**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 $^{19}F$ 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 rotationnelles avec $K = \frac{1}{2}$. L'application de cette méthode aux premières bandes rotationnelles de parité positive et négative du noyau $^{19}$ 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

June, 1969
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INTRODUCTION

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

The deformation in nuclei is usually interpreted as the effect of long-range correlations among the nucleons. In $SU(3)$ model of the nucleus one takes a long-range specialized 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 and will be followed in the present work.

The total angular momentum $J$ of the intrinsic wave function $\psi_k$ 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 $\Psi$ are not physical. The physical states are obtained by projecting (by exact projection or approximate projection technique) out of $\Psi$ 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 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 $^{19}$F. 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

$$H = \sum \langle \alpha | T | \beta \rangle c^+_\alpha c_\beta + \frac{1}{4} \sum \langle \beta | V | \gamma \rangle c^+_\alpha c^+_\beta c_\gamma c_\gamma$$  \hspace{1cm} (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 $V$. $\langle \alpha \rangle$, $\langle \beta \rangle$, 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 $\phi$ is assumed to have the form of a determinant of single particle orbitals $|i\rangle$, $|i_1\rangle$, $|i_2\rangle$, $\ldots$, $|i_A\rangle$. In the second quantised notation

$$|\psi\rangle = b^+_i b^+_i \ldots b^+_i |0\rangle$$  \hspace{1cm} (1.2)

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

$$|\psi\rangle = b^+_i b^+_i b^+_i |0\rangle$$  \hspace{1cm} (1.2a)

$|i\rangle$ can be expanded in the known single particle basis $\langle \alpha \rangle$, $\langle \beta \rangle$, $\ldots$.
\[ |\psi\rangle = \sum_{\lambda=\alpha_1,\ldots} \sum_{\mu} C_{i\lambda} |\lambda\rangle \]  

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

\[ E_{HF} = \langle \psi | H | \psi \rangle = \sum_i \langle i | T | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | V | ij \rangle \]  

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

\[ \frac{\partial}{\partial C_{i\lambda}} \left( E_{HF} - e_i \left( \sum_{\mu} C_{i\lambda} \lambda^2 - 1 \right) \right) = 0 \]  

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

\[ \sum_{\mu} \left[ \langle \lambda | T | \mu \rangle + \sum_i \langle \lambda i | V | \mu i \rangle \right] C_{\mu \lambda} = e_i C_{i\lambda} \]  

This is equivalent to an eigenvalue problem:

\[ h |i\rangle = e_i |i\rangle \]  

\[ \langle \lambda | h | \mu \rangle = \langle \lambda | T | \mu \rangle + \sum_i \langle \lambda i | V | \mu i \rangle \]

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,

\[ |m = \frac{1}{2}\rangle = |\frac{1}{2}\rangle = C_{\frac{1}{2} \frac{1}{2}} |d_{\frac{1}{2} \frac{1}{2}}\rangle + C_{\frac{1}{2} \frac{3}{2}} |d_{\frac{1}{2} \frac{3}{2}}\rangle + C_{\frac{1}{2} \frac{1}{2}} |d_{\frac{1}{2} \frac{1}{2}}\rangle \]
An iteration method is employed to determine these coefficients and the corresponding energies.

(a) Take H.F. orbitals $|i^{(0)}\rangle$ 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.

$$E_{\text{HF}} \text{ is given by}$$

$$E_{\text{HF}} = \frac{1}{2} \sum_i \left[ \langle i | T | i \rangle + e_i \right] \quad (1.9)$$

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 $e$ 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

$$V(r) = V_0 g(r) \left[ W + B P_r + H P_r P_x + M P_x \right] \quad (1.10)$$

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

\[ W + B + H + M = 1 \]  \hspace{1cm} (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>
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<th>Level</th>
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<td>$0d_3/2$</td>
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</tr>
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<td>$1s_{1/2}$</td>
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</tr>
<tr>
<td>$0p_{3/2}$</td>
<td>-15.65</td>
</tr>
<tr>
<td>$0s_{1/2}$</td>
<td>-21.8</td>
</tr>
<tr>
<td>Name</td>
<td>$g(r)$</td>
</tr>
<tr>
<td>--------</td>
<td>----------------</td>
</tr>
<tr>
<td>Gillet</td>
<td>$\exp(-\alpha r^2)$</td>
</tr>
<tr>
<td>Inoue</td>
<td>$\frac{\exp(-\alpha r)}{r}$</td>
</tr>
</tbody>
</table>
It is found that the H.F. wave functions $\phi_k$ 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 $\phi_k$ the components with angular momentum $J$.

