(1)}$) and two-body ($h^{(2)}$) parts. A similar expansion is possible for the angular momentum operator

$$\vec{J} = \vec{R} + \vec{j}$$

(3) The core wave function $|\chi_0\rangle$ defines a sharp orientation in space, i.e. $F(\beta) \equiv \langle\chi_0| e^{-i\beta R_y} |\chi_0\rangle$ is sharply peaked about $\beta=0$ and $\beta=\pi$. This is the usual condition for the validity of the Bohr-Mottelson model for even-even nuclei[10] and leads to a rotational spectrum of the projected core states[16], i.e. H_0 can be replaced by a pseudo-hamiltonian $E_0 + AR^2$.

(4) The single particle (hole) wave function varies with

orientation much more slowly than the core wave function

i.e. $f(\beta) \equiv \langle 0 | b_{\frac{1}{2}} e^{-i\beta J_y} b_{\frac{1}{2}}^+ | 0 \rangle$ decreases near $\beta = 0$ much

more slowly than $F(\beta)$. Furthermore $f(\beta)$ is very small

at back angles. We can thus write:

$f(\beta) \approx 1$ in the forward peak of $F(\beta)$

$ \approx 0$ in the backward peak of $F(\beta)$

It is very easy to show (see APPENDIX II) that with the

above approximations the energies E_J are given by:

$$E_J \approx \epsilon_0 + \epsilon_{\frac{1}{2}} + A\left[\sum_j j(j+1) |c_{j\frac{1}{2}}|^2 - \frac{1}{2} \right]$$
$$+ A\left[J(J+1) - (-)^{J+\frac{1}{2}} (J+\frac{1}{2}) \left(\sum_j (-)^{j+\frac{1}{2}} (j+\frac{1}{2}) |c_{j\frac{1}{2}}|^2 \right) \right]$$

$$(4.2)$$

Fig. 2 shows a plot of $f(\beta)$ for the positive parity

and negative parity orbitals of the missing proton compared

to $F(\beta)$ calculated for the Ne^{20} core. Clearly, the $K = \frac{1}{2}^-$

band satisfies all the criteria listed above and acceptable

agreement is both expected and observed between the result

of the approximate projection method and the strong coupling

model. In the $K = \frac{1}{2}^+$ band, however, the fourth assumption

fails badly. Although the derivation shown in the APPENDIX

II only proves that the above assumptions are sufficient

to obtain the strong coupling result (eqn. 4.2), it seems

very unlikely that an alternative approach might be able

to dispense with the fourth assumption, whose failure in

the case of the $K = \frac{1}{2}^+$ band can therefore be taken as the

reason for the failure of eqn. (4.1) to give an accurate

result for the decoupling parameter.

It is worth pointing out that if the core defines a

sharp spatial orientation, and if all the single particle

wave functions (both for the particles in the core and the

extra particle) vary with orientation much more slowly

than the total core wave function, then, due to the orthogonality
of the intrinsic single particle orbitals, which is effective
near $\beta=0$, one can to a good approximation separate J and H
into core and extra particle parts. It is also clear that
the Bohr-Mottelson result should improve rapidly as the number
N of the nucleons involved in the collective motion increases,
since one expects that $F(\beta)\approx f(\beta)^N$, neglecting exchange
effects, which in turn becomes an increasingly good approximation
for increasing N.

Conclusion

The method of approximate projection for calculating moment of inertia, band head and decoupling parameter has been tested on the F^{19} nucleus. It is found that there is agreement with the strong coupling model only for $K=\frac{1}{2}^-$ band of F^{19}. The lack of agreement for $K=\frac{1}{2}^+$ band of F^{19} has been attributed to the breakdown of one of the important assumptions employed in deriving the strong coupling model. The various assumptions for the strong coupling model can be summarised as follows:

(1) The nucleus can be regarded as a core and an extra particle (hole)

(2) The total Hamiltonian and angular momentum can be separated into core and extra particle (hole) parts.

(3) The core defines a sharp spatial orientation.

(4) The spatial orientation of the wave function of the particle (hole) varies much more slowly than the core.

In the $K=$ band the fourth assumption fails badly.

