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# THE WEAK COUPLING MODEL APPLIED TO THE NUCLEI WITH $A = 16\text{-}19$

## (I). Energy levels

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**Abstract:** We have formulated particle-hole states by coupling in $J$ and $T$ eigenfunctions resulting from diagonalization of $(sd)^{n_1}$ and $p^{n_2}$. A central particle-hole interaction is assumed and the results for the negative parity levels with $A = 16\text{-}19$ mostly compare well with experiment. In particular it is important to include three hole states in $^{17}O$. The structure of the positive parity levels in mass-18 is discussed.

## 1. Introduction

The shell model is well suited to the study of the low-lying energy levels of light nuclei. The basic approach is to choose a subspace of shell-model configurations which is assumed to represent the main degrees of freedom of the system. The task is then to predict as many nuclear properties as possible. The correctness of the configuration assignment is determined by a comparison between theory and experiment.

In the region of $^{16}O$ many calculations have been performed where the $^{16}O$ system is assumed to constitute a closed and spherical core. The degrees of freedom responsible for the nuclear properties are then attributed to the additional particles or holes outside the core. In this description one is restricted to energy levels with the same parity as the ground state. However, in several cases low-lying levels with different parity occur which can only be explained on the basis of excitations of the core. A particularly striking example of this is the $\frac{1}{2}^-$ level in $^{19}F$ at 0.11 MeV. In the case of energy levels with the same parity as the ground state, it has now become clear that particle-hole (p-h) excitations are important. Cohen *et al.* [1]) have demonstrated in their pseudonuclei calculations that many nuclear properties can be insensitive to the precise configurations involved, but the discovery [2]) of $0^+$ and $2^+$ levels at $\approx 5.3$ MeV in $^{18}O$ clearly shows the insufficiency of the original model in that it is unable to reproduce the correct number of levels. Other examples of "missing" levels [3-6]) include the $1^+$ level at 1.70 MeV in $^{18}F$, the $\frac{1}{2}^+$ level at 3.22 MeV in $^{19}O$ and the $0^+$ and $2^+$ levels at $\approx 7$ MeV in $^{20}Ne$. A study of electromagnetic transition rates in this region [7-9]) also shows the necessity of particle-hole excitations. The pseudonuclei calculations show the importance of comparing all possible data with model predictions, particularly the E2 rates.

In the last few years several calculations e.g. refs. [7-19]) have been done where core excitations are taken into account. The main problem is the large number of available configurations. To overcome this difficulty physical arguments are used to select a few particular excited modes of the $^{16}$O core which are assumed to be the dominant additional configurations in the wave function. The approach in selecting p-h configurations has been to use the $SU_3$ classification scheme or a deformed coupling scheme with a Nilsson-type single-particle potential well. The idea of deformation is connected with the fact that the p-h excitations produce energy spectra of the type $J(J+1)$ and large electric quadrupole transition rates.

In this situation it seems of interest to look for an alternative approach where the assumptions about the structure of the excited modes are less restrictive. The problem is to look for those p-h excitations which are energetically favoured and determine their energy positions relative to the particle configurations. In the approach presented here we have used as a starting point an idea discussed by Arima *et al.* [3]) which can be classified as a "weak coupling" model. The main assumption is that the correlations between particles in the same major shell are of predominant importance and the p-h interaction can be treated as a small perturbation. Accordingly we select our p-h states by combining eigenfunctions obtained by solving the $n_1$ particle problem in the sd-shell and the $(12-n_2)$ hole problem in the p-shell. We can then study the extent to which the p-h interaction destroys this simple picture and the ability of the model to reproduce experiment using a relatively small number of states. We shall restrict ourselves to consideration of the 1p and 2s-1d shells only, assuming that excitations involving the 1s or 1f-2p shells are of minor importance.

In sect. 2 we define the weak coupling model and point out the necessary steps in the calculation; these are then discussed in detail in sects. 3 and 4. In sect. 3 we give the solution to the eigenvalue problem for $n_1(n_2)$ particles in the sd(p) shell. Sect. 4 is devoted to the calculation of the required particle-hole matrix elements. The results are presented in sect. 5, starting with a general discussion and giving a detailed comparison with experiment in subsects. 5.1–5.5. Subsects. 5.1–5.4 deal with the negative parity levels in the nuclei with $A = 16-19$ and subsect. 5.5 the positive parity levels in mass-18. Our conclusions are presented in sect. 6.

## 2. The model

In the shell-model description we express the Hamiltonian of the system in the form

$$H = H_1 + H_2 + V_{12}, \qquad (1)$$

where $H_1(H_2)$ is the Hamiltonian operating on the coordinates of the sd(p) shell particles and $V_{12}$ gives the interaction between the p- and sd-shells. The basic form of the wave function is defined to be

$$|\Phi^{n_1 n_2}_{\nu J T M_T}\rangle = [|(\text{sd})^{n_1}\gamma_1 J_1 T_1\rangle|p^{n_2}\gamma_2 J_2 T_2\rangle]_{JM_J T M_T}$$

$$= \sum_{i_1 i_2} C(\gamma_1 \alpha_{i_1}) C(\gamma_2 \alpha_{i_2}) |(\text{sd})^{n_1}\alpha_{i_1} J_1 T_1, p^{n_2}\alpha_{i_2} J_2 T_2; JT\rangle, \quad (2)$$

where subscripts 1 and 2 label the sd- and p-shells respectively. Additional quantum numbers $v$ and $\gamma$ may be required and as indicated the latter represent in general a linear combination of basis functions with the chosen labels $\alpha$ (see sect. 3). The square brackets indicate that $J_1$ and $J_2$ are coupled to $J$, with $z$-component $M_J$, etc. We shall suppress the quantum numbers $M_J$ in the wave functions for simplicity. The wave function defined in eq. (2) will be referred to as a $n_1$ particle–$(12-n_2)$ hole state. We can then write for the ordinary shell-model basis with only the sd-shell unclosed;

$$|\Phi_{\gamma_1 J_1 T_1 M_{T_1}}^{n_1 12}\rangle = [|(\mathrm{sd})^{n_1}\gamma_1 J_1 T_1\rangle|\mathrm{p}^{12}J_2 = T_2 = 0\rangle]_{J_1 M_{J_1} T_1 M_{T_1}}. \qquad (3)$$

For our formulation the wave functions of eq. (2) are chosen as eigenstates of $H_1 + H_2$, so that

$$H_1|(\mathrm{sd})^{n_1}\gamma_1 J_1 T_1 M_{T_1}\rangle = E_{\gamma_1 J_1 T_1 M_{T_1}}^{n_1}|(\mathrm{sd})^{n_1}\gamma_1 J_1 T_1 M_{T_1}\rangle,$$

$$H_2|\mathrm{p}^{n_2}\gamma_2 J_2 T_2 M_{T_2}\rangle = E_{\gamma_2 J_2 T_2 M_{T_2}}^{n_2}|\mathrm{p}^{n_2}\gamma_2 J_2 T_2 M_{T_2}\rangle, \qquad (4)$$

where $E_{\gamma J T M_T}^{n}$ represents the binding energy of $n$ particles measured relative to a closed $^{16}\mathrm{O}$ core. The matrix elements of $H$ are thus

$$\langle\Phi_{vJTM_T}^{n_1 n_2}|H|\Phi_{v'JTM_T}^{n_1' n_2'}\rangle = \delta_{n_1 n_1'}\delta_{n_2 n_2'}\sum_{M_{T_1}(M_{T_2})} C(T_1 M_{T_1} T_2 M_{T_2}; TM_T)$$

$$\times C(T_1' M_{T_1} T_2 M_{T_2}; TM_T)\{(E_{\gamma_1 J_1 T_1 M_{T_1}}^{n_1} + E_{\gamma_2 J_2 T_2 M_{T_2}}^{n_2})\delta_{vv'}\delta_{T_1 T_1'}$$

$$- \langle\Phi_{\gamma_1 J_1 T_1 M_{T_1}}^{n_1 12}|V_{12}|\Phi_{\gamma_1' J_1' T_1' M_{T_1}}^{n_1 12}\rangle\delta_{\gamma_2\gamma_2'}\delta_{J_2 J_2'}\delta_{T_2 T_2'}\} + \langle\Phi_{vJTM_T}^{n_1 n_2}|V_{12}|\Phi_{v'JTM_T}^{n_1' n_2'}\rangle. \qquad (5)$$

In the case $n_1 = n_1'$, $n_2 = n_2'$ the last two terms together give the p-h interaction. The $M_T$ dependence of this equation is due to the Coulomb interaction. The final solution is therefore obtained by a diagonalization of $H$ within the chosen basis, the off-diagonal matrix elements being determined by $V_{12}$ only.

The necessary ingredients for the calculation are therefore the solutions of the eigenvalue problems posed in eq. (4) and the matrix elements of $V_{12}$.

## 3. The shell-model problem for $n$ particles in an oscillator shell

We shall formulate only the sd-shell case, pointing out any modifications required for the p-shell. The Hamiltonian has the usual form

$$H_1 = \sum_i \varepsilon_i + \sum_{i<j} V(r_{ij}), \qquad (6)$$

where the single-particle terms are adjusted to reproduce the experimental single-particle spectrum and $V(r_{ij})$ represents the residual two-body interaction. We shall use this interaction to determine the relative spacings of levels. We obtain ground state interaction energies which are very close to those deduced from experiment but we prefer to take the experimental values for the relevant binding energies relative to $^{16}\mathrm{O}$, thus including Coulomb effects empirically.

We use the $L$-$S$ coupling scheme and for the sd-shell the wave functions are further classified by the $(\lambda\mu)$ quantum numbers of the $SU_3$ group introduced by Elliott [20, 21]). This has the advantage that rather few terms are needed to provide a good description of the eigenfunctions. The calculation has been greatly facilitated by recent work on the $SU_3$ group. The orbital coefficients of fractional parentage ($SU_6 \supset SU_3$) have been calculated by Akiyama [22]) and the Wigner ($SU_3 \supset R_3$) and Racah coefficients of the $SU_3$ group have been tabulated by Vergados [23]) and Hecht [24]). We shall adopt the phase conventions of Vergados which have the advantage that the Wigner coefficients are all real.

We use the second quantization formalism and define a single-particle state by

$$|(\lambda 0)ljmm_t\rangle = a^\dagger_{(\lambda 0)ljmm_t}|0\rangle, \tag{7}$$

where $m$ and $m_t$ are the $z$-components of $j$ and the isospin and $\lambda = 2(1)$ for the sd(p) shell. The radial oscillator wave functions are as defined by Elliott [20]). The creation operator $a^\dagger_{(\lambda 0)ljmm_t}$ transforms as a $SU_3$ tensor $T^{(\lambda 0)}_{ljmm_t}$. The Hermitian conjugate $a_{(\lambda 0)ljmm_t}$ has the transformation properties

$$(-1)^{\frac{1}{2}(\lambda-l)+j-m+\frac{1}{2}-m_t} T^{(0\lambda)}_{lj-m-m_t}.$$

The form of our $n$-particle wave function is

$$|(sd)^n\alpha JT\rangle = |(sd)^n[f](\lambda\mu)\kappa LSJT\rangle, \tag{8}$$

where the partition $[f]$, labelling $SU_6$, specifies the orbital symmetry and $\kappa$ distinguishes states with the same $L$-value within a given $(\lambda\mu)$ representation. It is essential that $\kappa$ be an orthogonal label if we are to use the recoupling techniques in $SU_3$ analogous to the familiar Racah algebra of $R_3$. We therefore use the orthogonal $\kappa$-label introduced by Vergados which is closely related to Elliott's non-orthogonal $K$-label [23]). For simplicity $\kappa$ will be omitted unless it is needed for a complete specification. In the case of the p-shell $[f]$ and $(\lambda\mu)$ are equivalent since the states span a representation for a unitary transformation in three dimensions.

Using the two-particle coefficients of fractional parentage (c.f.p.) we can write the matrix elements of a two-body operator

$$\langle(sd)^n[f_1](\lambda_1\mu_1)\kappa_1 L_1 S_1 J_1 T_1| \sum_{i<j} V(r_{ij})|(sd)^n[f_1'](\lambda_1'\mu_1')\kappa_1' L_1' S_1' J_1 T_1\rangle$$

$$= \frac{1}{2}n(n-1) \sum \langle(n-2)[f''](\lambda''\mu'')S''T''; (\lambda_m\mu_m)S_m T_m|\}n[f_1](\lambda_1\mu_1)S_1 T_1\rangle_\rho$$

$$\times \langle(n-2)[f''](\lambda''\mu'')S''T''; (\lambda_m'\mu_m')S_m' T_m|\}n[f_1'](\lambda_1'\mu_1')S_1' T_1'\rangle_{\rho'}$$

$$\times \langle(\lambda''\mu'')\kappa''L'(\lambda_m\mu_m)L_m||(\lambda_1\mu_1)\kappa_1 L_1\rangle_\rho \langle(\lambda''\mu'')\kappa''L'(\lambda_m'\mu_m')L_m||(\lambda_1'\mu_1')\kappa_1' L_1'\rangle_{\rho'}$$

$$\times X \begin{pmatrix} L'' & L_m & L_1 \\ S'' & S_m & S_1 \\ J'' & J_m & J_1 \end{pmatrix} X \begin{pmatrix} L'' & L_m' & L_1' \\ S'' & S_m' & S_1' \\ J'' & J_m & J_1 \end{pmatrix}$$

$$\times \langle(sd)^2(\lambda_m\mu_m)L_m S_m; J_m T_m|V(r_{12})|(sd)^2(\lambda_m'\mu_m')L_m' S_m'; J_m T_m\rangle. \tag{9}$$

We follow the convention that when the summation indices are not specified the sum is to be taken over all labels which occur only on the right-hand side of the equation. The coefficients $X$ are defined in terms of the 9-$j$ symbol by

$$X \begin{pmatrix} A & B & C \\ D & E & F \\ G & H & I \end{pmatrix} = \hat{C}\hat{F}\hat{G}\hat{H} \begin{pmatrix} A & B & C \\ D & E & F \\ G & H & I \end{pmatrix}, \tag{10}$$

where $\hat{C} = \sqrt{2C+1}$ etc.