It can be seen very easily that H.F. wave functions with $K \neq 0$ can give projected states with $J = K, K+1, K+2, \ldots$. 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.

\[ |\phi_p\rangle = \sum_J a_J |J,0\rangle \]  \hspace{1cm} (2.1)

\[ \exp(-i\pi J) |\phi_p\rangle = \sum_{JM} a_J d^{JM}_{m0} (\pi) |JM\rangle \]

\[ = \sum_J a_J (-)^J |J,0\rangle \]
Now we prove that $|\phi_o\rangle$ should remain unchanged under application of the time reversal operator $\exp(-i\pi J_3)$.

Since $J_3 = \sum_{m=1}^{\Lambda} \langle \hat{J}_3 \rangle_{m}$, $\exp(-i\pi J_3) |\phi_o\rangle$ is itself a determinant. Thus we can write

$$\exp(-i\pi J_3) |\phi_o\rangle = (\exp(-i\pi \hat{J}_3) b_{k_1}^+ ) (\exp(-i\pi \hat{J}_3) b_{k_2}^+ ) \cdots |o\rangle$$

$$= b_{k_1}^+ (- b_{k_1}^+ ) \cdots \cdots \cdots \cdots |o\rangle$$

$$= b_{k_1}^+ b_{k_1}^+ \cdots \cdots \cdots \cdots |o\rangle$$

$$= |\phi_o\rangle$$

Thus

$$\sum_{J} a_J (-)^J |J 0\rangle = \sum_{J} a_J |J 0\rangle$$

(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 $P^M_J$ to be the angular momentum projection operator.

$$P^M_J = \sum_{JM} |JM\rangle \langle JM|$$

(2.3a)

$$( P^M_J )^2 = P^M_J$$

(2.3b)
where $|JM\rangle$ are a complete set of orthonormal eigenstates of $J^2$ and $J_z$.

To project states of good $J$ out of $\phi_k$, note
\[
|\phi\rangle = \sum_{JM} P^J_M |JM\rangle = \sum_{JM} a_{JM} |JM\rangle
\]  
(2.4)

Assuming $|JM\rangle$ to be normalised,
\[
|JM\rangle = \frac{P^J_M |\phi\rangle}{\sqrt{\langle \phi | P^J_M | \phi \rangle}}
\]  
(2.5)

\[
E_J = \langle JM | H | JM \rangle = \frac{\langle \phi | H P^J_M | \phi \rangle}{\langle \phi | P^J_M | \phi \rangle}
\]  
(2.6)

When $|\phi\rangle$ has axial symmetry it can be shown that
\[
\langle \phi | P^J_M | \phi \rangle = (J + \frac{1}{2}) \int_0^{\pi} \sin \theta \, d\theta \, d^J_{mm}(\theta) \langle \phi | e^{-i\theta J_y} | \phi \rangle
\]  
(2.7)
\[
\langle \phi | H P^J_M | \phi \rangle = (J + \frac{1}{2}) \int_0^{\pi} \sin \theta \, d\theta \, d^J_{mm}(\theta) \langle \phi | H e^{-i\theta J_y} | \phi \rangle
\]  
(2.8)

where $d^J_{mm}(\theta)$ is the reduced rotation matrix.

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

There are other methods of writing (2.7) and (2.8) (See Ref.10) and each is suited to a specific purpose.

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 extension (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

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

$$|\Phi\rangle = \sum_J a_J |J_{\frac{1}{2}}\rangle \quad (3.2)$$

Here $E_0$ is the band head, $A=\frac{1}{4J}$ where $J$ 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:

$$\hat{H} = E_0 + AJ+ Aa J_+ T \quad (3.3)$$

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

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

$$\langle \phi_{\frac{1}{2}} | (H - \mathcal{H}) \mathbb{J} \mathbb{J}_+ | \phi_{\frac{1}{2}} \rangle = 0 \quad (3.5)$$

$$\langle \phi_{\frac{1}{2}} | (H - \mathcal{H}) \mathbb{J}_+ \mathbb{J} | \phi_{\frac{1}{2}} \rangle = 0 \quad (3.6)$$

