THE G-BOSON AND SHELL MODEL MAPPINGS FOR THE INTERACTING BOSON MODEL

by

ANDREW STEPHEN COUCH

DEPARTMENT OF NATURAL PHILOSOPHY

Submitted for the degree of Master Of Science

to the Faculty Of Science at the University Of Glasgow.

JUNE 1986

ProQuest LLC.
789 East Eisenhower Parkway
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SUMMARY

This Thesis embodies the work I conducted whilst at Glasgow University between Sept 1984 and July 1986.

The project is an account of the current status of the Interacting Boson Model as applied to light nuclei, with an investigation into possible extensions of the current theory.

The IBM has been well investigated phenomenologically, but the provision of a microscopic theory with relation to the spherical shell model is still to some extent illusive.

Chapter 1 starts with a review of the general development of the model over the past decade, and then concentrates on two specific aspects of the model. The first is that of the IBM2, IBM3 and IBM4, in the SD shell. Here the results of other workers have been reproduced. The second topic is the g-boson.

Chapter 2 considers and reviews some of the earlier boson expansion methods, which although conceived as particle-hole excitation mechanisms, are shown to give valuable information on general mapping procedures and microscopic pairing relations of fermions.

Chapter 3 explains how a boson shell-model is constructed in the m-scheme, and the use of the Lanczos method discussing the relevant questions on convergence and fitting techniques. A new combinatorial procedure is described allowing the extension of current computer programs to include the g-boson (Glasgow-Lanczos-Morrison-Couch shell model code). A number of spectroscopic fits were carried out with various types of bosons in ^{24}Mg, which although not ruling out the sd-boson components

in the low lying states, did indicate that a g-boson is a useful modelling tool in this region. Following this the work described in chapter 2 for the SD shell was extended to include a g-boson in a weak coupling limit. Other than producing the low lying 4^+ state in ^{20}O known to have a large g-boson component, it produced little effect on the low lying spectra of other nuclei in the SD shell. It was concluded here, that the g-boson if introduced with sd-bosons should be placed in a stronger coupled calculation. In the spirit of renormalised interactions, a second calculation was performed, in which the g-boson alone was used. Here, at least for the more deformed nuclei, the best agreement with experiment to date was obtained, although the overbinding of the IBM2 increased by 50 %.

Chapter 4 presents the existing mapping procedures used in the IBM, and discusses two new approaches to this problem.
A final section presents the general conclusions reached in the main Thesis.

ACKNOWLEDGMENTS

I would like to thank my supervisor, Professor R. R. Whitehead for his guidance and advice during my first year of study.

I would like to express my gratitude to Dr A. Watt, my supervisor, for his guidance, advice and inspiration throughout my period of study.

I am also grateful to the rest of the Nuclear Physics Community for many valuable lectures and discussions, both at home and abroad.

I wish to acknowledge financial assistance from the Science and Engineering Research Council during the period of research, and from the Department with respect to attending Summer Schools.

PREFACE

In the mid-seventies, the introduction of the Interacting Boson Model (IBM) provided a unique tool, enabling calculations believed to reflect the collective nature of the low lying nuclear states to be applied systematically across large ranges of nuclei in cases where traditional shell model calculations were not feasible.

The main problem with the IBM has been its phenomenological roots, understanding why the model works so well, and relating this to a microscopic description in terms of the underlying fermion system.

The strength of the model lies to some extent in one's ability to select model Hamiltonians, which reflect the known favourable pairing mechanisms and their associated quadrupole interactions, and then produce analytic descriptions of the low lying nuclear levels. Certain parameters characterising these interactions of the nucleon pairs, were shown to vary systematically as one progresses across a range of nuclei. In this sense, the very least that the model provides is an excellent classification technique for large amounts of nuclear information.

The beauty and ease of application of group theory to the model is another of its strengths, for the simple IBM1 three symmetry limits exist. Each of these corresponds to a physical notion carried over from the earlier geometrical nuclear models. Later extensions of the basic model, to Bose-Fermi symmetries and Supersymmetries, provided further group theoretical applications, although physical interpretations here are more illusive.

In contrast to the above, the obvious gross violations of the Pauli exculsion principle has spurred forth the search for microscopic justifications of the success of the model. In this sense the model is often referred to as the Interacting Boson Approximation (IBA) to emphasise the fact that it is an approximation to the underlying fermion system. Here, as in most other works, no strict distinction is made between the use of the terms IBM and IBA.

CHAPTER 1

INTERACTING BOSON MODEL AND THE G-BOSON

1.1 A GENERAL REVIEW

The year 1975 saw the initial inception of the IBM in a series of four papers by ARIMA and IACHELLO (40, 9a, 9b, 9c), where the model was presented in three symmetry limits (CASTANOS (41), IACHELLO (3)).

The realisation of a model in a symmetry limit or more specifically a Hamiltonian for a nuclear system, stems from a number of sources. Of these the desire to see reflected in nature the beautiful structure of mathematics, namely group theory (HAMERMESH (44), WYBOURN (45), LIPKIN (46), ELLIOTT and DAWBER (56)), is foremost. It could be stated that a cooperative collective motion of nucleons, leading to a physical symmetry, be it spherical, triaxial or whatever, is evidence for symmetry in the Hamiltonian.

The roots of the IBM were in an extension of the ideas of JANNSSEN et al. (35) who provided an algebraic approach to handle a general collective Hamiltonian in five quadrupole shape variables. This came from the basic idea that certain nuclei would have quadrupole shape deformations, and each shape variable would correspond to one of the five magnetic sub-states of the quadrupole shape. These models were known to give the characteristic vibrational and rotational spectra which had been observed in many nuclei.

The Truncated Quadrupole Phonon Model (TQP) resulted from the desire for a truncation to a maximum number of phonons of excitation, to enable a finite matrix diagonalisation to be conducted. The problem however, was that there was no number conservation of the phonons. As a purely mathematical device a new object called an s-boson was introduced, which when taken with the quadrupole phonon or d-boson, led to number conservation. For N quanta, $N=N_d+N_s$, for N_s s-bosons and N_d d-bosons. This is referred to as a smooth truncation of the model.

Introduction of the s-boson created a six-dimensional vector space characterised by the group U(6), its sub-groups being used to describe analytical solutions for particular Hamiltonians.

This interpretation however, is not the one generally favoured today, although it has been re-introduced to some extent by PARK and ELLIOTT (52) to handle core polarisation effects.

The interpretation now adopted of the bosons, is that an s-boson is a pair of fermions coupled to a total angular momentum L=0 (usually no distiction is made between J and L for a boson pair, only the total angular momentum of the fermion pair being relevant), and a d-boson is a fermion pair coupled to L=2. More precisely, a boson is a representative coupling averaged over all possible fermion pairs.

Further evidence for the symmetry of the boson Hamiltonian comes from the group structure of the commutation relations for the underlying fermion pairs.

General reviews of the IBM are given in ELLIOTT (1), and ARIMA and IACHELLO (2), which deal with the transition between the various symmetry limits of the model. For example, this is

observed when one moves from a nucleus with only a few valence nucleons (vibrational limit), to a nucleus with many valence nucleons (well deformed, rotational limit).

The boson space characterised by the group U(6) has only three sub-group chains which end in the group O(3), and so give states with well defined angular momentum. At each stage moving through the sub-groups in the chain, we extract quantum numbers which specify our choice of representations, and so characterise the energy of the eigenstates. The symmetry limits are briefly outlined below.

U(5) LIMIT

The group chain $U(6) \supset U(5) \supset O(5) \supset O(3)$ represents the vibrational limit, with basis states denoted as $|N\ nd\ \tau\ LM\rangle$. The U(6) group gives the label N for the total number of bosons, U(5) gives the label nd for the number of d-bosons, O(5) the harmonic oscillator in five dimensions has the label τ, which plays the role of seniority with respect to the d-boson pairs coupled to L=0. Finally O(3) has the usual angular momentum and projection labels associated with the three dimensional rotation group. Some allowed values of L given τ are shown below.

$\tau = 0$ L=0

$\tau = 1$ L=2

$\tau = 2$ L=2, 4

$\tau = 3$ L=0, 3, 4, 6

Note: In addition an extra label is required as nd increases to distinguish certain states see IACHELLO (3).

O(6) LIMIT

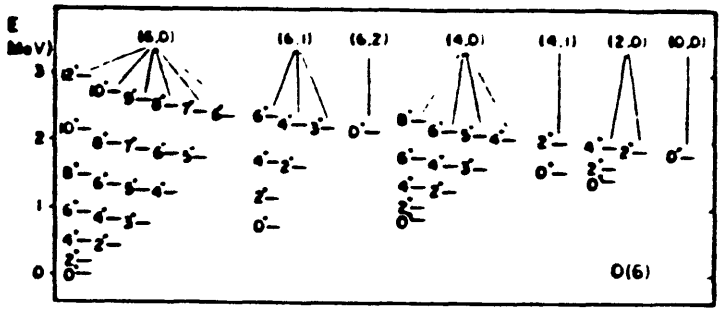
The group chain $U(6) \supset O(6) \supset O(5) \supset O(3)$, represents the so called gamma unstable limit. It corresponds to the geometrical picture of a nucleus with fixed beta deformation, and an energy of deformation independent of the angular coordinate gamma. It gives rise to states labelled as $|N \ \sigma \tau \ LM\rangle$, where N, L, τ and M are the same as in the U(5) limit, and σ the seniority label of O(6) is given as N, N-2, . . . 1 or 0, τ the label for O(5) takes the values $\sigma \ \sigma-1, \ . \ . \ . \ 1, \ 0$.

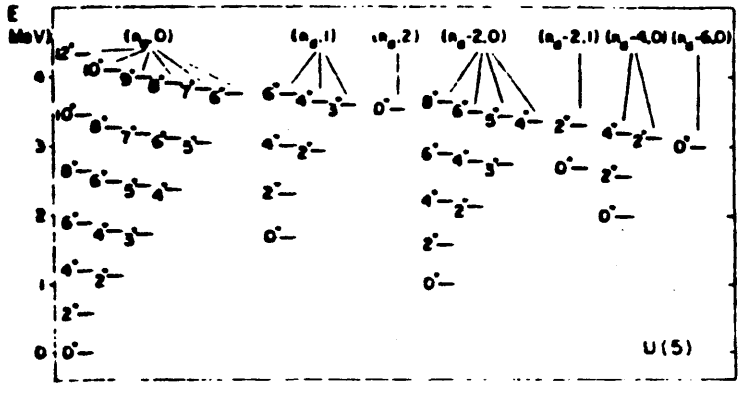
SU(3) LIMIT

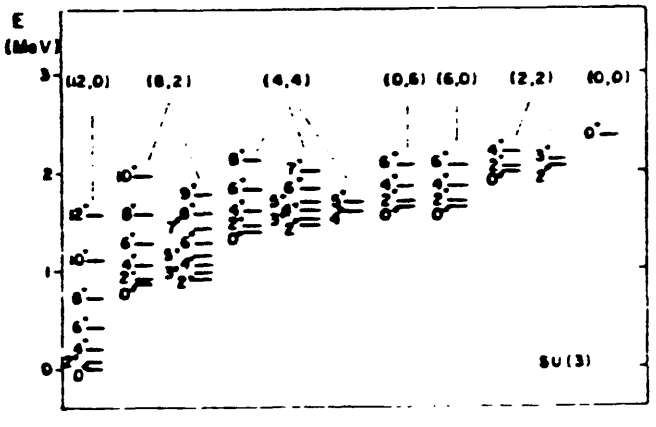
The group chain $U(6) \supset SU(3) \supset O(3)$, is appropriate in the rotational limit. Although the states can be labelled by N, L, M as in the O(6) limit, and the SU(3) labels (λ, μ) of ELLIOTT (10), an additional classification due to VERGADOS (11) tends to be used. The labels λ and μ can be related to the distribution of the oscillator quanta in various spatial directions (see ELLIOTT (1)).

In each case the energy of a state can be written in terms of the associated labels of a given symmetry limit. Examples of the characteristic spectra of the three limits described above can be seen in Figure 1, taken from ARIMA and IACHELLO (2).

FIGURE 1 SPECTRA FOR THE SYMMETRY LIMITS

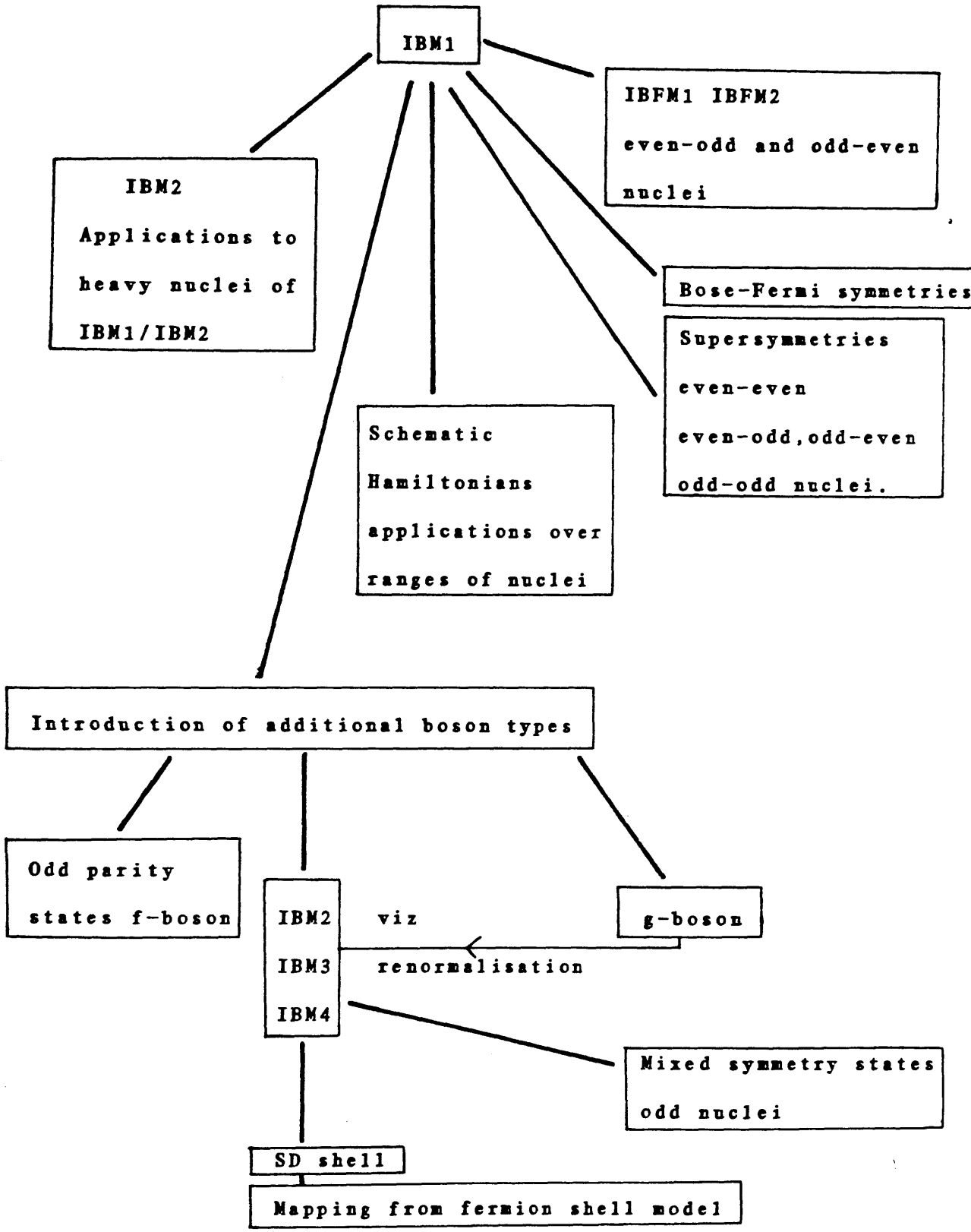






Leaving aside the connections between the IBM and older geometrical models (see IACHELLO (4), GINOCCHIO and KIRSON (39), and reviews of experimental comparisons for the model, of which CASTEN (7) is one of the best), the IBM had, by about 1980, reached a point of maturity at which it diversified into many areas. This is shown schematically in Figure 2.

FIGURE 2 DEVELOPMENT OF THE IBM



The application of the IBM1 is restricted to a large extent to nuclei with one type of valence nucleon. In the heavier nuclei the neutron and proton shells are well separated, and we have only nn and pp-boson types. This extension to the basic model is the IBM2 (see next section).

Published work on odd nuclei treats the extra nucleon as either weakly coupled to the collective core, or strongly coupled, as in the Nilsson model where all nucleons move in the same deformed potential. In the IBM, this is expressed in the IBFM1 (one type of boson), and IBFM2 (both nn and pp bosons), models which usually have only one extra nucleon outside an even-even boson core.

In the IBFM models the general Hamiltonian is written as shown below

$$H=H_F+ H_B+ H_{FB} \qquad \{1.1.1\}$$

Here H_F refers to the fermions,in this case the single particle energies, and H_B refers to the Hamiltonian of the even-even nucleus forming the boson core, with H_{FB} the interaction between the bosons and fermions (IACHELLO and SCHOLTEN (18)). This was applied with some success to Cs and odd neutron Xe isotopes with the IBFM2 by ARIAS, ALONSO and BRIJKER (19), and to many other nuclei in IACHELLO (5).

It was found to be of interest to consider systems with Bose-Fermi symmetries, in which the fermion and boson spaces have the same symmetry group,such as O(3) for the IBM and also for the spin orbit coupling in the fermion system. Other relations such

as for a j=3/2 fermion with O(6) symmetry were also attempted. (ELLIOTT (1)).