The method of approximate projection in the presence of decoupling is expected to be particularly useful in the study of light nuclei where the assumptions underlying the validity of the strong coupling model are more questionable than in the heavier nuclei where a large number of particles participate in the collective motion.
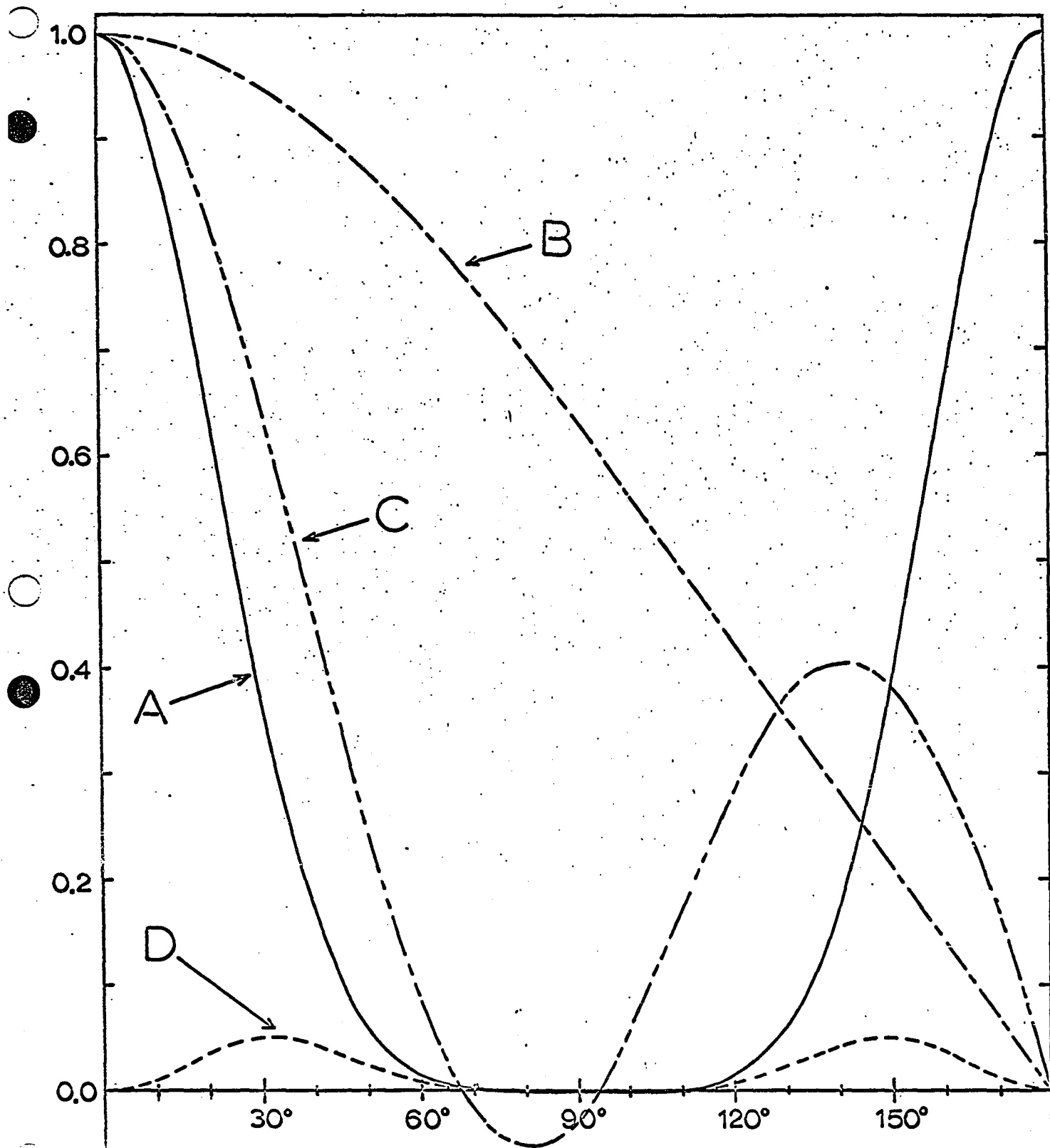
Fig 2: Curve A represents $F(\beta)$ for the Ne^{20} core, while curves B and C represent $f(\beta)$ for the $K=\frac{1}{2}^{-}$ and $K=\frac{1}{2}^{+}$ orbitals of the missing proton respectively. Curve D shows a typical off-diagonal matrix element $\langle x'| e^{-i\beta R_y} | \chi_0 \rangle$, as discussed in the APPENDIX II