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 $E_o$, $A$ and $a$. It is easy to see that

$$\langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}} \rangle = E_o + A \langle \phi_{\frac{1}{2}} | \mathbb{J}^2 | \phi_{\frac{1}{2}} \rangle + Aa \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J} | \phi_{\frac{1}{2}} \rangle \quad (3.7)$$

$$\langle \phi_{\frac{1}{2}} | H \mathbb{J}_+ \mathbb{J} | \phi_{\frac{1}{2}} \rangle = E_o \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J} | \phi_{\frac{1}{2}} \rangle + A \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J}^2 | \phi_{\frac{1}{2}} \rangle + Aa \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J}_+ \mathbb{J} | \phi_{\frac{1}{2}} \rangle \quad (3.8)$$

$$\langle \phi_{\frac{1}{2}} | H \mathbb{J}_+ \mathbb{J}_+ | \phi_{\frac{1}{2}} \rangle = E_o \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J}_+ | \phi_{\frac{1}{2}} \rangle + A \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J}_+ \mathbb{J}_+ | \phi_{\frac{1}{2}} \rangle + Aa \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J}_+ \mathbb{J}_+ \mathbb{J} | \phi_{\frac{1}{2}} \rangle \quad (3.9)$$

Note that

$$\langle \phi_{\frac{1}{2}} | H \mathbb{J}_+ \mathbb{J}_+ | \phi_{\frac{1}{2}} \rangle = \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J}_+ \mathbb{J}_+ | \phi_{\frac{1}{2}} \rangle$$

$$= \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J}_+ | \phi_{\frac{1}{2}} \rangle \langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}} \rangle$$

$$+ \sum'' \langle \phi_{\frac{1}{2}} | \mathbb{J}_+ \mathbb{J}_+ | \phi_{\frac{1}{2}} \rangle \langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}} \rangle \quad (3.10)$$

and
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).

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

\[ A = \frac{c_4}{c_5 + \alpha c_1} \]

\[ a = \frac{c_4 c_1 - c_3 c_5}{c_3 c_1 - c_4 c_2} \]

where

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

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

\[ C_3 = \sum'' \langle \phi_{\frac{1}{2}} | H | \phi_{\frac{1}{2}} \rangle \langle \phi_{\frac{1}{2}} | J_+ T | \phi_{\frac{1}{2}} \rangle \]
Thus the problem reduces to calculation of matrix elements $\langle \phi_{\frac{1}{2}} | \mathcal{J}_+ | \phi_{\frac{1}{2}} \rangle$, $\langle \phi_{\frac{1}{2}} | \mathcal{J}_+ | \phi_{\frac{1}{2}} \rangle$, 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 \( E_0 \), \( A \) 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

\[
a = - \sum_j (-)^{j+\frac{1}{2}} \langle j+\frac{1}{2} \mid \mathbf{C}_j \mid \frac{1}{2} \rangle^2
\]

where \( \mathbf{C}_j \) 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 \( 'a', A, E_0 \), 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>
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<th>( K=\frac{1}{2}^- )</th>
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<td></td>
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<td>( A )</td>
<td>( a )</td>
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<td>( A )</td>
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<td>2.69</td>
<td>-23.00</td>
<td>0.175</td>
<td>1.16</td>
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Fig. 1: Energy Level Diagram For $^{19}$F

EXPT.  CALC.

-20.90  -18.70
-19.04  13/2^+  
-19.29  7/2^+
-19.64  9/2^-
-19.68  7/2^-
-19.77  3/2

-21.72  9/2^+
-22.13  3/2^+
-22.22  3/2^-
-22.34  5/2^-

-23.08  1/2^-
-23.48  5/2^+
-23.57  1/2^-
-23.68  1/2^+

-23.86  1/2^+  

Fig. 1
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

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

where $|\chi_o\rangle$ 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 $\varepsilon_{\frac{1}{2}}$.

(2) The Hamiltonian can be written as

$$H = H_0 + h = H_0 + (u) + (a)$$

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 $|\chi_o\rangle$ defines a sharp orientation in space, i.e. $F(\beta) = \langle \chi_o | e^{-i\beta R_y} | \chi_o \rangle$ 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. $H$ can be replaced by a pseudo-hamiltonian $E_o + \Delta R^2$.

(4) The single particle (hole) wave function varies with
orientation much more slowly than the core wave function i.e.,

\[ f(\beta) \equiv \langle \beta | b_{\pm}^{-} \phi_{\pm} | 0 \rangle \]

decreases near \( \beta=0 \) much more slowly than \( F(\beta) \). Furthermore \( f(\beta) \) is very small at back angles. We can thus write:

\[ f(\beta) \approx 1 \quad \text{in the forward peak of } F(\beta) \]

\[ \approx 0 \quad \text{in the backward peak of } F(\beta) \]

It is very easy to show (see APPENDIX II) that with the above approximations the energies \( E_J \) are given by:

\[
E_J \approx E_0 + E_\pm + A \left[ \sum_j \frac{j (j+1)}{2} | C_j \rangle^2 \right] + A \left[ J(J+1) - \frac{1}{2} J^{+2} \left( \sum_j (-)^{j+\frac{1}{2}} (j+\frac{1}{2}) | C_j \rangle^2 \right) \right]
\]

