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POSITIVE PARITY GIANT MULTIPOLE RESONANCES IN ^{16}O

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Гигантские резонансы положительной четности в ^{16}O

В рамках оболочечной модели (n частиц – n дырок, n=0,1,2) были вычислены распределения спектроскопической изоскалярной и изовекторной силы для $J^{\pi}=0^+, 1^+, 2^+, 3^+$ и 4^+ в ядре ^{16}O. Изоскалярный квадрупольный резонанс фрагментирован, найдено восемь уровней в области 17-25 МэВ, которые исчерпывают 33% правила сумм с энергетическим весом. Этот результат хорошо согласуется с данными экспериментов по неупругому рассеянию ^3He и альфа-частиц. Гигантский монопольный изоскалярный (изовекторный) резонанс исчерпывает более 50% правила сумм в районе E* ≈ 30 МэВ (E* ≈ 40 МэВ). Предсказано существование коллективных состояний других мультипольностей в области энергии возбуждения 30 МэВ и в районе 50-60 МэВ. Учет корреляций в основном состоянии (2p-2h) приводит к значительному перераспределению спектроскопической силы по сравнению со случаем некоррелированного основного состояния.

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Positive Parity Giant Multipole Resonances in ^{16}O

Distributions of the ($J^{\pi}=0^+, 1^+, 2^+, 3^+, 4^+$) isoscalar and isovector strength in ^{16}O have been calculated in the n particle - n hole (n=0,1,2) shell model. The isoscalar quadrupole giant resonance comes out fragmentated over eight peaks which exhaust 33% of the EWSR between E* = 17 and 25 MeV. This result agrees nicely with the recent ^3He and alpha inelastic scattering experiments. Giant monopole isoscalar (isovector) resonance appears to exhaust more than 50% of the EWSR near E* = 30 MeV (E* = 40 MeV). Several collective states of other multipolarities are predicted either near to 30 MeV or between 50 and 60 MeV. The ground state correlations of the 2p2h type give rise to a considerable strength redistributions as compared with the case of the closed shell ground state.

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1. INTRODUCTION

It is perhaps the most surprising feature of the particle-hole (ph) model of the closed shell nuclei that it gives rise to collective states with specific and rich structure as a result of mixing very simple configurations. Experimentally such collective states may be excited by a large variety of low- and intermediate-energy projectiles such as photons, e^- , p , ^3He,... and, e.g., in the capture processes like μ^-- and radiative π^- -capture from the mesoatomic orbitals.

However different the particular properties of the above reactions may be, their physical universality manifests itself in a uniform response of the nuclear system, namely in the creation of the collective states frequently exhausting a considerable fraction of the respective sum rule (giant multipole resonances). Formally this universality may be traced to the fact that only a few elementary operators

$$Y_{LM}\tau_T, \quad [Y_L \cdot \sigma]_{LM}\tau_T, \tag{1}$$

where $\tau_0 = 1$ and $\tau_1 = \tau$, are supposed to mediate such transitions. A possible momentum dependence will be introduced later; σ and τ are the nucleon spin and isospin matrices, the angular momentum coupling is indicated by the square brackets. Though the spherical functions Y_{LM} arise from an infinite expansion of the wave describing motion of the incoming (outgoing) particle of impulse $\vec{k}$,

$$e^{-i\vec{k}\cdot\vec{r}} = 4\pi \sum_{L=0}^{\infty} \sum_{M=-L}^{L} (-i)^L j_L(kr) Y^*_{LM}(\Omega_{\vec{k}}) Y_{LM}(\Omega_{\vec{r}}), \quad (2)$$

the usual classification into monopole, dipole, quadrupole,... transitions is actually extremely useful, since only a few values of L are allowed when the operators (1) are to describe the excitation of the nuclear states with sharp total spin J.

The aim of the present paper is a theoretical search for the collective positive parity excitations in the ^{16}O nucleus as induced by the spin-, isospin-, and momentum-dependent transition operators. We examine in this respect a straightforward extension of the ph shell model, namely we diagonalize the nuclear residual force within the complete subspaces of the $2\hbar\omega$ configurations. Our interest in the problem was strongly stimulated by the experimental observation of the giant (isoscalar) quadrupole resonance. We devote major attention to this mode. Nevertheless, a possible collectivization of the positive parity $T=1$ states seems also to be of importance in several experimental situations. Such levels are expected to lie at higher energies than the isoscalar ones and the possible candidates in ^{16}O were, e.g., observed in electron scattering [1] (structures at 44.5 and 49 MeV) and in the radiative π^- capture, where the spin-quadrupole operator $[Y_2 \cdot \sigma]_{1^+,2^+,3^+}$ should be responsible for the whole upper half of the experimentally observed spectrum [2]. Indeed, this last example involves such high transferred momenta that they cannot be studied quantitatively within the long-wavelength limit. At the same time our approach is appropriate [3] for investigation of the giant magnetic (and spin-flip electric) resonances in backward e^- scattering. Similarly the model may be useful for the separation of isovector and isoscalar modes of the giant quadrupole resonance.

The idea of the possible existence of the spin- isospin- and spin-isospin-resonances goes back to the early sixties [4]. In ^{16}O such states were sought within the Tamm-Dancoff and random-phase approximation (1p1h) by Ellis and Osnes [5]. Most recently Liu and Brown [6] considered collective excitations in several closed shell nuclei including ^{16}O in an RPA-like model based on a specific choice of the nuclear interaction. The Skyrme potential, which is in fact a delta-shaped potential, has allowed them to include a large configuration space (1p-1h) via the response function technique.

Our approach is rather to keep a general nuclear interaction to avoid the inaccuracies in this sector. Simultaneously we are interested in the spreading of the collective states by coupling of the 1p1h and 2p2h configurations. In this respect and for the E2 excitations, our work is parallel to that by Knüpfer and Huber [7] and Hoshino and Arima [8]. Unlike them, however, we consider a wide class of isoscalar and isovector transition modes. The results change critically with the inclusion of the ground state correlations omitted in the mentioned papers and exhibit an unexpectedly [7] strong dependence on several single particle energy parameters. Also, we argue that phenomenological interactions used in refs. [7] and [8] may prove to be oversimplified for the work in large configuration spaces. Instead we have employed a realistic potential in the form due to Tabakin.

In sect. 2 we present a short review of the recent experimental and theoretical search for the giant quadrupole resonances. Sect. 3 contains some details of our calculations. Finally, in sect. 4 the results of the strength distributions of the individual J,T modes are summarized and discussed. Sect. 5 contains a summary of our work.