The SU$_3$ Wigner coefficients are defined by

$$|(\lambda_1\mu_1)\kappa_1 L_1 M_1\rangle_\rho = \sum_{\substack{\kappa''L'' \\ \kappa_m L_m}} \langle(\lambda''\mu'')\kappa''L''(\lambda_m\mu_m)\kappa_m L_m||(\lambda_1\mu_1)\kappa_1 L_1\rangle_\rho$$
$$\times [|(\lambda''\mu'')\kappa''L''\rangle|(\lambda_m\mu_m)\kappa_m L_m\rangle]_{L_1 M_1}, \tag{11}$$

where the label $\rho$ is needed because $(\lambda_1\mu_1)$ may occur more than once in the product $(\lambda''\mu'') \times (\lambda_m\mu_m)$ i.e. the product in general is not simply reducible. The coefficients which are not tabulated may be obtained by use of the known SU$_3$ Racah or recoupling coefficients [23,24] and the usual R$_3$ $U$-coefficients in the relation

$$\sum_\rho \langle(\lambda''\mu'')\kappa''L''(\lambda_m\mu_m)\kappa_m L_m||(\lambda_1\mu_1)\kappa_1 L_1\rangle_\rho$$
$$\times U((\lambda''\mu'')(\lambda_\alpha\mu_\alpha)(\lambda_1\mu_1)(\lambda_\beta\mu_\beta); (\lambda'\mu')(\lambda_m\mu_m))_\rho$$
$$= \sum_{\substack{\kappa_\alpha L_\alpha \\ \kappa_\beta L_\beta \\ \kappa'L'}} \langle(\lambda''\mu'')\kappa''L''(\lambda_\alpha\mu_\alpha)\kappa_\alpha L_\alpha||(\lambda'\mu')\kappa'L'\rangle\langle(\lambda'\mu')\kappa'L'(\lambda_\beta\mu_\beta)\kappa_\beta L_\beta||(\lambda_1\mu_1)\kappa_1 L_1\rangle$$
$$\times \langle(\lambda_\alpha\mu_\alpha)\kappa_\alpha L_\alpha(\lambda_\beta\mu_\beta)\kappa_\beta L_\beta||(\lambda_m\mu_m)\kappa_m L_m\rangle U(L'L_\alpha L_1 L_\beta; L'L_m), \tag{12}$$

where we have suppressed the $\rho$-labels on the right since we shall be dealing with cases where they are not needed, i.e. $\lambda_\alpha$ or $\mu_\alpha$ is zero and $\lambda_\beta$ or $\mu_n$ is zero.

The two-particle c.f.p. may be obtained from the one-particle c.f.p. by the relation

$$\langle(n-2)[f''](\lambda''\mu'')S''T''; (\lambda_m\mu_m)S_m T_m|\}n[f_1](\lambda_1\mu_1)S_1 T_1\rangle_\rho$$
$$= \sum \langle(n-2)[f''](\lambda''\mu'')S''T''; (20)\tfrac{1}{2}\tfrac{1}{2}|\}(n-1)[f'](\lambda'\mu')S'T'\rangle$$
$$\times \langle(n-1)[f'](\lambda'\mu')S'T'; (20)\tfrac{1}{2}\tfrac{1}{2}|\}n[f_1](\lambda_1\mu_1)S_1 T_1\rangle$$
$$\times U((\lambda''\mu'')(20)(\lambda_1\mu_1)(20); (\lambda'\mu')(\lambda_m\mu_m))_\rho$$
$$\times U(S''\tfrac{1}{2}S_1\tfrac{1}{2}; S'S_m)U(T''\tfrac{1}{2}T_1\tfrac{1}{2}; T'T_m), \tag{13}$$

and the one-particle c.f.p. is factored following Jahn and van Wieringen [25]

$$\langle(n-1)[f'](\lambda'\mu')S'T'; (20)\tfrac{1}{2}\tfrac{1}{2}|\}n[f_1](\lambda_1\mu_1)S_1 T_1\rangle$$
$$= \left(\frac{n_f}{n_f}\right)^{\frac{1}{2}} \langle[f'](\lambda'\mu'); (20)|\}[f_1](\lambda_1\mu_1)\rangle\langle[\tilde{f}']S'T'; \tfrac{1}{2}\tfrac{1}{2}|\}[\tilde{f}_1]S_1 T_1\rangle! \tag{14}$$

TABLE 1

Eigenfunctions and eigenvalues for $(sd)^{n_1}$ [a]

| $n_1$ | $T_1$ | $J_1$ | Eigenvalue | Configuration [b] | Configuration | Configuration | Configuration | Configuration |
|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 1 | 0.00 | 0.931 (40)002 | -0.171 (40)022 | -0.255 (02)002 | -0.199 (21)110 | |
|   |   | 3 | 1.15 | 0.981 (40)022 | -0.111 (02)022 | -0.158 (21)130 | | |
|   |   | 5 | 1.46 | 1.000 (40)042 | | | | |
|   |   | 2 | 3.33 | 0.940 (40)022 | -0.112 (02)022 | 0.322 (21)120 | 0.158 (02)022 | 0.298 (21)110 |
|   |   | 1* | 3.76 | 0.275 (40)002 | -0.164 (40)022 | 0.885 (02)002 | 0.338 (21)130 | |
|   |   | 3* | 4.94 | 0.158 (40)022 | -0.030 (40)042 | 0.927 (02)022 | | |
|   |   | 4* | 6.13 | 1.000 (40)042 | | | | |
|   |   | 1** | 6.51 | 0.147 (40)002 | 0.847 (40)022 | 0.275 (02)002 | -0.176 (02)022 | -0.393 (21)110 |
|   |   | 2* | 7.00 | -0.016 (40)022 | 0.929 (02)022 | 0.370 (21)120 | | |
| 2 | 1 | 0 | 0.00 | 0.842 (40)000 | -0.411 (02)000 | 0.349 (21)112 | 0.214 (21)122 | |
|   |   | 2 | 2.01 | 0.797 (40)020 | -0.301 (02)020 | 0.444 (21)112 | 0.179 (21)132 | |
|   |   | 4 | 3.46 | 0.683 (40)040 | 0.730 (21)132 | | | |
|   |   | 0* | 3.65 | 0.489 (40)000 | 0.855 (02)000 | -0.172 (21)112 | 0.411 (21)122 | |
|   |   | 2* | 3.98 | 0.410 (40)020 | 0.690 (02)020 | -0.399 (21)112 | -0.167 (21)132 | |
|   |   | 3 | 4.78 | 1.000 (21)122 | | | | |
|   |   | 4* | 7.86 | 0.730 (40)040 | -0.683 (21)132 | | | |
| 3 | 1/2 | 1/2 | 0.00 | 0.960 (60)001 | -0.048 (22)001 | 0.185 (41)111 | 0.205 (41)113 | 0.224 (41)123 |
|   |   | 3/2 | 0.28 | 0.892 (60)021 | -0.321 (22)021 | 0.160 (22)221 | 0.157 (41)113 | 0.220 (41)123 |
|   |   | 5/2 | 1.51 | 0.885 (60)021 | -0.306 (22)021 | 0.148 (22)221 | -0.231 (41)121 | 0.171 (41)143 |
|   |   | 7/2 | 2.92 | 0.880 (60)041 | -0.146 (22)041 | 0.398 (41)133 | 0.130 (41)141 | -0.265 (22)023 |
|   |   | 1/2* | 4.85 | 0.295 (60)021 | 0.745 (22)021 | -0.446 (22)221 | 0.298 (41)113 | 0.205 (22)231 |
|   |   | 3/2* | 5.02 | -0.339 (60)041 | -0.382 (22)231 | 0.826 (41)123 | -0.123 (41)131 | |
|   |   | 11/2 | 5.03 | 0.796 (60)061 | 0.606 (41)153 | | | |
|   |   | 5/2* | 5.27 | 0.119 (60)001 | 0.940 (22)001 | -0.149 (41)111 | -0.205 (41)113 | -0.197 (22)001 |
|   |   | 7/2* | 5.72 | 0.770 (60)041 | -0.316 (22)231 | 0.100 (41)123 | -0.469 (41)131 | 0.276 (22)023 |
| 3 | 3/2 | 1/2 | 0.00 | 0.714 (41)121 | -0.358 (41)131 | 0.257 (22)021 | 0.469 (22)221 | -0.276 (11)121 |
|   |   | 3/2 | 0.21 | -0.712 (41)111 | 0.374 (41)121 | -0.483 (22)221 | 0.252 (11)111 | 0.239 (30)013 |
|   |   | 5/2 | 0.52 | -0.293 (41)111 | 0.907 (22)001 | -0.132 (11)111 | -0.105 (30)013 | -0.253 (03)113 |
| 4 | 0 | 0 | 0.00 | 0.913 (80)000 | -0.207 (42)000 | 0.209 (04)000 | 0.276 (61)112 | -0.064 (23)112 |
|   |   | 2 | 1.65 | 0.932 (80)020 | -0.188 (42)020 | 0.145 (61)112 | 0.237 (61)122 | 0.138 (61)132 |
|   |   | 4 | 4.17 | 0.884 (80)040 | -0.290 (42)040 | 0.154 (42)240 | 0.232 (61)132 | 0.237 (61)142 |
|   |   | 0* | 5.98 | 0.292 (80)000 | 0.877 (42)000 | -0.298 (04)000 | -0.025 (61)112 | 0.236 (23)112 |
|   |   | 6 | 8.76 | 0.896 (80)060 | -0.115 (42)060 | 0.397 (61)152 | -0.162 (61)162 | |

⋮

| | | | | |
|---|---|---|---|---|
| 4 | 1 | 2 | 0.00 | 1.000 (61)112 ᶜ) |
| 5 | | | 0.00 | 1.000 (81)111 ᵈ) |
| | | | 0.35 | 1.000 (81)121 ᵈ) |
| | | | 1.75 | 1.000 (81)131 ᵈ) |
| | | | 2.80 | 1.000 (62)001 ᵈ) |

ᵃ) $J$, $J*$, $J**$ refer to the first, second and third states having the same $J$ but increasing excitation energy.

ᵇ) The configurations are specified by $(\lambda_1\mu_1)\kappa_1$, $L_1$, $2 \times S_1$. The partition $[f_1]$ corresponds to the most symmetric orbital wave function consistent with the $(\lambda_1\mu_1)$ and spin-isospin quantum numbers, except for the two cases labelled $(\bar{2}\bar{2})$ where $[f_1] = [21]$ e.g. for $n_1 = 4T_1 = 0$ the configuration (23)112 indicates $(\lambda_1\mu_1) = (23)$, $\kappa_1 = 1$, $L_1 = 1$, $S_1 = 1$ and $[f_1] = [31]$ (rather than [211]). We have retained a maximum of five components in the eigenfunctions, see text.

ᶜ) Ref. [29]).    ᵈ) Ref. [30]).

TABLE 2

Eigenfunctions and eigenvalues for $p^4z$

| $n_2$ | $T_2$ | $J_2$ | Eigenvalue | Configuration ᵃ) | Configuration | Configuration | Configuration | Configuration |
|---|---|---|---|---|---|---|---|---|
| 10 | 0 | 1 | 0.00 | 0.042 (02)002 | 0.959 (02)022 | −0.280 (10)010 | | |
| | | 1* | 3.92 | 0.959 (02)002 | 0.039 (02)022 | 0.280 (10)010 | | |
| | | 2 | 7.05 | 1.000 (02)022 | 1.000 (02)022 | | | |
| | | 3 | 10.12 | 1.000 (02)022 | 1.000 (02)022 | | | |
| 10 | 1 | 0 | 0.00 | 0.847 (02)000 | 0.532 (10)012 | | | |
| | | 2 | 7.14 | 0.933 (02)020 | −0.359 (10)012 | | | |
| 9 | ½ | ½ | 0.00 | 0.830 (03)111 | 0.414 (11)111 | −0.152 (11)113 | 0.341 (11)123 | |
| | | 3/2 | 3.68 | 0.946 (03)111 | −0.267 (11)113 | 0.184 (11)121 | | |
| 8 | 0 | 0 | 0.00 | 0.883 (04)000 | 0.407 (12)012 | 0.162 (20)000 | 0.125 (20)024 | |
| | | 2 | 4.66 | 0.947 (04)020 | −0.190 (12)012 | −0.215 (12)222 | 0.143 (12)032 | −0.111 (01)112 |

ᵃ) The notation is as given in the footnote to table 1. The partition $[f_2]$ is uniquely specified by $(\lambda_2\mu_2)$ and $n_2$ i.e. $[f_2] = [\lambda_2+\mu_2+x, \mu_2+x, x]$ with $x = \frac{1}{3}(n_2-\lambda_2-2\mu_2)$.

where $n_f$ is the dimension of the irreducible representation $[f]$ of the symmetric group and $[f]$ and $[\tilde{f}]$ are conjugate representations. We use the spin-isospin c.f.p. tabulated by Jahn and van Wieringen [25]) and the orbital c.f.p. tabulated by Akiyama [22]). For the p-shell we, of course, requires to replace $(\lambda\mu) = (20)$ by $(\lambda\mu) = (10)$ in eqs. (13) and (14) and since the label $[f]$ is redundant the orbital c.f.p. are unity.