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 $F(\beta) \sim f(\beta)$, 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 $^{19}$F nucleus. It is found that there is agreement with the strong coupling model only for $K=\frac{1}{2}^-$ band of $^{19}$F. The lack of agreement for $K=\frac{1}{2}^+$ band of $^{19}$F 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 $K=\frac{1}{2}^-$ 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 $\langle \chi' | \sigma^z \beta_{xy} | \chi \rangle$, 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 $\alpha^+_a$, $\alpha_a$, or $b^+_a$, $b_a$ where $\alpha$ summarises all the quantum numbers $n_\alpha$, $l_\alpha$, $j_\alpha$, $m_\alpha$, $m_{\alpha}$. $a$'s and $b$'s are related.

\[
\begin{align*}
 b^+_a &= \alpha^+_a \\
 b_a &= \alpha_a \\
 b^+_A &= \alpha^+_A = (-)^{j_A + m_A + \frac{1}{2} + m_{t_A}} \cdot \alpha^-_A \\
 b_A &= \alpha^+_A
\end{align*}
\]

(b) Deformed Basis

It is denoted by $\tilde{b}^+_\alpha$, $\tilde{b}_\alpha$

\[
\tilde{b}^+_\alpha = \sum c_{\alpha\gamma} b^+_\gamma \quad \text{(A.1a)}
\]

or

\[
\tilde{b}^+_\gamma = \sum (\tilde{c}')_{\gamma\alpha} \tilde{b}^+_\alpha = \sum c_{\alpha\gamma} b^+_\gamma \quad \text{(A.1b)}
\]
Hamiltonian (spherical basis)

\[ H = \sum \epsilon_\alpha : a^\dagger_\alpha a^\dagger_\alpha : + \frac{1}{4} \sum V_{\alpha \beta \gamma \delta} : a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a^\dagger_\delta : \]

\[ \sum \epsilon_\alpha : a^\dagger_\alpha a^\dagger_\alpha : = \sum_\alpha \epsilon_\alpha : a^\dagger_\alpha a^\dagger_\alpha : + \sum_\lambda \epsilon_\lambda : a^\dagger_\lambda a^\dagger_\lambda : \]

\[ = \sum_\alpha \epsilon_\alpha b^\dagger_\alpha b_\alpha + \sum_\lambda \epsilon_\lambda b^\dagger_\lambda b_\lambda \]

\[ = \sum_\alpha \epsilon_\alpha b^\dagger_\alpha b_\alpha + \sum_\lambda \epsilon_\lambda b^\dagger_\lambda b_\lambda \]

where \( \epsilon_\alpha = \epsilon_\alpha \)

\( \epsilon_\lambda = -\epsilon_\lambda \)

similarly

\[ \sum V_{\alpha \beta \gamma \delta} : a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a^\dagger_\delta : = \sum U_{\alpha \beta \gamma \delta} b^\dagger_\alpha b^\dagger_\beta b^\dagger_\gamma b^\dagger_\delta \]

where

\[ U_{abcd} = V_{abcd} \]

\[ U_{ABCD} = V_{\delta \epsilon \theta \lambda} = (-)^{j_A + j_B + j_C + j_D} V_{-D,-C,-B,-A} \quad (A.2) \]

\[ U_{\alpha \beta \delta \lambda} = -V_{\alpha \delta \beta \lambda} = (-)^{j_A + m_B + j_C + m_D + m_{\alpha} m_{\beta} m_{\delta} m_{\lambda}} V_{\alpha,-C,-D,-\lambda} \]

We have made use of the fact that \( m_A + m_B + m_C + m_D \) and
therefore

\[ (-)^{m_A+m_B+m_C+m_D} = 1 \]

\[ H = \sum_b \epsilon_{\alpha} b_{\alpha}^{+} b_{\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \nu_{\alpha\beta\gamma\delta} b_{\alpha}^{+} b_{\beta}^{+} b_{\gamma} b_{\delta} \]  \hspace{1cm} (A.2b)