2. GIANT QUADRUPOLE RESONANCE IN ^{16}O

2.1. Experimental Work

A detailed review of the recent efforts to observe and understand the quadrupole resonance in ^{16}O may be found in lectures by Hanna [9]. Probably the most important earlier experiments are those with gamma rays [(γ,p),(γ,α)] and with polarized protons, the reaction $(\vec{p},\gamma)$. They seem to suggest an enormous concentration of the isoscalar E2 strength well below 20 MeV and that of isovector strength above 20 MeV. Decisive, however, must be the inelastic scattering experiments. For the (^{3}He, ^{3}He′) reaction the measurements [10] show strong peaking of the E2 strength at 19 MeV. The (α,α′) process is selective for the excitation of the T=0 model if we disregard the small Coulomb effects.

Knöpfle et al. [11] observed scattering of 146 MeV alpha particles and found 65% of the E2 energy weighted sum rule (EWSR) to be concentrated between 15.9 and 27.3 with its centroid at 20.7 MeV. Harakeh et al. [12] using 104 MeV alpha particles observed 40^{+20}_{-10} % of the isoscalar EWSR to be exhausted between 17 and 25 MeV. Some levels observed above 22 MeV are, however, possibly octupole (3^-) and/or monopole (0^+) excitations. Due to a better energy resolution Harakeh et al. [12] observed transitions to the individual nuclear levels. Since they found also multipolarities different from 2^+ in the region below 27 MeV which Knöpfle et al. [11] interpreted as a single quadrupole excitation, the sizable difference of the results obtained by the two groups can be understood.

Strong support to the Harakeh et al. [12] results is given by the most recent work on the ^{3}He inelastic scattering [13]. In this reaction the isovector excitations are considerably depressed (by a factor of ≈ 1/30) and the cross section may be entirely attributed to the T=0 mode. The individual transition strengths observed [13] are in good agreement with those reported in ref. [12]. Similarly, the 2^+0 excited states between 17 and 25 MeV exhaust [13] 37% of the EWSR supporting the Harakeh et al. value 40^{+20}_{-10} %.

To conclude this shortened list of experimental results we should just mention that Hotta et al. [14] by inelastic electron scattering observed 43% of the E2 sum below 20 MeV and about 20% in the region between 20 and 30 MeV. Indeed isoscalar snd isovector com - ponents cannot be disentagled in such a work.

2.2. Theories

There exist several attempts to investigate theoretically the distribution of E2 (and E0) strength for ^{16}O in the giant resonance region. The works based on the 1p1h excitations [15] of $2\hbar\omega$ type place a major isoscalar strength in a compact peak at about 22 MeV. This might be identified with the resonance seen in the (γ, p_0) reaction (in fact T=1 interpretation is more likely true). Then, the other isoscalar E2 strength spread out over the lower excitation energies lacks explanation. A better theory should provide a broad distribution (rather than a single peak) shifted towards lower energies. Insufficient broadening of about 2 MeV was obtained by taking into account the coupling with the continuum [15]. The effects of 2p-2h admixtures in the excited states were studied by Knüpfer and Huber [7] and by Hoshino and Arima [8]. They indeed demonstrated considerable spreading of the E2 isoscalar strength distribution in qualitative agreement with experiment. Nevertheless, the detailed calculated strength distribution differs considerably from the data [12,13]. In particular, Hoshino and Arima [8] found 88% of the EWSR to be exhausted between 20 and 30 MeV.

3. DETAILS OF CALCULATION

3.1. The ^{16}O Nuclear Wave Functions

Both ground and excited state wave functions were constructed within the complete subspaces of definite $J^{\pi}T$ including 1p-1h and 2p-2h of $0\hbar\omega + 2\hbar\omega$ unperturbed energy.

By a detailed analysis [16] Brown and Green found less than 2% admixtures of the 4p-4h configurations in the ^{16}O ground state. Omission of these 4p4h components should not spoil the calculated ground state wave function (g.s.w.f.). As for the excited states it must be remembered, however, that our model is unable to account for some important low-lying states such as the well known $2^+T=0$ level at 6.92 MeV which have predominantly 4p-4h structure. In the early investigation of the positive parity 2p-2h states in ^{16}O an attempt (numerically successful) was made to describe such states by an artificial choice of the interaction potential [17]. We do not follow this line. The two-body residual interaction was taken in the form of Tabakin's realistic interaction constructed so as to fit nucleon-nucleon scattering data (0 - 320 MeV) and deuteron properties. We use $^1P_1$ channel parameters of the potential as modified by Clement and Baranger [18]. The harmonic oscillator basis corresponds to the size parameter $b=(\hbar/m\omega)^{1/2} = 1.67$ fm. In view of the rather large number of components included explicitly in the diagonalization, we decided not to consider any renormalization correction.

Calculation of the Hamiltonian matrix is straight forward. Unsettled, however, remains the choice of single particle energies (s.p.e.) in the "upper" (0f1p) shell. Commonly [7,8,17] are used the modifications of a set suggested by Jolly [1] in 1963. It might be expected that the calculation of positive parity states within (rather large) complete $2\hbar\omega$ model space is insensitive to these parameters, for they only influence some of the

1p1h components which are few in number and strongly spread out over many excited states. Even a numerical estimate in favour of this argument has been made[7]. We have observed, however, that the above is true for the density of states only. In fact, the calculated eigenvectors (and strength distributions) vary rapidly even with a very moderate change of the fp shell s.p.e.

The choice by Jolly[1] cannot be considered satisfactory for our needs, since it was made "ad hoc" for use in an oversimplified ph calculation which disregards any configuration mixing, not to speak of higher (2p2h) components which are present in our model space. The set[1] is partly based on the $^{16}O(p,p')^{16}O^*$ data. Actually, the scattering on A=15 system would be more appropriate here. The two differ by the target isospin T_A, and it is well-known[19] that the isospin term $\vec{t}\cdot\vec{T}_A$ of the optical potential may easily account for the results which differ by a few MeV in both cases.

To elucidate the problem of s.p.e. parameters in our model we use first the s.p.e. set I of table 1 which is near to Jolly's choice and then repeat the calculations with a slightly modified set II: the positions of the fp orbitals were shifted down by 25% in the second series.

The definition of our basis vectors and procedure used to eliminate the spurious states arising due to the centre-of-mass motion are described in Appendix A. The excited state wave functions obtained by the diagonalization are too lengthy to be listed here. It might be useful, however, to have at least the ground and isoscalar giant

Table 1

The single particle spectrum (MeV)

Set	$0s_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	$0d_{5/2}$	$1s_{1/2}$
I,II	-45.0	-21.8	-15.65	-4.15	-3.27

Set	$0d_{3/2}$	$0f_{7/2}$	$1p_{3/2}$	$0f_{5/2}$	$1p_{1/2}$
I	0.93	11.7	17.7	18.7	24.7
II	0.93	8.7	13.3	14.0	18.5

monopole resonance vectors in the explicit form. We show them in table 2.