APPENDIX I

Calculation of Matrix Elements

Notation

Greek indices denote arbitrary states

Small Roman denote particles

Capital Roman denote holes

Basis

(a) Spherical Basis

It is denoted by a_α^+, a_α or b_α^+, b_α where α summarises all the quantum numbers n_α, l_α, j_α, m_α, $m_{t\alpha}$. a's and b's are related.

$$b_\alpha^+ = a_\alpha^+$$

$$b_\alpha = a_\alpha$$

$$b_A^+ = a_{\bar{A}} = (-)^{j_A + m_A + \frac{1}{2} + m_{t_A}} \cdot a_{-A}$$

$$b_A = a_{\bar{A}}^+$$

(b) Deformed Basis

It is denoted by ℓ_α^+, ℓ_α

$$\ell_\alpha^+ = \sum C_{\alpha\gamma} b_\gamma^+ \tag{A.1a}$$

or

$$b_\gamma^+ = \sum (\bar{c}')_{\gamma\alpha} \ell_\alpha^+ = \sum C_{\alpha\gamma} \ell_\alpha^+ \tag{A.1b}$$

Hamiltonian (spherical basis)

$$H = \sum_\alpha \epsilon_\alpha : a_\alpha^+ a_\alpha : \;+\; \frac{1}{4} \sum V_{\alpha\beta\gamma\delta} : a_\alpha^+ a_\beta^+ a_\gamma a_\delta$$

$$\sum_\alpha \epsilon_\alpha : a_\alpha^+ a_\alpha : \;=\; \sum_\alpha \epsilon_\alpha : a_\alpha^+ a_\alpha : \;+\; \sum_A \epsilon_A : a_A^+ a_A :$$

$$=\; \sum_\alpha \epsilon_\alpha \, b_\alpha^+ b_\alpha \;+\; \sum_A \epsilon_A : b_{\bar{A}} \, b_{\bar{A}}^+ :$$

$$=\; \sum_\alpha \epsilon_\alpha \, b_\alpha^+ b_\alpha \;+\; \sum_A \epsilon_A \, b_{\bar{A}}^+ b_{\bar{A}}$$

$$=\; \sum_\alpha \epsilon_\alpha \, b_\alpha^+ b_\alpha \qquad\qquad \text{where}\quad \epsilon_\alpha = \epsilon_\alpha$$
$$\epsilon_A = -\epsilon_A$$

similarly

$$\sum V_{\alpha\beta\gamma\delta} : a_\alpha^+ a_\beta^+ a_\gamma a_\delta : \;=\; \sum U_{\alpha\beta\gamma\delta} \, b_\alpha^+ b_\beta^+ b_\gamma b_\delta$$

where

$$U_{abcd} \;=\; V_{abcd}$$

$$U_{ABCD} \;=\; V_{\bar{D}\bar{C}\bar{B}\bar{A}} \;=\; (-)^{j_A + j_B + j_C + j_D} \cdot V_{-D-C-B-A} \qquad (A.2)$$

$$U_{aBcd} \;=\; -V_{a\bar{C}\bar{B}d} \;=\; -(-)^{j_B + m_B + j_C + m_C + 1 + m_{t_B} + m_{t_C}} \cdot V_{a,-c,-B,d}$$

We have made use of the fact that $m_A + m_B = m_C + m_D$ and

therefore

$$(-)^{m_A + m_B + m_C + m_D} = 1$$

$$H = \sum_\alpha \epsilon_\alpha b_\alpha^+ b_\alpha + \frac{1}{4} \sum V_{\alpha\beta\gamma\delta} b_\alpha^+ b_\beta^+ b_\gamma b_\delta \qquad (A.2b)$$

Operators J_+, J_-, J_-J_+ in spherical basis

$$J_\pm = \sum_{\alpha,\delta} \langle \alpha | j_\pm | \delta \rangle : a_\alpha^+ a_\delta :$$

$$= \sum_{a,d} \langle a | j_\pm | d \rangle b_a^+ b_d + \sum_{A,D} \langle \bar{D} | j_\pm | \bar{A} \rangle b_A^+ b_D \qquad (A.3)$$

where

$$\langle \bar{D} | j_\pm | \bar{A} \rangle = (-)^{j_A + m_A + j_D + m_D + 1 + m_{t_A} + m_{t_D}} \cdot \langle -D | j_\pm | -A \rangle$$