For the one-body operator we can derive an expression analogous to eq. (9) where instead of the two-particle c.f.p. we use the one-particle c.f.p. and the factor $\frac{1}{2}n(n-1)$ is replaced by $n$.

## 3.1. PARAMETERS AND RESULTS

For the p-shell the single-particle parameters are taken to reproduce the $p_{\frac{1}{2}}^{-1}$–$p_{\frac{3}{2}}^{-1}$ splitting of 6.16 MeV in $^{15}O$ and the two-body matrix elements are taken from the results of the fit to the p-shell data carried out by Cohen and Kurath (case (8-16) 2BME), ref. [26]).

In the sd-shell we use for the $d_{\frac{5}{2}}$–$s_{\frac{1}{2}}$ and $d_{\frac{5}{2}}$–$d_{\frac{3}{2}}$ splittings 0.87 and 5.08 MeV respectively, obtained from the experimental $^{17}O$ spectrum. For the two-body matrix elements we use a version of those Kuo and Brown have calculated from the Hamada-Johnston potential which closely resemble the values quoted by Kuo [27]). The dimensions of the energy matrices increase rapidly through the sd-shell and we found it necessary to reduce the basis somewhat. The $SU_3$ scheme is well suited to this and from the results of Flores and Pérez [6,28]) we find that the omitted configurations typically contribute $\approx 1\%$ to the low-lying eigenfunctions and less than 0.1 MeV to the eigenvalues.

For later computational convenience we have restricted the eigenfunctions to have a maximum of five components, renormalizing and slightly adjusting for orthogonality where necessary. Some very small amplitudes have also been omitted and the omitted configurations contributed a total of 12(1)% for the sd(p) shell in the worst case. The relevant eigenvalues and eigenvectors for the sd- and p-shells given in tables 1 and 2 respectively should therefore be a good approximation. For the purposes of estimation $^{20}F$ and $^{21}Ne$ have been represented by only one component suggested by the work of refs. [29,30]). We shall use throughout the notation $J, J^*, J^{**}$ to refer to the first, second, third states having the same $J$, but increasing excitation energy.

## 4. Calculation of the particle-hole matrix elements

We now require to calculate the matrix elements of $V_{12}$ in order to evaluate the last two terms of eq. (5). We distinguish two types: the matrix elements diagonal in particle number (DPN) where $n_1 = n_1'$ and $n_2 = n_2'$ and the matrix elements off-diagonal in particle number (ODPN) where $n_1 = n_1' + 2$ and $n_2 = n_2' - 2$. We shall discuss the case of an interaction which is scalar in the space, spin and isospin variables. Extension to more general cases is straightforward.

## 4.1. THE DPN MATRIX ELEMENTS

We can write the potential in the form

$$V_{12} = \sum \hat{\mathscr{J}} \hat{\mathscr{T}} \mathscr{V}_D\{(\bar{\lambda}_1\bar{\mu}_1)\bar{\kappa}_1(\bar{\lambda}_2\bar{\mu}_2); \mathscr{L}\mathscr{S}\mathscr{T}\}$$
$$\times [[a^{\dagger}_{(20)} a_{(20)}]_{(\bar{\lambda}_1\bar{\mu}_1)\bar{\kappa}_1 \mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}} [a^{\dagger}_{(10)} a_{(10)}]_{(\bar{\lambda}_2\bar{\mu}_2)\mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}}]_{J=T=0}. \quad (15)$$

The quantities $\mathscr{V}_D$ are given in terms of antisymmetrized two-particle matrix elements by

$$\mathscr{V}_D\{(\bar{\lambda}_1\bar{\mu}_1)\bar{\kappa}_1(\bar{\lambda}_2\bar{\mu}_2); \mathscr{L}\mathscr{S}\mathscr{T}\}$$
$$= \sum_{\substack{ll'L \\ ST}} (-1)^{\frac{1}{2}l' + \bar{\lambda}_2 + \mathscr{S} + \mathscr{T} + L + S + T} \hat{L}\hat{S}\hat{T}(\hat{\mathscr{L}}\hat{\mathscr{S}}\hat{\mathscr{T}})^{-1}$$
$$\times \langle (20)l(02)l'||(\bar{\lambda}_1\bar{\mu}_1)\bar{\kappa}_1 \mathscr{L}\rangle U(ll'11; \mathscr{L}L)$$
$$\times U(\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}; \mathscr{S}S)U(\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}; \mathscr{T}T)\langle l1; LST|V_{12}|l'1; LST\rangle_{AS}, \quad (16)$$

where we have used the relation $\langle(10)1(01)1||(\bar{\lambda}_2\bar{\mu}_2)\mathscr{L}\rangle = (-1)^{\bar{\lambda}_2 + \mathscr{L} + 1}$.

The $(\bar{\lambda}\bar{\mu})$ quantum numbers take the values:

sd-shell: $(\bar{\lambda}_1\bar{\mu}_1) = (20) \times (02) = (00) + (11) + (22)$,

p-shell: $(\bar{\lambda}_2\bar{\mu}_2) = (10) \times (01) = (00) + (11)$.

We can then write for the matrix elements of $V_{12}$

$$\langle(sd)^{n_1}\alpha_1 J_1 T_1, p^{n_2}\alpha_2 J_2 T_2; JT|V_{12}|(sd)^{n'_1}\alpha'_1 J'_1 T'_1, p^{n'_2}\alpha'_2 J'_2 T'_2; JT\rangle$$
$$= \sum \mathscr{V}_D\{(\bar{\lambda}_1\bar{\mu}_1)\bar{\kappa}_1(\bar{\lambda}_2\bar{\mu}_2); \mathscr{L}\mathscr{S}\mathscr{T}\}\hat{J}_2\hat{T}_2(\hat{J}'_2 \hat{T}'_2)^{-1}$$
$$\times U(J_2 J \mathscr{J} J'_1; J_1 J'_2)U(T_2 T \mathscr{T} T'_1; T_1 T'_2)$$
$$\times A(n_1 \alpha_1 J_1 T_1 \alpha'_1 J'_1 T'_1; (\bar{\lambda}_1\bar{\mu}_1)\bar{\kappa}_1 \mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T})$$
$$\times A(n_2 \alpha_2 J_2 T_2 \alpha'_2 J'_2 T'_2; (\bar{\lambda}_2\bar{\mu}_2)\mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}), \quad (17)$$

where

$$A(n_\nu \alpha_\nu J_\nu T_\nu \alpha'_\nu J'_\nu T'_\nu; (\bar{\lambda}_\nu\bar{\mu}_\nu)\bar{\kappa}_\nu \mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T})$$
$$= \tfrac{1}{2}n_\nu \hat{\mathscr{J}}\hat{\mathscr{T}} X \begin{pmatrix} L'_\nu & \mathscr{L} & L_\nu \\ S'_\nu & \mathscr{S} & S_\nu \\ J'_\nu & \mathscr{J} & J_\nu \end{pmatrix} \sum_{\substack{\rho[f'] \\ (\lambda'_\nu\mu'_\nu)S'T'}} \langle(\lambda'_\nu\mu'_\nu)\kappa'_\nu L'_\nu(\bar{\lambda}_\nu\bar{\mu}_\nu)\bar{\kappa}_\nu \mathscr{L}||(\lambda_\nu\mu_\nu)\kappa_\nu L_\nu\rangle_\rho$$
$$\times f_\rho((\lambda_\nu\mu_\nu)(\lambda'_\nu\mu'_\nu)(\lambda'\mu')(\bar{\lambda}_\nu\bar{\mu}_\nu))U(\mathscr{S}\tfrac{1}{2}S_\nu S'; \tfrac{1}{2}S'_\nu)U(\mathscr{T}\tfrac{1}{2}T_\nu T'; \tfrac{1}{2}T'_\nu)$$
$$\times \langle(n_\nu-1)[f'](\lambda'\mu')S'T'; (\Lambda_\nu 0)\tfrac{1}{2}\tfrac{1}{2}|\}n_\nu[f_\nu](\lambda_\nu\mu_\nu)S_\nu T_\nu\rangle$$
$$\times \langle(n_\nu-1)[f'](\lambda'\mu')S'T'; (\Lambda_\nu 0)\tfrac{1}{2}\tfrac{1}{2}|\}n_\nu[f'_\nu](\lambda'_\nu\mu'_\nu)S'_\nu T'_\nu\rangle,$$

$$f_\rho((\lambda_\nu\mu_\nu)(\lambda'_\nu\mu'_\nu)(\lambda'\mu')(\bar{\lambda}_\nu\bar{\mu}_\nu)) = (-1)^{\frac{1}{2}(\Lambda_\nu - \lambda'_\nu + \mu'_\nu + \lambda' - \mu')}$$
$$\times \left(\frac{\dim(\lambda'_\nu\mu'_\nu)}{\dim(\lambda'\mu')}\right)^{\frac{1}{2}} U((\lambda'_\nu\mu'_\nu)(0\Lambda_\nu)(\lambda_\nu\mu_\nu)(\Lambda_\nu 0); (\lambda'\mu')(\bar{\lambda}_\nu\bar{\mu}_\nu))_\rho,$$

the dimension of an $SU_3$ representation

$$\dim (\lambda\mu) = \tfrac{1}{2}(\lambda+1)(\mu+1)(\lambda+\mu+2) \quad \text{and} \quad \Lambda_1 = 2, \Lambda_2 = 1.$$

## 4.2. THE ODPN MATRIX ELEMENTS

For these matrix elements we write $V_{12}$ in the form

$$V_{12} = \sum (-1)^{\mathscr{L}+1} \hat{\mathscr{J}} \hat{\mathscr{T}} \mathscr{V}_{\text{OD}}\{(\bar{\lambda}_1\bar{\mu}_1)(\bar{\lambda}_2\bar{\mu}_2); \mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}\}$$
$$\times [[a^\dagger_{(20)} a^\dagger_{(20)}]_{(\bar{\lambda}_1\bar{\mu}_1)\mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}}[a_{(10)} a_{(10)}]_{(\bar{\lambda}_2\bar{\mu}_2)\mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}}]_{J=T=0}. \tag{18}$$

The quantities $\mathscr{V}_{\text{OD}}$ are given in terms of the two-body matrix elements by

$$\mathscr{V}_{\text{OD}}\{(\bar{\lambda}_1\bar{\mu}_1)(\bar{\lambda}_2\bar{\mu}_2); \mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}\} = \tfrac{1}{4}(1-(-1)^{\mathscr{L}+\mathscr{S}+\mathscr{T}})$$
$$\times \sum_{ll'} \langle(20)l(20)l'\|(\bar{\lambda}_1\bar{\mu}_1)\mathscr{L}\rangle\langle(sd)^2 ll'; \mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}|V_{12}|p^2; \mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}\rangle, \tag{19}$$

where we have used the relation $\langle(01)1(01)1\|(\bar{\lambda}_2\bar{\mu}_2)\mathscr{L}\rangle = (-1)^{\mathscr{L}}$. The $(\bar{\lambda}\bar{\mu})$ quantum numbers take the values

$$\text{sd-shell}; \ (\bar{\lambda}_1\bar{\mu}_1) = (20)\times(20) = (40)+(02)+(21),$$
$$\text{p-shell}; \ (\bar{\lambda}_2\bar{\mu}_2) = (01)\times(01) = (02)+(10).$$

The ODPN matrix elements then take the form

$$\langle(sd)^{n_1+2}\alpha_1 J_1 T_1, p^{n_2}\alpha_2 J_2 T_2; JT|V_{12}|(sd)^{n_1}\alpha_1' J_1' T_1', p^{n_2+2}\alpha_2' J_2' T_2'; JT\rangle$$
$$= \sum (-1)^{J_2+J_2'-\mathscr{J}+T_2+T_2'-\mathscr{T}+\frac{1}{2}(\bar{\lambda}_2+\bar{\mu}_2-\mathscr{L})} \mathscr{V}_{\text{OD}}\{(\bar{\lambda}_1\bar{\mu}_1)(\bar{\lambda}_2\bar{\mu}_2); \mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}\}$$
$$\times U(T_2 T \mathscr{T} T_1'; T_1 T_2')U(J_2 J \mathscr{J} J_1'; J_1 J_2')$$
$$\times B(n_1 \alpha_1 J_1 T_1 \alpha_1' J_1' T_1'; (\bar{\lambda}_1\bar{\mu}_1)\mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T})$$
$$\times B(n_2 \alpha_2' J_2' T_2' \alpha_2 J_2 T_2; (\bar{\mu}_2\bar{\lambda}_2)\mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T}), \tag{20}$$

where

$$B(n_\nu \alpha_\nu J_\nu T_\nu \alpha_\nu' J_\nu' T_\nu'; (\bar{\lambda}_\nu\bar{\mu}_\nu)\mathscr{L}\mathscr{S}\mathscr{J}\mathscr{T})$$
$$= ((n_\nu+2)(n_\nu+1))^{\frac{1}{2}} X \begin{pmatrix} L_\nu' & \mathscr{L} & L_\nu \\ S_\nu' & \mathscr{S} & S_\nu \\ J_\nu' & \mathscr{J} & J_\nu \end{pmatrix}$$
$$\times \sum_\rho \langle(\lambda_\nu'\mu_\nu')\kappa_\nu' L_\nu'(\bar{\lambda}_\nu\bar{\mu}_\nu)\mathscr{L}\|(\lambda_\nu\mu_\nu)\kappa_\nu L_\nu\rangle_\rho$$
$$\times \langle n_\nu[f_\nu'](\lambda_\nu'\mu_\nu')S_\nu' T_\nu'; (\bar{\lambda}_\nu\bar{\mu}_\nu)\mathscr{S}\mathscr{T}|\}(n_\nu+2)[f_\nu](\lambda_\nu\mu_\nu)S_\nu T_\nu\rangle_\rho.$$

The application of eqs. (17) and (20) is simplified by noting that the contributions from the sd-shell $(A_1, B_1)$ and the p-shell $(A_2, B_2)$ can be evaluated separately and may be required several times during the course of a calculation. Eqs. (12)–(14) and the appropriate c.f.p. [refs. [22,25])] are also needed.