3.2. The Transition Operator

The nuclear collective excitations caused by operators of the type (1) are considered in the long-wave length limit

$$j_L(kr) \xrightarrow[k\to 0]{} \frac{(kr)^L}{(2L+1)!!}. \qquad (3)$$

Following Ellis and Osnes[5] we generalize slightly the operators (1) by inclusion of an ℓ-dependence. We consider the general form

$$O_{TJM}(Lr\mathcal{L}S) = \sum_i r_i^L [[Y_L(\Omega_i)\ell_r(i)]_{\mathcal{L}} \sigma_S(i)]_{JM} \tau_T(i), \qquad (4)$$

where the sum goes over the individual nucleons. The square brackets symbolize the angular momentum coupling and a symmetrized

Table 2

Ground state and T=0 giant monopole resonance wave functions of ^{16}O. The configuration is labelled $[(p\bar{p})JT(h\bar{h})JT]_{00}$; s.p. orbitals are $2 \equiv 0p_{3/2}$, $3 \equiv 0p_{1/2}$, $4 \equiv 0d_{5/2}$, $5 \equiv 1s_{1/2}$, $6 \equiv 0d_{3/2}$. Configuration is omitted if $|a_i| < 0.1$ for all listed states. Diagonalization was performed with the s.p.e. set II of table 1

E(MeV) / %EWSR	ground / -	24.2 / 4.4	27.9 / 19.1	30.2 / 17.6	31.7 / 19.8
0p0h	0.8856	-0.0724	-0.0683	0.0397	0.2075
$1s_{\frac12}0s_{\frac12}^{-1}$	0.08I7	-0.26I3	-0.I729	-0.2074	-0.3I09
$1p_{\frac12}0p_{\frac12}^{-1}$	0.I762	-0.I3I4	-0.3689	-0.395I	-0.4067
$1p_{\frac12}Cp_{\frac12}^{-1}$	0.0I57	-0.0330	-0.2387	-0.2I34	-0.3I67
$p\bar{p}$ $h\bar{h}$ JT	Two particle - two hole components				
44 22 0I	0.0528	0.0829	0.I926	-0.003I	-0.2098
44 33 0I	0.I677	0.II75	0.4082	0.0725	-0.4308
44 22 I0	-0.0I20	0.0477	0.I007	-0.030I	-0.I050
44 23 I0	-0.I247	-0.0545	-0.2739	-0.0599	0.I996
44 22 2I	-0.0II3	0.0I83	-0.I350	-0.II28	0.0070
44 23 2I	0.II33	-0.0I64	-0.0I98	0.0403	0.2693
44 22 30	0.0487	-0.0I49	-0.I024	-0.0429	0.I206
45 23 20	0.0058	-0.0732	-0.020I	0.I5I5	-0.0925
45 23 2I	-0.0277	-0.2665	0.0336	0.I2I5	-0.0306
45 22 30	0.0I27	-0.I544	-0.0339	0.067I	-0.0535
46 22 I0	-0.I257	-0.0323	-0.I30I	0.0I32	0.0240
46 23 I0	0.I456	0.I249	0.25I8	-0.0353	-0.I298
46 33 I0	0.0208	0.0054	0.200I	-0.2229	-0.0594
46 23 II	-0.0879	-0.0047	-0.I7I4	-0.0896	0.00I7
46 23 20	0.I443	-0.0I88	-0.I357	0.0348	0.0942
46 23 2I	-0.0I28	-0.0265	-0.I478	-0.0628	0.096I
55 22 0I	0.0048	0.236I	-0.0364	-0.I0I3	0.0205
55 33 0I	0.023I	0.628I	-0.2260	-0.0522	-0.0736
55 22 I0	0.0040	0.I288	0.0I85	-0.I366	0.0676
55 23 I0	-0.05I7	-0.4464	0.0554	0.2558	-0.I235
55 33 I0	0.055I	0.I98I	-0.3948	0.7I33	-0.3II8
56 33 I0	0.0544	0.I887	0.0002	-0.0356	0.0409
66 22 0I	0.III2	0.0263	0.0958	0.0232	-0.0342
66 33 0I	-0.0I22	0.0677	0.II84	-0.0I53	-0.I678

product $[Y_L \ell_r] = \frac{1}{2}([Y_L \ell_r] + [\ell_r Y_L])$ is inderstood. The symbol $\ell_1(\ell_0)$ denotes the angular momentum operator (unit operator). The meaning of σ_S and τ_T is analogous. The radial dependence r^L will be changed in the monopole case where we take r^2 form. More about the earlier use of the operator (4) may be found in the paper by Ellis and Osnes[5]. They also give an explicit expression for the single particle reduced matrix elements of the operator (4).

Multiplicative factors (like Z^2/A^2 for the $\Delta T = 0$ transition) were suggested by Nathan and Nilson[20] and recently used, e.g., by Liu and Brown[6] with the aim of effectively describing the collective motions in which neutron and proton matter move together. Since these factors do not change the relative (% EWSR) transition strength attributed to particular excited states which are alone discussed in this paper, we shall use the unrenormalized operator (4). Note that for $L = 0$ we simply use the unit operator instead of $Y_{00} = (4\pi)^{-1/2}$. The transition matrix element for the np-nh initial and final states is given in Appendix B.

3.3. The Sum Rules

The energy weighted sum rule for the operators O_{0JM}(JOJO) can be calculated in a model independent way. We shall characterize the degree of collectivity of our $J^+T=0$ nuclear levels by the percentage of the EWSR they exhaust. Following Lane[4] we have

$$S_{TJ} = \sum_n (E_n - E_0) |\langle n | O_{TJ0} | 0 \rangle|^2 , \qquad (5)$$

$$S_{0J} = \frac{\hbar^2 A}{8\pi m} J(2J+1)\langle r^{2J-2}\rangle . \qquad (6)$$

With our value of the harmonic oscillator constant (b= 1.67 fm) we obtain S_{02} = = 1643 MeV fm^4 if the correlated ground state wave function of table 2 is used to calculate $\langle r^2 \rangle$. Effect of the ground state correlations (g.s.c.) on the $\langle r^2 \rangle$ value is, however, less than 1%. We discuss, therefore all our results in terms of the above EWSR. For the J=4 subspace we have S_{04} = 6.7 x x 10^5 MeV fm^8. The J=0 sum rule may easily be calculated with the result

$$S_{00} = \frac{\hbar^2 A}{2m} 4\langle r^2 \rangle = 8307 \text{ MeV}\cdot\text{fm}^4 . \qquad (7)$$

The sum rules corresponding to the transition operators which contain spin and/or isospin matrices should always be evaluated within the chosen nuclear model. Since our results for these transitions are of an exploratory nature, we rather follow another path. The degrees of collectivity of these states will be given as fractions of the energy weighted model sum (EWMS) which we define through eq. (5) restricting, however, the sum to the calculated nonspurious excited states of the given angular momentum, parity and isospin as displayed in table 3. The model spaces are large enough to ensure a reasonable correspondence of the EWSR and EWMS values. The only exception found in our work concerns the J=4 case; we discuss it in detail below (subsect. 4.2).