since

$$j_A = j_D \quad , \qquad m_{t_A} = m_{t_D} \quad , \qquad m_A = m_D \pm 1$$

$$(j_\pm)_{\bar{D}\bar{A}} = - (j_\pm)_{-D,-A}$$

$$(j_+)_{\alpha\delta} = \delta_{n_\alpha n_\delta} \delta_{\ell_\alpha \ell_\delta} \delta_{j_\alpha j_\delta} \delta_{m_{t_\alpha} m_{t_\delta}} \delta_{m_\alpha, m_\delta + 1} \sqrt{(j_\delta - m_\delta)(j_\delta + m_\delta + 1)}$$

$$(j_-)_{\alpha\delta} = \delta_{n_\alpha n_\delta} \delta_{\ell_\alpha \ell_\delta} \delta_{j_\alpha j_\delta} \delta_{m_{t_\alpha} m_{t_\delta}} \delta_{m_\alpha, m_\delta - 1} \sqrt{(j_\delta + m_\delta)(j_\delta - m_\delta + 1)}$$

Using eqns.(A.3)

$$(J_- J_+) = \sum_\alpha (j_- j_+)_\alpha \, b_\alpha^+ b_\alpha + \sum_A (j_+ j_-)_{\bar{A}} \, b_A^+ b_A$$

$$+ \sum_{abcd} (j_-)_{ad} \, (j_+)_{bc} \, b_a^+ b_b^+ b_c b_d + \sum_{ABCD} (j_-)_{\bar{D}\bar{A}} (j_+)_{\bar{C}\bar{B}} \, b_A^+ b_B^+ b_C b_D$$

$$- \sum_{\substack{a\,d \\ B\,c}} \left[(j_-)_{\bar{C}\bar{B}} \, (j_+)_{ad} + (j_+)_{\bar{C}\bar{B}} \, (j_-)_{ad} \right] b_B^+ b_c^+ b_a^+ b_d \qquad (A.4)$$

$$(j_- j_+)_\alpha = (j_\alpha - m_\alpha)(j_\alpha + m_\alpha + 1)$$

$$(j_+ j_-)_{\bar{A}} = (j_A - m_A)(j_A + m_A + 1)$$

Hamiltonian (deformed basis)

$$H = \sum_{\alpha'} \epsilon_{\alpha'} \, b_{\alpha'}^+ b_{\alpha'} + \frac{1}{4} \sum U_{\alpha'\beta'\gamma'\delta'} \, b_{\alpha'}^+ b_{\beta'}^+ b_{\gamma'} b_{\delta'} \qquad (A.5)$$

Using eqn. (A.1b)

$$H = \sum \tilde{\epsilon}_{\alpha\delta} \, b_\alpha^+ b_\delta + \frac{1}{4} \sum \tilde{U}_{\alpha\beta\gamma\delta} \, b_\alpha^+ b_\beta^+ b_\gamma b_\delta \qquad (A.5a)$$

where

$$\tilde{\epsilon}_{\alpha\delta} = \sum_{\alpha'} \epsilon_{\alpha'} \, C_{\alpha\alpha'} \, C_{\delta\delta'} \qquad (A.6)$$

$$\tilde{U}_{\alpha\beta\gamma\delta} = \sum C_{\alpha\alpha'} \, C_{\beta\beta'} \, C_{\gamma\gamma'} \, C_{\delta\delta'} \, U_{\alpha'\beta'\gamma'\delta'} \qquad (A.6a)$$

Operator $J_- J_+$ (deformed basis)

$$J_- J_+ = \sum_{\alpha\delta} \widetilde{(j_- j_+)}_{\alpha\delta} \, b_\alpha^+ b_\delta + \sum \widetilde{(j_-)}_{\alpha\delta} \, \widetilde{(j_+)}_{\beta\gamma} \, b_\alpha^+ b_\beta^+ b_\gamma b_\delta \qquad (A.7)$$

where

$$\widetilde{(j_- j_+)}_{ad} = \sum_{\alpha'} C_{a\alpha'} \, C_{d\alpha'} \, (j_- j_+)_{\alpha'} \qquad (A.8a)$$

$$\widetilde{(J_- J_+)}_{AD} = \sum_{A'} C_{AA'} C_{DA'} (J_+ J_-)_{\overline{A}'} \tag{A.8b}$$

$$\widetilde{(J_\pm)}_{ad} = \sum_{a'd'} C_{aa'} C_{dd'} (J_\pm)_{a'd'} \tag{A.8c}$$

$$\widetilde{(J_\pm)}_{AD} = -\sum_{A'D'} C_{AA'} C_{DD'} (J_\pm)_{\overline{D}'\overline{A}'} \tag{A.8d}$$