Supersymmetry was introduced to provide a representation with either an even number of nucleons and J even, or an odd number of nucleons and J odd.This implied group operators which changed boson states denoted $|\alpha\rangle$ into fermion states denoted $|i\rangle$. We define the following set of operators,and their adjoints, using the fermion operators a_i and boson operators b_α.

$$G_{\alpha\alpha'}=b^+_\alpha b_{\alpha'} , \quad G_{ii'}=a^+_i a_{i'} , \quad F_{i\alpha}=a^+_i b_\alpha \qquad [1.1.2]$$

Assume that the b^+_α, b_α commute with the a^+_i, a_i, and we have the usual fermion anti-commutation relations and boson commutation relations for their respective parts, namely

$$(b_\alpha , b^+_{\alpha'})=\delta_{\alpha\alpha'} , \quad (b^+_\alpha , b^+_{\alpha'})=(b_\alpha , b_{\alpha'})=0 \qquad [1.1.3]$$

$$\{a_i , a^+_{i'}\}=\delta_{ii'} , \quad \{a^+_i , a^+_{i'}\}=\{a_i , a_{i'}\}=0 \qquad [1.1.4]$$

For n boson states and m fermion states we define the product group U(m)*U(n), this is the usual Bose-Fermi group. We find upon inclusion of the F and F^+ operators with the G and G^+ operators, that we require the commutator of F and G to produce F and yet the anti-commutator of F and F to produce G. To obtain this we require a graded Lie algebra denoted as the supergroup U(n/m). For example the boson U(6), and a d3/2 fermion (U(2j+1)) U(4), we have the supergroup U(6/4), and subgroups $U(6)_B*U(4)_F \supset O(6)_B*O(6)_F \supset O(6)_{BF}$. Here the labels B and F indicate the Bose and Fermi spaces respectively.

The distinction between Bose-Fermi symmetries involving a simultaneous transformation in the boson and fermion spaces, and a supersymmetry which contains both the bosons and fermions in the same multiplet is emphasised.

These techniques allow the treatment of odd-odd, even-odd and odd-even partners of a given even-even nucleus to be treated such as VAN ISACKER et al. (14) for ^{196}Pt ^{197}Pt ^{197}Au ^{198}Au which fit well into this scheme. The U(6/12) presents a possible manifestation of U(5) supersymmetry in the Hg isotopes (SUN, FRANK and VAN ISACKER (12), VERGNES et al. (16)), for the Rh isotopes (VAN ISACKER et al. (15)), and the odd-mass Os (WARNER et al. (13)). The sub-group structure of U(6/12) is extensively investigated in VAN ISACKER, FRANK and SUN (17). Obviously the group theoretical problem becomes far more complex in these situations as compared to the simple IBM, and various approximations have to be made.

Worthy of note in connection with the applications of the IBM for schematic Hamiltonians, is the work of CASTEN, FRANK and BRENTANO (34), who carried out calculations for about 100 nuclei in the A=100 to 200 regions. They required only seven parameters of which four were constant for the 100 nuclei, and one parameter taking three values in each of three regions. B(E2) values and the lowest lying levels were investigated.

This examination was over the spherical (vibrational) to deformed transformation with the Hamiltonian shown below, for nd d-bosons and a quadrupole-quadrupole interaction.

$$H = \epsilon nd - kQ.Q \qquad [1.1.5]$$

$$Q = (s^{\dagger}\tilde{d} + d^{\dagger}s) + \frac{\sqrt{7}}{2}\chi(d^{\dagger}\tilde{d})^{(2)} \qquad (1.1.6)$$

Where the operator $\tilde{d}$ is defined to be $(-)^{\mu}d_{-\mu}$, so as to transform as a spherical tensor under rotations.

A new parametrisation, with N_{π} the number of proton bosons and N_{ν} the number of neutron bosons was used, so reducing an IBM2 calculation to an effective IBM1 calculation. The relationship is

$$\varepsilon = \varepsilon_{o}\exp(-\theta\{N_{\pi}N_{\nu} - N_{b}\}) \qquad (1.1.7)$$

with the parameter N_{b} taking different values in each region of nuclei, and the four fixed parameters being ε_{o}, θ, x, k. This shows the classification power of the IBM.

IBM1 HAMILTONIAN

With two types of bosons, we have two single particle energies constituting the one-body part of the Hamiltonian. As the boson pair wave function must be symmetric with respect to particle exchange, we find that the following seven two-body matrix elements exist.

$$\langle sd|V|d^2\rangle_2 \;,\; \langle d^2|V|d^2\rangle_{0,2,4} \;,\; \langle s^2|V|s^2\rangle_0 \qquad (1.1.8)$$

$$\langle sd|V|sd\rangle_2 \;,\; \langle s^2|V|d^2\rangle_0$$

The matrix elements are taken as normalised and symmetrised, and as seen in Appendix B our many body Hamiltonian can be written as follows.

$$H = \frac{1}{(n-1)} \sum_{\substack{i \le j \\ k \le l}} \frac{(\varepsilon_i + \varepsilon_j)}{(1+\delta_{ij})} \delta_{il}\delta_{jk} b_i^\dagger b_j^\dagger b_k b_l$$

$$+ \sum_{\substack{i \le j \\ k \le l \\ JM}} \frac{\sqrt{(1+\delta_{j_1 j_2})(1+\delta_{j_3 j_4})}}{(1+\delta_{j_1 j_2}\delta_{m_1 m_2})(1+\delta_{j_3 j_4}\delta_{m_3 m_4})} \langle j_1 m_1 j_2 m_2 | JM \rangle \qquad (1.1.9)$$

$$\times \langle j_3 m_3 j_4 m_4 | JM \rangle \langle (j_1 j_2) J | V | (j_3 j_4) J \rangle b_i^\dagger b_j^\dagger b_k b_l$$

1.2 IBM2/3/4 IN THE SD SHELL

IBM2

In the IBM2 the distinction is made between valence protons forming proton bosons with subscripts π , and valence neutrons forming neutron bosons with subscripts ν . The pair states here are $|s_\nu s_\pi 0\rangle$, $|s_\nu d_\pi 2\rangle$, $|d_\nu s_\pi 2\rangle$ and $|d_\nu d_\pi L\rangle$ for L=0,1,2,3,4. In this case the schematic Hamiltonians are often constructed with a Majorana term, in order to place states antisymmetric in the neutron proton labels to higher energies. An additional label introduced in this model is F-spin, assigned F=1/2 for any boson, and M_F=1/2 for a nn-boson and M_F=-1/2 for a pp-boson. States of maximum F-spin are further assumed to lie at the lowest energies (IACHELLO (4), OTSUKA, ARIMA and IACHELLO (25)).

IBM3

In 1980 it was suggested by ELLIOTT and WHITE (48) that to enable calculations in light nuclei to be performed, and so reflect the fact that the proton and neutron shells have similar energies, an np-boson with T=1 and M_T=0 was required, so completing the boson T=1 triplet. The boson pair being required to be totally symmetric could now have the symmetry restriction removed from its constituent spaces of T and sd, and so new states, not occurring in the previous IBM1/2 would be present. From a group theoretical point of view, the group was now U3(T)*U6(sd). The boson interaction was required to be isospin invariant , although different for pairs coupled to T=0, 1, 2 . The interaction could be written as follows.

$$V(ij)=(1/2)(V1+V2)+(1/6)(2V0+V2-3V1)P_{ij}+(1/3)(V2-V0)(t_i.t_j) \qquad (1.2.1)$$

Where V(ij) is the interaction between bosons i and j, P_{ij} is an exchange operator in the T-space, and t_i is a 3*3 matrix instead of the usual 2*2 Pauli spin matrices, and V0, V1, V2 are the interactions in the T=0, 1, 2, states. For V0 and V2 as in the IBM1 we have seven parameters. However, due to overall symmetry V1 has only three parameters as follows.

$$\langle sd|V1|sd\rangle_1 \ , \ \langle d^2|V1|d^2\rangle_1 \ , \ \langle sd|V1|d^2\rangle_1 \qquad (1.2.2)$$

IBM4

Following this it was suggested that if the T=1 np-boson existed then a T=0 np-boson completing the isospin triplet and singlet should be possible (ELLIOTT and EVANS (47)). They concluded that T=0 implies the need for an intrinsic spin S=1 for the bosons , and for T=1 we require S=0.

If we consider an LS coupling scheme for the fermions, then for two nucleons in a state l , the lowest states have L=0 and 2, with T=1 and S=0 or T=0 and S=1, due to the anti-symmetry, and so we have now six types of bosons $^3s_1$, $^3d_1$, $^3d_2$, $^3d_3$ with S=1 and $^1s_0$, $^1d_2$ for S=0, in the notation of $^{2S+1}l_J$.

From a group theoretical point of view we now have U6(TS)*U6(sd). The new group U6(TS) contains U3(T), and SU4 the Wigner super multiplet, we have the classification U6(TS) $\supset$ SU4 $\supset$ SU2(T)*SU2(S). This work was later followed by that of HALSE, ELLIOTT and EVANS (50), where the first half of the SD shell $16<A<28$ was examined, and binding energies relative to the ^{16}O core, spectra and E2 transitions were calculated.

The technique used in this case was to obtain the boson energies from the mass 18 isotopes, and the matrix elements from the mass 20 isotopes.

Using the following projection technique with certain assumptions, it was possible to reduce the IBM2/3/4 calculations to an effective IBM1 calculation which was then used to compute the spectra.

A general two-body interaction between particles i and j is given as

$$V(ij)=\sum_{\alpha} P_{\alpha}(ij)\ V_{\alpha}(ij) \qquad \{1.2.3\}$$

Where $P_{\alpha}(ij)$ are projection operators in the symmetric two-boson charge spin space, satisfying constraints such as isospin invariance imposed on V, and V_{α} are corresponding operators in the sd space.

Denoting the N boson state by $|N\ E\ n\ \rangle$ where E and n are labels for the charge-spin and sd spaces respectivly, then it follows that

$$\langle N\ E\ n'|V(ij)|N\ E\ n\rangle=\sum_{\alpha}\langle N\ E|P_{\alpha}(ij)|N\ E\rangle\langle N\ n'|V_{\alpha}(ij)|N\ n\rangle$$

$$=\langle N\ n'|V_{NE}^{eff}\ (ij)|N\ n\rangle \qquad \{1.2.4\}$$

$$\text{where} \qquad V_{NE}^{eff}\ (ij)=\sum_{\alpha}\langle N\ E|P_{\alpha}(ij)|N\ E\rangle V_{\alpha} \qquad \{1.2.5\}$$

V_{NE}^{eff} defines the effective interaction for a choosen N and E. Since states are symmetric in both spaces (assumed to lie at lowest energy) the choice is independent of i j, and noting that the number of interactions is N(N-1)/2, we obtain

$$\langle N\ E\ |P_{\alpha}(ij)|N\ E\rangle=\left[2/(N(N-1))\right]\langle N\ E\ |\sum_{i<j} P_{\alpha}(ij)|n\ E\ \rangle \qquad \{1.2.6\}$$

The conclusions of this paper are that the IBM4 is a better choice than the IBM2/3 for the SD shell, although for the lowest few states the IBM2 works quite well. The main difference between using the IBM4 and IBM2, is that the IBM2 overbinds nuclei by about 10 to 40 MeV.

In order to test our model program, capable of performing IBM1 calculations, the calculation of (48) for the IBM2 were repeated, for which we obtained agreement except that for ^{22}Ne, the J assignments to the second 2^+ and first 6^+ require to be interchanged being incorrectly assigned in (48), see figure 3.

IBM2 CALCULATION

Only T=1 states are present. The single particle energies of the ^1s_o and $^1d_2$ were obtained from the lowest 0^+ and 2^+ states of ^{18}O, ^{18}Ne and T=1 states of ^{18}F, which all give essentially the same results (Coulomb corrected with respect to the ^{16}O core). With only two types of boson the interaction $V_{\nu\nu}$ was obtained from ^{20}O and $V_{\pi\pi}$ from ^{20}Ne. We take $V_{\nu\nu}=V_{\pi\pi}$.

With bosons t=1, we obtain $T=t_1+t_2=0,2$, where T=1 is rejected on grounds of being of mixed symmetry character, and we assume that such states of mixed symmetry lie at higher energies.

With the further assumption that $M_T=T$ for the lowest states, it is shown in (48) that the effective interaction for the IBM2 calculation can be written as

$$V_{\nu\pi}^{eff} = V_{\nu\nu} + (N-T)(N+T)(V_{\nu\pi} - V_{\nu\nu})/\{2N(N-1)\} \qquad \{1.2.7\}$$

As shown in ref (48) the determined values of $V_{\nu\nu}$ and $V_{\nu\pi}$ are combined in the above to produce the above seven matrix elements for an IBM1 calculation. The levels below 10MeV were obtained for ^{22}Ne, ^{24}Ne ,^{24}Mg ,^{26}Mg are shown in Figures 3,4,5,6, with the corresponding experimental spectra. The agreement obtained with experiment is fair, and the presence of a number of obviously incorrect states points to the need for a mapping procedure, to eradicate the unphysical components from such states, or the states themselves (see chapter 4).

Further applications of the IBM4 were to odd-odd nuclei using a strong non-central interaction in the SD shell, by HALSE (49), in an investigation of ^{22}Na and ^{26}Al.