Table 3

Dimensions of the $2\hbar\omega$ J^+T subspaces in ^{16}O

Type (JT)	=00	0I	I0	II	20	2I	30	3I	40	4I
1p1h	3	3	7	7	8	8	6	6	3	3
2p2h	40	42	76	I22	II0	I43	87	I3I	67	84
Spurious	5	5	II	I2	I3	I3	9	9	4	4

4. RESULTS AND DISCUSSION

4.1. Isoscalar Quadrupole Resonance

The calculated E2 isoscalar strength distributions are presented in table 4 together with the recent high-resolution (150 keV) data from the 104 MeV (α,α') reaction. We would like to draw readers' attention to the parameter dependence of the results. The first series of calculations (columns 2-4) was performed with s.p.e. set I of table 1 which practically follows the choice of ref./7/ and differs little from those of ref./8/. In agreement with the earlier studies the main E2 isoscalar strength is located between 23 and 30 MeV which is at variance with the experiment /12,13/. Our second series of calculations (table 4, columns 5-7) was performed with set II of the s.p.e. where the fp shell orbitals were shifted down by 25%. The resulting eigenenergies agree in these two cases within ≈0.5 MeV. Nevertheless, the distribution of the spectroscopic E2 strength is in the second series unambiguously transferred to the levels around 20 MeV. It is indeed a lucky coincidence that the results of our second series quantitatively almost agree with the experiment, since the above 25% reduction was attempted in a purely

Table 4

Distribution of isoscalar quadrupole strength in percentage of the EWSR eq. (6), S_{02} = =1643 MeV fm^4.

Energy (MeV)	s.p.e. set I $N^{a)}$	s.p.e. set I no g.s.c.	s.p.e. set I g.s.c.	s.p.e. set II $N^{a)}$	s.p.e. set II no g.s.c.	s.p.e. set II g.s.c.	(α,α') at 104 MeV $N^{a)}$	(α,α') at 104 MeV %EWSR[b]	(α,α') at 104 MeV %EWSR[b]
<17	1	2.8	5.5	1	6.1	8.7	4	12.6	25.2
17-20	2	2.6	2.5	2	11.2	8.4	2	4.7	9.4
19.5							(1)[c]	(1.3)	(2.6)
20-22	2	3.5	3.4	2	19.1	12.7	3	6.9	13.8
22-25	2	40.7	26.9	4	19.9	11.1	(4)[c]	(10.4)	(20.8)
22-25[d]	5	1.9	1.4	3	1.1	0.9			
17-25	11	48.7	34.2	11	51.3	33.1	10	23	47
25-30	17	19.0	10.5	17	7.0	2.9	-	-	-
<60	105	83.0	53.5	105	73.0	47.3	-	-	-

a) Number of individual levels.
b) See ref.[12].
c) Non-quadrupole (L=3, L=0) identification is also possible.
d) Non-collective levels.

modelistic approach just to see the trend of results. It shows, however, that a responsible choice of s.p. energies of the shell nucleons may easily resolve the disagreement quoted by Harakeh et al.[12] between the

observed distribution of the isoscalar strength and that obtained[7,8] by the diagonalization within complete $2\hbar\omega$ shell model space.

The main problem studied quantitatively in this investigation is the influence of the higher admixtures in the ground state wave function on the transition strength distribution. By comparing columns 3 and 4 (6 and 7) of table 4, significant effects of the g.s.c. can be seen. Besides the tendency to reduction of the EWSR percentage exhausted in the studied region also a redistribution of the strength towards the low-lying states is observed. In order to study the sensitivity of this change to the particular form of the g.s.w.f., we have repeated the calculations with the g.s.w.f. obtained by Ellis and Zamick[21]. The latter was constructed in a manner similar to ours, the difference being in their choice of the residual interaction (Kallio-Kolltveit force). The results are remarkably stable. Redistribution of the E2 strength obtained for two forms of correlated g.s.w.f. does not exceed 0.5-1% in the cases we have compared.

Two sets of experimental values for the E2 strength distribution are given by Harakeh et al.[12] We reproduce them in table 4. The smaller ones (column 9) are the results of their measurements. Those of the other set (column 10) were renormalized by a factor of 2 "... so that the isoscalar transition rate of the 6.92 MeV level is equal to the electromagnetic transition rate"[12]. Our calculated distributions seem to suggest at the most a less drastic renormalization procedure.

This is also in agreement with the most recent ^3He inelastic scattering experiment, ref. /13/.

We have already stressed that the present model cannot provide proper description of some low-lying levels in ^{16}O which are known to have mainly 4p-4h structure. At the same time 4p-4h admixtures in the ^{16}O ground state are certainly small. Then the spectroscopic strength attributed by experiment to the 2^+ levels at 6.92 MeV and 10.52 MeV has to be accounted for via 1p1h and 2p2h components of these excited states because the matrix elements $\langle [4p4h]_{2^+0} | 0_{020} | [2p2h]_{g.s.} \rangle$ vanish. It is gratifying that almost 10% of the EWSR is concentrated at the calculated 2^+ "level" at 16 MeV despite the crudeness of our model for this low-energy region.

Four levels have been observed /12/ between 22 and 25 MeV with possible L=2 assignment. The octupole (monopole for the 23.85 MeV structure) assignment is the discussed /12/ alternative. A strong (1p-1h) isoscalar 3^- level was obtained with our interaction at 23.86 MeV. Among monopole excitations, the lowest nonspurious isoscalar level comes out at 24.1-24.2 MeV and may carry about 5% of its own EWSR (see table 8).

The calculated isoscalar quadrupole states in the region 17-25 MeV exhaust 33-34% of the sum rule limit if the ground state correlations are included. This has to be compared with the experimental estimates 40^{+20}_{-10} % from ref. /12/ and 37% of the EWSR reported in ref. /13/. The results contrast strongly with some earlier calculations, e.g., Hoshino and Arima /8/ obtained 82% of the EWSR located between 19 MeV and 28 MeV; they agree, however,

roughly with findings by Knüpfer and Huber /7/ who quote 40% of the EWSR exhausted in the energy region 20-40 MeV. The paper /8/ (most probably that of ref. /7/ as well) does not consider the ground state correlations; therefore our corresponding value 49-51% of the EWSR is probably a fairer counterpart of their results. We did not obtain any noticeable concentration of the isoscalar S=0 E2 strength in the region between 30 MeV and 60 MeV where our model predicts 76 more excited levels.

4.2. Search for New Collective States

We shall present here only selected results in condensed form illustrating the qualitative features and possible trends towards collectiveness in the groups of positive parity excitations. In tables 5 and 6 we show the percentage distributions of the spectroscopic strength in transitions induced by the operators (4). Note that tables 5 and 6 are calculated in terms of the EWMS introduced in subsect. 3.3. In the preparation of the tables we omitted numerous contributions of the levels which add less than 2% of the EWMS. Each table entry then summarizes contributions of typically 2-5 nuclear excited states within the energy interval of 2.5 MeV. The latter was chosen with respect to the expected broadening of the possible new giant resonances which may be of the order of 5-7 MeV by analogy with the observed giant dipole and quadrupole resonances.