Operators \( J_+, J_-, J_- J_+ \) in spherical basis:

\[ J_\pm = \sum_{\alpha, \beta} \langle j_\pm | s \rangle \cdot a_{\alpha}^{\pm} a_{\beta}^{\pm} = \sum_{\alpha, \beta} \langle a_{\alpha}^{\pm} b_{\beta}^{\pm} + \sum_{\alpha, \beta} \langle a_{\alpha}^{\pm} b_{\beta}^{\pm} \rangle \]  \hspace{1cm} (A.3)

where

\[ \langle a_{\alpha}^{\pm} b_{\beta}^{\pm} \rangle = (-)^{j_A+m_A+j_B+m_B+1+1} \langle -D | j_\pm-\Lambda \rangle \]

since

\[ j_A = j_B , \quad m_A = m_B , \quad m = m_B \pm 1 \]

\[ \langle j_\pm | s \rangle = - \langle j_\pm | -s, -\Lambda \rangle \]

\[ (j_\pm)^{\pm} = \delta_{m_A m_B} \delta_{j_A j_B} \delta_{m_{A} m_{B}} \delta_{m_{A} m_{B}+1} \sqrt{(j_{A}-m_{A})(j_{B}+m_{B})} \]

\[ (j_\pm)^{-} = \delta_{m_A m_B} \delta_{j_A j_B} \delta_{m_{A} m_{B}} \delta_{m_{A} m_{B}+1} \sqrt{(j_{A}+m_{A})(j_{B}-m_{B})} \]

Using eqns. (A.3)
\( (\mathcal{J} \mathcal{J}^\dagger) = \sum_{\alpha} (j_{-} j_{+})_{\alpha} b_{\alpha}^{+} b_{\alpha} + \sum_{A} (j_{+} j_{-})_{A} b_{A}^{+} b_{A} \)

\[ + \sum_{abcd} (j_{-})_{a,b} (j_{+})_{b,c} b_{a}^{+} b_{c} b_{d} + \sum_{ABCDE} (j_{-})_{A,B} (j_{+})_{B,C} b_{A}^{+} b_{C} b_{D} \]

\[ - \sum_{ad \in B} [(j_{-})_{e,f} (j_{+})_{a,d} + (j_{+})_{e,f} (j_{-})_{a,d}] b_{a}^{+} b_{c}^{+} b_{d} \quad (A.4) \]

\( (j_{-} j_{+})_{\alpha} = (j_{\alpha} - m_{\alpha})(j_{\alpha} + m_{\alpha} + 1) \)

\( (j_{+} j_{-})_{A} = (j_{A} - m_{A})(j_{A} + m_{A} + 1) \)

\textbf{Hamiltonian (deformed basis)}

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

Using eqn. (A.1b)

\[ H = \sum_{\alpha\delta} \tilde{\epsilon}_{\alpha\delta} b_{\alpha}^{+} b_{\delta} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \tilde{U}_{\alpha\beta\gamma\delta} b_{\alpha}^{+} b_{\beta}^{+} b_{\gamma} b_{\delta}, \quad (A.5a) \]

where

\[ \tilde{\epsilon}_{\alpha\delta} = \sum_{\alpha'} \epsilon_{\alpha'} c_{\alpha\alpha'} c_{\delta\delta'}, \quad (A.6) \]

\[ \tilde{U}_{\alpha\beta\gamma\delta} = \sum_{\alpha\beta\gamma\delta} c_{\alpha\alpha'} c_{\beta\beta'} c_{\gamma\gamma'} c_{\delta\delta'}, \quad (A.6a) \]

\textbf{Operator } \( \mathcal{J}_{-} \mathcal{J}_{+} \) (deformed basis)

\[ \mathcal{J}_{-} \mathcal{J}_{+} = \sum_{\alpha\delta} (j_{-} j_{+})_{\alpha\delta} b_{\alpha}^{+} b_{\delta} + \sum_{\alpha\beta\gamma\delta} (j_{-} j_{+})_{\alpha\beta\gamma\delta} b_{\alpha}^{+} b_{\beta}^{+} b_{\gamma} b_{\delta}, \quad (A.7) \]

where

\[ (j_{-} j_{+})_{\alpha\beta} = \sum_{\alpha'} c_{\alpha\alpha'} c_{\beta\beta'} (j_{-} j_{+})_{\alpha'} \quad (A.8a) \]

...
\[
\langle \phi_k | (\vec{J}_- \vec{J}_+ | \phi_k \rangle = \sum_{\alpha} (\vec{J}_- \vec{J}_+)_{\alpha\alpha} \langle \phi_k | b_{\alpha}^+ b_{\alpha} | \phi_k \rangle
\]
\[
+ \sum (\vec{J}_-)_{\alpha\beta} (\vec{J}_-)_{\beta\alpha} \langle \phi_k | b_{\beta}^+ b_{\beta} b_{\alpha} b_{\alpha} | \phi_k \rangle
\]
\[
= \sum_{\alpha} (\vec{J}_- \vec{J}_+)_{\alpha\alpha} n_{\alpha} - \sum_{\alpha} (\vec{J}_-)_{\alpha\beta} (\vec{J}_-)_{\beta\alpha} n_{\alpha} n_{\beta} (A.9)
\]

since

\[
(\vec{J}_-)_{\alpha\alpha} = 0
\]

Also

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

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

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

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 $(\frac{3}{2} (j^+)^i) T$ is a product of $T^i$. 