FIGURE 3 Spectrum ^{22}Ne

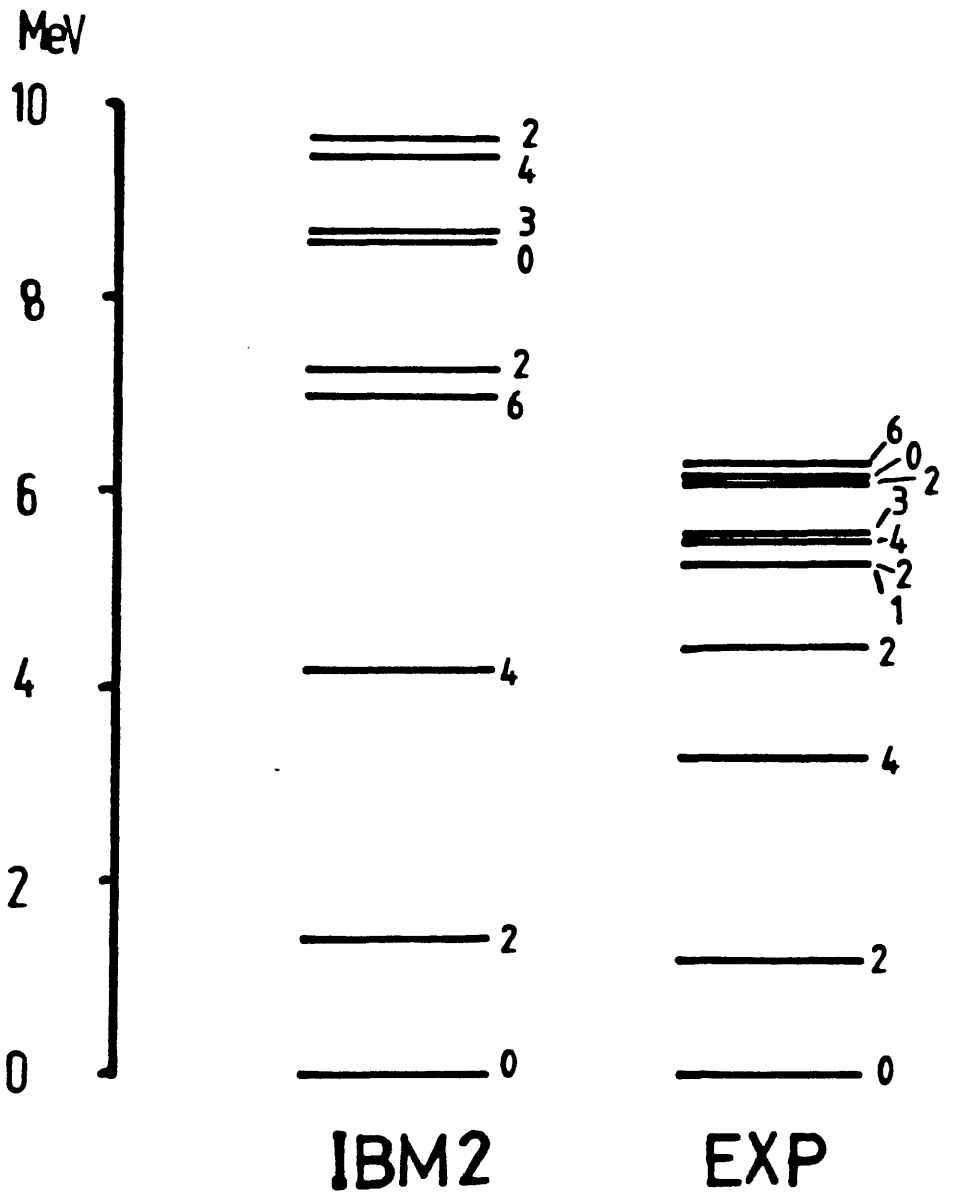


FIGURE 4 Spectrum ^{24}Ne

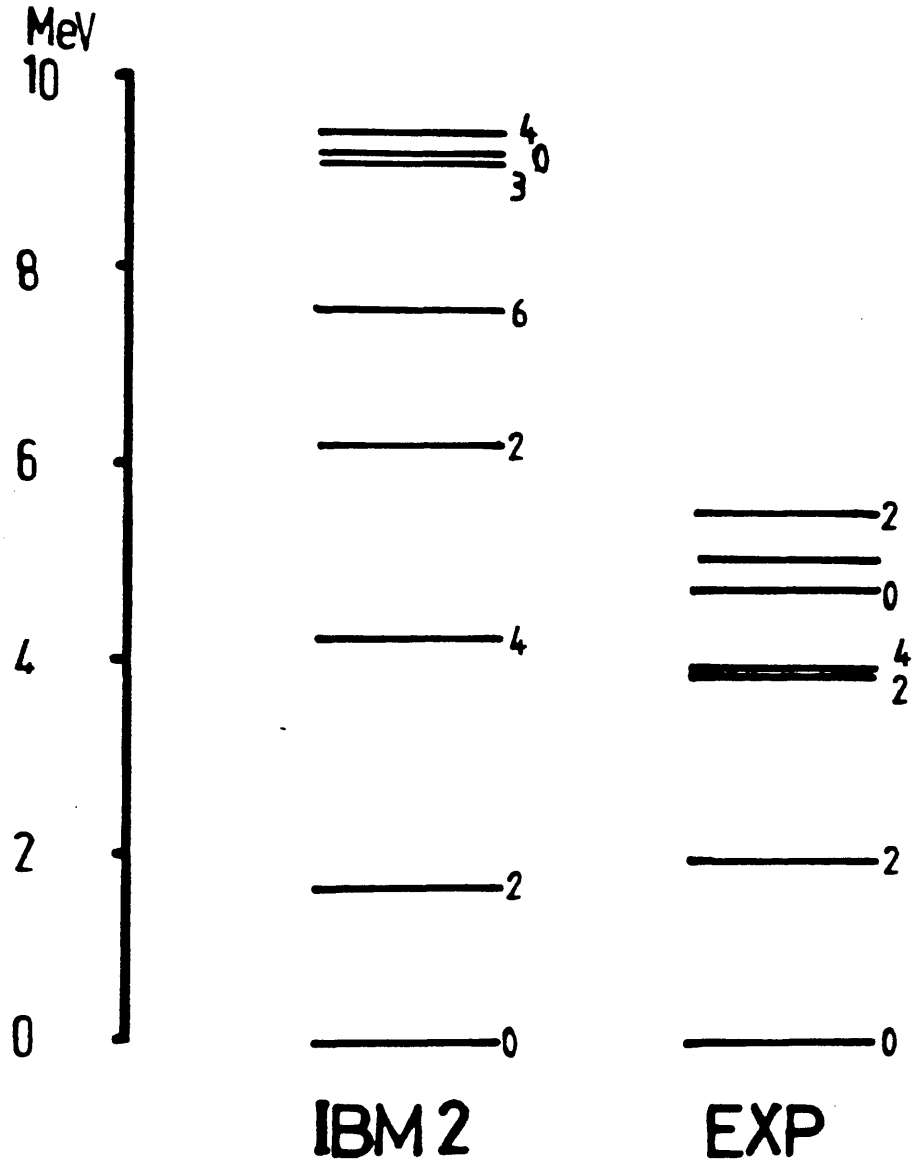


FIGURE 5 Spectrum ^{24}Mg

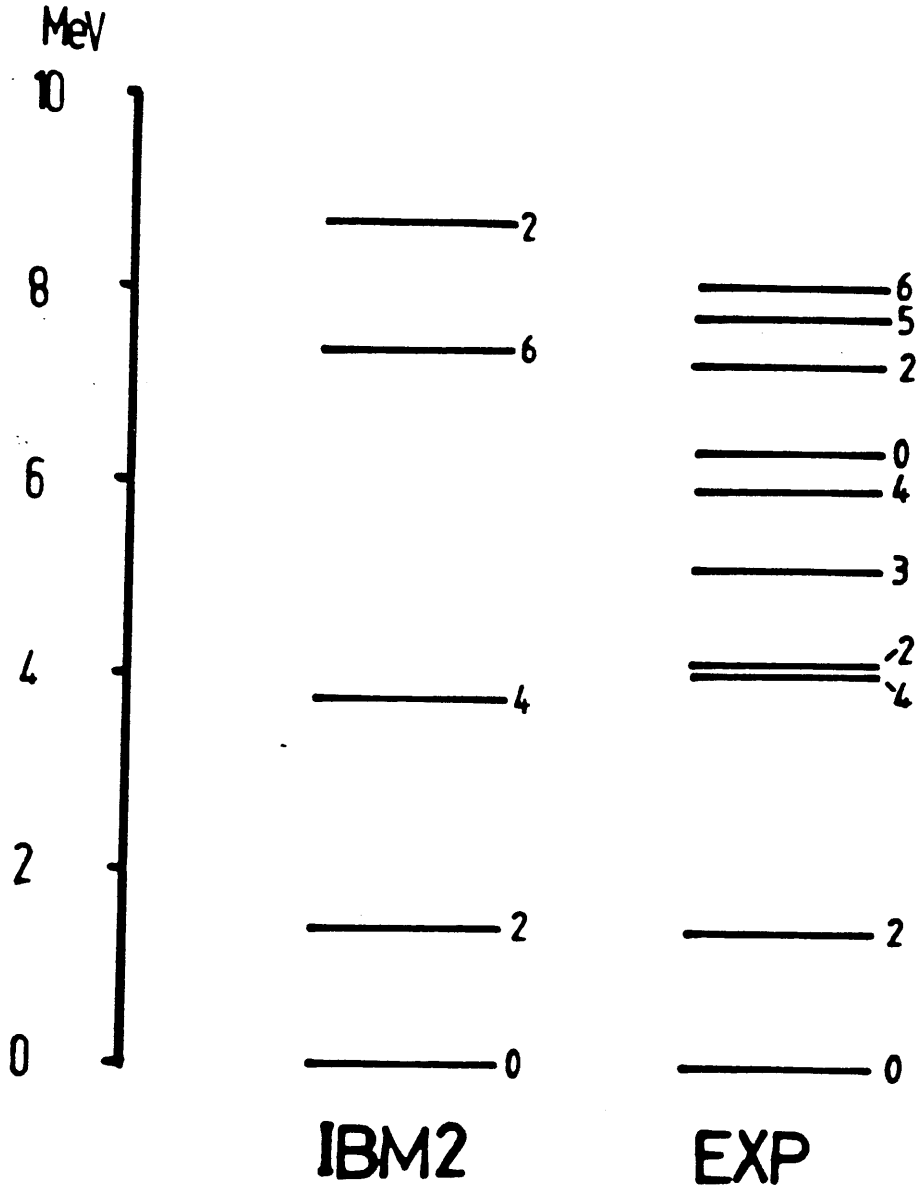
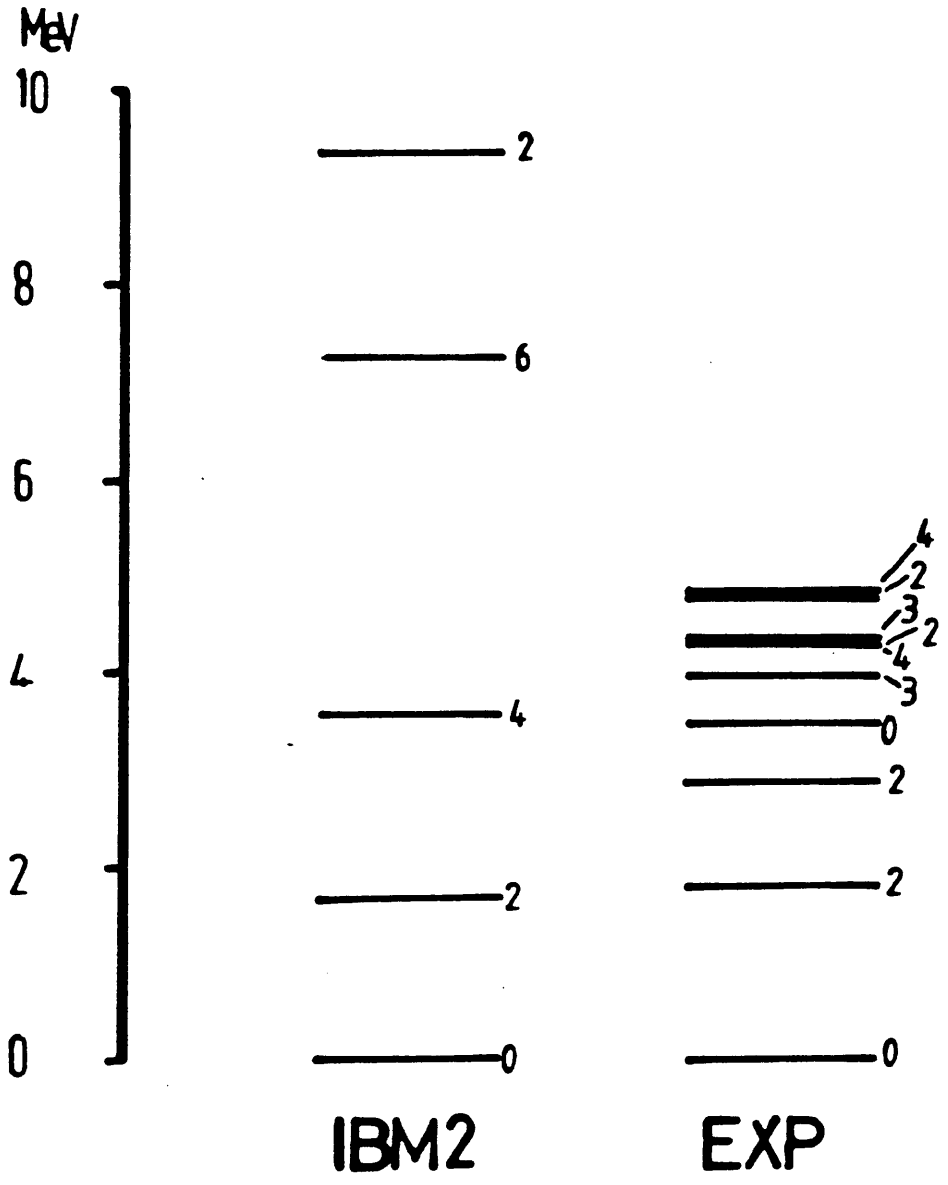


FIGURE 6 Spectrum ^{26}Mg



1.3 G-BOSON

The significance of the g-boson in calculations is still to some extent an open question. One question which is still unclear is whether the g-boson could be used instead of say extending a model from IBM3 to IBM4. Or, whether other higher order s' and d' bosons are required such as those by VAN ISACKER et al. (27). One argument for the introduction of g-boson components is evidenced from the two-body density matrices for a fermion calculation on ^{24}Mg, where components such as J=4 fermion pairs would seem to be very important even in the ground state. The argument put forward by some is that the boson Hamiltonian is renormalised for such effects, but even if this is the case, certain states will not be present in a renormalised calculation, and so other states may be incorrectly assigned.

Published work on the g-boson is quite scarce, mainly due to the difficulties of performing anything other than a perturbative calculation. OTSUKA (30) maintains that the effect of a g can be renormalised, and this effect is small in any case in the low lying states. Similarly, OTSUKA , ARIMA and YOSHINAGA (32), in an earlier work considered the intrinsic state in a Nilsson model and concluded that 0^+ 2^+ pairs dominate, while 4^+ 6^+ pairs decrease in importance as one progresses from spherical to deformed nuclei. However, BES et al. (23) do not agree, and maintain that the 4^+ pairs are of importance even in the low lying states. SAGE and BARRETT (33) suggest a perturbative approach and a number of calculations have been performed with this in mind, such as HUA (29), HEYDE et al. (28), HUA and XIAO (31), and VAN ISACKER et al. (27).

The Glasgow-Lanczos-Morrison-Couch method is not restricted to such perturbation methods (see chapter 3).

CHAPTER 2

BOSON EXPANSION TECHNIQUES

2.1 MICROSCOPIC PAIRING OF FERMIONS

The favourable mechanism of pairing fermions in time reversed orbits leading to a superfluid state in nuclear matter, is a well known phenomenon. The pairing we shall discuss here is of a more general nature, and as a simplification we only consider a single j-shell.

The basic idea in Boson Expansion (BE) techniques is to look at the fermion pair commutation relations and attempt to approximate these relations by those of bosonic objects. In this context the BE methods relate to particle -hole excitations, believed to be responsible for the observed collective behaviour in nuclei. (BELIAEV and ZELEVINSKY (58)). This idea was taken across to particle-particle cases by LI, DREIZLER and KLEIN (54).

In this section we outline some of the BE ideas as applied to the particle-particle case, in a single j-shell.

We begin by defining the pair operators

$$A^{+J}_M = \frac{1}{\sqrt{2}} \sum_{m_1(m_2)} \langle j^{m_1}, j^{m_2} | JM \rangle a^+_{m_1} a^+_{m_2}$$

$$B^J_M = \frac{1}{(\hat{J})^{1/2}} \sum_{m_1(m_2)} \langle j^{m_1}, j_{-m_2} | JM \rangle (-)^{j-m} a^+_{m_1} a_{m_2}$$

The A, A^+ operators obey the commutation relations

$$[A_1, A_2] = [A^+_1, A^+_2] = 0$$

$$[A_1, A^+_2] = \delta_{12} - 2 \sum_3 Y(123) (\hat{J}_3)^{1/2} B^+_3 \qquad \{2.1.1\}$$

Where Y(123) are numerical factors defined in Appendix A.

This can be written in terms of a smallness parameter $1/\Omega$, where Ω is the maximum number of pairs that can be formed in a given j-shell, and in the limit when Ω tends to infinity we can write

$$Y(123) \propto \frac{1}{(2\Omega)^{1/2}} \qquad (2.1.2)$$

Further it can be shown that the expectation value of the B operator can be related to Ω in the vacuum as

$$\langle B^{J}_{M}(ab) \rangle \propto \left(\frac{N}{2\Omega}\right) \qquad (2.1.3)$$

Consequently if the number of particles N is small compared to Ω, then the above operator becomes small, and Y(123) can be neglected, giving

$$[A_1, A_2^{+}] \simeq \delta_{12} \qquad (2.1.4)$$

The operator A^{+} can be approximated by the boson operator a^{+}, with the commutation relations as shown

$$[a_1, a_2^{+}] = \delta_{12}\,, \quad [a_1^{+}, a_2^{+}] = [a_1, a_2] = 0 \qquad (2.1.5)$$

This appears to be intuitive, as we would expect the Pauli exclusion priciple to be weak when a shell has few nucleons in it.

It is seen that for the case of a single j-shell the term δ_{12}, becomes

$$\delta_{12} = \tfrac{1}{2}\,\delta_{J_1 J_2}\delta_{M_1 M_2}\left\{\delta_{a_1 a_2}\delta_{b_1 b_2} - \delta_{a_1 b_2}\delta_{a_2 b_1}\right\} \qquad \{2.1.6\}$$

And the underlying fermion nature of this boson is still present.

2.2 MAPPING FROM FERMION TO BOSON SPACES

In order to improve upon the approximations of the last section, a number of techniques were developed, some of which are briefly described below.

BELIAEV ZELEVINSKY METHOD

This technique is outlined in LI, DREIZLER and KLEIN (54), and was initially proposed in the paper by BELIAEV and ZELEVINSKY (58). Further modifications to correctly include all effects of the Pauli principle were proposed by MARSHALEK (55,53).

Here one approximates the fermion pair operator A^+ to higher orders, with the boson operators a^+, and for a third order term we would obtain

$$A_1^+ = a_1^+ + \sum_{234} g^{(1)}_{234}\, a_2^+ a_3^+ a_4 + O(5) \qquad \{2.2.1\}$$

This is then substituted into the $A^{\dagger}$ commutation relations and values for $g^{(\eta)}_{234}$ are obtained. Repeating this procedure at each order, an infinite convergent expansion is obtained. The Pauli principle will not be violated provided that the expansion is taken to all orders.

MARUMORI METHOD

An alternative to the BZ method is that of Marumori. Here one identifies an image of the fermion space in the boson space, this sub-space being referred to as the physical space, all other states being referred to as unphysical states. The mapping used is actually not unitary, although it is treated as being unitary. Fermion operators are then mapped into their boson counterparts. Convergence here depends upon the choice of model space.

Mapping operator V

$$\begin{aligned} V|f\rangle &= |b) \\ V^{\dagger}|b) &= |f\rangle \\ V^{\dagger}|b \text{ unphysical}) &= 0 \end{aligned} \qquad (2.2.2)$$

The fermion operators are then constructed in the boson space so as not to connect into the unphysical part of the space.

DYSON METHOD

Another way around the problem posed by the commutation relations, is to define non-hermitian operators, and so satisfy

the commutation relations exactly. The problem here is that the Hamiltonian is then non-hermitian. This technique has uses as an intermediate form, used by other methods.

HOLSTEIN-PRIMAKOFF METHOD

This is yet another technique, specifically used in the quasi-spin formalism (JANSSEN, DONAU and FRAUENDORF (57)).

A unification of the BE methods in the language of complex vector spaces can be found in the works of DOBACZEWSKI (59,60), and applications include those of TAMURA, WEEKS and KISHIMOTO (20), HECHT, McGRORY and DRAAYER (6).

In summary, these techniques whilst not always directly related to the IBM, do give a feeling for the sort of problems likely to be incurred when handling fermion and boson spaces.

CHAPTER 3

SHELL MODEL CALCULATION WITH BOSONS

3.1 BOSON SHELL MODEL AND THE LANCZOS METHOD

The most popular boson calculations have been performed with the aid of the code PHINT by SCHOLTEN (8), which is characterised by its use of coefficients of fractional parentages.