The exceptional concentration of the monopole strength, both isoscalar and isovector,

Table 5

Distribution of isoscalar strength in ^{16}O corresponding to the transition operators of eq. (4). Only contributions larger than 2% of the EWMS are summarized within the energy intervals of 2.5 MeV. The s.p.e. set I of table 1

E_x (MeV)	20 - 30				30 - 40				40 - 50				> 50	
r^2		4		8	7	63	4	2	2					
$r^2[\ell.\sigma]_{00}$				3	3	2	4		16		9		4	35[a)]
$r^2\ell$					13	21	25	5	9					
$r^2\sigma$				4	5	5	15	8	4	8	3		17	8
$r^2[\ell\,\sigma]_{10}$		2	5	21	18	2	8	6		3	4			
$r^2[Y_2.\sigma]_{10}$				2	2	5	3	28	4	14	2	3	7	5
r^2Y_{20}	7[b)]	50	6	5										
$r^2[\ell.\sigma]_{20}$			5	7		5	8	10	15	4		6		
$r^2[Y_2.\sigma]_{20}$						3	2		2	2	7	4	3	37[c)]
$r^2[[Y_2.\ell]_3.\sigma]_{20}$						4	3	11	6	15	6	2		
$r^2[Y_2.\ell]_{30}$				6	5	15	21	2	11		3	5		
$r^2[Y_2.\sigma]_{30}$			4	4	5	26	11		9	2				
$r^2[[Y_2.\ell]_3.\sigma]_{30}$			3	8		6	14	5	6	4	7	11		
$r^4[Y_4.\sigma]_{30}$				2		5	17	5	17	8	3	2		
r^4Y_{40}			8	24	15		5			5				
$r^4[Y_4.\sigma]_{40}$			10	2			2	8		35	9		6	
$r^2[[Y_2.\ell]_3.\sigma]_{40}$			7		9	15	31			9				

a) The levels at E_x=56,57 and 58 MeV exhaust 18%, 5% and 8% of the EWMS, respectively.
b) Additional 15% of the EWMS is located below E_x=20 MeV.
c) The levels at E_x= 53, 56, 57 and 58 MeV exhaust 10%, 7%, 14% and 6% of the EWMS, respectively.

Table 6

Distribution of isovector strength in ^{16}O corresponding to the transition operators of eq. (4). Only contributions larger than 2% of the EWMS are summarized within the energy intervals of 2.5 MeV. The s.p.e. set I of table 1

E_x (MeV)	20-30				30-40				40-50				> 50	
$r^2\tau$		6	7	2		2	4	10	41	4	15			
$r^2[\ell.\sigma]_{00}\tau$			6	35	7	8	13		4	5				
$r^2\ell\,\tau$			5		8	9	9	17	6					
$r^2\sigma\,\tau$							5	5	3	6		15	4	24[a)]
$r^2[\ell.\sigma]_{10}\tau$		5	5	9	6	8	2	6	4	8				
$r^2[Y_2.\sigma]_{10}\tau$							7	7	13	2	5		5	18[a)]
$r^2Y_{20}\tau$							16	4		3	12		13	
$r^2[\ell.\sigma]_{20}\tau$	4	7	5		3	9	8	12						
$r^2[Y_2.\sigma]_{20}\tau$				2	2		8	3	3	7	6		12	3
$r^2[[Y_2.\ell]_3.\sigma]_{20}\tau$					2	6	9	8	20	3	2		3	
$r^2[Y_2.\ell]_{30}\tau$			3		7		10	16	5			3		
$r^2[Y_2.\sigma]_{30}\tau$				8	6	4	11	5					9	
$r^2[[Y_2.\ell]_3.\sigma]_{30}\tau$				5	6	6	8	4	7		5	10	3	
$r^4[Y_4.\sigma]_{30}\tau$				3	11	6	3	7	5	8		3		
$r^4Y_{40}\tau$					5	5	9	9	8	11	4	4		
$r^4[Y_4.\sigma]_{40}\tau$			6	5	6	9	8	5	7	9	6	5		
$r^2[[Y_2.\ell]_3.\sigma]_{40}\tau$	3		3	6	9	17	17	7	2					

a) Two levels near E_x = 56 MeV exhaust 8% of the EWMS.

is immediately seen and is quite comparable with that reported in subsect. 4.1 for the GQR. If observed experimentally, the isoscalar monopole mode may provide direct information on the nuclear compressibility which is one of the least known nuclear characteristics. The nuclear hydrodynamics suggests for the energy of breathing mode the following expression:

$$E_{B.M.} = \left(\frac{\hbar^2}{m}\frac{K}{r^2}\right)^{1/2}, \qquad (8)$$

where m is the nucleon mass, K represents the nuclear compressibility and r is the rms nuclear radius.

The distribution of the isoscalar monopole strength is shown in table 7. From comparison of the displayed variants it can be seen that the details of the strength distribution again strongly depend on the choice of the s.p.e. Similarly the fraction of the EWSR exhausted in the model space changes sizably with the change of s.p.e., it overdraws even the sum rule limit (see also table 8) if s.p.e. set I are used. Nevertheless, we find always the monopole T=0 strength concentrated on 3-4 levels which exhaust 50-60% of the EWSR near $E \approx 30$ MeV excitation energy. Substituting into eq. (8) our calculated rms radius $\langle r^2 \rangle = 6.22$ fm^2 we end up with a reasonable estimate of the compression modulus $K \approx 140$ MeV which agrees nicely with the result quoted by Bethe /22/ ($K = 146$ MeV).

Ground state correlations, if included, cause again (with the operator r^2) a considerable reduction of the spectroscopic strength located in our model space and redistribution of the strength towards low-

Table 7

Distribution of isoscalar monopole strength in ^{16}O

State[a] (MeV)	S[b] (fm^4)	EWSR[b] (%)	S[c] (fm^4)	EWSR[c] (%)	State[d] (MeV)	S[c] (fm^4)	EWSR[c] (%)
24.1	8.3	2.4	10.1	2.9	24.2	15.3	4.4
28.3	14.0	4.8	18.1	6.1	27.9	57.0	19.1
30.5	12.3	4.7	14.9	5.5	30.2	48.5	17.6
33.3	70.1	28.0	46.2	18.5	31.7	52.1	19.8
33.8	106.8	43.2	72.2	29.2	33.6	1.6	0.6
35.1	10.8	4.6	6.6	2.8	35.2	0.3	9.1
26-36		87.7		65.0	24-36		61.6
36-70		19.7		11.0	36-70		4.9

The sum rule of eq. (7) is $S_{00} = 8307$ MeV fm^4.
a) the s.p.e. of table 1, set I.
b) No ground state correlation.
c) Ground state correlations included.
d) The s.p.e. of table 1, set II.

lying levels. This is rather a general tendency, we shall not stress it further in connection with other excitation modes. The important exception, however, has been found for the transitions induced by the operators like $r^2[\ell\cdot\sigma]_{0^+,1^+,2^+}\tau_T$ and $r^2\ell\tau_T$ (T=0,1). In the absence of the angular dependence

Table 8

Calculated values of the energy weighted model sum (EWMS) as defined in eq. (5) in units of MeV fm^4 s.p.e. set I of table 1 were used.