Positive parity states of $F^{19}$

$|\phi_{HF}\rangle = \sum \frac{1}{2} b^{+}_{\frac{1}{2}} b^{+}_{\frac{1}{2}} b^{+}_{\frac{1}{2}} 0^6\rangle$

$\therefore T|\phi_{HF}\rangle = \sum \frac{1}{2} b^{+}_{\frac{1}{2}} b^{+}_{\frac{1}{2}} b^{+}_{\frac{1}{2}} (\frac{3}{2}) (-\frac{3}{2}) 0^6\rangle$

$= b^{+}_{\frac{1}{2}} b^{+}_{\frac{1}{2}} b^{+}_{\frac{1}{2}} 0^6\rangle$

$= \sum b^{+}_{\frac{1}{2}} b^{+}_{\frac{1}{2}} \phi_{HF}\rangle$

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

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

$\quad - \sum_{A^{\prime},a^{\prime},d^{\prime}} (J_+)^{a'A^{\prime}} C_{A^{\prime}a'^{\prime}} C_{dd'} \langle \phi_{HF}|b^{+}_A b^{+}_d T|\phi_{HF}\rangle$

Second term is zero. Also

$\eta_k = 1$

$\eta_{\frac{1}{2}} = 0$

$\therefore \langle \phi_{HF}|J_+T|\phi_{HF}\rangle = \sum_{a',d'} (J_+)^{a'd'} C_{a'a'} C_{dd'}$

Other matrix elements for this case are listed in

APPENDIX III.B
Negative parity states of $F^{19}$

$$T | \Phi_{HF} \rangle = \hat{g}_{K}^{+} \hat{v}_{K} | \Phi_{HF} \rangle$$

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

As before

$$\langle \Phi_{HF} | J_{+} T | \Phi_{HF} \rangle = - \sum_{A', D'} (J_{+})_{A' A} C_{KA'} C_{RD}$$

(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)

\[ E_J = \frac{\langle \phi^{\frac{1}{2}} | H | \phi^{\frac{1}{2}} \rangle}{\langle \phi^{\frac{1}{2}} | P^{J}_{\frac{1}{2}} | \phi^{\frac{1}{2}} \rangle} \]

where \( P^{J}_{\frac{1}{2}} \) is the angular momentum projection operator.

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

\[ H \approx \epsilon_0 + A J^2 + h \]

\[ = (\epsilon_0 + A \frac{J^2}{2} - 2 A J J_z) - A J_+ J_- - A J_+ J_- + (h + A J^2) \]

The overlap integral can be written:

\[ \langle \phi^{\frac{1}{2}} | P^{J}_{\frac{1}{2}} | \phi^{\frac{1}{2}} \rangle = \frac{2 J + 1}{2} \int_0^{\beta_{\text{max}}} d\beta \sin \beta dJ_{\frac{1}{2}} \langle \phi^{\frac{1}{2}} | e^{-iJ_{y}J_{y}} | \phi^{\frac{1}{2}} \rangle \]

\[ \approx \frac{2 J + 1}{2} \int_0^{\beta_{\text{max}}} d\beta \sin \beta dJ_{\frac{1}{2}} \langle \chi_{\epsilon_{\text{max}}} | e^{-iJ_{y}J_{y}} | \chi_{\epsilon_{\text{max}}} \rangle \]

where \( \beta_{\text{max}} \) is a value of \( \beta \) outside the peak of \( F(\beta) \).

The matrix elements of the Hamiltonian can be calculated term by term.