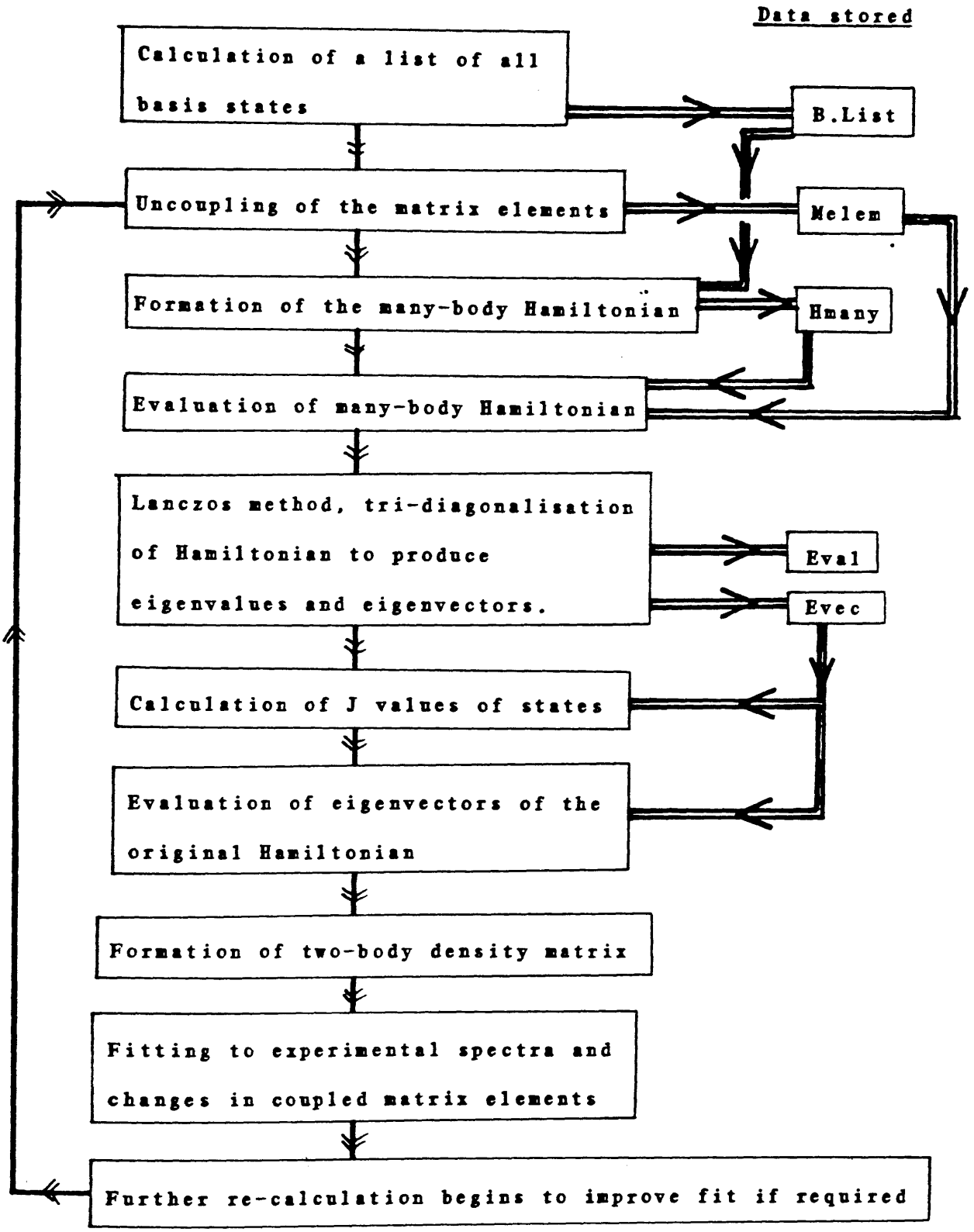
The methods used here were similar to those developed for earlier fermion calculations of WHITEHEAD, WATT, COLE, MORRISON (37). These are performed in the m-scheme which with its realisation of the second quantisation in the orbital representation, provides a very natural form for use on computers. Figure 7 shows in a block form the various operations performed in a calculation. Three areas can be targeted in a calculation which demand the main computation, these are as follows.

a) The formation of the many-body Hamiltonian (for a chosen nucleus this need only be constructed once, and subsequent calculations do not require this to be repeated, the calculation of the exact form of the resulting matrix however, must be recomputed if the initial matrix elements are changed).

b) Execution of the Lanczos method in tri-diagonalising the Hamiltonian.

c) Fitting the matrix elements to the experimental data, here again a matrix diagonalisation is the main source of computation.

FIGURE 7 OUTLINE OF A SHELL MODEL CALCULATION



From a computational point of view the main strength of these algorithms is the manner in which the Lanczos method extracts the lowest eigenvalues first , which readily converge, without the need to produce every state in a calculation.

A weakness of the technique, excluding the fitting which any method must cope with, is the need to form the entire many-body Hamiltonian, although in the boson case this is less of a problem due to the smallness of the model space compared to the fermion calculations, and the time required here is only a small fraction of the time required for the iterations.

MATRIX ELEMENTS AND THE MANY-BODY HAMILTONIAN

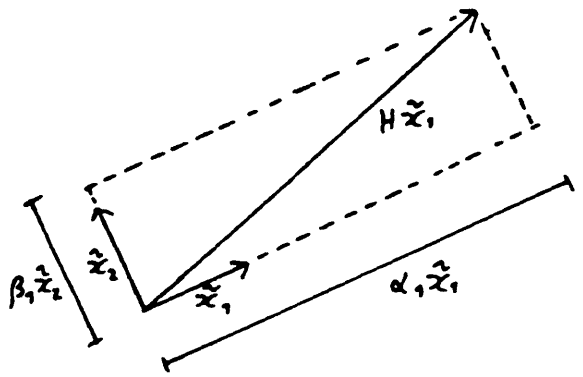
The choice of normalisation for the matrix elements and the associated form of the Hamiltonian are shown in Appendix B.

The many-body Hamiltonian is stored in an upper-triangular form, as it is real symmetric. Its rows and columns are labled by the basis states. And in its formation all the required combinations of $b_i^\dagger b_j^\dagger b_k b_l$ are applied to connect one state to another. The resulting matrix element (m,n) represents the interaction as derived from the one and two-body matrix elements between states m and n.

LANCZOS METHOD

Vector $\tilde{x}_1$ is assumed to be normalised $\tilde{x}_1 . \tilde{x}_1 = 1$, and for a real-symmetric operator H, we produce an orthogonal vector $\tilde{x}_2$, by applying H to $\hat{x}_1$, as shown below in Figure 8.

FIGURE 8



$$\hat{x}_1 . \hat{x}_2 = 0, \quad H\tilde{x}_1 = \alpha_1\hat{x}_1 + \beta_1\tilde{x}_2, \quad \hat{x}_1 H\tilde{x}_1 = \alpha_1, \quad \tilde{x}_2 H\hat{x}_1 = \beta_1 \qquad [3.1.1]$$

repeating this operation for $\hat{x}_2$ orthogonal to $\hat{x}_1$ and normalised we obtain

$$H\hat{x}_2 = \gamma\hat{x}_1 + \alpha_2\tilde{x}_2 + \beta_2\tilde{x}_3 \qquad [3.1.2]$$

$$\tilde{x}_1 H\tilde{x}_2 = \gamma = \beta_1 \qquad \text{as H is hermitian}$$

$$\tilde{x}_2 H\tilde{x}_2 = \alpha_2 \qquad [3.1.3]$$

$$\tilde{x}_3 H\tilde{x}_2 = \beta_2$$

repeating this, we span the vector space resulting in the following matrix representation of the Hamiltonian H

$$H_T = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & \beta_3 & \\ & & \beta_3 & \alpha_4 & \beta_4 \\ & & & \ddots & \ddots \end{pmatrix} \qquad [3.1.4]$$

For the operation on the k^{th} vector we obtain

$$H\tilde{x}_k = \beta_{k-1}\tilde{x}_{k-1} + \alpha_k\hat{x}_k + \beta_k\hat{x}_{k+1} \qquad (3.1.5)$$

The choice of starting vector $\tilde{x}_1$ is important, and will be discussed in the section 3.2.

By forming the scalar products above, and performing a re-orthogalisation for each new vector $\tilde{x}_k$ to all other vectors, and then normalising $\tilde{x}_k$, the Hamiltonian is placed in the desired form.

At this point the eigenvectors and eigenvalues of the tri-diagonal Hamiltonian are evaluated (see ORTEGA (43)).

We now have obtained the following

$$H_T v_i = \lambda_i v_i \qquad (3.1.6)$$

We still require the eigenvectors of the original Hamiltonian

$$Hu_i = \lambda_i u_i \qquad (3.1.7)$$

Let V be the matrix of the Lanczos vectors $V=\{\tilde{x}_1, \tilde{x}_2, \hat{x}_3 \ldots\}$

The we find that

$$u = Vv \qquad (3.1.9)$$

CALCULATION OF THE J VALUES FOR STATES

The basis states used in a calculation have a definite projection of angular momentum M, the same for all states. This implies that only nuclear states with $J \geq M$ can be recovered from the calculation. The angular momentum of a given state is evaluated as follows with the use of the standard raising and lowering operators.

$$J_{\pm}|jm\rangle = \left[(j \mp m)(j \pm m + 1)\right]^{1/2} |j\, m \pm 1\rangle \qquad \{3.1.10\}$$

We can write

$$J^2 = J_- J_+ + J_0(J_0+1) \qquad \{3.1.11\}$$

Where we have

$$\langle J_0(J_0+1)\rangle = M(M+1) \qquad \{3.1.12\}$$

Our states can be written as follows

$$|\phi\rangle = \sum_k a_k |k\rangle \qquad \{3.1.13\}$$

$$|k\rangle = |n_1, n_2, n_3 \ldots\ldots n_n\rangle \qquad \{3.1.14\}$$

for basis state $|k\rangle$, orbital occupation numbers $n_1, n_2 \ldots n_n$.

As $J_- J_+$ is a linear operator we have

$$J_- J_+ = \sum_{kl} \langle k|J_- J_+|l\rangle a_k^* a_l \qquad \{3.1.15\}$$

And

$$\langle J^2 \rangle = J(J+1) \qquad (3.1.16)$$

Thus we obtain our final expression for J as

$$J = \frac{\left(1 + 4\langle J_- J_+ \rangle + 4M(M+1)\right)^{1/2} - 1}{2} \qquad (3.1.17)$$

3.2 CONVERGENCE AND SPANNING THE VECTOR SPACE

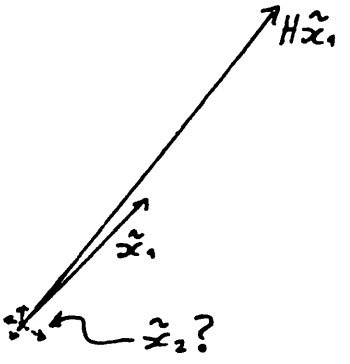
SPANNING THE VECTOR SPACE

The Lanczos method normally continues until it spans the space of eigenvectors represented in the starting vector† With a random vector this is usually the entire space.
However, we examined the extension of a two boson calculation from sd-bosons to sdg-bosons, where the g-bosons introduced initially with a very small interaction with the sd-bosons, so that the original sd states would be reproduced. It was found that the original sd states could not be recovered as would be expected. The problem was traced back to a lack of othogonality in the states. The re-orthogonalisation was unable to take care of this. The problem occurs due to the Hamiltonian only shifting the new vector upon which it acts by a small amount. The presence of rounding errors have two effects. The advantage is that in this context they allow the calculation to extend into a

† Or eigenvectors of the desired lowest states have converged.

sub-space of the total space, which had no components in the original starting vector, which is a desireable effect. The second effect which is undesireable is that the vectors are no longer orthogonal. This is shown schematically in Figure 9 below, where characteristically the norm of $\tilde{x}_2$ is small, being comparable with numerical accuracy.

FIGURE 9



The problem was overcome by setting a criteria that if the norm of the new vector was small, then re-orthogonalisation was used, however if the norm was very small then the vector space was manually spanned. This is achieved by forcing each component of the vector in turn to be one and all other components zero, until a linearly independent vector has been found.

IMPROVED CONVERGENCE THROUGH A WELL CHOOSEN STARTING VECTOR

Due to the iterative nature of the fitting calculations in obtaining converged fits, an improvement in computation can be made in all but the first iteration. In the first iteration a starting vector with all its components set to one is selected, in order to maximise the overlap of the starting

vector with the eigenvectors, at this point unknown, which span the vector space.

The method here is simply to sum the eigenvectors of the states to be fitted as produced by the first iteration normalise, and then use this as the starting vector for the second iteration Figures 10 and 11 show the improvement of this method over the existing technique in which the starting vector is always the same. In both figures two vectors are selected and summed to give the new starting vector.

Selecting two vectors ϕ_1 and ϕ_2 orthonormal, and forming the normalised sum Ψ , we obtain

$$\Psi = \frac{1}{\sqrt{2}}(\phi_1+\phi_2) \qquad \{3.2.1\}$$

With an energy given as follows

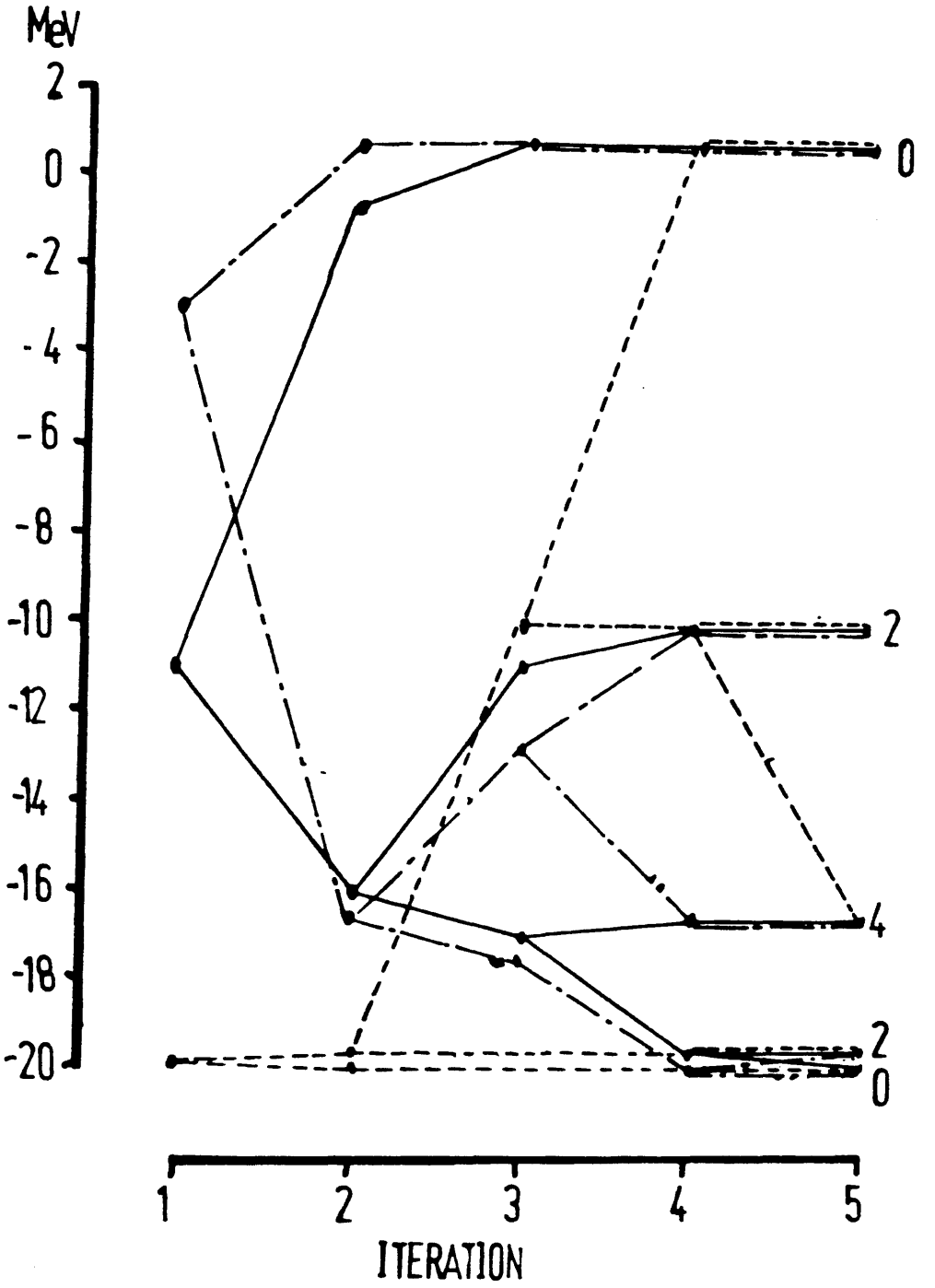
$$H\Psi = \frac{1}{\sqrt{2}}(E_1\phi_1+E_2\phi_2) \qquad \{3.2.2\}$$

$$E=\langle\Psi|H|\Psi\rangle=\frac{1}{2}(E_1+E_2) \qquad \{3.2.3\}$$

This is visible in Figure 10 where the first approximation to an eigenvalue appears to lie midway between the two eigenvalues produced in the second iteration.

However, it does not appear to be the case in Figure 11. This can be understood by realising that after each iteration the Hamiltonian changes, and so the above relationship is only approximate.

FIGURE 10 2 Bosons

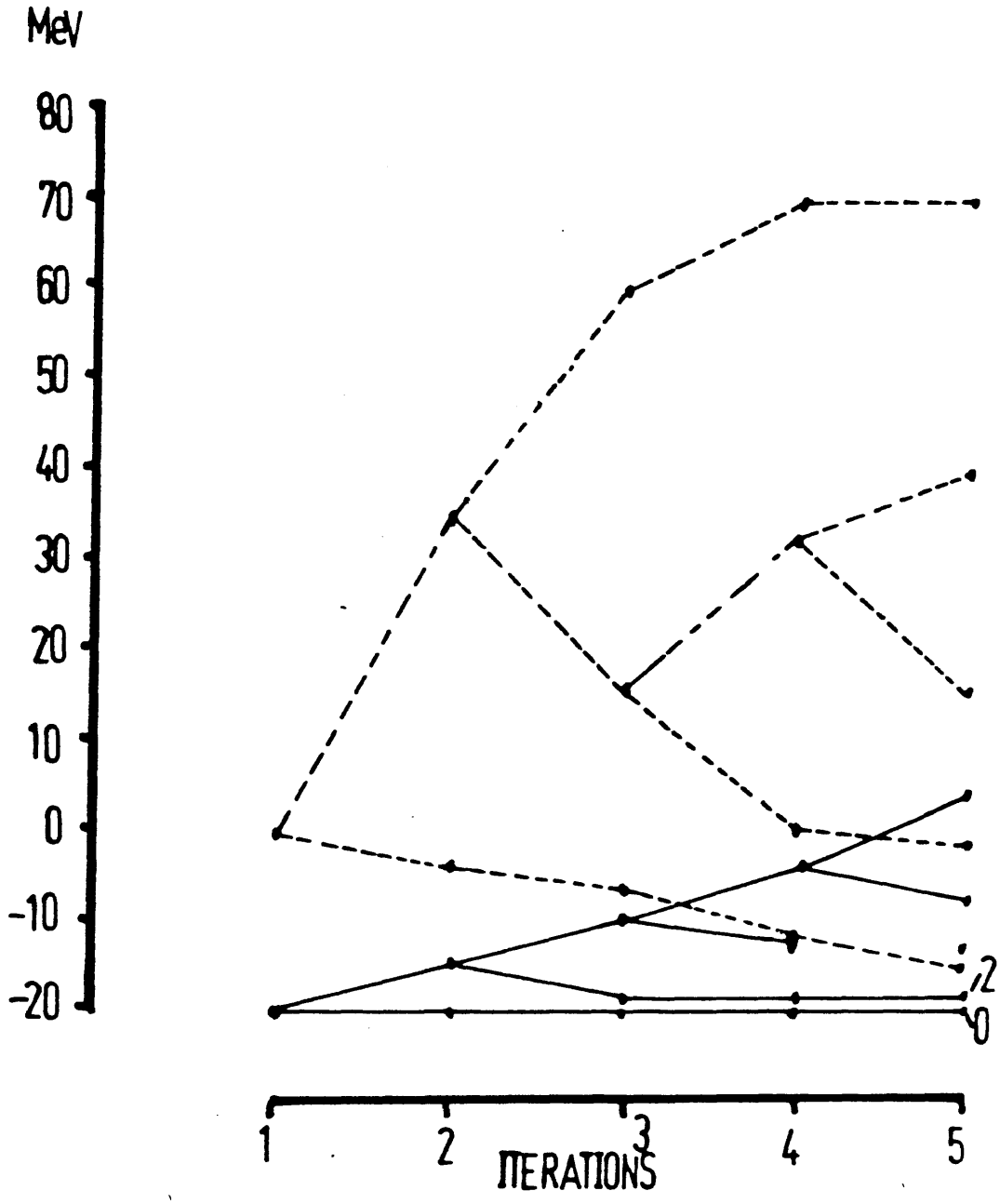


—— Starting vector all 1's

------ sum of 0^+ & 2^+ eigenvectors for starting vector.