### 4.3. THE INTERACTION $V_{12}$

For the DPN matrix elements, which involve the same number of holes, we use for $V_{12}$ the Gillet potential [31]) which is of the form

$$V_0(W + MP_{ij}^M + BP_{ij}^B - HP_{ij}^\tau)e^{-r^2_{ij}/\mu^2}.$$

Gillet fitted the interaction to the 1 particle-1 hole (1p-1h) negative parity states in $^{16}O$, obtaining the following parameters: $V_0 = -40$ MeV, $W = M = 0.35$, $H = 0.40$, $B = -0.10$ and $b/\mu = 1.0$ $(b = (\hbar/m\omega)^{\frac{1}{2}})$.

For the ODPN matrix elements it is unlikely that the effective central interaction would be exactly the same and indeed use of the Gillet interaction results in matrix elements which seem too small. We therefore use for $V_{12}$ a Rosenfeld interaction which would be roughly appropriate for (sd)$^{n_1}$, namely

$$v = V_0(W + MP_{ij}^M + BP_{ij}^B - HP_{ij}^\tau) \frac{e^{-r_{ij}/\mu}}{r_{ij}/\mu},$$

where the Rosenfeld parameters [32]) are $W = -0.13$, $M = 0.93$, $H = -0.27$ and $B = 0.47$ and we take $V_0 = -55$ MeV and $b/\mu = 1.3$. Using the Kallio-Kolltveit interaction [33]) with a reasonable value of $b$ we get closely similar matrix elements, except that there is no interaction in odd states. This difference is not important here.

These matrix elements with the Rosenfeld interaction seem somewhat too large, but we believe this may be attributed to spurious state effects. If one considers the problem of 2p-2h states in $^{16}O$, it has been pointed out [34]) that a state exists which simultaneously has a large overlap with the 2s spurious state and a large off-diagonal matrix element with the 0p-0h state (9 MeV with our Rosenfeld interaction, $v$). Of course the completely spurious 2s state has zero matrix element with the 0p-0h state, the cancellation being effected by the 1p-1h 2$\hbar\omega$ excitations. These 1p-1h states are necessary to completely separate the 2$\hbar\omega$ c.m. excitation. The above large matrix element means that if the 0p-0h state is allowed to mix with the complete set of 2p-2h states, the admixture in the resulting ground state eigenfunction will contain a considerable spurious component. This extra spurious mixing can be removed either by taking away the largely spurious states or by replacing $v_{ij}$ with $\tilde{v}_{ij} = v_{ij} + \alpha r_i \cdot r_j/b^2$ for the ODPN matrix elements ($\alpha = 0.95$ MeV for the Rosenfeld interaction $v$), in which case one must still take care that excited states do not have large spurious components. The operator $r_i \cdot r_j$ is proportional to the two-body piece of $R^2$ (where $R = (1/A) \sum_i r_i$). We note that because of the properties of oscillator wave functions and the fact that $R$ operates on the c.m. coordinates, $R^2$ will only give non-zero matrix elements between the 0p-0h state and the 2s spurious state with the same relative wave function i.e. $R^2$ picks out the amount of 2s spurious state in a given wave function. Physically this procedure corresponds to subtracting the expectation value of the c.m. kinetic energy (which is related to $\langle R^2 \rangle$) so that the Hamiltonian contains kinetic and potential terms, both of which are functions of relative coordinates only.

Now we wish to consider the mixing, for example, of 2p-1h and 4p-3h states. We can clearly expect that components in the 4p-3h states which can be formed by operating on the 2p-1h wave functions with the 2s c.m. raising operator will give a non-negligible effect, even though the intensity of spurious states in our wave functions is small. We must therefore use $\tilde{v}_{ij}$, but since exclusion principle effects can be expected to play a role here the best value for $\alpha$ is unclear. However, we note that for our *particular* purposes taking $\tilde{v}_{ij}$ instead of $v_{ij}$ gives essentially identical results to simply reducing the strength of the potential, $V_0$. We therefore used a potential $v'$, where the strength, $V_0 = -42$ MeV, was adjusted to give the lowest $\frac{1}{2}^-$ in $^{17}$O at the experimental energy. This would correspond to a value of $\alpha$ a little smaller ($\approx 10\%$) than suggested above, but of the same order of magnitude. We believe that this same procedure gives a more reliable estimate of the mixing of $n$-hole and $(n+2)$-hole states. We shall quote eigenvectors obtained using $v'$ only, since those obtained from $v$ are closely similar, although the energies may differ significantly.

It is also necessary to include the Coulomb interaction, which gives very small off-diagonal matrix elements, but can make a significant contribution to the diagonal matrix elements e.g. in $^{17}$O for the 4p-3h states with $T_1 = 0$ and $T_2 = \frac{1}{2}$, a contribution of $-1.7$ MeV. Since the Coulomb interaction gives scalar, vector and tensor terms in the isospin, some extension of eqs. (15)–(20) is required.

## 5. Application

A number of interesting features emerge from the Gillet p-h interaction. The diagonal matrix elements can be approximated to within $\approx 1$ MeV by retaining only space scalar terms with $(\bar{\lambda}_1\bar{\mu}_1) = (\bar{\lambda}_2\bar{\mu}_2) = (00)$. Of these the terms with $\mathscr{S} = 0$ and $\mathscr{T} = 0$ or 1 give important contributions as shown by Zamick [35]), but the $\mathscr{S} = \mathscr{T} = 1$ term can also give a significant effect (see ref. [36]) where simple expressions are given for most of the space scalar matrix elements of interest). As regards the off-diagonal matrix elements which involve the same number of holes, the largest values are obtained between states with the same $(\lambda\mu)$ structure i.e. $(\lambda'_\nu\mu'_\nu) = (\lambda_\nu\mu_\nu)$; $\nu = 1, 2$. Here contributions from space scalar and $(\bar{\lambda}_1\bar{\mu}_1) = (\bar{\lambda}_2\bar{\mu}_2) = (11)$, $\mathscr{L} = 2$ terms are predominant. It is not then too surprising that the matrix elements turn out to be insensitive to the small components in the linear combinations adopted for the p- and sd-shell eigenfunctions, justifying the retention of only five terms in tables 1 and 2.

Although the p-h matrix elements are insensitive to the precise linear combinations adopted, this is not true for the particle-particle and hole-hole matrix elements. Thus it is more favorable energy-wise to couple the linear combinations of tables 1 and 2, rather than the states of $(sd)^{n_1}$ with $(\lambda_1\mu_1) = (2n_1, 0)$ and $p^{n_2}$ with $(\lambda_2\mu_2) = (0, 12-n_2)$. Assuming these pure configurations rather than the actual linear combinations, we can analyse the low-lying eigenvectors obtained from diagonalization with a given $n_1$ and $n_2$. We often obtain $\approx 0.9$ overlap with a state coupled to total $(\lambda\mu) = (2n_1, 12-n_2)SJK_SK_J$. (Here we have followed Harvey [17]) in taking fixed $K_J$, the

projection of $J$ on the intrinsic axis, which implies a sum over $L$ for $S \neq 0$.) The "real" overlap, however, is smaller because the amplitudes of $(2n_1, 0)$ and $(0, 12-n_2)$ are usually less than 1. We have also considered the coupling of $[f_1]$ and $[f_2]$ to total $[f]$ – this, however, does not seem to be indicated in general.
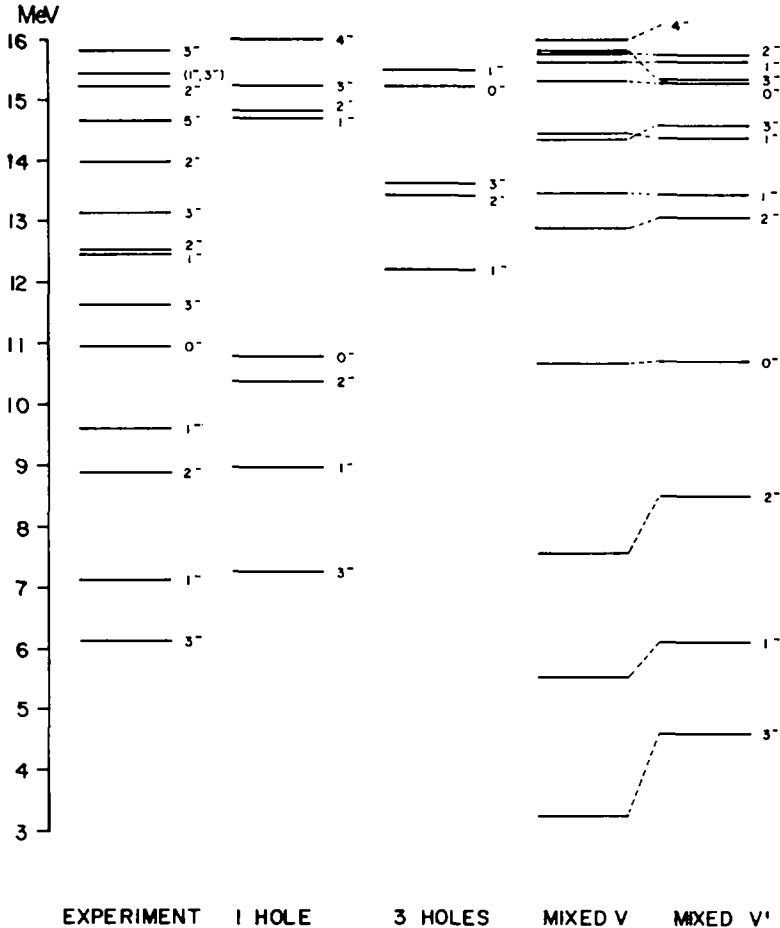


Fig. 1. The calculated and experimental $T = 0$ negative parity levels of $^{16}$O, relative to the $0^+$ ground state. Experimental levels which have not been assigned negative parity and $T = 0$ are omitted.

In the following our method of cutting the basis will be to include all p-h states up to a given excitation energy. After examining a number of other configurations we also include those which give a significant effect on the low-lying spectrum. In view of the above remarks, for a given number of holes one must examine those configurations which have the same $(\lambda \mu)$ structure as the low-lying states.

We should point out here that our states contain components where the c.m. is not in a $1s$ state. Usually the intensity of such spurious components is small ($\approx 5 \%$) and it is always less than 15 % in the states of interest so we shall not comment further.

TABLE 3

Wave functions for the negative parity states of $^{16}O$ with $T = 0$, $T_1 = T_2 = \frac{1}{2}$

| $J$ | 1 hole | | | 3 hole | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.99 | | | 0.11 | | | | | | |
| 1 | 0.72 | 0.19 | | 0.36 | 0.37 | 0.11 | | | | |
| 1* | −0.64 | 0.46 | 0.32 | 0.45 | 0.16 | 0.18 | 0.31 | | 0.15 | |
| 1** | 0.29 | 0.47 | | −0.70 | 0.44 | | | | | |
| 2 | 0.75 | 0.18 | 0.33 | 0.23 | 0.30 | −0.18 | 0.34 | 0.34 | | |
| 2* | −0.63 | 0.42 | 0.37 | 0.35 | 0.12 | −0.16 | 0.34 | | | |
| 3 | 0.81 | 0.29 | −0.21 | 0.33 | −0.24 | 0.21 | | | | |
| 3* | −0.48 | 0.76 | −0.21 | 0.11 | 0.12 | −0.16 | 0.31 | | | |
| 5 | | | | 0.99 | 0.13 | | | | | |
| 6 | | | | 0.85 | 0.53 | | | | | |
| 7 | | | | 1.00 | | | | | | |

a) The wave functions are given in terms of the eigenvectors of $(sd)^{1}$ and $p^{-2}$ which are labelled $J_1 T_1$ and $J_2 T_2$ respectively (see tables 1 and 2). $J$, $J^*$, $J^{**}$ refer to the first, second, third states having the same $J$ but increasing excitation energy. Components with amplitudes < 0.1 have been omitted.