Now we are in a position to calculate the various matrix elements. For example,

$$\langle \phi_k | J_- J_+ | \phi_k \rangle = \sum_{\alpha\delta} \widetilde{(J_- J_+)}_{\alpha\delta} \langle \phi_k | b_\alpha^+ b_\delta | \phi_k \rangle$$

$$+ \sum \widetilde{(J_-)}_{\alpha\delta} \widetilde{(J_-)}_{\beta\gamma} \langle \phi_k | b_\alpha^+ b_\beta^+ b_\gamma b_\delta | \phi_k \rangle$$

$$= \sum_\alpha \widetilde{(J_- J_+)}_{\alpha\alpha} n_\alpha - \sum_{\alpha\beta} \widetilde{(J_-)}_{\alpha\beta} \widetilde{(J_+)}_{\beta\alpha} n_\alpha n_\beta \tag{A.9}$$

Since

$$\widetilde{(J_+)}_{\alpha\alpha} = 0$$

Also

$$n_\alpha = \langle \phi_{HF} | b_\alpha^+ b_\alpha | \phi_{HF} \rangle$$

$$n_\alpha = 1 \quad \text{if } \alpha \text{ is occupied}$$
$$= 0 \quad \text{if } \alpha \text{ is not occupied}$$

$$|\phi_k^*\rangle = b_\alpha^+ b_\delta |\phi_k\rangle \quad , \quad |\phi_k^{**}\rangle = b_\alpha^+ b_\beta^+ b_\gamma b_\delta |\phi_k\rangle$$

Other matrix elements are given in APPENDIX III.A

Matrix Elements Involving T

Such matrix elements are dependent on a particular nuclear configuration. T unlike J_+ is a many particle operator. This means that while J_+ is a sum of single particle operators $(\sum_i (j_+)^i)$ T is a product $(\pi_i T^i)$.

Positive parity states of F^{19}

$$|\phi_{HF}\rangle = b^+_{\frac{1}{2}\frac{1}{2}} \, b^+_{\frac{1}{2}-\frac{1}{2}} \, b^+_{-\frac{1}{2}-\frac{1}{2}} \, |0^{16}\rangle$$

$$\therefore T|\phi_{HF}\rangle = b^+_{\frac{1}{2}\frac{1}{2}} \, b^+_{-\frac{1}{2}-\frac{1}{2}} \, (-b^+_{+\frac{1}{2}-\frac{1}{2}}) |0^{16}\rangle$$

$$= b^+_{-\frac{1}{2}\frac{1}{2}} \, b^+_{\frac{1}{2}-\frac{1}{2}} \, b^+_{-\frac{1}{2}-\frac{1}{2}} \, |0^{16}\rangle$$

$$= b^+_{\tilde{k}} \, b_{k} \, |\phi_{HF}\rangle$$

where k stands for particle state with $m_k = -m_{\tilde{k}} = \frac{1}{2}$

$$\langle \phi_{HF}|J_+ T|\phi_{HF}\rangle = \sum_{\substack{a,d \\ a'd'}} (j_+)_{a'd'} \, C_{aa'} \, C_{dd'} \, \langle \phi_{HF}| b^+_a b_d \, T|\phi_{HF}\rangle$$

$$- \sum_{AD,AD'} (j_+)_{D'\bar{A}'} \, C_{AA'} \, C_{DD'} \, \langle \phi_{HF}| b^+_A b_D \, T|\phi_{HF}\rangle$$

Second term is zero. Also

$$n_k = 1$$

$$n_{\tilde{k}} = 0$$

$$\therefore \langle \phi_{HF}|J_+ T|\phi_{HF}\rangle = \sum_{a'd'} (j_+)_{a'd'} \, C_{ka'} \, C_{\tilde{k}d'}$$

Other matrix elements for this case are listed in APPENDIX III.B

Negative parity states of F^{19}

$$T|\phi_{HF}\rangle = b_{\tilde{k}}^{+} b_{k} |\phi_{HF}\rangle$$

K stands for hole (unpaired) state with $m_{K} = -m_{\tilde{K}} = \frac{1}{2}$

As before

$$\langle \phi_{HF}| J_{+}T| \phi_{HF}\rangle = -\sum_{A'D'} (j_{+})_{\tilde{D}'\tilde{A}'} C_{kA'} C_{\tilde{K}D'} \qquad (A.11)$$