—·— sum of 0^+ & 2^+ Lanczos vectors for starting vector.

FIGURE 11 10 Bosons



—— sum of first two eigenvectors 0 & 2 for starting vector.

----- starting vector all 1's

In figure 10 it can be seen that if one sums the Lanczos vectors as opposed to the eigenvectors, the convergence is not improved. This can be understood by noting that the Hamiltonian changes between fits†, and whereas this is not very important for the eigenvectors, the Lanczos vectors may change dramatically. It is found that even if the eigenvalues of the previous calculation are changed by quite large amounts, the eigenvectors are comparatively stable.

3.3 FITTING PROCEDURE AND THE DENSITY MATRIX

DENSITY MATRIX

Whilst the information on nuclear levels can be conveyed in terms of the state vectors, an alternative formulation of the state information is in the language of the density matrix.

For each nuclear level there exist a set of two-body density matrix elements, which when combined with the interaction matrix elements yield the energy of the state. Indeed all the state information can be conveyed using the set of 1,2...N-body density matrix elements.

The Hamiltonian may be written as

$$H = \sum_j \hat{H}_j h_j \qquad \{3.3.1\}$$

Here the quantities $\hat{H}j$ are operators of the form $A_1^+ A_2^+ A_3 A_4$ the subscript j being a convenient label to represent this combination. The quantities h_j are pure numbers defining the interaction.

The density matrix element for a state I with respect to interaction matrix elements denoted j is written

$$\rho_j^{(I)} = \langle \Psi_I | \hat{H}_j | \Psi_I \rangle \qquad \{3.3.2\}$$

† The Hamiltonian matrix changes as the matrix elements on which it depends change.

giving $$E^{(I)} = \langle \psi_I | H | \psi_I \rangle = \sum_j \rho_j^{(I)} h_j \qquad (3.3.3)$$

A further property of $\rho^{(I)}$ is that its trace corresponds to the number of interactions, and as ρ is a two body density matrix,

$$Tr(\rho^{(I)}) = \frac{1}{2} N(N-1) \qquad (3.3.4)$$

where $Tr(\rho^{(I)})$ is a sum over $\rho_j^{(I)}$, corresponding to diagonal matrix elements such as $\langle s^2 | V | s^2 \rangle$, but not off-diagonal elements such as $\langle sd | v | d^2 \rangle$.

Further the state $\psi^{(I)}$ can be written in terms of its basis states

$$|\psi^{(I)}\rangle = \sum_m C_m^{(I)} |\varphi_m\rangle \qquad (3.3.5)$$

Where

$$(\varphi_m, \varphi_n) = \delta_{mn} \qquad (3.3.6)$$

$$\langle H \rangle = \langle \psi^I | \hat{H} | \psi^I \rangle = E(\rho) \qquad (3.3.7)$$

$$= \sum_{mn} C_m^{*(I)} C_n^{(I)} \varphi_n \hat{H} \varphi_m$$

$$= \sum_{mn} \rho_{mn} H_{mn} \qquad (3.3.8)$$

The density matrix ρ_{mm} measures the amount of the basis state φ_m in the nuclear state $\psi^{(i)}$.

In the above treatment we considered $\hat{H}$ to be a many-body operator, where as in {3.3.1} our Hamiltonian is a two-body operator.

The relationship between a two-body density matrix and the many-body density matrix can be written as follows

$$\rho^2 = \frac{1}{(N-2)!} \sum_{\substack{k_1,k_2 \\ \cdots k_{N-2}}} \rho^N (i_1' i_2' k_1^+ k_2^+ \cdots k_N \, j_1 j_2 k_1 k_2 \cdots k_N) \qquad \{3.3.9\}$$

FITTING PROCEDURE

Hamiltonian is a linear operator and can be written as

$$H = \sum_k \hat{H}_k h_k \qquad \{3.3.10\}$$

$$E^{(i)} = \sum_k \rho_k^{(i)} h_k \qquad \{3.3.11\}$$

We have a Hamiltonian described by the operators $\hat{H}_j$ and the set of numbers h_j and require to obtain the correction h_j',† $h_j^N = h_j + h_j'$, such that we minimise the differences between the calculated and experimental energy levels.

We form

$$S = \sum_i \left(E_i^{(c)} - E_i^{(exp)} \right)^2 \qquad \{3.3.12\}$$

† h_j' are phenomenological variations chosen to fit the data.

and minimise this with respect to h'_j. Assume that ρ^i_j does not vary appreciably with variation in h_j.

Our first calculation gave

$$E_i^{(c')} = \sum_j \rho^i_j h_j \qquad \{3.3.13\}$$

assume our improved calculation gives

$$E_i^{(c)} = \sum_j \rho^i_j [h_j + h'_j] \qquad \{3.3.14\}$$

then we have

$$S = \sum_i \left(\sum_j \rho^i_j h_j + \sum_j \rho^i_j h'_j - E_i^{(exp)} \right)^2 \qquad \{3.3.15\}$$

and minimising this

$$\frac{\partial S}{\partial h'_j} = \frac{\partial}{\partial h'_j} \sum_i \left(E_i^{(c')} - E_i^{(exp)} + \sum_j \rho^i_j h'_j \right)^2 \qquad \{3.3.16\}$$

Let $\delta E_i = E_i^{(exp)} - E_i^{(c')}$, then we obtain

$$\sum_k \left(\sum_i \rho^i_j \rho^i_k \right) h'_k = \sum_i \rho^i_j \delta E_i \qquad \{3.3.16\}$$

which can be written in matrix form as

$$M \underset{\sim}{h'} = \underset{\sim}{\delta} \qquad \{3.3.18\}$$

Since M is real symmetric it can be diagonalised by a unitary matrix U, as follows

$$U D U^{-1} \underset{\sim}{h}' = \underset{\sim}{\delta} \qquad \{3.3.19\}$$

$$U^{-1} \underset{\sim}{h}' = D^{-1}(U^{-1}\underset{\sim}{\delta}) = \underset{\approx}{\Delta}$$

vector increment is

$$\underset{\sim}{h}' = U \underset{\approx}{\Delta} \qquad \{3.3.20\}$$

And our new Hamiltonian is given as

$$h_j^N = h_j + h_j' \qquad \{3.3.21\}$$

Our program could in addition weight the fitting by the accuracy of each experimental level, this could be used to bias a fit to a selection of levels.

When a fit to experimental spectra is undertaken, it is linear combinations of the matrix elements that are fitted, and from these the respective changes in matrix elements is deduced. It is almost always the case that the number of linear combinations which contain information, is less than the number of matrix elements. This is determined by looking at the eigenvalues D of the matrix M after diagonalisation. A linear combination with a small eigenvalue compared to the others is rejected as it contains no reliable information.

3.4 COMBINATORIAL METHOD FOR BOSONS

The representation of a basis state in the m-scheme for fermions was investigated in WHITEHEAD, WATT, COLE and MORRISON (37) and general approaches to such representations of numbers for computer storage are considered in BECKENBACH (42). The ideas of (37) have now been extended to the case of bosons.

In the m-scheme we construct a sub-set of all possible basis states, namely those with a given M value. The orbital or box like representation is most appropriate for the action of operators such as $b_i^+ b_j^+ b_k b_l$ which change the numbers of objects in the boxes i, j, k, l.

The simple IBM1 has only six orbitals for each state, and so a partial bit code representation is appropriate, with four bits per orbital, that is up to a maximum of fifteen bosons, a 32 b[illegible] word is sufficient. However, with the addition of a g-boson fifteen orbitals are required, and so this representation becomes insufficient for states with more than three bosons (at two bits per orbital in a 32 bit word).

The technique to be outlined here, being the most efficient form of storage for the set with all basis states, is only limited by the total number of basis states being less than the computers maximum integer storage (around 10^9).

The extra computation required in coding and the subsequent decoding of basis states outweighs that which would be required for other forms of storage in the larger calculations.

The number of permutations for the distribution of N bosons over n orbitals is given by

$$ {}^{N+n-1}C_n = \frac{(N+n-1)!}{(N-1)!\,n!} \qquad (3.4.1) $$

Table 1 shows a list of such states for the simple case of 2 bosons and 3 orbitals.

TABLE 1

State Code	Permutation
1	2 0 0
2	1 1 0
3	1 0 1
4	0 2 0
5	0 1 1
6	0 0 2

The numbers 1 to 6 being stored as the code for a given permutation. We require a general method, so that given either the distribution of bosons we can code a state, or given a coded state we can determine the distribution of bosons.

As shown in Appendix C an algorithm for coding a state can be found, and this can be transformed into operations on a simple table of Binomial coefficients, shown in table 2. Any element in a given row is easily constructed from the previous element in the same row.

TABLE 2

Box sums	number of objects in a box sum					
	n	n-1	n-2	n-3	.....	0
n1	$^{N-2}C_{-1}$	$^{N-1}C_{0}$	$^{N}C_{1}$	$^{N+1}C_{2}$	.....	$^{N+n-2}C_{n-1}$
n1+n2	$^{N-3}C_{-1}$	$^{N-2}C_{0}$	$^{N-1}C_{1}$	$^{N}C_{2}$	.....	$^{N+n-3}C_{n-1}$
n1+n2+n3	$^{N-4}C_{-1}$	$^{N-3}C_{0}$	$^{N-2}C_{1}$	$^{N-1}C_{2}$		$^{N+n-4}C_{n-1}$
.....	.....	.....	.....	.....	.....	.....
n1+n2+n3... +nN-1	$^{0}C_{-1}$	$^{1}C_{0}$	$^{2}C_{1}$	$^{3}C_{2}$	.....	$^{n}C_{n-1}$

As a simple example consider the case of the state code for 011000, that is, two bosons and 6 boxes. To encode this state we must first form the row sums, which we see are as follows

(n1=0, n2=1, n3=1, n4=0, n5=0, n6=0)

n1=0

n1+n2=1

n1+n2+n3=2

n1+n2+n3+n4=2

n1+n2+n3+n4+n5=2

The appropriate form of table 2 in this case is shown in table 3.

TABLE 3

Box sums	number of objects			
	2	1	0	
n1	0	1	6*	
n1+n2	0	1*	5	
n1+n2+n3	0*	1	4	
n1+n2+n3+n4	0*	1	3	
n1+n2+n3+n4+n5	0*	1	2	

* Indicates subtractions during the row search yield the result ≥ 0.

For the given box sums, adding together the corresponding elements from table 3 we obtain the state code of 6+1+0+0+0=7.

In order to decode state 7 with the table starting with the first row search the table from right to left along the row, subtracting off the corresponding value in the table from the state code, here 7, and when the result is ≥ 0 the appropriate row sum is noted, in this case 0,1, or 2. Then proceed to the next row of the table ,and continue the process with the result of the first subtraction, in this case 1, we then manipulate the row sums to obtain the values n1,n2....nN-1, and establish nN from the known total number of bosons.

3.5 ^{24}Mg: THE EVIDENCE FOR A G-BOSON

In order to investigate the possibility of extending the sd-boson model in the SD shell, three cases of fitting to experimental spectra were examined. These fits did not consider the binding energies or BE2's, and so the single particle energies were of no importance, as they could be absorbed in the diagonal matrix elements.

^{24}Mg was selected due to its deformation in the ground state this being consistent with the idea that deformation would tend to break the s pairs, and so there would be more likelihood of g pairs being present. In figures 12, 13, 14 the resulting spectra are shown.