Operator	Isoscalar ($\tau_0 = 1$)		Isovector ($\tau_1 = \tau$)	
	uncorrel. g.s.	correl. g.s.	uncorrel. g.s.	correl. g.s.
$r^2\tau_T$	8930[a)]	6340	I0000	6690
$r^2[\ell\cdot\sigma]_{00}\tau_T$	6780	9480	4060	6600
$r^2\ell\tau_T$	4530	3400	4950	6850
$r^2\sigma\tau_T$	II040	8230	II600	8I00
$r^2[\ell\cdot\sigma]_1\tau_T$	4740	6680	50I0	6040
$r^2[Y_2\cdot\sigma]_{10}\tau_T$	2050	I420	2290	I470
$r^2Y_{20}\tau_T$	I360[a)]	880	2II0	I430
$r^2[\ell\cdot\sigma]_{20}\tau_T$	5070	6400	4840	59I0
$r^2[Y_2\cdot\sigma]_{20}\tau_T$	2390	I580	2II0	I4I0
$r^2[[Y_2\cdot\ell]_3\cdot\sigma]_{20}\tau_T$	II90	860	II60	820

a) The s.p.e. set II produces the EWMS of 7940 MeV fm^4 (1200 MeV fm^4) as compared with the EWSR of 8310 MeV fm^4 (1660 MeV fm^4) in the monopole (quadrupole) case.

(Y_{00} = const.) their reduced matrix elements, e.g. $\langle p||r^2[\ell\cdot\sigma]||p\rangle$ of the valence (sd)-shell particles are by an order-of-magnitude larger than valence-hole matrix elements of the type $\langle p||r^2[\ell\cdot\sigma]||h\rangle$. Then the transition strength is determined predominantly by the $(2p2h)_{g.st.} \longrightarrow (2p2h)_{exc.st.}$ processes. Percen-

tage of the EWSR obtained in such cases may be enhanced by 20-60% if the g.s.c. are taken into account. The examples are given in table 8. In the case of operators r^2 and $r^2\tau$ the enhancement does not appear due to an (accidental) cancellation of the large matrix elements of the valence shell nucleons: actually the expression $\langle j||r^2\tau_T||j\rangle/(2j+1)^{1/2}$ which enters into eq. (B9) is independent of j for the $d_{5/2}, s_{1/2}$ and $d_{3/2}$ orbitals.

The existence of the monopole isovector giant resonance is also interesting not only as a new specific form of the collective nuclear motion but also for the possible implications in the understanding of the so-called Nolen-Schiffer anomaly. It was suggested recently[/23/] that much of the anomaly concerning the Coulomb energy differences in mirror nuclei may be explained by the coupling of the odd nucleon with a strongly collective isovector $J=0$ level. The details of the strength distribution for this mode are given in fig. 1 and complement the data of tables 7 and 8. Again the location of the resonance may be shifted by a few MeV due to the uncertainties in the single particle spectrum. The appearance of the resonance is strikingly similar to that of the isoscalar GQR. It extends over a region of about 6 MeV being split into several (≈ 6) levels of different strength.

Transitions with $S=1$ are rarely considered in the closed shell nuclei since the $(0\hbar\omega)$ spin-flip configurations $[(\ell_{j=\ell+1/2})^{-1}\ell_{j=\ell-1/2}]_{J^+}$ are absent in this case. Recently the spin-flip transitions $(2\hbar\omega)$ in ^{16}O have been observed in the backward electron scattering[/24/]. We show

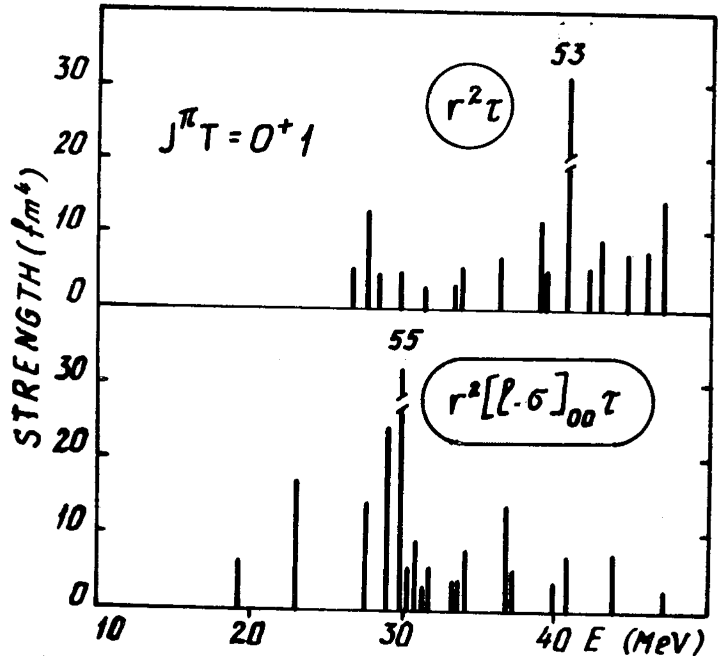

Fig. 1. Distribution of the T=1 monopole strength in ^{16}O. The s.p.e. set I of table 1 used in the calculations.

in fig. 2, as an example, the strength distributions for three independent spin-flip operators of the 2^+0 subspace. Correlated g.s.w.f. was used. The results obtained with two s.p.e. sets differ quantitatively at lower energies. The strong concentration of the strength corresponding to the $r^2[Y_2 \cdot \sigma]_2$ operator ($\approx 35\%$ of the EWMS) around 55 MeV is stable against such a change. Similarly the operators $r^2[Y_2 \cdot \sigma]_J$ with $J = 1,3$ bring about sizable concentrations of the spectroscopic strength (see table 5).