TABLE 4

Wave functions for the negative parity states of $^{17}O$ with $T = \frac{1}{2}$, $T_2 = \frac{1}{2}$

| $J$ | 1 hole | | | 3 hole | | |
|---|---|---|---|---|---|---|
| | $T_1 = 0$ | | $T_1 = 1$ | $T_1 = 0$ | | |
| | | | | | | |
| $\frac{1}{2}$ | −0.24 | −0.23 | 0.73 | 0.11 | 0.57 | 0.11 |
| $\frac{1}{2}*$ | | | −0.60 | 0.15 | 0.68 | 0.26 |
| $\frac{3}{2}$ | 0.77 | 0.21 | 0.17 | 0.33 | 0.47 | |
| $\frac{3}{2}*$ | −0.15 | −0.15 | 0.63 | | 0.71 | 0.21 |
| $\frac{5}{2}$ | −0.28 | −0.16 | 0.74 | 0.12 | 0.56 | −0.12 |
| $\frac{7}{2}$ | 0.87 | 0.15 | 0.11 | 0.24 | 0.38 | |
| $\frac{9}{2}$ | −0.36 | −0.21 | 0.85 | | 0.31 | 0.11 | 0.28 |
| $\frac{9}{2}*$ | 0.76 | 0.21 | 0.50 | | −0.24 | 0.26 | 0.13 |
| $\frac{11}{2}$ | 0.95 | | 0.17 | | 0.25 | |

a) See footnote to table 3.

## 5.1. THE NEGATIVE PARITY LEVELS OF $^{16}$O WITH $T = 0$

In fig. 1 we compare experiment [37-40]) and theory for the $T = 0$ negative parity states of $^{16}$O. Column two gives the results of diagonalizing the complete 1p-1h basis where we have removed the $1^-$ spurious state exactly. Following Mavromatis *et al.* [41]) the $d_{\frac{5}{2}}$-$d_{\frac{3}{2}}$ splitting was modified slightly to the value of 5.58 MeV – the weighted mean of the two strong states seen by Salisbury and Richards [42]). The $0^-$ and $3^-$ levels were used to determine the parameters of the Gillet interaction [31]) so that effects due to 3p-3h states may be included. Nevertheless it is of interest to see whether such states lie sufficiently low to explain the experimental levels not given in the one-hole basis.

We have taken a minimum of all 3p-3h states with $T_1 = T_2 = \frac{1}{2}$ which are expected to lie below 20 MeV. The lowest 3p-3h states with $T_1 = T_2 = \frac{3}{2}$ lie at $\approx 25$ MeV and the off-diagonal matrix elements with the 3p-3h states with $T_1 = T_2 = \frac{1}{2}$ are small, although they can have large matrix elements with the 1p-1h states. Such effects we assume to be included in the effective interaction. The results of diagonalizing the 3p-3h basis are given in fig. 1, column 3 and it is seen that the levels do not come sufficiently low in energy. We have examined a number of configurations but were unable to produce any further lowering. In particular we considered the off-diagonal matrix elements of the lowest 5p-5h states with $T_1 = T_2 = \frac{1}{2}$, taking the configuration assignments for the five holes from the work of Boyarkina [43]). These turn out to be small and since the states lie at $\approx 22$ MeV their effect is negligible.

The results of diagonalizing the 1 and 3 hole states together are given in fig. 1, columns 4 and 5 and table 3, and we obtain significant mixing. Clearly the 3p-3h states are able to give large depressions for the lowest $1^-$, $2^-$ and $3^-$ levels, whereas the RPA depresses only the $3^-$ significantly [31,41]). The eigenvalues are more reasonable for $v'$ but the agreement for the $J = 1$ and 3 levels is still poor, although we do produce a $2^*$ at approximately the correct energy. As regards states with $J > 4$, our lowest $5^-$, $6^-$ and $7^-$ levels lie at 17.3, 20.2 and 19.2 MeV respectively. Experimentally levels with $J = 5^-$ and $7^-$ have been observed at 16.9 and 20.9 MeV. However, whereas we predict no other $5^-$ levels below 20 MeV, there are three additional $5^-$ assignments [39,40]), including one at 14.7 MeV. It seems unlikely that a 3p-3h basis could explain all these states, at least with this p-h interaction.

## 5.2. THE NEGATIVE PARITY LEVELS OF $^{17}$O

We have taken a minimum of all 2p-1h and 4p-3h states lying below 9 MeV. Since there is rather little $f_{\frac{5}{2}}$ strength in the levels of interest [44]) the configuration consisting of a $f_{\frac{5}{2}}$ particle outside a closed $^{16}$O core has not been included. The states formed by coupling the $2^+$ ground state of four particles with $T_1 = 1$ and the $\frac{1}{2}^-$ ground state of the three-hole system with $T_2 = \frac{1}{2}$ produce $\frac{3}{2}^-$ and $\frac{5}{2}^-$ states with total $T = \frac{1}{2}$ at 13.9 and 13.0 MeV respectively. They were not included as little mixing is expected with the low-lying states. Also not included were the 4p-3h states with $T_1 = 1$ or 2 and $T_2 = \frac{1}{2}$ coupled to $T = \frac{1}{2}$, the lowest of which are expected at $\approx 23$ MeV.

The results of diagonalizing the one-hole and three-hole bases separately and together are compared with experiment [37,44,45]) in fig. 2 and the eigenfunctions for the mixed case are given in table 4. The 2p-1h states do not come low enough to explain the experimental spectrum, confirming the results of Margolis and de Takacsy [46]). It is encouraging to note that their results using the complete $1\hbar\omega$ basis and ours using a
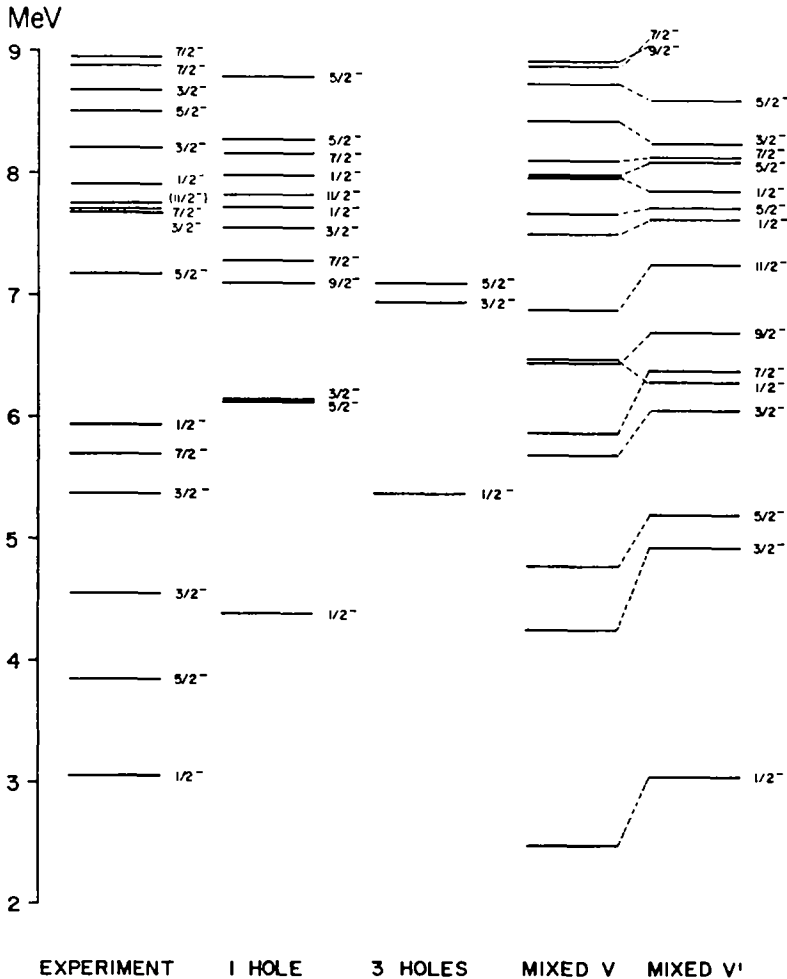


Fig. 2. The calculated and experimental negative parity levels of $^{17}$O, relative to the $\frac{5}{2}^+$ ground state. Experimental levels which have not been assigned negative parity are omitted.

cut 2p-1h basis agree quite well. Inclusion of the 4p-3h states yields quite good agreement with experiment, although we have not managed to depress the $\frac{5}{2}^-$ state sufficiently. For the higher levels the only serious disagreement occurs for the $\frac{3}{2}^-$ levels – we are missing two from the spectrum of $^{17}$O and also the analogues of the two $\frac{3}{2}^-$ levels at $\approx 7$ MeV in $^{17}$F have yet to be identified [42]). Also one must expect to find

the analogue in $^{17}$O of the $(\frac{1}{2}, \frac{1}{2})^-$ level at 6.43 MeV in $^{17}$F [ref. [47]], this may correspond to the additional theoretical $\frac{1}{2}^-$ predicted at $\approx 7.5$ MeV. There is an additional theoretical $\frac{1}{2}^-$ level at 9.4 MeV, but in order to explain this experimental data it is probably necessary to greatly expand the basis including, for example, all (sd)$^2$ and (sd)$^4$ eigenfunctions which have predominantly $(\lambda_1 \mu_1) = (02)$ and (42) respectively, although present indications are not too hopeful. These states would, however, mix very little with the lowest $\frac{1}{2}^-$ levels.

As regards states with high spin, the $^{15}$N($\alpha$, d)$^{17}$O reaction is expected to populate strongly levels which have the structure (sd)$^2$ $J_1 = 5$ $T_1 = 0$, coupled to a p$_{\frac{1}{2}}$ hole [48]). This leads to identifications of $(\frac{11}{2}^-)$ for a level at 7.74 MeV, in good agreement with our predictions, and $(\frac{9}{2}^-)$ for a level at 9.14 MeV. This latter level should be identified with our $\frac{9}{2}^{*-}$ which lies at 9.05 MeV and has 58 % of the above configuration, rather than the $\frac{9}{2}^-$ at 6.7 MeV, which is mainly (sd)$^2$ $J_1 = 4$ $T_1 = 1$ coupled to a p$_{\frac{1}{2}}$ hole (see table 4).

The off-diagonal Coulomb matrix elements are very small and the diagonal ones are essentially constant for fixed $n_1$, $n_2$, $T_1$, $T_2$, $T$ and its $z$-component $M_T$, implying constant Coulomb matrix elements. We can therefore easily estimate the difference in excitation energy of the negative parity levels in $^{17}$F as compared to $^{17}$O relative to their respective ground states. We get contributions from the differences in the relevant experimental binding energies and the sign of the vector part of the Coulomb interaction. Together these give the following adjustments for $^{17}$F as compared to $^{17}$O: $-$ 2p-1h ($T_1 = 0$) $+0.42$ MeV; 2p-1h ($T_1 = 1$) $-0.05$ MeV, and 4p-3h ($T_1 = 0$, $T_2 = \frac{1}{2}$) $+0.33$ MeV. Using our wave functions these values give shifts of the right sign which are $\approx 100$ keV greater than experiment. The only exception is the $\frac{1}{2}^-$ at 5.7 MeV in $^{17}$O which experimentally is shifted by $-0.03$ MeV in $^{17}$F, theoretically by $+0.37$ MeV. It should be noted that most of the relevant levels in mass-17 are unbound and our treatment ignores the asymptotic behaviour of the wave functions, as is usual in shell-model analyses.