FIGURE 12 d-boson fit ^{24}Mg

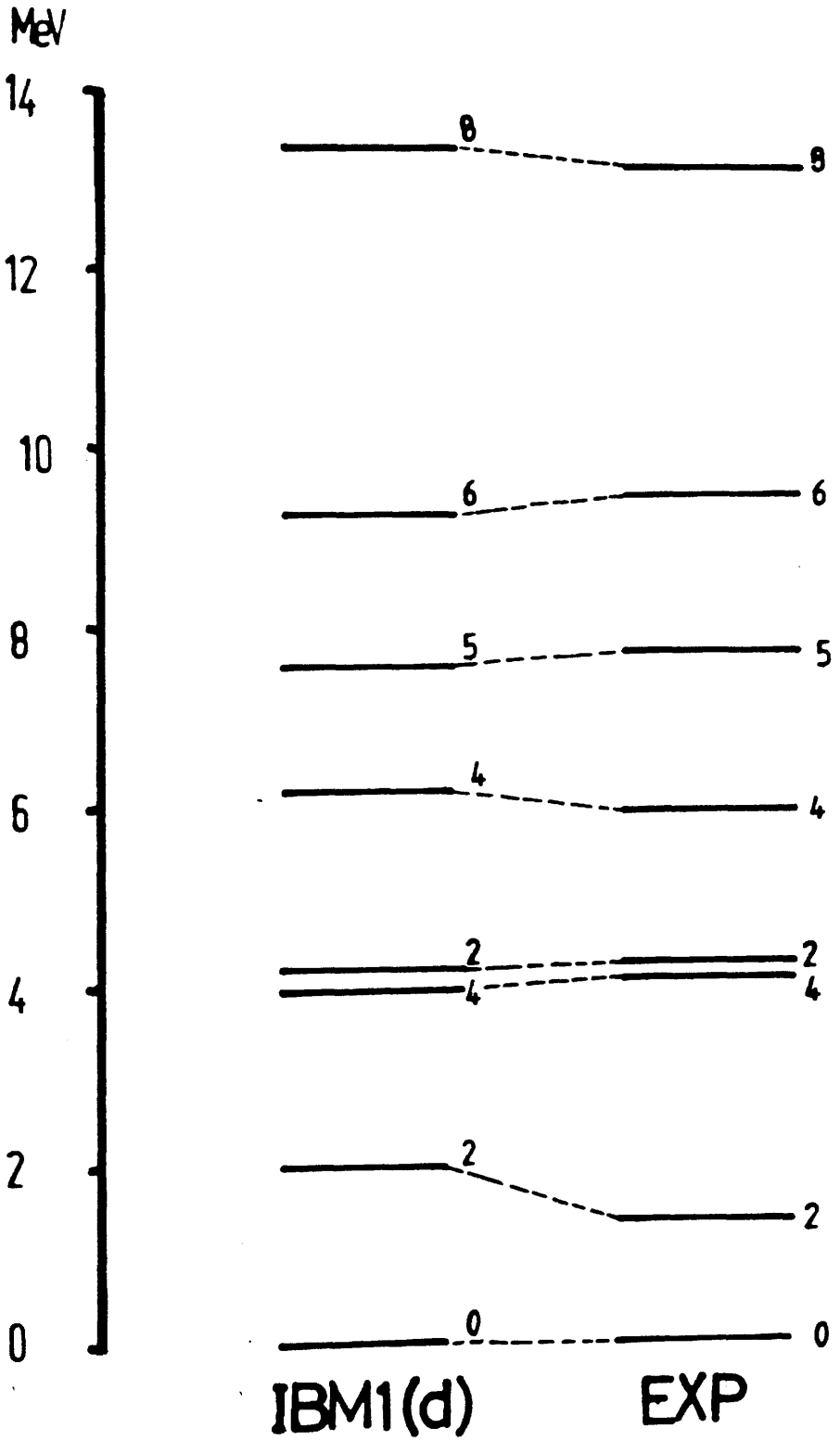


FIGURE 13 sd-boson fit ^{24}Mg

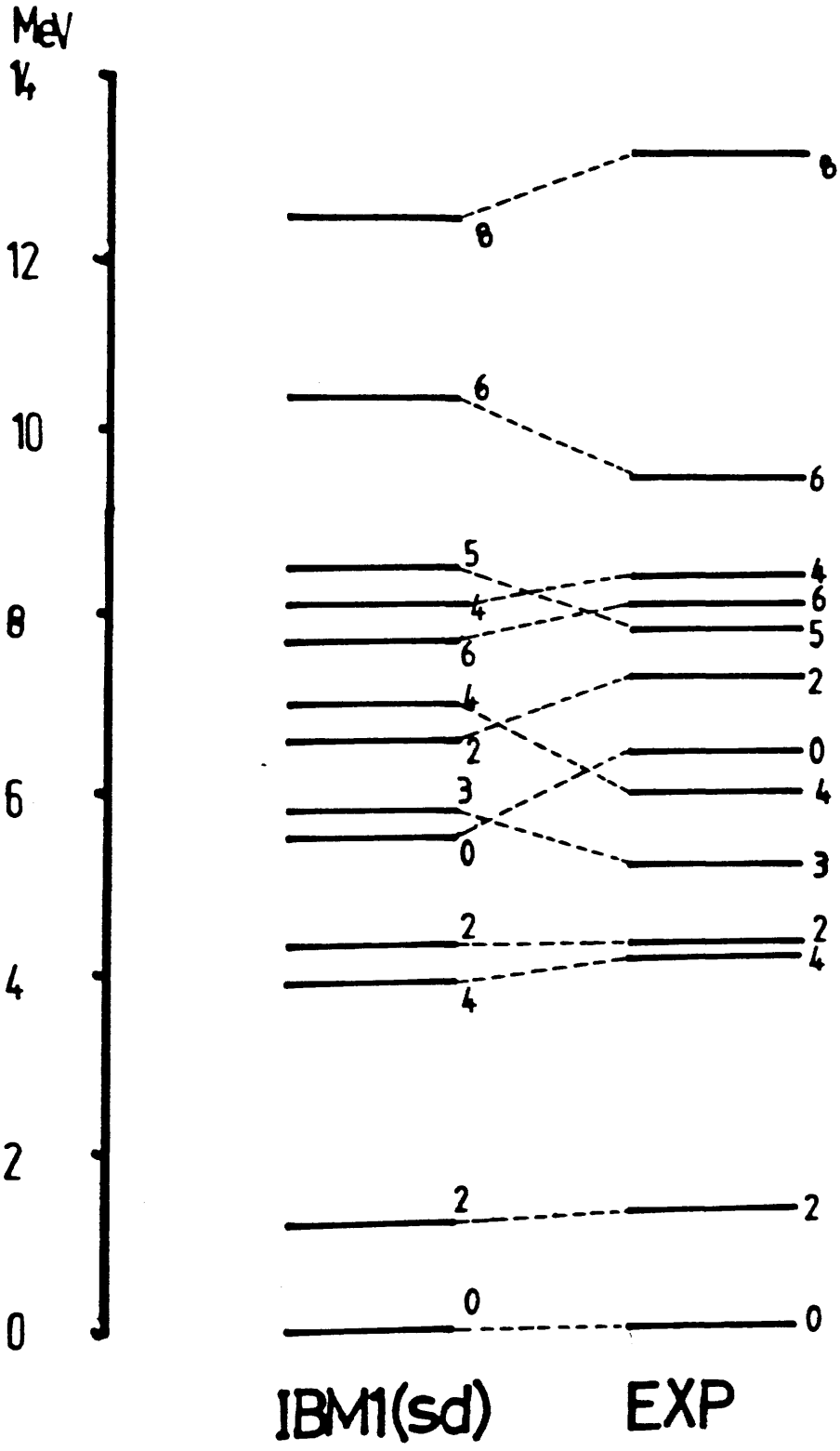
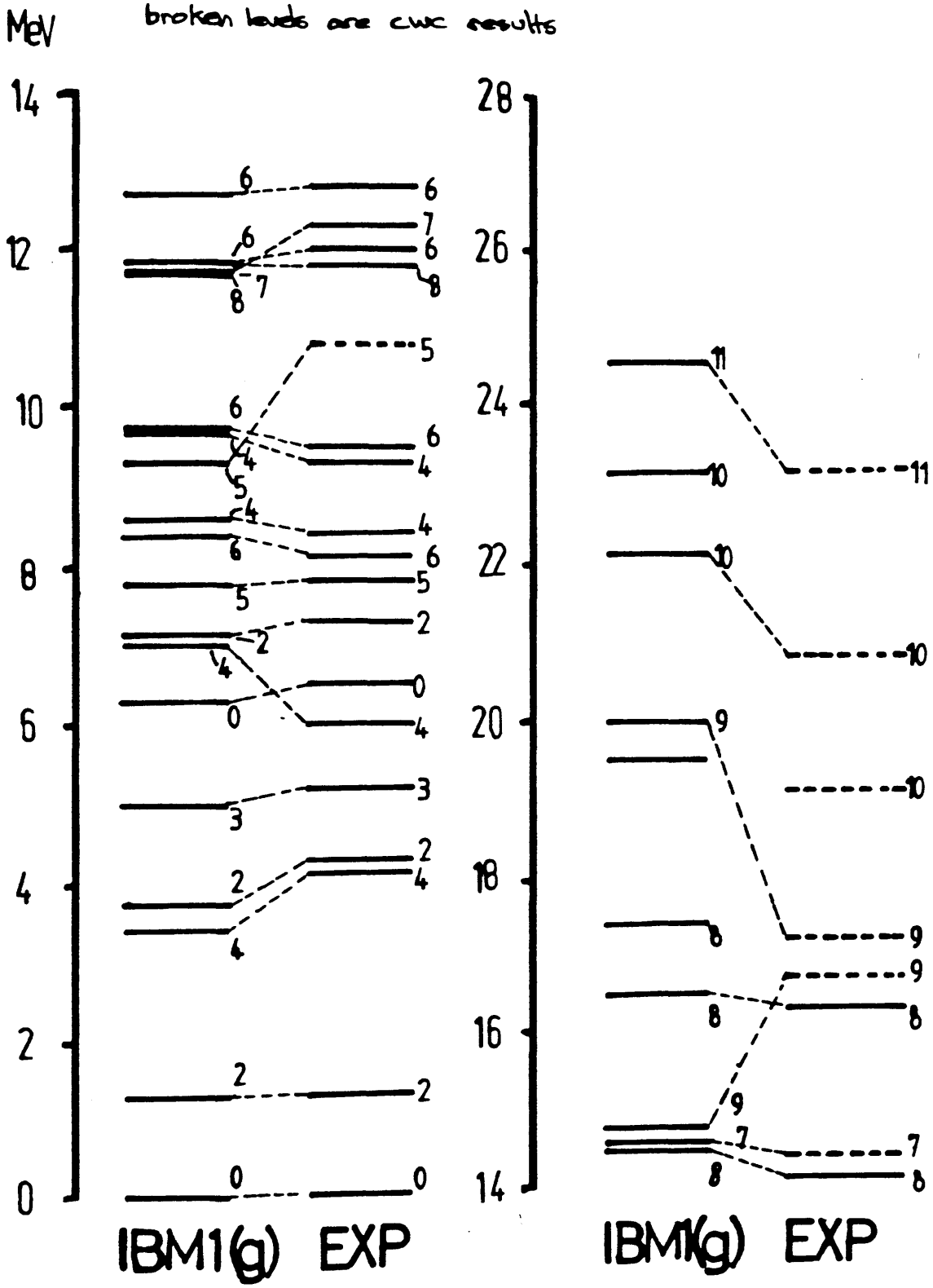


FIGURE 14 g-boson fit ^{24}Mg



DESCRIPTION OF FIGURE 12

The model space consisted of d-bosons only, this resulted in 8 levels, all of which were fitted to experimental levels, using 3 linear combinations of the 4 parameters. The resulting fit was very good, with only the lowest 2^+ state out by about 0.6MeV, all other states being within about 0.2MeV of their experimental values. The fit can be characterised by a χ^2 measure, which we set in this case to the value of one.

DESCRIPTION OF FIGURE 13

The model space in this case consisted of sd-bosons, with a full space of 17 levels, of which 13 could be fitted to experimental levels. The remaining four had energies in excess of 60Mev, and consequently were probably of an unphysical nature. The fit again was generally good, with the highest 6^+ and 8^+ differing by about 1MeV from the experimental values, and the other levels accurate to about 0.5MeV on average. The 13 levels were fitted with 5 linear combinations of the 9 parameters, and the relative χ^2 was about 10.

DESCRIPTION OF FIGURE 14

The model space in this case consisted of only g-bosons producing 33 levels, of which 19 were fitted using 5 linear combinations of the 6 parameters. In addition a further 6 levels could be found to correspond approximately to the predicted

results of KELVIN,WATT,WHITEHEAD (38) for CWC interaction in ^{24}Mg. An average variation in the accuracy of the levels was about 0.4MeV, with a 1MeV difference in the second 5^+ state. The relative χ^2 was about 5.

It is concluded that the g-boson provides a good model of ^{24}Mg giving good agreement with a large number of levels. The ratio of the number of levels fitted to number of linear combinations of the parameters, were for the d, sd and g, 2.6, 1.8, 3.8.

3.6 THE G-BOSON IN THE SD SHELL

Following the work described in the last section in the SD shell, an attempt was made to introduce a g-boson into this type of calculation. Assuming that the sd-bosons are required for this style of calculation, the g can only be put into the calculation in a weak coupling limit. This is simply because the number of parameters that would be required for a strongly coupled calculation, would far outstrip the available experimental information required to determine the parameters. In this weak coupling limit it is found that the overbinding of nuclei by the IBM2 remains unchanged.

The sd matrix elements were taken as in the previous calculations, and the five g matrix elements $\langle g^2|V|g^2\rangle_L$, with L=0,2,4,6,8 were set up to reflect the formation of the g at a higher energy than the s and d-bosons. The level assignments were made from the spectra as shown in Figures 15 and 16.

DESCRIPTION OF FIGURE 15

The broken levels, as in the earlier calculations are ignored as they are believed to be particle-hole structures. As we have a weak coupling limit there is an overlap in assigning both the sd and g matrix elements to the second 0^+ and 2^+ levels, due to no other low lying 0^+ and 2^+ levels to use for the g matrix elements. This results in two near degenerate pairs of levels being produced in the calculation, one being of sd-type and the other of g-type in each pair.

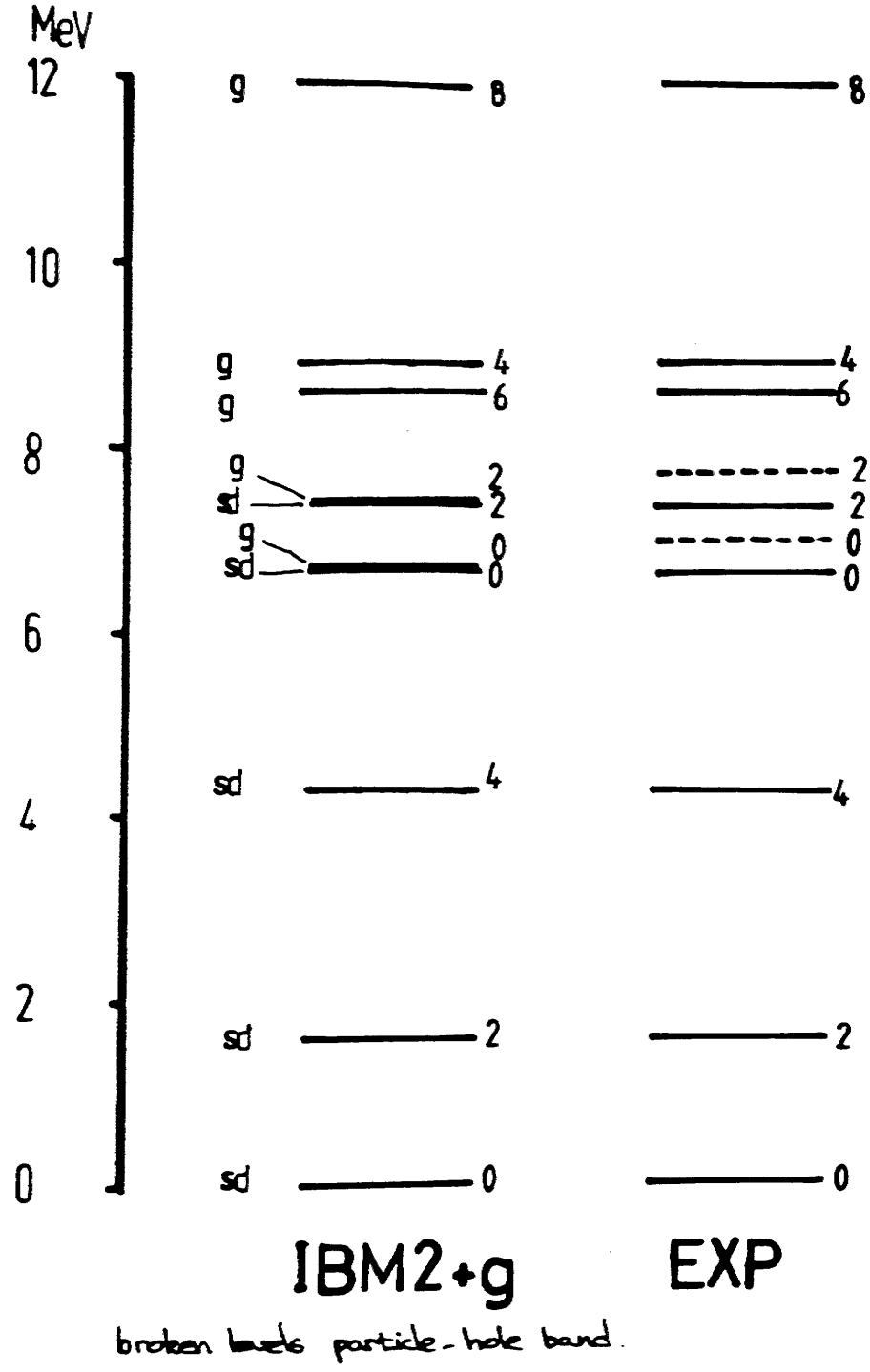
DESCRIPTION OF FIGURE 16

In fixing up the sd matrix elements the first 4^+ state is ignored as it is believed to be dominated by g components. The g matrix elements are again set to produce states above the sd ones. Again a problem of overlap exists for the second 0^+ state of the g-band, and for the same reason as before a pair of near degenerate levels are produced, round-off error prevents exact degeneracy. A problem here, is that no experimental 6^+ and 8^+ levels exist for ^{20}O, and so these levels were inferred from the ^{20}Ne spectrum. The sudden and unexpected appearance in this spectrum of a low lying 4^+ state, near the experimental 4^+ state believed to have a large g component Otsuka (24) is a significant advance, indicating that the techniques used here are a definite improvement.

The g matrix elements obtained here, and the single particle energy of the g obtained from mass 18 isotopes are shown in table 4, the matrix elements for $V_{y\pi}$ were coulomb corrected to the same extent as those used in the sd case.

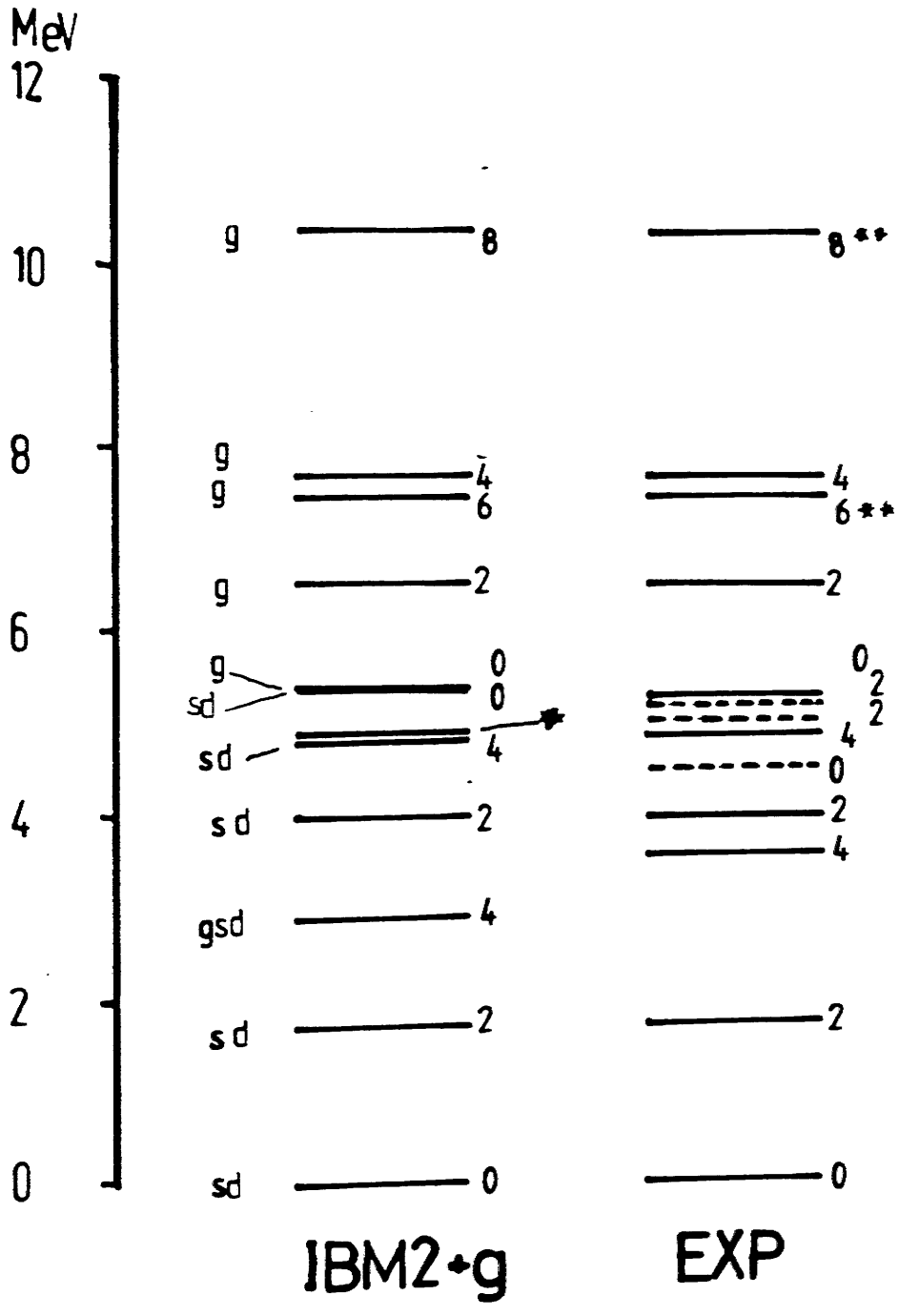
Calculations were performed for ^{22}Ne, ^{24}Ne and ^{24}Mg. In all three cases no low lying levels were to be found with any g-boson contribution. This can be understood as the pure g states lying at very high energy, and the mixed sdg states forced to high energy due to the large single particle energies and the interaction for the sd-g spaces being switched off. This indicates that future calculations should be performed with a stronger coupling between the model spaces in order to lower the energy of such mixed states. It might be expected that in such a stronger coupled calculation that the energy of the low lying 4^+ state in ^{20}O would shift closer to the experimental value.

FIGURE 15 Spectrum ^{20}Ne



broken bands particle-hole band.

FIGURE 16 Spectrum ^{20}O



* five degenerate levels broken levels particle-hole band.

** inferred levels from ^{20}Ne as described p55.

TABLE 4

J	^{20}O $V_{\nu\nu}$	^{20}Ne $V_{\nu\pi}$
0	-1.11	-16.70
2	0.06	-16.00
4	1.26	-14.39
6	1.00	-14.64
8	4.17	-11.47

Single particle energy -8.63 MeV

THE G-BOSON RENORMALISED FOR SD-BOSON EFFECTS

The question as to whether one can model the nuclei in the SD-shell using a g-boson renormalised for sd-boson effects, is addressed here. This style of calculation is one that had not been previously performed, and was evaluated here in a similar manner to the sd-boson calculations, as follows.