\[ \langle \phi^{\frac{1}{2}} | (\epsilon_0 + A \frac{J^2}{2} - 2 A J J_z) P^{J}_{\frac{1}{2}} | \phi^{\frac{1}{2}} \rangle = (\epsilon_0 + A J (J + 1) - \frac{1}{2} A) \langle \phi^{\frac{1}{2}} | P^{J}_{\frac{1}{2}} | \phi^{\frac{1}{2}} \rangle \]

\[ \langle \phi^{\frac{1}{2}} | A J_+ J_- P^{J}_{\frac{1}{2}} | \phi^{\frac{1}{2}} \rangle = A \left[ (J + \frac{1}{2}) (J + \frac{3}{2}) \right]^{\frac{1}{2}} \int_0^{\beta_{\text{max}}} d\beta \sin \beta dJ_{\frac{1}{2}} \langle \chi_{\epsilon_{\text{max}}} | e^{-iJ_{y}J_{y}} | \chi_{\epsilon_{\text{max}}} \rangle \]

\[ \approx 0 \quad \text{since} \quad \tilde{d}_{\frac{1}{2}}^J (\beta) \rightarrow 0 \quad \text{for small} \ \beta \]
\[ \langle \phi^+_{\frac{J}{2}} | A J J \bar{J} \frac{P_{\frac{J}{2}}^+}{\frac{J}{2}} | \phi^+_{\frac{J}{2}} \rangle = A \left( J+\frac{1}{2} \right) \left( J+\frac{1}{2} \right) \int d\beta \sin \beta d\frac{J}{2} \left( \beta \right) \langle \chi_0 \mid e^{-i\beta R_y} \mid \chi_0 \rangle \]

\[ \cdot \langle 0 \mid b_{\frac{J}{2}}^- J^+ e^{-i\beta y} b_{\frac{J}{2}}^+ | 0 \rangle \]

\[ = A \left( J+\frac{1}{2} \right) \left( J+\frac{1}{2} \right) \int d\beta \sin \beta d\frac{J}{2} \left( \beta \right) \langle \chi_0 \mid e^{-i\beta y} | \chi_0 \rangle \]

\[ \cdot \langle 0 \mid b_{\frac{J}{2}}^- J^+ e^{-i\beta y} b_{\frac{J}{2}}^+ | 0 \rangle \]

\[ \approx A \left( J+\frac{1}{2} \right) \left( J+\frac{1}{2} \right) \left[ \sum_\mu \langle C_{\frac{J}{2}} \mid \hat{\chi} \rangle \langle \phi^+_{\frac{J}{2}} | P_{\frac{J}{2}}^+ | \phi^+_{\frac{J}{2}} \rangle \right] \]

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

\[ \langle \phi^+_{\frac{J}{2}} | h(\mu) \frac{P_{\frac{J}{2}}^+}{\frac{J}{2}} | \phi^+_{\frac{J}{2}} \rangle = \sum_{\mu \nu \rho \tau} \mathcal{V}_{\mu \nu \rho \tau} \left( J+\frac{1}{2} \right) \int d\beta \sin \beta d\frac{J}{2} \left( \beta \right) \langle \chi_0 \mid a^+_{\mu} e^{-i\beta R_y} \mid \chi_0 \rangle \]

\[ \cdot \langle 0 \mid a^+_{\nu} a^-_{\rho} e^{-i\beta y} b_{\frac{J}{2}}^+ | 0 \rangle \]

The \( \mathcal{V}_{\mu \nu \rho \tau} \) are antisymmetrised matrix elements of the two-body potential and the operators \( a^+_{\mu}, a^-_{\mu} \) are the creation and annihilation operators for a particle with quantum numbers \( \mu \). We can thus write

\[ \langle \chi_0 \mid a^+_{\mu} a^-_{\rho} e^{-i\beta R_y} \mid \chi_0 \rangle = \langle \chi_0 \mid a^+_{\mu} a^-_{\tau} \mid \chi_0 \rangle \langle \chi_0 \mid e^{-i\beta R_y} \mid \chi_0 \rangle \]

\[ + \sum' \langle \chi_0 \mid a^+_{\mu} a^-_{\tau} \mid \chi' \rangle \langle \chi' \mid e^{-i\beta R_y} \mid \chi_0 \rangle \]

where \( |\chi'\rangle \) are excited intrinsic core states. The first term evidently gives the Hartree-Fock potential energy corresponding to \( b_{\frac{J}{2}}^+ \), while the second term contains the off-diagonal matrix element \( \langle \chi' \mid e^{-i\beta R_y} \mid \chi \rangle \) which is very small (see Ref. 16 and Fig. 2), and can be neglected.
We can therefore write that
\[
\langle \phi_{\frac{1}{2}} | (h + v_c + A_{\tau}^{-1}) P_{\frac{1}{2} \frac{1}{2}} | \phi_{\frac{1}{2}} \rangle \approx \left[ \epsilon_{\frac{1}{2}} + A \sum_j d_j d_{j+1}^* | c_{\frac{1}{2}} |^2 \right] \langle \phi_{\frac{1}{2}} | P_{\frac{1}{2} \frac{1}{2}} | \phi_{\frac{1}{2}} \rangle
\]