## 5.3. THE NEGATIVE PARITY STATE OF $^{18}$F AND $^{18}$O

For $^{18}$F we have taken a minimum of all 3p-1h states with $T_1 = T_2 = \frac{1}{2}$ and $T = 0$ expected to lie below 8 MeV. The comparison with the known experimental negative parity levels [37,49,50]) on the left of fig. 3 shows that the 1$^-$ compares reasonably with experiment and also the 3$^-$ if we associate it with the most likely experimental candidate [49]) at 3.79 MeV. On the other hand, the 0$^-$ and 2$^-$ agree poorly with experiment being $\approx 2$ MeV too high. From the wave functions given in table 5 we see that the main component of the 0$^-$ wave function is (sd)$^3$ [3] (60) $L_1 = 0$, $S_1 = J_1 = \frac{1}{2}$ coupled to a p$_{\frac{1}{2}}$ hole. We have evaluated the off-diagonal matrix elements between this and the rest of the complete set of 3p-1h states. Assuming a constant energy separation of 6 MeV, usually an underestimate, first order perturbation theory gives a depression of the lowest 0$^-$ of only $\approx 0.2$ MeV. Thus the error does not seem to be in the cutting of the basis. Configurations of type (sd)(fp) do not give a significant

effect and the low-lying 5p-3h states with $T_1 = T_2 = \frac{1}{2}$ also seem unable to give an effect of the magnitude required. The lowest of these 5p-3h states given by coupling the ground states of $(sd)^5$ with $J_1 = \frac{1}{2}^+$ and $p^{-3}$ with $J_2 = \frac{1}{2}^-$ leads to $1^-$ and $2^-$ states at $\approx 8$ MeV. Interaction with other three-hole states is expected to give depressions $\approx 1$ MeV and it may be important to include the 5p-3h states to explain the four levels at 5.5 to 6.5 MeV. Two of these are probably analogues of the $^{18}$O $1^-$ and $3^-$ levels and since they have all been seen [50]) in $^{14}$N$(\alpha, \alpha)^{14}$N considerable isobaric spin
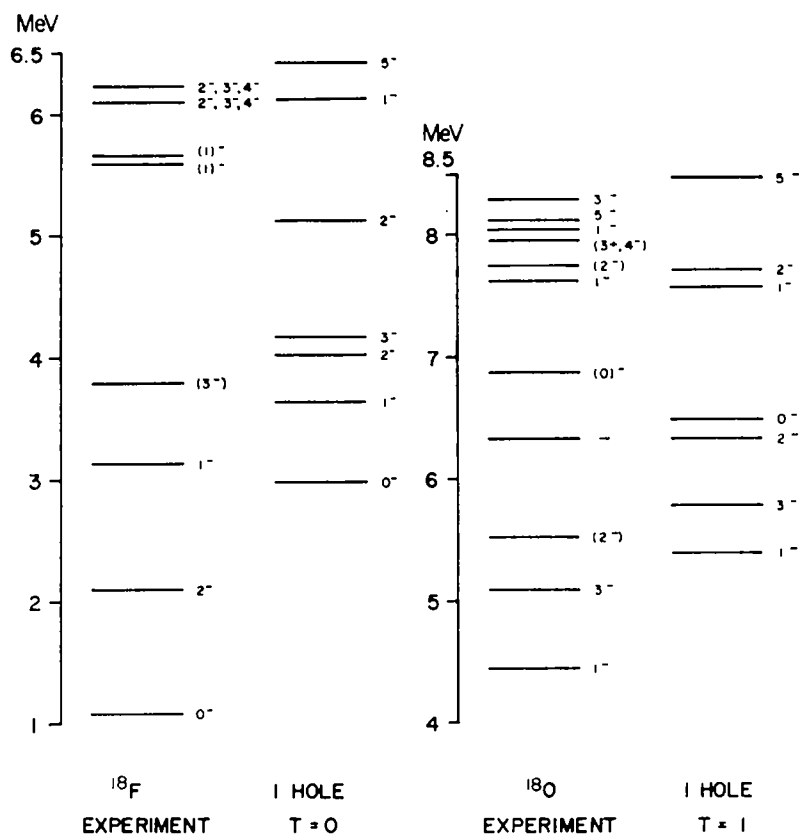


Fig. 3. The calculated and experimental negative parity levels of $^{18}$F and $^{18}$O, relative to their respective ground states. Experimental levels which have not been assigned negative parity are omitted.

mixing is indicated. Thus we require $1^-$ and $3^-$ $T = 0$ levels in the vicinity, whereas the 2p-1h basis provides only the former. On the other hand this argument is contradicted by the recent work of Mangelson et al. [51]) who suggest a $(4^+)$ $T = 0$ assignment for the lower member of this quartet so that the situation still appears fluid. The 5p-3h states with $T_1 = T_2 = \frac{1}{2}$ were not considered since the lowest occurs at $\approx 23$ MeV.

For $^{18}$O we have taken a minimum of all 3p-1h states with $T_1 = T_2 = \frac{1}{2}$ coupled to $T = 1$ lying below 11 MeV. The comparison on the right of fig. 3 with the experimental levels for which negative parity has been assigned [37, 52–55]) shows rather reasonable agreement. In saying this we note that the proton pick-up reaction from $^{19}$F, which could be expected to populate levels with $J = 0^- - 2^-$, does in fact populate all the experimental levels in fig. 3, except the 5.52 MeV ($2^-$) and the 8.04 MeV $1^-$ levels [55]). The latter is expected to be a 3p-1h state with $T_1 = \frac{1}{2}$ (see below) and as regards the former only a rather tentative assignment of negative parity has been made. Harvey [56]) has interpreted the lowest levels in terms of a $[4^4 2]$ (61) band, however, we find that such a band lies at a somewhat higher excitation energy than he suggests and our wave functions (see table 5) contain roughly equal amounts of $[4^4 2]$ and $[4^3 3^2]$. The 3p-1h states with $T_1 = T_2 = \frac{1}{2}$ are expected to mix little with those having $T_1 = \frac{3}{2}$, $T_2 = \frac{1}{2}$ the lowest of which being a $3^-$ level at 8.15 MeV formed by coupling the $(sd)^3$ $J_1 = \frac{5}{2}^+$ ground state with a $p_{\frac{1}{2}}$ hole. A $J = 1^-$ level may be obtained at 8.26 MeV with a similar isotopic spin structure and $J_1 = \frac{1}{2}^+$ coupled to $(0.96p_{\frac{1}{2}}^{-1} + 0.29p_{\frac{3}{2}}^{-1})$. We can tentatively identify these with the experimental $3^-$ and $1^-$ levels at 8.29 and 8.04 MeV, although for the $1^-$ we have used the theoretical $\frac{1}{2}^+$ excitation energy which is 0.9 MeV less than the experimental value in $^{19}$O. However, some further depression of this state is expected due to the 5p-3h states. The lowest 5p-3h states with $T_1 = T_2 = \frac{1}{2}$, $T_1 = \frac{1}{2}$ and $T_2 = \frac{3}{2}$, and $T_1 = T_2 = \frac{3}{2}$ lie at $\approx 10$, 19 and 29 MeV respectively and will mix very little with the 3p-1h states having $T_1 = T_2 = \frac{1}{2}$. On the other hand we can expect the lowest $0^- - 3^-$ levels of fig. 3 to be pushed down by roughly 0.5 MeV with 5 % mixing due to the 5p-3h states with $T_1 = \frac{3}{2}$ and $T_2 = \frac{1}{2}$. These are given by coupling the $J_1 = \frac{5}{2}^+$ and $\frac{3}{2}^+$ states (assumed $[32]$ (62) $\kappa = 0, L = 2$ and 0) to the $J_2 = \frac{1}{2}^-$ ground state and lie at $\approx 15$ MeV.

We would predict the excitation energy of the negative parity levels in $^{18}$Ne to be larger by $+0.32$ MeV than in $^{18}$O. The experimental value of $+0.15$ has the same sign, but is much smaller. Here we have used the probable assignment of $1^-$ for the 4.59 MeV level in $^{18}$Ne due to L'Ecuyer et al. quoted in ref. [57]).

## 5.4. THE NEGATIVE PARITY STATES OF $^{19}$F

We have included all states of 4 particles with $T_1 = 0$ and $J_1 = 0, 0^*, 2, 4, 6$ coupled to a $p_{\frac{1}{2}}$ or $p_{\frac{3}{2}}$ hole. The theoretical results for $^{19}$F are shown in fig. 4 together with the known experimental levels [55, 58]) below 6.5 MeV. Table 5 gives the eigenfunctions for these levels and also the $\frac{5}{2}^{*-}$ and $\frac{7}{2}^{*-}$ levels, which lie at $\approx 8$ MeV. If the $J = 0, 2$ and 4 states of $^{20}$Ne were pure (80) our lowest eigenfunctions would give overlaps $\approx 0.93$ with the (81) $K_J = \frac{1}{2}$ band considered by Harvey [17]). Our relative spacings agree fairly well with his as the effect of diagonalizing the $J = 0, 2$ and 4 matrices for $^{20}$Ne is to push down all the (80) states by $\approx 2$ MeV and the corresponding 20 % mixing of other configurations leaves the p-h matrix elements essentially unchanged. We find that our states which are equivalent to Harvey's $K_J = \frac{1}{2}$ band start at 6.4 MeV with the $\frac{3}{2}^*$. This is higher than he predicts and the reason is that it is

more favourable to have a larger percentage of $p_{\frac{1}{2}}$ hole in the low-lying levels than the (81) $K_J = \frac{1}{2}$ coupling scheme would allow.

TABLE 5

Wave functions for the negative parity states of $^{18}O$, $^{18}F$ and $^{19}F$

| $J$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ [a]) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $^{18}F$ 3p-1h $\quad T = 0$, $T_1 = T_2 = \frac{1}{2}$ | | | | | | | | | | | | |
| 0 | 1.00 | $\frac{1}{2}$ | $\frac{1}{2}$ | | | | | | | | | |
| 1 | 0.98 | $\frac{1}{2}$ | $\frac{1}{2}$ | −0.16 | $\frac{1}{2}$ | $\frac{3}{2}$ | | | | | | |
| 1* | 0.95 | $\frac{3}{2}$ | $\frac{1}{2}$ | −0.29 | $\frac{5}{2}$ | $\frac{3}{2}$ | | | | | | |
| 2 | −0.43 | $\frac{3}{2}$ | $\frac{1}{2}$ | 0.91 | $\frac{5}{2}$ | $\frac{1}{2}$ | | | | | | |
| 2* | 0.91 | $\frac{3}{2}$ | $\frac{1}{2}$ | 0.43 | $\frac{5}{2}$ | $\frac{1}{2}$ | | | | | | |
| 3 | 0.99 | $\frac{5}{2}$ | $\frac{1}{2}$ | 0.14 | $\frac{7}{2}$ | $\frac{3}{2}$ | | | | | | |
| 5 | 1.00 | $\frac{9}{2}$ | $\frac{1}{2}$ | | | | | | | | | |
| $^{18}O$ 3p-1h $\quad T = 1$, $T_1 = T_2 = \frac{1}{2}$ | | | | | | | | | | | | |
| 0 | 0.99 | $\frac{1}{2}$ | $\frac{1}{2}$ | −0.15 | $\frac{3}{2}$ | $\frac{3}{2}$ | | | | | | |
| 1 | 0.97 | $\frac{1}{2}$ | $\frac{1}{2}$ | 0.20 | $\frac{1}{2}$ | $\frac{3}{2}$ | 0.14 | $\frac{5}{2}$ | $\frac{3}{2}$ | | | |
| 1* | −0.11 | $\frac{1}{2}$ | $\frac{1}{2}$ | 0.97 | $\frac{3}{2}$ | $\frac{1}{2}$ | 0.18 | $\frac{1}{2}$ | $\frac{3}{2}$ | | | |
| 2 | 0.42 | $\frac{3}{2}$ | $\frac{1}{2}$ | 0.84 | $\frac{5}{2}$ | $\frac{1}{2}$ | −0.10 | $\frac{1}{2}$ | $\frac{3}{2}$ | 0.32 | $\frac{5}{2}$ | $\frac{3}{2}$ |
| 2* | 0.87 | $\frac{3}{2}$ | $\frac{1}{2}$ | −0.46 | $\frac{5}{2}$ | $\frac{1}{2}$ | −0.17 | $\frac{3}{2}$ | $\frac{3}{2}$ | | | |
| 3 | 0.98 | $\frac{5}{2}$ | $\frac{1}{2}$ | −0.14 | $\frac{3}{2}$ | $\frac{3}{2}$ | 0.11 | $\frac{7}{2}$ | $\frac{3}{2}$ | | | |
| 5 | 1.00 | $\frac{9}{2}$ | $\frac{1}{2}$ | | | | | | | | | |
| $^{19}F$ 4p-1h $\quad T = \frac{1}{2}$, $T_1 = 0$, $T_2 = \frac{1}{2}$ | | | | | | | | | | | | |
| $\frac{1}{2}$ | 0.98 | 0 | $\frac{1}{2}$ | 0.17 | 2 | $\frac{3}{2}$ | | | | | | |
| $\frac{1}{2}$* | 1.00 | 0* | $\frac{1}{2}$ | | | | | | | | | |
| $\frac{3}{2}$ | 0.96 | 2 | $\frac{1}{2}$ | −0.20 | 0 | $\frac{3}{2}$ | 0.18 | 2 | $\frac{3}{2}$ | | | |
| $\frac{3}{2}$* | 0.86 | 0 | $\frac{3}{2}$ | 0.49 | 2 | $\frac{3}{2}$ | | | | | | |
| $\frac{5}{2}$ | 0.99 | 2 | $\frac{1}{2}$ | 0.12 | 4 | $\frac{3}{2}$ | | | | | | |
| $\frac{5}{2}$* | 0.99 | 2 | $\frac{3}{2}$ | 0.16 | 4 | $\frac{3}{2}$ | | | | | | |
| $\frac{7}{2}$ | 0.94 | 4 | $\frac{1}{2}$ | −0.27 | 2 | $\frac{3}{2}$ | 0.22 | 4 | $\frac{3}{2}$ | | | |
| $\frac{7}{2}$* | 0.15 | 4 | $\frac{1}{2}$ | 0.89 | 2 | $\frac{3}{2}$ | 0.43 | 4 | $\frac{3}{2}$ | | | |
| $\frac{9}{2}$ | 0.99 | 4 | $\frac{1}{2}$ | | | | | | | | | |

[a]) See footnote to table 3.