For other matrices of this case, see APPENDIX III.C

APPENDIX II

We shall now derive eqn. (4.2) from the exact expression for the energies of the projected states (eqn. 2.6)

$$E_J = \langle \phi_{\frac{1}{2}} | H\, P^J_{\frac{1}{2}\frac{1}{2}} | \phi_{\frac{1}{2}} \rangle \Big/ \langle \phi_{\frac{1}{2}} | P^J_{\frac{1}{2}\frac{1}{2}} | \phi_{\frac{1}{2}} \rangle$$

where $P^J_{\frac{1}{2}\frac{1}{2}}$ is the angular momentum projection operator.

With the assumptions listed in Chapter IV, we have for the Hamiltonian:

$$H \approx \varepsilon_0 + A \vec{R}^2 + h$$

$$= \left(\varepsilon_0 + A \vec{J}^2 - 2A\, j_z J_z \right) - A\, j_- J_+ - A\, j_+ J_- + \left(h + A \vec{j}^2 \right)$$

The overlap integral can be written:

$$\langle \phi_{\frac{1}{2}} | P^J_{\frac{1}{2}\frac{1}{2}} | \phi_{\frac{1}{2}} \rangle = \frac{2J+1}{2} \int_0^\pi d\beta\, \sin\beta\, d^J_{\frac{1}{2}\frac{1}{2}}(\beta) \langle \phi_{\frac{1}{2}} | e^{-i\beta J_y} | \phi_{\frac{1}{2}} \rangle$$

$$\approx \frac{2J+1}{2} \int_0^{\beta_{max}} d\beta\, \sin\beta\, d^J_{\frac{1}{2}\frac{1}{2}}(\beta) \langle \chi_0 | e^{-i\beta J_y} | \chi_0 \rangle$$

where $\beta_{max} < \frac{\pi}{2}$ is a value of β outside the peak of $F(\beta)$. The matrix elements of the Hamiltonian can be calculated term by term.

$$\langle \phi_{\frac{1}{2}} | \left(\varepsilon_0 + A \vec{J}^2 - 2A\, j_z J_z \right) P^J_{\frac{1}{2}\frac{1}{2}} | \phi_{\frac{1}{2}} \rangle = \left(\varepsilon_0 + A J(J+1) - \frac{1}{2} A \right) \langle \phi_{\frac{1}{2}} | P^J_{\frac{1}{2}\frac{1}{2}} | \phi_{\frac{1}{2}} \rangle$$

$$\langle \phi_{\frac{1}{2}} | A\, j_- J_+ P^J_{\frac{1}{2}\frac{1}{2}} | \phi_{\frac{1}{2}} \rangle = A \left[(J-\tfrac{1}{2})(J+\tfrac{3}{2}) \right]^{1/2} \cdot \frac{2J+1}{2} \int_0^\pi d\beta\, \sin\beta\, d^J_{\frac{3}{2}\frac{1}{2}}(\beta)$$

$$\cdot \langle \chi_0 | e^{-i\beta R_y} | \chi_0 \rangle \langle 0 | b_{\frac{1}{2}}\, j_-\, e^{-i\beta j_y}\, b^+_{\frac{1}{2}} | 0 \rangle$$

$$\approx 0 \qquad \text{since } d^J_{\frac{3}{2}\frac{1}{2}}(\beta) \longrightarrow 0 \text{ for small } \beta$$

$$\langle \phi_{\frac{1}{2}} | A j_+ j_- P_{\frac{1}{2}\frac{1}{2}}^J | \phi_{\frac{1}{2}} \rangle = A (J+\tfrac{1}{2})^2 \int_0^{\pi} d\beta \sin\beta \, d_{-\frac{1}{2}\frac{1}{2}}^J (\beta) \langle \chi_0 | e^{-i\beta R_y} | \chi_0 \rangle$$

$$\cdot \langle 0 | b_{\frac{1}{2}} j_+ \, e^{-i\beta j_y} b_{\frac{1}{2}}^+ | 0 \rangle$$