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

\[ \langle \phi_k^* | J^+ J_+ | \phi_k \rangle = (1 - m_\alpha) n_\delta \left[ (\bar{J}^{-} J_+)_\alpha^{\delta} - \sum_{\rho'} n_{\rho'} \left\{ (\bar{J}^{-})_{\alpha \rho'} (\bar{J}_+)^{\rho'}_{\delta} \right\} \right. \]

\[ + (\bar{J}_-)_{\alpha \rho'} \left( \bar{J}^+ \right)^{\rho'}_{\delta} \]

\[ \langle \phi_k^{**} | J^+ J_+ | \phi_k \rangle = n_\delta n_{\rho'} (1 - m_\alpha) (1 - m_\rho) \left[ (\bar{J}^{-})_{\alpha \delta} (\bar{J}_-)^{\rho'}_{\delta} - (\bar{J}^{-})_{\rho_\delta} (\bar{J}_+)^{\rho'}_{\delta} \right. \]

\[ - (\bar{J}^{-})_{\alpha \rho'} (\bar{J}_-)^{\rho'}_{\delta} + (\bar{J}^{-})_{\rho_\delta} (\bar{J}_+)^{\rho'}_{\delta} \]

\[ \langle \phi_k^{**} | H | \phi_k \rangle = (1 - m_\alpha) (1 - m_\rho) n_\delta n_\delta \bar{U}_{\alpha \beta \rho \delta} \]
APPENDIX III.B

If \( \alpha, \beta \) are particles

\[
\langle \phi_{HF}^* | J_+ T | \phi_{HF} \rangle = - \sum_{a', d'} (j+)_{a' d'} [ C_{h a'} C_{d d'} \eta_a \delta_{h k} - C_{a a'} C_{i a'} (1 - \eta_a) \delta_{i k} ]
\]

If \( \alpha, \beta \) are holes

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

If \( \alpha, \beta, \gamma, \delta \) are particles

\[
\langle \phi_{HF}^* | J_+ T | \phi_{HF} \rangle = + \sum_{a', d'} (j+)_{a' d'} \left[ - \eta_c (1 - \eta_a) C_{a a'} C_{d d'} \delta_{c k} \delta_{d k} + \eta_c (1 - \eta_a) C_{a a'} C_{d d'} \delta_{c k} \delta_{d k} 
+ \eta_c (1 - \eta_a) C_{a a'} C_{d d'} \delta_{c k} \delta_{d k} - \eta_c (1 - \eta_a) C_{a a'} C_{d d'} \delta_{c k} \delta_{d k} \right]
\]

If \( \alpha, \beta, \gamma, \delta \) are holes

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

If \( \alpha, \beta \) are particles and \( \gamma, \delta \) are holes

\[
\langle \phi_{HF}^* | J_+ T | \phi_{HF} \rangle = - \sum_{A', D'} (1 - \eta_a) \eta_c C_{B A'} C_{D D'} (j+)_{B' A'} \delta_{D h} \delta_{A k} \]

APPENDIX III.C

If $\alpha, \beta$ are particles

$$\langle \phi_{\text{HF}}^x | J^+ | \phi_{\text{HF}} \rangle = 0$$

If $\alpha, \beta$ are holes

$$\langle \phi_{\text{HF}}^x | J^+ | \phi_{\text{HF}} \rangle = \sum_{A', B'} (j+)_{B'}^{A'} \left[ C_{A\alpha}^A C_{B\beta}^B (1-\eta) S_{A \alpha} - C_{A\alpha}^A C_{B\beta}^B \eta_\beta S_{A \alpha} \right]$$

If $\alpha, \beta, \gamma, \delta$ are particles

$$\langle \phi_{\text{HF}}^{x*} | J^+ | \phi_{\text{HF}} \rangle = 0$$

If $\alpha, \beta, \gamma, \delta$ are holes

$$\langle \phi_{\text{HF}}^{x*} | J^+ | \phi_{\text{HF}} \rangle = \sum_{A', B'} (j+)_{B'}^{A'} \left[ \eta_\gamma S_{A \gamma} - \eta_\gamma (1-\eta) \eta_\delta S_{A \gamma} + \eta_\gamma (1-\eta) \eta_\delta S_{A \gamma} \right]$$

If $\alpha, \beta$ are particles and $\gamma, \delta$ are holes

$$\langle \phi_{\text{HF}}^{x*} | J^+ | \phi_{\text{HF}} \rangle = \sum_{A', B'} (1-\eta) \eta_{\alpha} C_{A \alpha} C_{B \delta} (j+)_{A'}^{B'} S_{A \alpha} S_{B \delta}$$
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