Our theoretical calculation accounts very well for all the known negative parity levels up to 4.5 MeV, although the $\frac{3}{2}^-$, $\frac{7}{2}^-$ doublet is inverted. However, above 4.5 MeV there are many more levels than theory predicts. Additional 4p-1h states can be formed by coupling the $2^+$ ground state of 4 particles with $T_1 = 1$ to a $p_{\frac{1}{2}}$ hole which gives rise to $\frac{3}{2}^-$ and $\frac{5}{2}^-$ p-h states at 7.9 and 7.2 MeV respectively. Obviously coupling holes to the low lying levels of $^{20}F$ can produce a number of p-h states, but they should mix little with states based on $^{20}Ne$. It is also unlikely that this will result in new states below 5.5 MeV.

As regards the 6p-3h states the lowest of those with $T_1 = 0$ $T_2 = \frac{1}{2}$ and $T_1 = 1$ $T_2 = \frac{1}{2}$ are calculated to be at 12.5 and 9.2 MeV respectively. In both cases we have assumed the structure [42](82) $\kappa = 0$, $L = 0, 2, 4$ for the particles with $J_1 = 1, 3, 4$ for $T_1 = 0$ and $J_1 = 0, 2, 4$ for $T_1 = 1$. Such configurations may influence the 4p-1h
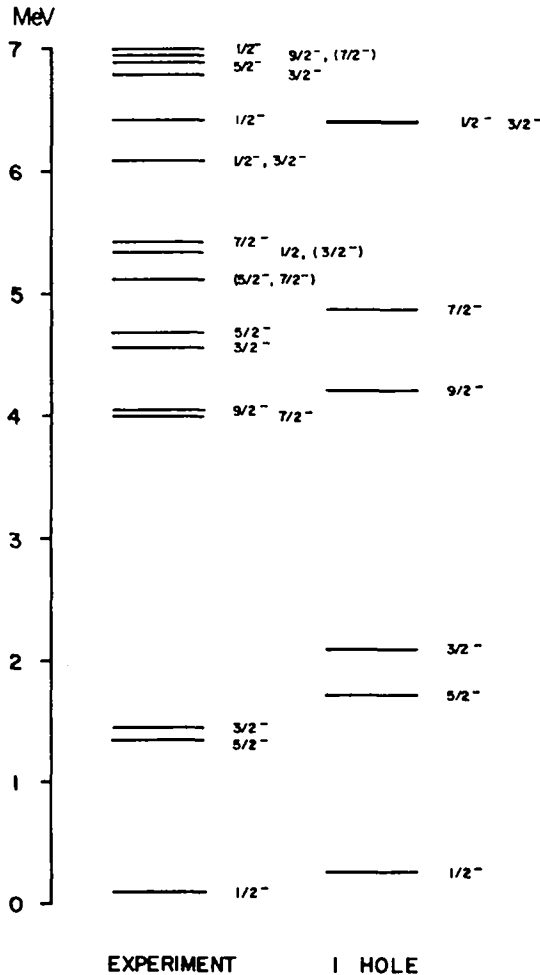


Fig. 4. The calculated and experimental negative parity levels of $^{19}$F, relative to the $\frac{1}{2}^+$ ground state. Experimental levels which have not been assigned negative parity are omitted.

states and lower their energy positions. In one case we obtained as much as 0.5 MeV by only 5 % mixing of a 6p-3h configuration. Several of these effects have to be investigated further. Preliminary indications are that such considerations will not alter the relative spacings within, for example, the $\frac{1}{2}^-$, $\frac{3}{2}^-$, etc. group of levels but may alter the spacing between groups i.e. the $\frac{1}{2}^- - \frac{1}{2}^{*-}$ splitting may be somewhat modified.

Benson and Flowers [59]) have recently obtained results which are similar to ours. However, in order to get the lowest $\frac{1}{2}^-$ state in the correct position they need a $p_{\frac{1}{2}}$–$d_{\frac{5}{2}}$ splitting some 4.4 MeV less than the experimental value. This is due to the neglect of the Coulomb p-h interaction which contributes $-0.9$ MeV and the use of Kallio-Kollt-veit interaction. For this interaction the complete scalar term with $\mathscr{L} = \mathscr{S} = \mathscr{T} = 0$ in eq. (15) is more strongly repulsive than for the Gillet potential [36]) and results in about 3.3 MeV more repulsion in diagonal matrix elements. To reproduce the nega-tive parity levels in the 4-6 MeV region Benson and Flowers [59]) take a $p_{\frac{1}{2}}$–$p_{\frac{3}{2}}$ splitting some 2 MeV less than the experimental $^{15}$N value. This may be understood as an approximate procedure to include effects from high-lying 4p-1h and particularly 6p-3h states as discussed above.

In common with Benson and Flowers [59]) we find the 3.91 MeV level, known to have $J = \frac{3}{2}$, difficult to understand. If it has negative parity our $\frac{3}{2}^{*-}$ lies at too great an excitation energy and although Benson and Flowers predict a lower energy, this state should be populated strongly in the proton pick-up reaction on $^{20}$Ne, which is not the case for the 3.91 MeV level [55]). As regards positive parity candidates, the (sd)$^3$ basis, which otherwise appears to give reasonable agreement up to 5 MeV, pro-duces a $\frac{3}{2}^{*+}$ level at 6.9 MeV. The lowest core excited 5p-2h state $(T_1 = \frac{1}{2}, T_2 = 1)$ is predicted at 6.5 MeV, again much too high.

Our formulation predicts that the excitation energy of the negative parity states in $^{19}$Ne be larger by $+0.38$ MeV than in $^{19}$F whereas the experimental figure is $+0.15$ MeV. Again we have the correct sign, but the magnitude is too large.

As we have suggested the Coulomb p-h interaction can be accurately approximated by a constant, $c$, multiplied by the number of proton particles and holes, averaged with the square of the appropriate isospin Clebsch-Gordan coefficients. We have used a value of $c = 0.43$ MeV, calculated with $b = 1.7$ fm. Then, as we have seen, the theo-retical displacements of the members of a given isospin multiplet are much larger than given experimentally, although generally of the right sign. Except for the $\frac{1}{2}^-$ level in mass-17 which remains an anomaly, agreement with experiment can be achieved (to within $\approx 50$ keV) either by reducing the value of $c$ to 0.29 MeV or by adopting an $A^{-\frac{1}{3}}$ dependence for the displacement energy between the $T_z = -\frac{1}{2}$ and $+\frac{1}{2}$ members of the $T = \frac{1}{2}$ doublets of one and three holes (i.e. for mass-19 the Coulomb displace-ment energy of a hole in the p-shell is reduced by a factor $(\frac{15}{19})^{\frac{1}{3}}$ from the experimental value). The former procedure does not seem to be indicated since with oscillator wave functions it corresponds to taking the unreasonable value of $b = 2.5$ fm and the use of Woods-Saxon wave functions appears to lead to only a very small reduction in the parameter $c$.

### 5.5. THE POSITIVE PARITY STATES IN MASS-18

Consider first the positive parity levels in $^{18}$O. In columns 1–3 of fig. 5 we give the experimental spectrum [54]) and the results of diagonalizing the 2p-0h and 4p-2h con-figurations separately. In the 4p-2h case we have found it necessary to include at least

4 particles with $T_1 = 0$ and $J_1 = 0, 2, 4$ coupled to two holes with $T_2 = 1$ and $J_2 = 0, 2$. Although the main components of the low-lying $0^+$ and $2^+$ states have the 2 holes coupled to $J_2 = 0$, they have been pushed down by 0.9 and 0.6 MeV respectively by mixing with states involving coupling of the holes to $J_2 = 2$. In estimating the energies of the 4p-2h configurations it does not therefore seem a good approximation to restrict the holes to the $p_{\frac{1}{2}}^{-2}$ configuration.

TABLE 6

Wave functions for the positive parity states of $^{18}$O, $T = 1$

| | 0 hole | | | | | | | 2 hole | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $T_1 = 1, J_2 = T_2 = 0$ | | | | | | | $T_1 = 0, T_2 = 1$ | | | | | | | | |
| $J$ | | $J_1$ | | $J_1$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ *) |
| 0 | 0.96 | 0 | | | −0.30 | 0 | 0 | | | | | | | | | |
| 0* | 0.26 | 0 | −0.36 | 0* | 0.85 | 0 | 0 | 0.17 | 0* | 0 | 0.22 | 2 | 2 | | | |
| 0** | 0.92 | 0* | | | 0.35 | 0 | 0 | 0.13 | 2 | 2 | | | | | | |
| 2 | 0.96 | 2 | | | −0.25 | 2 | 0 | | | | | | | | | |
| 2* | 0.95 | 2* | | | −0.25 | 2 | 0 | | | | | | | | | |
| 2** | 0.23 | 2 | 0.26 | 2* | 0.89 | 2 | 0 | 0.17 | 0 | 2 | −0.17 | 2 | 2 | 0.14 | 4 | 2 |
| 3 | 1.00 | 3 | | | | | | | | | | | | | | |
| 4 | 0.99 | 4 | | | −0.16 | 4 | 0 | | | | | | | | | |
| 4* | 0.14 | 4 | 0.51 | 4* | 0.81 | 4 | 0 | 0.19 | 2 | 2 | −0.17 | 4 | 2 | | | |

*) See footnote to table 3.

The results of diagonalizing the zero- and two-hole states together are given in fig. 5. Here all the 2p-0h levels have been shifted in energy without changing their relative positions. This has been done in order to obtain the final ground state after diagonalization at zero energy which on our energy scale is the position of the physical ground state. The shifts are 0.4 MeV for $^{18}$O and 1.0 MeV for $^{18}$F using potential $v'$ and show the increase in binding energy due to the p-h admixtures. We note that nearly the same increase in binding energy is obtained from Kuo's matrix elements [27] by including 4p-2h excitations in a perturbation calculation. It is also interesting to note that our shifts are not incomparable with those found by Kahana et al. [60] when the bare $G$-matrix elements are calculated with Woods-Saxon rather than harmonic oscillator wave functions. Our final eigenfunctions given in table 6 are hardly affected by this procedure, except for the $0^{*+}$. Here the shift removes a near degeneracy between the unperturbed 2p-0h and 4p-2h positions so that the $0^{*+}$ becomes largely 4p-2h. This is strongly favoured by the $\gamma$· transitions. The spectrum is reasonable below 5.5 MeV except that we do not obtain sufficient splitting between the 0* and 0**.

The lowest 4p-2h states with $T_1 = 1, T_2 = 1$ and 0 lie at 11 and 13 MeV respectively and are not expected to give a significant effect. As regards the 4p-2h states with $T_1 = 2$ $T_2 = 1$, the lowest of which lies at 10.6 MeV, zero off-diagonal matrix elements are given with our 4p-2h states with $T_1 = 0$, but the off-diagonal matrix ele-

ments with our 2p-0h states are very large as pointed out by Brown and Green [10]). Since the effect of such states is to push down the 2p-0h levels by roughly the same amount, we have not further considered them.

In the 5.5–7.5 MeV region of excitation energy we see that there are four levels found experimentally which have not been assigned definite negative parity and which do not fit in with our negative parity predictions (see fig. 3). Of these the 7.12 MeV $4^+$
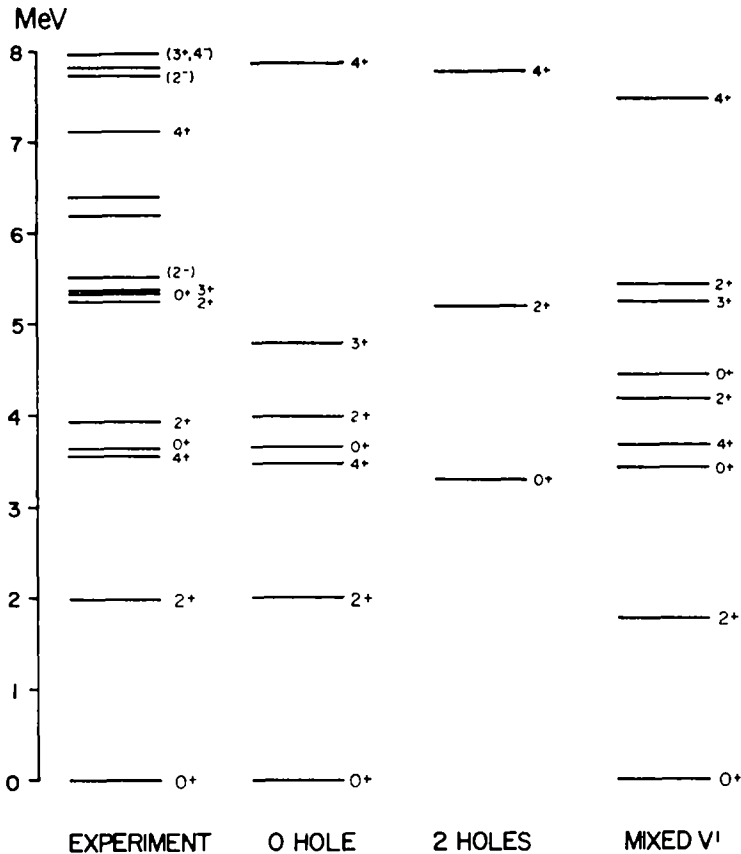


Fig. 5. The calculated positive parity levels of $^{18}$O and the experimental spectrum (levels assigned definite negative parity are omitted).

level probably corresponds to the theoretical $4^{*+}$ state. We expect no additional 2p-0h or 4p-2h states in this region and estimate the lowest 6p-4h state ($T_1 = 1$, $T_2 = 0$) at $\approx 10$ MeV. Thus the structure of the remaining three levels remains unclear.