$$= A (-)^{J+\frac{1}{2}} (J+\tfrac{1}{2})^2 \int_0^{\pi} d\beta' \sin\beta' d_{\frac{1}{2}\frac{1}{2}}^J (\beta') \langle \chi_0 | e^{-i\beta R_y} | \chi_0 \rangle$$

$$\cdot \langle 0 | b_{\frac{1}{2}} \, j_+ \, e^{-i\pi j_y + i\beta' j_y} b_{\frac{1}{2}}^+ | 0 \rangle$$

$$\approx A (-)^{J+\frac{1}{2}} (J+\tfrac{1}{2}) \left[\sum_j (-)^{j+\frac{1}{2}} (j+\tfrac{1}{2}) |C_{j\frac{1}{2}}|^2 \right] \langle \phi_{\frac{1}{2}} | P_{\frac{1}{2}\frac{1}{2}}^J | \phi_{\frac{1}{2}} \rangle$$

We have made use of the fact that $\langle \chi_0 | e^{-i\beta' R_y} | \chi_0 \rangle$ is symmetric about $\frac{\pi}{2}$ to change to $\beta' = \pi - \beta$.

$$\langle \phi_{\frac{1}{2}} | h^{(2)} P_{\frac{1}{2}\frac{1}{2}}^J | \phi_{\frac{1}{2}} \rangle = \sum_{\mu\nu\sigma\tau} V_{\mu\nu\sigma\tau} (J+\tfrac{1}{2}) \int_0^{\pi} d\beta \sin\beta \, d_{\frac{1}{2}\frac{1}{2}}^J (\beta) \langle \chi_0 | a_\mu^+ a_\tau e^{-i\beta R_y} | \chi_0 \rangle$$

$$\cdot \langle 0 | b_{\frac{1}{2}} a_\nu^+ a_\sigma \, e^{-i\beta j_y} b_{\frac{1}{2}}^+ | 0 \rangle$$

The $V_{\mu\nu\sigma\tau}$ are antisymmetrised matrix elements of the two-body potential and the operators a_μ^+, a_μ are the creation and annihilation operators for a particle with quantum numbers μ. We can thus write

$$\langle \chi_0 | a_\mu^+ a_\tau e^{-i\beta R_y} | \chi_0 \rangle = \langle \chi_0 | a_\mu^+ a_\tau | \chi_0 \rangle \langle \chi_0 | e^{-i\beta R_y} | \chi_0 \rangle$$

$$+ \sum' \langle \chi_0 | a_\mu^+ a_\tau | \chi' \rangle \langle \chi' | e^{-i\beta R_y} | \chi_0 \rangle$$

where $|\chi'\rangle$ are excited intrinsic core states. The first term evidently gives the Hartree-Fock potential energy corresponding to $b_{\frac{1}{2}}^+$, while the second term contains the off-diagonal matrix element $\langle \chi' | e^{-i\beta R_y} | \chi \rangle$ which is very small (see Ref. 16 and Fig. 2), and can be neglected.

We can therefore write that

$$\langle \phi_{\frac{1}{2}} | (h^{(1)} + h^{(2)} + A \vec{j}^2) \, P_{\frac{1}{2}\frac{1}{2}}^{J} | \phi_{\frac{1}{2}} \rangle \approx \left[\epsilon_{\frac{1}{2}} + A \sum_{j} j(j+1) |C_{j\frac{1}{2}}|^2 \right] \langle \phi_{\frac{1}{2}} | P_{\frac{1}{2}\frac{1}{2}}^{J} | \phi_{\frac{1}{2}} \rangle$$

where $\epsilon_{\frac{1}{2}}$ is the Hartree-Fock energy of the orbital corresponding to $b_{\frac{1}{2}}^{+}$. Getting all these relevant terms we obtain the eqn. 4.2

APPENDIX III.A

$$\langle \phi_k^* | J_- J_+ | \phi_k \rangle = (1-n_\alpha)\, n_\delta \left[\widetilde{(J_- J_+)}_{\alpha\delta} - \sum_{\beta'} n_{\beta'} \left\{ (\widetilde{J_-})_{\alpha\beta'} (\widetilde{J_+})_{\beta'\delta} \atop + (\widetilde{J_+})_{\alpha\beta'} (\widetilde{J_-})_{\beta'\delta} \right\} \right]$$