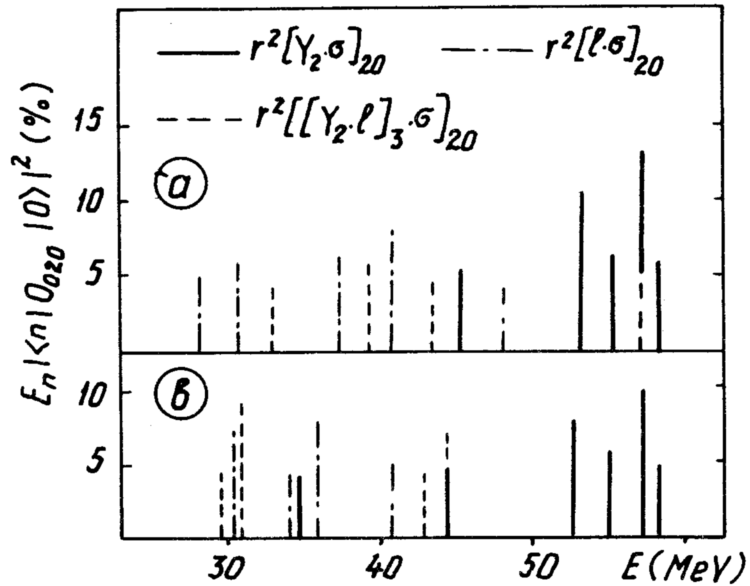

Fig. 2. Distribution of the T=0 quadrupole strength expressed in % of the EWMS defined in eq. (5). a) s.p.e. set I of table 1; b) s.p.e. set II of table 1.

It may be appropriate to compare our results with those obtained by Ellis and Osnes [5]. They also used a realistic interaction (Sussex matrix elements), the model space, however, differs from our. In their study of the 1p1h ($2\hbar\omega + 4\hbar\omega$) configuration mixing, the strong collective excitations always lie below 40 MeV. The levels of the second group which they obtain above ≈ 55 MeV all bear only negligible strength. In our calculation the collective states populate also the 50-60 MeV region. It is perhaps worth noting that strong collective levels near 50 MeV excitation energy in ^{16}O were observed already in 1962 by Bishop and Isabelle[1] in the e^- inelastic scattering experiment.

In general the isovector strength (except for the monopole one) is considerably more fragmentated than in the isoscalar case. By comparing the respective entries of tables 5 and 6 we can easily see that the isoscalar and isovector quadrupole modes are clearly separated in energy. Less than 3% of the isoscalar strength induced by the operator r^2Y_{20} extends beyond 30 MeV. At the same time the operator $r^2Y_{20}\tau$ exhausts less than 7% of its limit in this region being fragmentated over 28 levels. The collective isovector quadrupole states are all obtained above 35 MeV excitation energy.

Three of the isoscalar excitation operators (r^2, r^2Y_{20} and r^4Y_{40}) allow the model independent calculation of the EWSR limits. The monopole and quadrupole cases show that our model sums (table 8) represent at least 80% of the EWSR limit (65% taking into account g.s.c.). The hexadecapole transitions however represent an interesting exception. The $J=4$ nuclear states calculated within our model space exhaust only 17% of the EWSR limit (10% of g.s.c. are included). From the results reported by Liu and Brown[6] we conclude that the $4\hbar\omega$ (1p1h) configurations become strongly dominant, the r^4 factor in the radial integrals ensures there a reasonable overlapping. Since such components are absent in our model space we should add, that the seemingly strong concentrations of the hexadecapole isoscalar strength seen in table 5 at 30, 35 and 45 MeV excitation

energy are to be interpreted with caution.

5. CONCLUSIONS

The positive parity collective states in ^{16}O have been investigated within the n particle- n hole ($n=0,1,2$) shell model which incorporates the ground state correlation effects. The concentration of the spectroscopic strength of the giant resonance type has been found for the monopole ($T=0$ and $T=1$) and quadrupole isoscalar modes. In the latter case 33-34% of the EWSR is concentrated between $E^*=17$ and 25 MeV. This is in good agreement with the inelastic alpha[12] and ^3He[13] scattering experiments which show 40^{+20}_{-10} % and 37% of the EWSR, respectively. The isovector quadrupole strength is located above $E^*=35$ MeV and strongly fragmentated over numerous levels. The detailed strength distributions for the individual nuclear states are very sensitive to the choice of single particle energies of the fp shell orbitals.

The 2p2h admixtures in the ^{16}O excited states provide approximately correct spreading of the strength in the giant resonance regions. The ground state correlations of the 2p2h type bring about an important redistribution of the strength and usually lower the percentage of the EWSR located on the calculated levels. In cases where the monopole term Y_{00} of the plane wave expansion (2) is considered separately, e.g., in the operators $[\ell\cdot\sigma]_{0^+,1^+,2^+}$ and $[\ell\cdot\sigma]_{0^+,1^+,2^+}\tau$, the incorporation of the g.s.c. may, however, cause a very strong (20-60%) enhancement of the EWSR fraction located in the model space. Indeed both $(2p2h)_{g.s.} \longrightarrow (1p1h)_{exc.s}$ and $(2p2h)_{g.s.} \longrightarrow (2p2h)_{exc.s.}$ processes contribute to the described effects together with the weighting factor $(0.88)^2$ of the dominant process $(0p0h)_{g.s.} \longrightarrow (1p1h)_{exc.s.}$.

The concentrations of spectroscopic strength reaching 5-12% of the EWSR for the individual levels and possible grouping of such levels has been predicted for several spin-, isospin- and ℓ-dependent transition operators. As expected, the $[Y_2 \cdot \sigma]_J$ $([Y_2 \cdot \sigma]_J \tau)$ operator is of special interest in this respect.

Unlike the other examples, we found for the hexadecapole excitations that the $2\hbar\omega$ model space is insufficient to describe the collective nuclear properties in ^{16}O. The $4\hbar\omega$ components have to be involved in order to exhaust a reasonable fraction of the corresponding EWSR.

APPENDIX A

For the purpose of establishing our phase convention we denote the 1p1h and 2p1h kets by

$$|ph\,JMTQ> = \sum_{\substack{m_p m_h \\ q_p q_h}} (-)^{j_h - m_h + \frac{1}{2} - q_h} \begin{bmatrix} j_p & j_h & J \\ m_p & -m_h & M \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & T \\ q_p & -q_h & Q \end{bmatrix} a^+_\pi a_\chi |C>,$$

$$|(p_1 p_2) J_P T_P (h_1 h_2) J_H T_H, JMTQ>$$

$$= n(p_1 p_2) n(h_1 h_2) \sum_{\substack{m_i q_i \\ M_P M_H Q_P Q_H}} (-)^{J_H + M_H} \begin{bmatrix} p_1 & p_2 & J_P \\ m_{p_1} & m_{p_2} & M_P \end{bmatrix} \begin{bmatrix} h_1 & h_2 & J_H \\ m_{h_1} & m_{h_2} & -M_H \end{bmatrix} \times$$

$$\times \begin{bmatrix} J_P & J_H & J \\ M_P & M_H & M \end{bmatrix} \times \qquad \text{(A2)}$$

$$\times (-)^{T_H + Q_H} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & T_P \\ q_{p_1} & q_{p_2} & Q_P \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & T_H \\ q_{h_1} & q_{h_2} & -Q_H \end{bmatrix} \begin{bmatrix} T_P & T_H & T \\ Q_P & Q_H & Q \end{bmatrix} a_{\pi_1} a_{\pi_2} a_{\chi_1} a_{\chi_2} |C>$$

We have used $\left[\begin{smallmatrix} \cdots \\ \cdots \end{smallmatrix} \right]$ to denote Clebsch-Gordan coefficients, the symbol $|C>$ represents the closed shell g.s. and $n(a,b) = (1+\delta_{ab})^{-1/2}$. The harmonic oscillator orbitals positive near origin have been chosen and the order of coupling is $\vec{\ell} + \vec{s} = \vec{j}$.