For $^{18}$F we shall discuss only the $T = 0$ levels, since the $T = 1$ levels are the analogues of those already discussed for $^{18}$O. We have considered 4p-2h states with $T_1 = T_2 = 0$ and $J_1 = 0, 2, 4, 6$ coupled to $J_2 = 1, 1^*, 2, 3$. The 4p-2h states with

TABLE 7

Wave functions for the positive parity states of $^{18}$F $(T = 0)$ and $^{17}$O $(T = \tfrac{1}{2})$

| | 0 hole ($J_2=0$) | | | | 2 hole | | | | | | | | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| | $T_1=0, T_2=0$ | | | | $T_1=\tfrac{1}{2}, T_2=\tfrac{1}{2}$ | | | | | | $T_1=0, T_2=0$ | | | | | | *) | | |
| $J$ | | $J_1$ | | $J_1$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ | | $J_1$ | $J_2$ |
| **$^{18}$F, $T=0$** | | | | | | | | | | | | | | | | | | | |
| 1 | 0.94 | 1 | | | −0.33 | 0 | 1* | 0.26 | 2 | 1 | 0.12 | 0* | 1 | 0.17 | 2 | 1* | 0.13 | 2 | 2 |
| 1* | 0.96 | 1* | | | 0.93 | 0 | 1 | −0.26 | 0* | 1* | | | | | | | | | |
| 1** | 0.15 | 1 | 0.14 | 1* | 0.11 | 2 | 1* | 0.78 | 2 | 1 | 0.42 | 0 | 1* | | | | | | |
| 1*** | −0.14 | 1 | 0.72 | 1** | −0.16 | 0 | 1 | −0.47 | 2 | 1* | −0.12 | 0* | 1* | −0.38 | 2 | 1* | | | |
| 1**** | | | | | −0.42 | 0 | 1* | −0.37 | 2 | 1* | | | | 0.20 | 2 | 2 | | | |
| 2 | 0.80 | 2 | | | −0.47 | 2 | 1 | −0.11 | 0 | 2 | | | | | | | | | |
| 2* | 0.49 | 2 | | | 0.85 | 2 | 1 | | | | | | | | | | | | |
| 2** | 0.99 | 2* | | | | | | | | | | | | | | | | | |
| 2*** | | | | | | | | | | | | | | | | | | | |
| 3 | 0.95 | 3 | | | −0.30 | 2 | 1* | 0.16 | 4 | 1 | | | | | | | | | |
| 3* | 1.00 | 3* | | | 0.97 | 2 | 1 | | | | 0.16 | 4 | 1* | | | | | | |
| 3** | | | | | −0.64 | 4 | 1 | −0.38 | 4 | 1* | | | | | | | | | |
| 4 | 0.67 | 4 | | | −0.23 | 4 | 1* | | | | | | | | | | | | |
| 5 | 0.97 | 5 | | | 0.99 | 4 | 1 | 0.13 | 6 | 1* | | | | | | | | | |
| 5* | | | | | | | | | | | | | | | | | | | |
| **$^{17}$O, $T=\tfrac{1}{2}$** | $T_1=\tfrac{1}{2}, T_2=0$ | | | | $T_1=\tfrac{1}{2}, T_2=0$ | | | $T_1=\tfrac{1}{2}, T_2=1$ | | | $T_1=\tfrac{1}{2}, T_2=1$ | | | | | | | | |
| $\tfrac{1}{2}$ | 0.87 | $\tfrac{1}{2}$ | | | −0.32 | $\tfrac{1}{2}$ | 1* | −0.25 | $\tfrac{1}{2}$ | 0 | 0.28 | $\tfrac{1}{2}$ | 0 | | | | | | |
| $\tfrac{1}{2}$ | 0.92 | $\tfrac{1}{2}$ | | | −0.20 | $\tfrac{1}{2}$ | 1* | −0.24 | $\tfrac{1}{2}$ | 0 | −0.24 | $\tfrac{1}{2}$ | 0 | | | | | | |

*) See footnote to table 3.

$T_1 = T_2 = 1$ are not expected to be important, the lowest lying at $\approx 10$ MeV. In fig. 6 we give the results of diagonalizing the 2p-0h and 4p-2h states separately and together. These results are compared with the experimental spectrum [49,61]), where we have omitted negative parity and $T = 1$ levels. The wave functions are given in table 7.
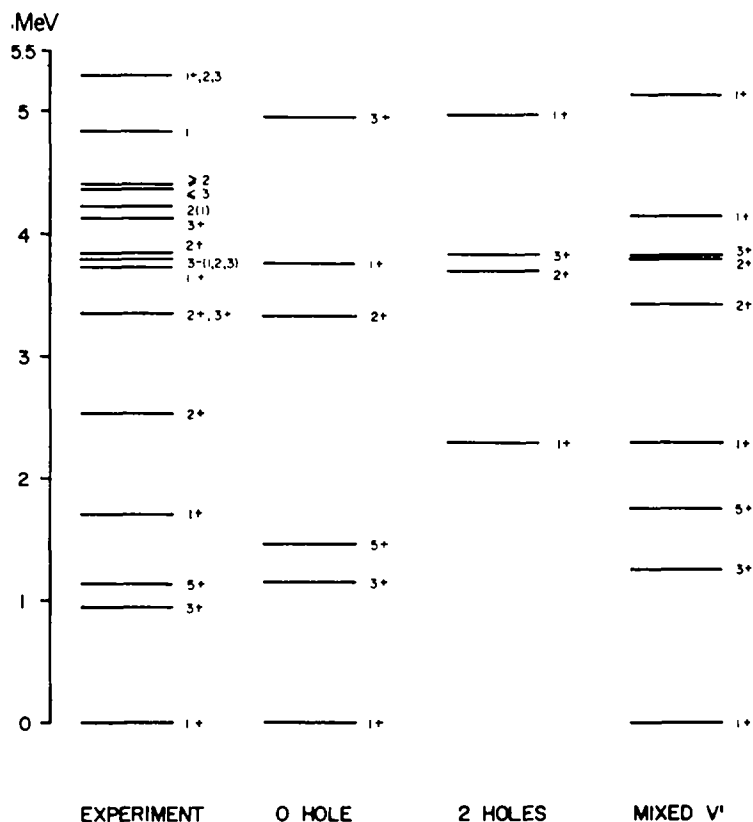


Fig. 6. The calculated positive parity $T = 0$ levels of $^{18}$F and the experimental spectrum (levels assigned definite negative parity or $T = 1$ are omitted).

The $1^+$ ground state wave function is largely 2p-0h and contains rather little of the dominant configuration of the $1^{*+}$ i.e. 4p-2h with $J_1 = 0$, $J_2 = 1$. The reason for this small mixing is that as would be expected in the $j$-$j$ coupling limit, the $1^+$ ground state of $^{14}$N has as the dominant piece of the wave function (02) with $L = 2$ rather than $L = 0$ (see table 2). Hence, in the limit of pure $SU_3$ wave functions the relevant matrix element vanishes. The low-lying $3^+$ and $5^+$ levels are largely of a 2p-0h nature and their excitation energies are somewhat greater than suggested by experiment.

Experimentally $2^+$ levels are observed at 2.52 and 3.84 MeV and both the $^{16}O(^3He, p)^{18}F$ and $^{14}N(^7Li, t)^{18}F$ reactions [51,61]) suggest a 4p-2h structure for the lower level and a 2p-0h structure for the higher one. In contrast we predict $2^+$ levels

at 3.4 and 3.8 MeV with 63 % and 24 % 2p-0h admixtures respectively. Clearly this indicates that our two-hole $2^+$ level lies too high. The ($^7$Li, t) data further suggests that the level at 3.36 MeV ($J^\pi = 2^+, 3^+$) has a 4p-2h structure with $J^\pi = 3^+$, which is in agreement with our prediction for the $3^{*+}$. The 4.12 MeV $3^+$ level should then presumably correspond to our $3^{**+}$ which is largely 2p-0h, although the excitation energy (5.9 MeV) is not in good agreement. The ($^3$He, p) work seems consistent with a 2p-0h structure for either state.

It seems reasonable to associate our mostly 2p-0h $1^{**+}$ level with the experimental $1^{(+)}$ level seen at 3.72 MeV. Since only the level at 4.84 MeV has been assigned definite $J = 1$ and we do not expect a negative parity level in this region, we tentatively make the correspondence with our $1^{***+}$ level. This level is largely 4p-2h and contains 61 % of the configuration with $J_1 = 2$, $J_2 = 1$ which might be expected to be strongly excited by the ($^7$Li, t) reaction. However, the ($^7$Li, t) data shows large cross sections for the 4.23 MeV level ($J = 2(1)$) and the 5.30 MeV level ($J^\pi = 1^+, 2, 3$). As regards the 4.23 MeV level, it has a 12 % branch to the 2.1 MeV $2^-$ level [49]) and this may indicate negative parity as suggested by Benson and Flowers [59]). We note that the ($^7$Li, t) reaction does sometimes populate negative parity levels quite strongly e.g. the 2.1 MeV $2^-$ level and also that we predict a $2^-$ level at 5.1 MeV (see fig. 3) for which this level appears the best candidate. The origin of the large cross section for the 5.30 MeV level is not clear. It may be that this is the $1^{***+}$, in which case it would seem unreasonable to associate the 4.84 MeV level with our next predicted $1^+$ level at 6.3 MeV, although this does have only very small components involving the ground state of $^{14}$N. Middleton et al. [61]) take this 5.3 MeV level to have a 4p-2h configuration with $J_1 = 4$, $J_2 = 1$ coupled to $J^\pi = 3^+$, although our calculation indicates that this configuration lies at approximately 8 MeV.

Thus taking the assignment of $3^-$ for the 3.79 MeV level we have an explanation of all the levels up to 4 MeV although the theoretical excitation energies are usually somewhat larger than the experimental ones, sometimes markedly so. Above 4 MeV the comparison between theory and experiment is difficult, in particular the doublet at 4.4 MeV does not fit in with our predictions.

It seems clear that agreement with experiment would be improved by lowering all our 4p-2h states with $T = 0$ uniformly, while leaving those with $T = 1$ unchanged. Benson and Flowers [59]) have essentially done this by taking the $p_{\frac{1}{2}}$–$d_{\frac{1}{2}}$ splitting as a free parameter in their calculations. They need a value substantially smaller than that deduced from the experimental binding energies, as was the case in $^{19}$F also. Bearing in mind this difference their results are rather similar to ours. This suggests a lack of sensitivity to the precise details of the calculation.

In table 7 we give for later use the wave functions of the 4, $1^{****}$ and $5^*$ triplet which lies at 6.25 MeV and the $2^{**}$ level predicted at $\approx$ 8 MeV. We also give the wave functions we have obtained for the ground and first excited states of $^{17}$O. We comment only that they contain approximately the same amounts of 0, 2 and 4 (close to zero) hole configurations as obtained by Brown and Green [10]).

## 6. Conclusions

We conclude that the weak coupling model generally gives a good description of the low-lying p-h states. It appears to be most favourable only to couple in $J$ and $T$ the eigenfunctions obtained by diagonalizing $(sd)^{n_1}$ and $p^{n_2}$. The additional p-h interaction gives mainly diagonal matrix elements in this basis which simply lead to an energy shift. This shift is very insensitive to the exact form of the particle and hole wave functions, whereas for $n$ particles in an oscillator shell small admixtures can affect the energy considerably; we conclude that the most important correlations are those between particles and holes separately. Our final states can therefore be approximately identified by their appropriate particle and hole eigenfunctions. By this procedure we are able to reduce the shell-model basis rather severely. The off-diagonal matrix elements between states with the same number of holes are generally small, except for the special cases where both states have the same $(\lambda\mu)$ structure for the particles and the holes. This, however, does not produce states which have total $(\lambda\mu)$ as a good quantum number. In the rather few cases where configurations with different numbers of particles are nearly degenerate the off-diagonal matrix elements (ODPN) may produce considerable mixing.

Shell-model calculations which include excitations between different oscillator shells can produce spurious states due to c.m. excitations. We have pointed out that this is likely to give a sizeable effect and for our particular purposes a reduction of the ODPN matrix elements is indicated.

We expect our method to give the main components of the wave functions, since we have included the states lying in the region of interest. However, we have found a number of states at high excitation energies which have large off-diagonal matrix elements with low-lying states containing a smaller number of holes. Brown and Green [10]) have compared such effects to the unlinked clusters of perturbation theory which lower the energies of all states uniformly without affecting the relative spacings. The role of these effects, however, in a consistent shell-model framework is not clear.

As regards specific predictions, the major discrepancies occur for the $^{16}O$ $J = 1^-$ and $3^-$ levels and the $^{18}F$ $J = 0^-$ and $2^-$ levels where we are not able to get the p-h states sufficiently low in energy. At least for the $^{18}F$ $J = 0^-$ level the trouble does not seem to lie in the cutting of the basis. We therefore examined the matrix elements $\mathscr{V}_D$ of the Gillet potential to see if some modification of them could improve agreement with experiment. We were unable to find such a modification and it seems likely that this simple form of potential is too restrictive.

As remarked, the electromagnetic transition rates are important quantities to compare with experiment. These will be discussed, together with the spectroscopic factors, in a later paper.

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