$$\langle \phi_k^{**} | J_- J_+ | \phi_k \rangle = n_\delta\, n_\gamma (1-n_\alpha)(1-n_\beta) \left[(\widetilde{J_-})_{\alpha\delta} (\widetilde{J_+})_{\beta\gamma} - (\widetilde{J_-})_{\beta\delta} (\widetilde{J_+})_{\alpha\gamma} \right.$$
$$\left. - (\widetilde{J_-})_{\alpha\gamma} (\widetilde{J_+})_{\beta\delta} + (\widetilde{J_-})_{\beta\gamma} (\widetilde{J_+})_{\alpha\delta} \right]$$

$$\langle \phi_k^{**} | H | \phi_k \rangle = (1-n_\alpha)(1-n_\beta)\, n_\gamma\, n_\delta\, \widetilde{u}_{\alpha\beta\gamma\delta}$$

APPENDIX III.B

If α, ∂ are particles

$$\langle \phi_{HF}^{*} | J_{+}T | \phi_{HF} \rangle = -\sum_{a'd'} (j_{+})_{a'd'} \left[C_{ka'} C_{dd'} \eta_{a} \delta_{a\tilde{k}} - C_{aa'} C_{\tilde{k}d'} (1-\eta_{a}) \delta_{dk} \right]$$

If α, ∂ are holes

$$\langle \phi_{HF}^{*} | J_{+}T | \phi_{HF} \rangle = 0$$

If α, β, γ, ∂ are particles

$$\langle \phi_{HF}^{**} | J_{+}T | \phi_{HF} \rangle = +\sum_{a'd'} (j_{+})_{a'd'} \left[-\eta_{a}(1-\eta_{b}) C_{ba'} C_{dd'} \delta_{ck} \delta_{a\tilde{k}} + \eta_{a}(1-\eta_{a}) C_{aa'} C_{dd'} \delta_{ck} \delta_{d\tilde{k}} \right.$$
$$\left. + \eta_{c}(1-\eta_{a}) C_{aa'} C_{cd'} \delta_{dk} \delta_{a\tilde{k}} - \eta_{c}(1-\eta_{a}) C_{aa'} C_{cd'} \delta_{dk} \delta_{b\tilde{k}} \right]$$

If α, β, γ, ∂ are holes

$$\langle \phi_{HF}^{**} | J_{+}T | \phi_{HF} \rangle = 0$$

If α, ∂ are particles and β, γ are holes

$$\langle \phi_{HF}^{**} | J_{+}T | \phi_{HF} \rangle = -\sum_{A'D'} (1-\eta_{B}) \eta_{c} C_{BA'} C_{CD'} (j_{+})_{\bar{D}'\bar{A}'} \delta_{dk} \delta_{a\tilde{k}}$$

APPENDIX III.C

If α, ∂ are particles

$$\langle \phi_{HF}^{*} | J_+ T | \phi_{HF} \rangle = 0$$

If α, ∂ are holes

$$\langle \phi_{HF}^{*} | J_+ T | \phi_{HF} \rangle = \sum_{A'D'} (j_+)_{\bar{D}'\bar{A}'} \left[C_{AA'} C_{\tilde{K}D'} (1-\eta_A) \delta_{D,K} - C_{KA'} C_{DD'} \eta_D \delta_{A\tilde{K}} \right]$$

If α, β, γ, ∂ are particles

$$\langle \phi_{HF}^{**} | J_+ T | \phi_{HF} \rangle = 0$$

If α, β, γ, ∂ are holes

$$\langle \phi_{HF}^{**} | J_+ T | \phi_{HF} \rangle = \sum_{A'D'} (j_+)_{\bar{D}'\bar{A}'} \left[\eta_D (1-\eta_B) C_{BA'} C_{DD'} \delta_{C,K} \delta_{A\tilde{K}} - \eta_D (1-\eta_A) C_{AA'} C_{DD'} \delta_{CK} \delta_{B\tilde{K}} \right.$$
$$\left. - \eta_C (1-\eta_B) C_{BA'} C_{CD'} \delta_{DK} \delta_{A\tilde{K}} + \eta_C (1-\eta_A) C_{AA'} C_{CD'} \delta_{DK} \delta_{B\tilde{K}} \right]$$

If α, ∂ are particles and β, γ are holes

$$\langle \phi_{HF}^{**} | J_+ T | \phi_{HF} \rangle = \sum_{a'd'} (1-\eta_a) \eta_d C_{aa'} C_{dd'} (j_+)_{a'd'} \delta_{C,K} \delta_{B,\tilde{K}}$$

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