The single particle energy of the g-boson was taken as the first 4^+ state in ^{18}O, and the matrix elements calculated from the spectra of ^{20}Ne and ^{20}O as in the previous IBM2 calculations.

The energy levels in ^{20}Ne, used to calculate the g matrix elements, had to be Coulomb corrected for the two protons outside the ^{16}O core. It is known that the IBM2 fails to predict the binding energies well, and so with this in mind the Coulomb correction was evaluated in an approximate manner. More

sophisticated methods exist for corrections which vary with the excitation energy of the nucleus. The Coulomb energy of valence particles is evaluated using the form given by DE SHALIT and TALMI (62), the expression for Z' valence protons is as follows.

$$E(Z') = CZ' + Z'(Z'-1)A/2 + \{Z'/2\}B \qquad [3.5.1]$$

Here $\{Z'/2\}$ is the largest integer not exceeding $Z'/2$, and for 2s1/2 protons GLAUDEMANS, WIECHERS and BRUSSARD (63) give values for the constants A, B, C, as 0.519MeV, -0.018MeV, 5.659MeV respectivly. This gives the energy of the two protons as 11.881MeV.

Taking the binding energy of ^{20}Ne as -32.0079MeV with respect to the ^{16}O core, and Coulomb correcting this gives the ground state energy as -43.8889MeV. For a level of excitation energy ΔE_J, the matrix elements for the neutron-proton boson interaction can be determined as follows.

$$E_J = -43.8889 + \Delta E_J = 2\epsilon_g + \langle g^2 | V | g^2 \rangle_J \qquad [3.5.2]$$

The matrix elements for J=0, 2, 4, 6, 8 are then established, and are shown in table 5, taken from the lowest 0^+, 2^+, 4^+, 6^+, 8^+ levels in ^{20}Ne.

In a similar manner the matrix elements for $V_{\nu\nu}$ are evaluated from the spectra of ^{20}O, although here due to the lack of 6^+ and 8^+ levels in the spectra, the matrix elements for J=6, 8 had to be estimated. They were chosen so as to give the same difference to J=4 matrix elements as observed in the ^{20}Ne case.

The matrix elements are shown in table 5, taken from the lowest 0^+, 2^+, 4^+ levels in ^{20}O.

The spectra obtained in the resulting "effective" IBM1 calculation are shown for ^{22}Ne, ^{24}Ne, ^{24}Mg in figures 17, 18, 19.†

† This is an IBM2 calculation performed with an effective IBM1 interaction in an IBM1 model space, denoted IBM2g in the figures.

FIGURE 17 G-BOSON ^{22}Ne

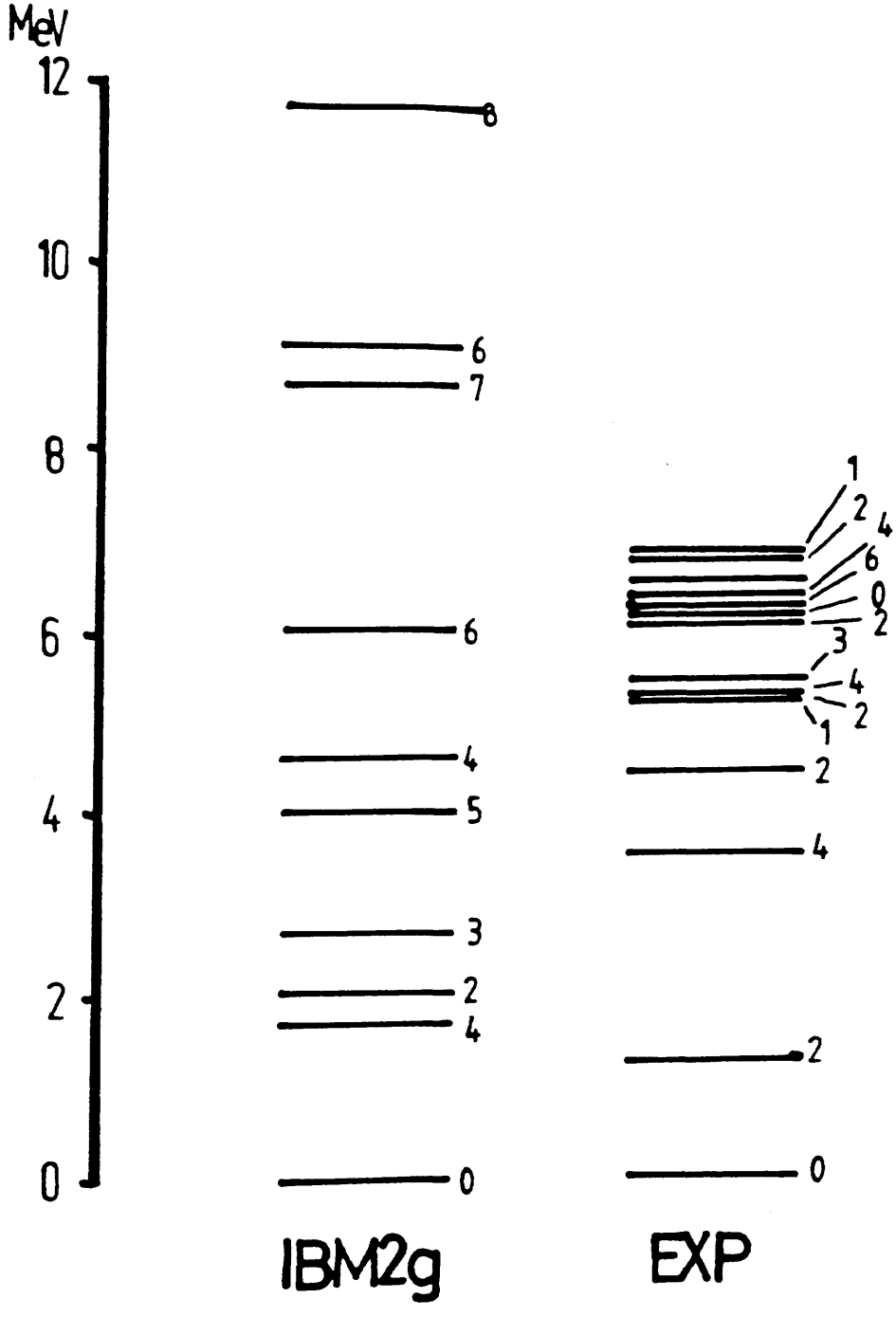


FIGURE 18 G-BOSON ^{24}Ne

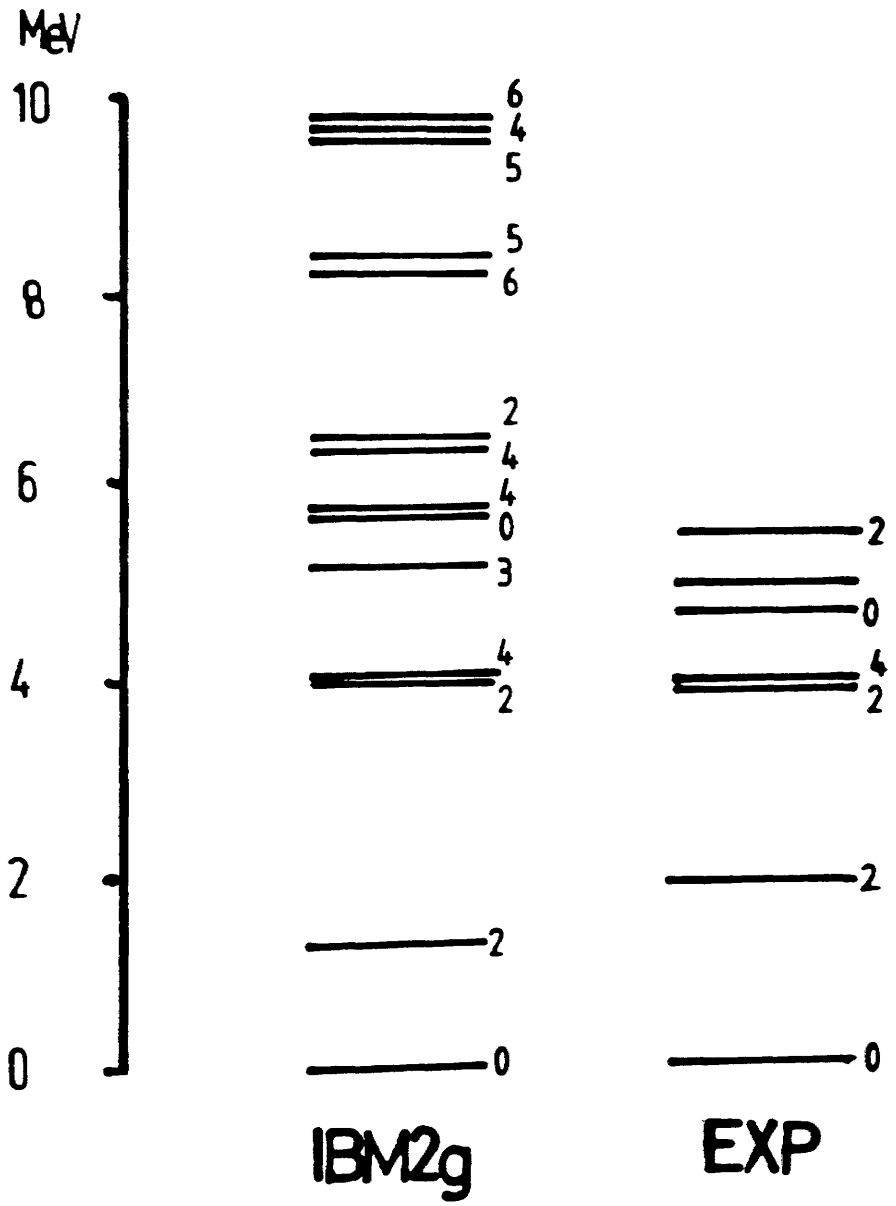


FIGURE 19 G-BOSON ^{24}Mg

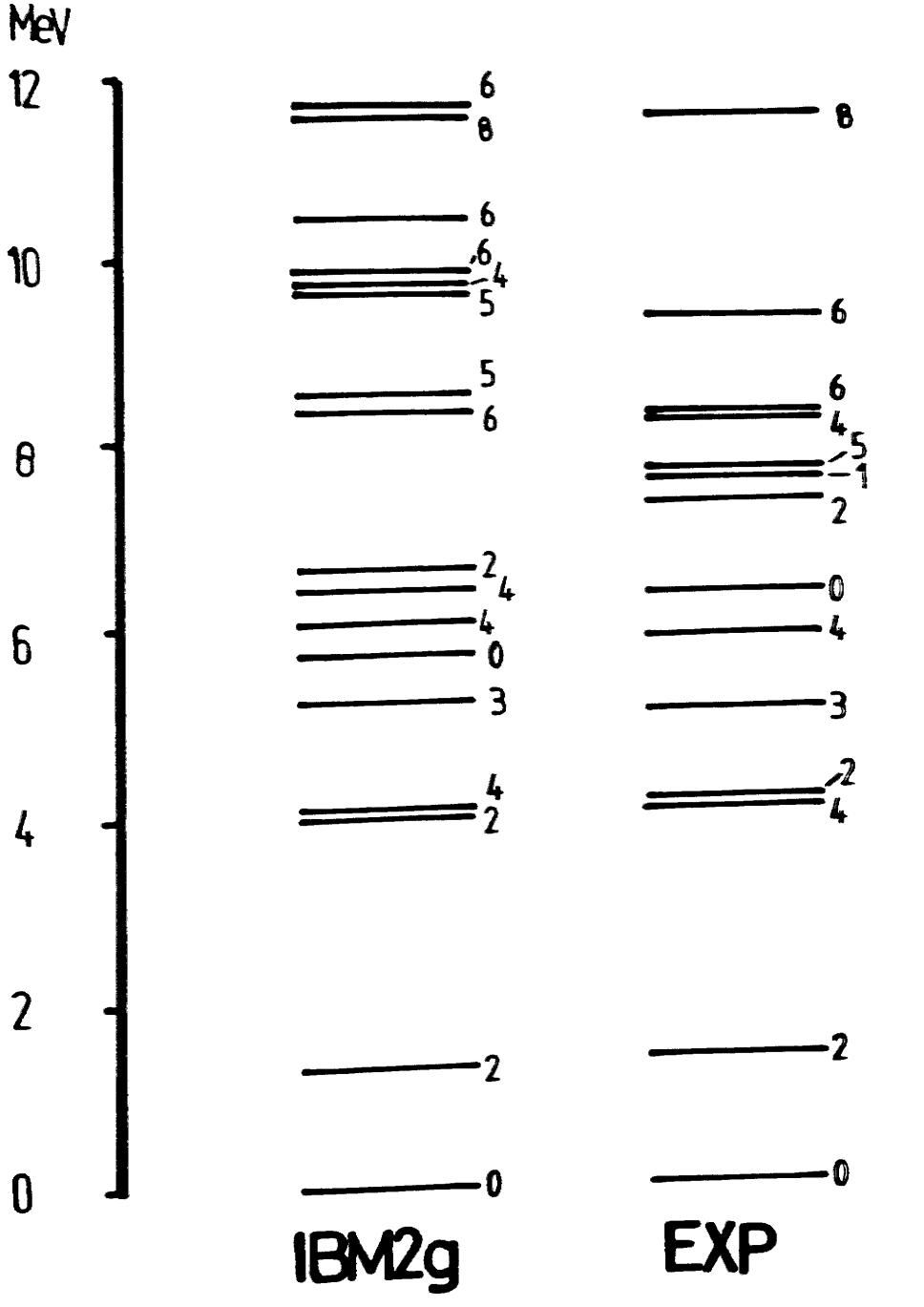


TABLE 5

J	^{20}O $V_{\nu\nu}$	^{20}Ne $V_{\nu\pi}$
0	-6.4937	-26.6289
2	-4.8200	-24.9952
4	-2.9237	-22.3812
6	1.6053	-17.8522
8	4.7786	-14.6789

single particle energy -8.63 MeV

The resulting binding energies exceed those of the IBM2 sd-boson calculations by about 5 to 20 Mev resulting in an increase in the overbinding of the IBM2 by about 50%. The spectra for ^{22}Ne shows a number of unphysical states at low energy, however, for ^{24}Ne and ^{24}Mg a marked improvement in the spectra is observed. In the case of Mg an additional six levels above 12Mev were found to be close to experimental values. A similar calculation for ^{26}Mg, not shown, gave little improvement on the sd-boson calculations. The calculated ground state has J=4, but there is also a nearly degenerate state with J=0. This could be understood as the Pauli exclusion principle becomes more prominent for five bosons, and consquently states of J=4 lying at low energy are unphysical.

CHAPTER 4

BOSON MAPPING TECHNIQUES

4.1 SYMMETRY LIMIT MAPPINGS

Upon examination of the spectra shown in the earlier chapters, it is evident that certain states at low energy having no experimental counterparts are in gross violation of the Pauli exclusion principle (P.E.P). These configurations may be realised with bosons of new types s'and d'-bosons, involving fermions in higher shells for example, although the configurations would correspondingly be at a higher energy (VAN ISACKER (27) et al.). The desire to eliminate such unphysical basis states which will mix into the other low lying states is at the centre of the mapping techniques for state vectors.

It is evident from other work such as LI, DREIZLER and KLEIN (54), that in the vibrational limit the approximation of a number of single j-shells by a effective j-shell with the same number of orbitals, is a good approximation and consequently the problem of such states as described above may not be so critical.

No techniques yet exist for the mapping of fermions to bosons outside of a symmetry limit. Indeed the earlier Boson Expansion methods were used in symmetry limits. Many techniques have now been used in the vibrational limit, mapping in a seniority scheme, and BONATOS, KLEIN (51) have extended this to the deformed rotational case, at least in the case of a p shell with SO(7)) SU(3) symmetry.

4.2 THE O.A.I. METHOD AND ITS EXTENSIONS

The O.A.I mapping technique was first proposed in ARIMA, OTSUKA, IACHELLO, TALMI (21,22) and applied by OTSUKA, ARIMA, IACHELLO (24). This provided a new approach to the mapping problem. Here collective SD fermion pair states are isolated, and found to correspond to certain boson states in a vibrational limit with a seniority scheme. This amounts to a truncation of the fermion space to a collective space.

Firstly one constructs modified pair operators $D^{\dagger}_{\mu} = PA^{(2)\dagger}_{\mu}$, where the operator P acts to project a state of maximum seniority from the action of $A^{(2)\dagger}$ on a state of maximum seniority. These states are then constructed by successive application of the $D^{\dagger}$ operators followed by $S^{(0)\dagger}$ pair operators. The resulting collective SD space states can be written as follows, where α denotes the intermediate angular momentum coupling scheme.

$$| S^{n}(S^{(n-\nu)/2} D^{\nu/2}), \alpha, L, M \rangle \qquad [4.2.1]$$

In the above the operators $D^{\dagger}$ commute when operating on states of maximum seniority, and the above states can be placed in correspondence to the boson states as follows, where γ_d, n_Δ, L, M, are the labels of SU(5) ⊃ O(5) ⊃ O(3) symmetry limit.

$$| s^{n_s} d^{n_d}, \gamma_d, n_\Delta, L, M) \qquad [4.2.2]$$

Here one identifies the total number of bosons with half the number of fermions, and the number of d-bosons with half the fermion seniority.

Fermion operators can be mapped into the boson space in a zeroth order approximation, where an n-body fermion operator maps to an n-body boson operator.

An extension to the above method is described in EVANS, ELLIOTT, SZPIKOWSKI (26) in the f7/2 shell.

A test of the O.A.I. against the older boson expansion techniques is described in ARIMA, YOSHIDA, GINOCCHIO (61), in which it is found that the O.A.I method is the better method. This shows that the choice of Hamiltonian determines the type of symmetry limit mapping to be applied.

4.3 A NEW MAPPING APPROACH

In this section a new proposed mapping technique is outlined, for the mapping of both state vectors and operators from fermion spaces to the IBM, outside of a symmetry limit. This is to some extent an extension of the B.Z. mapping procedure, and is carried out in a Zeroth approximation as is the O.A.I.

A one body hamiltonian for a single j-shell is mapped as follows. It is of the form

$$H_F = \varepsilon_j \sum_m a_m^\dagger a_m \qquad [4.3.1]$$

and can be written for a state of n fermions as

$$H_F = \frac{\varepsilon_j}{(n-1)} \sum_{mk} a_m^\dagger a_k^\dagger a_k a_m \qquad [4.3.2]$$

Where $\sum_k a_k^\dagger a_k$ is the number operator.

Coupling these pairs we obtain

$$H_F = \frac{\varepsilon_j}{(n-1)} \sum_{JM} A^{\dagger(J)}_M(mk) A^{(J)}_M(mk) \qquad [4.3.3]$$

and so the boson Hamiltonian in the zeroth order becomes

$$H_B = \frac{\varepsilon_j}{(n-1)} \sum_{JM} b^{\dagger(J)}_M b^{(J)}_M \qquad [4.3.4]$$

and if we require that

$$\langle \phi_f | H_F | \phi_f \rangle = \langle \phi_B | H_B | \phi_B \rangle \qquad [4.3.5]$$

this implies that the number of bosons is given by

$$n_B = \frac{1}{2} n(n-1) \qquad [4.3.6]$$

Then the number of bosons corresponds to the number of fermion interactions.

For the case of a two-body fermion operator we proceed in a similar manner to the above, as follows

$$H_F = \sum_{\substack{i \le j \\ k \le l}} V_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l \qquad [4.3.7]$$

$$H_F = \frac{2}{(n-2)(n-3)} \sum_{\substack{i \le j \\ k \le l \\ m \le n}} V_{ijkl}\, a_i^\dagger a_j^\dagger a_m^\dagger a_n^\dagger a_n a_m a_k a_l \qquad [4.3.8]$$

and the pairs of operators can be coupled giving

$$H_F \propto \frac{2V_{ijkl}}{(n-2)(n-3)} \left(A^{\dagger(J_1)}_{m_1} A^{\dagger(J_2)}_{m_2} \right)_{JM} \left(A^{(J_2)}_{m_2} A^{(J_3)}_{m_3} \right)_{JM} \quad [4.3.9]$$

The consideration of symmetry and coupling factors would also be required, although this is not shown here.

State vectors would be mapped by taking two fermion pair operators in all combinations, and expressing them as a sum of bosons pair operators, this would then be expanded, and finally the P.E.P imposed on the resulting boson configuration. This could be used as a technique for the eradication of the unphysical basis configurations. These techniques appear to offer the basis for a new mapping procedure. However, considerable effort is still required before it would be possible to judge the effectiveness of the method.

4.4 BOSON DRIVEN SHELL MODEL CALCULATIONS

Another proposed extension to the IBM is that of using a fermion calculation to produce the boson pair wave functions, as follows.

1) Assume a fermion interaction eg. P.W. and perform a shell model calculation for the two fermion systems. Record the energies and wave functions of the states.

2) Assume the energies of the lowest 0^+ and 2^+ states correspond to e_s and e_d, and that the boson states correspond to the eigenstates

$$S^\dagger |0\rangle = \sum \alpha^S_{kl} a^\dagger_k a^\dagger_l |0\rangle$$

$$D^\dagger |0\rangle = \sum \alpha^D_{ij} a^\dagger_i a^\dagger_j |0\rangle \qquad \{4.4.1\}$$

3) Construct boson pair states as follows

$$|B_\lambda\rangle = (D^\dagger S^\dagger)_2 |0\rangle = (\sum \alpha^D_{ij} a^\dagger_i a^\dagger_j)(\sum \alpha^S_{kl} a^\dagger_k a^\dagger_l)|0\rangle \qquad \{4.4.2\}$$

with similar expressions for $S^\dagger S^\dagger |0\rangle$ and $(D^\dagger D^\dagger)_L |0\rangle$.

These correspond to four fermion states, and matrix elements of the P.W. interaction can be calculated using standard fermion techniques. These values would then be interpreted as matrix elements between two-boson systems, which can then be used in many-boson calculations.

Finally, the eigenstates of a many-boson state can be transformed into fermion wavefunctions in the same way. These should provide excellent approximations to fermion eigenstates and would be used as initial vectors in a Lanczos procedure, for instance.

4.5 CONCLUSIONS

It was first shown in chapter 3 section 3.5, that on a purely phenomenological basis the g-boson could be used in ^{24}Mg to give a good account of the spectrum. The long standing question of whether the g is important in the low lying states of deformed nuclei will not be answered until more calculations like the above have been performed. It would also be possible to perform a g calculation and renormalise for the sd-boson effects.

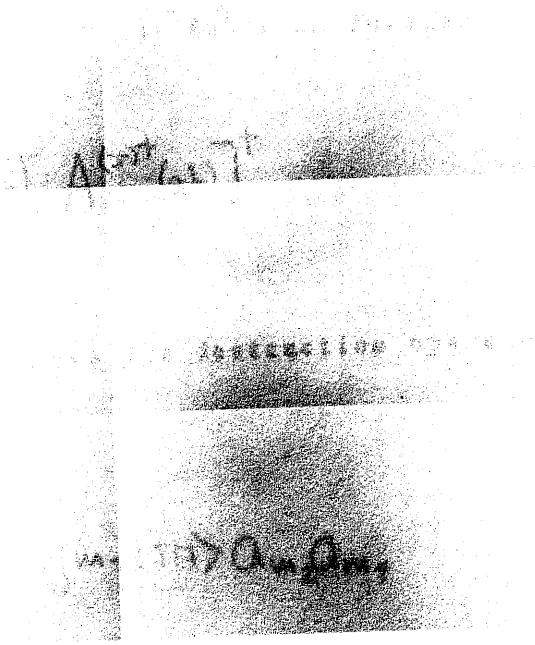
In chapter 3 section 3.6 the g-boson was put into an SD-shell calculation in a weak coupling limit. The results here indicated that a stronger coupling limit would be more appropriate.

A final calculation in section 3.6, in which the g-boson was used in the SD-shell being renormalised for sd-boson effects, gave a significant improvement in spectra for the more deformed nuclei, although the over binding of the IBM2 increased by 50%. This would seem to indicate that as we move to more deformed nuclei the higher order bosons become more significant as might be expected. In general, when introducing other types of bosons, the need for a mapping technique to replace the current perturbational methods is required to keep the number of matrix elements and basis states to a manageable size, this would also be in keeping with the idea that the IBM characterises the most collective states and so maintains a moderate sized model space.

In the last two sections, new work was suggested, the first of which offered a new interpretation to the IBM1 and provided a symmetry independent mapping approximation method. Whilst the

other section offered an alternative style of calculation to those currently undertaken.

The IBM still has a large number of new extensions, many not fully explored.



APPENDIX A

PAIR OPERATORS AND COMMUTATION RELATIONS

We summarise here some of the results from LI, DREIZLER and KLEIN (54), for pairs of fermions in a single j-shell.

We adopt the convention that summation indices shown as (m), indicate that the variable is actually fixed by the values of other quantum numbers.

Define a normalised pair operator as

$$A^{(J)\dagger}_{M} = \frac{1}{\sqrt{2}} \sum_{m_1(m_2)} \langle j m_1 j m_2 | JM \rangle a^{\dagger}_{m_1} a^{\dagger}_{m_2} \qquad \{a1\}$$

The phase of these operators is taken as follows

$$A^{(J)}_{M}(ab) = \left[A^{(J)\dagger}_{M}(ab) \right]^{\dagger} \qquad \{a2\}$$

As a result of this we have the destruction operators given as

$$A^{(J)}_{M} = \frac{1}{\sqrt{2}} \sum_{m_1(m_2)} \langle j m_1 j m_2 | JM \rangle a_{m_2} a_{m_1} \qquad \{a3\}$$

An additional operator is then defined as

$$B^{(J)}_{M} = \frac{1}{(\hat{J})^{1/2}} \sum_{m_1(m_2)} \langle j m_1 j -m_2 | JM \rangle (-)^{j-m} a^{\dagger}_{m_1} a_{m_2} \qquad \{a4\}$$

Taking the above operators we can evaluate their commutation relations which are found to be as follows (see EDMONDS (36)).

$$\left[A_1^{\dagger}, A_2^{\dagger}\right] = 0 \qquad \{a5\}$$

$$\left[A_1, A_2^{\dagger}\right] = \delta_{12} - 2\sum_3 Y(123)(\hat{J}_3)^{1/2} B_3^{\dagger} \qquad \{a6\}$$

$$\left[B_1^{\dagger}, A_2^{\dagger}\right] = \frac{2}{(\hat{J}_1)^{1/2}} \sum_3 Y(231)\, A_3^{\dagger} \qquad \{a7\}$$

$$\left[B_1^{\dagger} B_2\right] = \frac{1}{(\hat{J}_2\hat{J}_3)^{1/2}} - \sum_3 \left(1 - (-)^{J_1+J_2+J_3}\right) \times Y(123)(\hat{J}_3)^{1/2} B_3^{\dagger} \qquad \{a8\}$$

Where the following definitions apply

$$A_1^{\dagger} = A_{M_1}^{(J_1)\dagger} \qquad \{a9\}$$

$$Y(123) = (-)^{2j+J_2+J_3}(\hat{J}_2\hat{J}_3)^{1/2} \langle J_2 M_2 J_3 M_3 | J_1 M_1 \rangle \times \begin{Bmatrix} J_2 & J_3 & J_1 \\ j & j & j \end{Bmatrix} \qquad \{a10\}$$

Where $\begin{Bmatrix} & \end{Bmatrix}$ is the 6j symbol

$$\delta_{12} = \frac{1}{2}\delta_{J_1 J_2}\delta_{M_1 M_2}\left[\delta_{a_1 a_2}\delta_{b_1 b_2} - \theta(a_1 b_1 J_1)\delta_{a_1 b_2}\delta_{a_2 b_1}\right] \qquad \{a11\}$$

$$\theta(abJ) = (-)^{j_a + j_b - J} \qquad \{a12\}$$

$$\hat{J} = J(J+1)$$

{•13}

APPENDIX B

NORMALISATION OF BOSON MATRIX ELEMENTS

The one-body Hamiltonian for the bosons can be written as

$$H_B = \sum_i \varepsilon_i b_i^\dagger b_i \qquad \{b1\}$$

For a state with n bosons, we can express this in the form

$$H_B = \frac{1}{2} \sum_{ij} \frac{(\varepsilon_i + \varepsilon_j)}{(n-1)} b_i^\dagger b_j^\dagger b_j b_i \qquad \{b2\}$$

For the purpose of calculations we impose the resriction that $i \leq j$, in which case we obtain

$$H_B = \sum_{i \leq j} \frac{(\varepsilon_i + \varepsilon_j)}{(n-1)(1+\delta_{ij})} b_i^\dagger b_j^\dagger b_j b_i \qquad \{b3\}$$

We can also introduce two additional indices, giving

$$H_B = \sum_{\substack{i \leq j \\ k \leq l}} \frac{\delta_{il}\delta_{jk}}{(n-1)} \frac{(\varepsilon_i + \varepsilon_j)}{(1+\delta_{ij})} b_i^\dagger b_j^\dagger b_k b_l \qquad \{b4\}$$

We now consider the two-body part of the Hamiltonian.

First a general normalised pair state is defined as

$$|(j_1 j_2)JM\rangle = \frac{1}{(1+\delta_{j_1 j_2})^{1/2}}\left[\sum_{m_1 m_2}\langle j_1 m_1 j_2 m_2 | JM\rangle b^{+}_{m_1} b^{+}_{m_2}\right]|0\rangle \qquad \{b5\}$$

It is then assumed that the normalised matrix elements are of the form

$$\langle (j_1 j_2)J | H' | (j_3 j_4)J\rangle \qquad \{b6\}$$

The uncoupled Hamiltonian is chosen as

$$\hat{H} = \sum_{\substack{i\le j \\ k\le l}}{}' V_{ijkl}\, b^{+}_i b^{+}_j b_k b_l \qquad \{b7\}$$

The following condition is then required to be satisfied for the uncoupled and coupled Hamiltonians

$$\langle (j_1 j_2)J | \hat{H} | (j_3 j_4)J\rangle = \langle (j_1 j_2)J | H' | (j_3 j_4)J\rangle \qquad \{b8\}$$

This leads to an expression for V as follows

$$V_{j_1^{m_1} j_2^{m_2} j_3^{m_3} j_4^{m_4}} = \sum_{JM} \frac{\sqrt{(1+\delta_{j_1 j_2})(1+\delta_{j_3 j_4})}}{(1+\delta_{j_1 j_2}\delta_{m_1 m_2})(1+\delta_{j_3 j_4}\delta_{m_3 m_4})} \qquad \{b9\}$$

$$\times \langle j_1^{m_1} j_2^{m_2} | JM\rangle \langle j_3^{m_3} j_4^{m_4} | JM\rangle \langle (j_1 j_2)J | H' | (j_3 j_4)J\rangle$$

Finally the complete Hamiltonian can be written as follows

$$\hat{H} = \frac{1}{(n-1)} \sum_{\substack{i \le j \\ k \le l}} \frac{(\varepsilon_i + \varepsilon_j)}{(1+\delta_{ij})} \delta_{il}\delta_{jk}\, b_i^\dagger b_j^\dagger b_k b_l$$

$$+ \sum_{\substack{i \le j \\ k \le l \\ J\Pi}} \frac{\sqrt{(1+\delta_{j_1 j_2})(1+\delta_{j_3 j_4})}}{(1+\delta_{j_1 j_2}\delta_{m_1 m_2})(1+\delta_{j_3 j_4}\delta_{m_3 m_4})} \langle j_1^{m_1} j_2^{m_2} | J\Pi \rangle \qquad \text{(b10)}$$

$$\times \langle j_3^{m_3} j_4^{m_4} | J\Pi \rangle \langle (j_1 j_2) J | H' | (j_3 j_4) J \rangle b_i^\dagger b_j^\dagger b_k b_l$$

APPENDIX C

COMBINATORIAL TECHNIQUES FOR BOSONS

Given n distinguishable objects distributed over N boxes, with no restriction on the number of objects per box, the problem is one of determining the number of permutations for the n objects and N-1 partitions that separate the groups of objects associated with each box. (.object, | partition)

.....|...|.....|.....|..

With a total of (n+N-1) entities to be permuted and requiring the n objects and the N-1 partitions to be two indistinguishable groups of elements, the number of distinct permutations is

$$ {}^{N+n-1}C_{n} = \frac{(N+n-1)!}{(N-1)!\,n!} \qquad \{c1\} $$

Let the boxes 1,2...N contain n1,n2....nN bosons.
It follows from a sequential ordering of the states that

State code for some chosen configuration n1,n2,n3.....nN
= number of permutations with n,n-1,...n1+1 objects
distributed over orbital 1
+ number of permutations with n1 fixed and the now
remaining n-n1,n-n1-1,.....n2+1 objects
distributed over orbital 2
+ number of permutations with n1 and n2 fixed and

now remaining n-n1-n2,n-n1-n2-1.....n3+1 objects distributed over orbital 3

+ .....

+ number of permutations with n1,n2,n3.....nN-1 fixed and the remaining nN objects distributed over orbital N, which is 1

{c2}

Then the total number of states (or permutations) with n to n1+1 objects distributed over orbital 1 is equivalent to the total number of states with 0 to n-(n1+1) remaining objects distributed over the remaining 2,3.....N orbitals. So our state code can now be written as follows

State code for n1,n2,n3....nN

= the total number of states with (0,1.....n-n1-1) objects distributed over the (2,3.....N) orbitals

+ (0,1.....n-n1-n2-1) objects distributed over the (3,4.....N) orbitals

+ .....

+ (0,1.....(n-n1-n2...-ni-1) objects distributed over (i.....N) orbitals

+ 1

{c3}

An expression is required for the total number of remaining permutations when some set of orbitals contain a fixed distribution of objects.

Consider a state with some chosen number of objects in the first orbital n1c. We now have a remaining N-1 orbitals ie N-2 partitions and n-n1c objects, this leads to the following expression for the number of remaining permutations.

$$ {}^{N-2+n-n1c}C_{n-n1c} \qquad \{c4\} $$

The total number of such permutations where n1c ranges from n to n1+1. Let r=n-n1c, then this is just

$$ \sum_{r=0}^{n-n1} {}^{N-2+r}C_r \qquad \{c5\} $$

Similarly, for n1 in the first orbital and n2c in the second, and where n2c ranges from n-n1 to n2+1 and k=n-n1-n2c we obtain

$$ \sum_{k=0}^{n-n1-n2-1} {}^{N-3+k}C_k \qquad \{c6\} $$

giving for the ith orbital

$$ \sum_{s=0}^{n-\sum_{j=1}^{i} n_j - 1} {}^{N-i-1+s}C_s \qquad \{c7\} $$

Where s is defined as

$$ s = n - \sum_{j=1}^{i-1} n_j - n_i \qquad \{c8\} $$

The state code can now written as

$$\text{State Code} = \sum_{r=0}^{n-n_1-1} {}^{(N-2)+r}C_r + \sum_{r=0}^{n-n_1-n_2-1} {}^{(N-3)+r}C_r + \ldots$$

$$+ \ldots + \sum_{r=0}^{n-\sum_{j=1}^{i} n_j - 1} {}^{(N-1-i)+r}C_r + \ldots + 1 \qquad \{c9\}$$

The above can be simplified with the use of the following result.

$$\sum_{r=0}^{R} {}^{N+r}C_r = {}^{N+R+1}C_R \qquad \{c10\}$$

And so our final expression for the state code is

$$\text{State Code} = {}^{(N-2+n-n_1)}C_{(n-n_1-1)} + {}^{(N-3+n-n_1-n_2)}C_{(n-n_1-n_2-1)} + \ldots$$

$$+ \ldots + {}^{N-1-i+n-\sum_{s=1}^{i} n_s}C_{n-\sum_{s=1}^{i} n_s - 1} + \ldots + 1 \qquad \{c11\}$$

NOTE The factor of 1 in the above can be omitted as it occurs for all states. This will change the state numbering from 1,2....to 0,1....

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