The entirely spurious vectors corresponding to the $1\hbar\omega$ $(2\hbar\omega)$ centre-of-mass excitations have been constructed /24/ by the action of the raising operator $A^{+(1)}$ on the non-spurious ($1\hbar\omega$ spurious) 1p1h states $|p'h'\, J'=J, J\pm 1, T'=T>$. Calculating overlaps with the basis states (A1) and (A2), we obtain for the components

$$\xi_i = \left[\frac{2J'+1}{A}\right]^{1/2} [\delta_{hh'} <p||a^+||p'> W(j_p j_h 1 J'; J j_{p'}) \qquad \text{(A3)}$$

$$+ (-)^{J+J'} \delta_{pp'} <h'||a^+||h> W(j_p j_h J' 1; J j_{h'})],$$

$$i = 1, \ldots, n_1 .$$

and

$$\xi_i = \frac{n(p_1p_2)n(h_1h_2)}{\sqrt{A}}(-)^{J'+J}\hat{J}_P\hat{J}_H\hat{J}'\hat{T}_P\hat{T}_H\delta_{TT'}W(T_P\tfrac{1}{2}T\tfrac{1}{2};\tfrac{1}{2}T_H)$$

$$\times P(p_1p_2J_PT_P)P(h_1h_1J_HT_H)\times \qquad (A4)$$

$$\times[\delta_{p'p_2}\delta_{h'h_2}\begin{Bmatrix} j_{p1} & j_{p2} & J_P \\ j_{h1} & j_{h2} & J_H \\ 1 & J' & J \end{Bmatrix} \langle p_1||a^+||h_1\rangle],$$

$i=n_1+1,\ n_1+2,\ldots,n$.

Here A is the number of particles, $W(\ldots;\ldots)$ and $\{\because\}$ stand for the Racah and 9j-symbols, respectively, P is the exchange operator $P(abJT)f(a,b)=f(a,b)+(-)^{j_a+j_b+J+T}f(b,a)$. We use the usual notation $\hat{a}=(2a+1)^{1/2}$. n_1 is the number of 1p1h components, n is the dimension of the complete subspace for the given J,T. For definition of the reduced matrix elements of the harmonic oscillator raising operator a^+, see ref. /25/.

Let H_{ij} be the Hamiltonian matrix constructed in the original (partly spurious) basis eqs. (A1) and (A2). Let $\xi_i^{(k)}$ be the i-th component of the k-th ($k=1,2,\ldots,m$) spurious state as given by eqs. (A3) and (A4). The diagonalization of the new matrix

$$M=R^{(m)}R^{(m-1)}\ldots R^{(k)}\ldots R^{(1)}HR^{(1)}\ldots R^{(k)}\ldots R^{(m)} \qquad (A5)$$

produces $n-m$ (nonzero) eigenvalues and eigenvectors free of any spuriousness /26/. The remaining m purely spurious eigenvectors correspond to the (m-fold degenerate) zero eigenvalue. Here the auxiliary matrices $R^{(k)}$ are defined as

$$R_{ij}^{(k)}=\delta_{ij}-S_{ij}^{(k)}=\delta_{ij}-\xi_i^{(k)}\xi_j^{(k)}. \qquad (A6)$$

A substantial economy of the computational efforts may be achieved if the relation (A5) is not viewed as a matrix multiplication but rather in the form (recurrently)

$$RHR=(I-S)H(I-S)=H-SH-HS+SHS.$$

In this way the time consuming matrix operations are substituted by much quicker multiplication of a matrix by a vector, e.g.,

$$(HS)_{ij}=\sum_\ell H_{i\ell}\xi_\ell^{(k)}\xi_j^{(k)}=K_i^{(k)}\xi_j^{(k)},\ldots \text{ etc.}$$

In addition the large quadratic matrices $R^{(k)}$ need not be stored.

Finally one additional technical comment. The $[1p1h]_{J=T=0}$ components ($2\hbar\omega$) have nonzero matrix elements of the Hamiltonian with the unperturbed (0p0h) state. These m.e. actually measure the violation of the self-consistency by our harmonic oscillator basis. The problem was already considered by Mavromatis /27/, note, however, a missing factor $\sqrt{2}$ in eq. (1a) of ref. /27/.

APPENDIX B

The above construction leaves us with the model wave functions in the form

$$|np-nh,JMTQ\rangle=a|C\rangle+\sum_i b_i|ph\,JMTQ,i\rangle+ \qquad (B1)$$

$$+\sum_j d_j|(p_1p_2)J_PT_P(h_1h_2)J_HT_H;JMTQ,j\rangle.$$

In what follows the respective quantities of the ground state vector will bear a prime.

For a one-body transition operator of the form:

$$\hat{F}_{tr}^{k\kappa} = \sum_{\alpha\beta} \langle \alpha | F_{tr}^{k\kappa} | \beta \rangle a_\alpha^+ a_\beta \qquad (B2)$$

the (ground state) $\longrightarrow$ (excited state) transition matrix element is given as

$$\langle np-nh, JMTQ | \hat{F}_{tr}^{k\kappa} | np'-nh', J_i = T_i = 0 \rangle = \frac{\delta_{Jk}\, \delta_{Tt}\, \delta_{M\kappa}\, \delta_{Qr}}{\hat{k}\hat{t}}$$

$$\times [\delta_{J0}\delta_{T0}\, a \sum_k b_k' M_{01}(k) + \sum_i b_i a' M_{10}(i) + \qquad (B3)$$

$$+ \sum_{i,k} b_i b_k' M_{11}(i,k) + \sum_{i,\ell} b_i d_\ell' M_{12}(i,\ell) +$$

$$+ \sum_{j,k} d_j b_k' M_{21}(j,k) + \sum_{j,\ell} d_j d_\ell' M_{22}(j,\ell)].$$

The transitions between the individual subspaces amount to

$$M_{01}(k) = \langle C | \hat{F} | p'h'\, 00, k \rangle = \langle h || F || p \rangle, \qquad (B4)$$

$$M_{10}(i) = \langle phJT, i | \hat{F} | C \rangle = \langle p || F || h \rangle, \qquad (B5)$$

$$M_{11}(i,k) = \langle phJT, i | \hat{F} | p'h'\, 00, k \rangle =$$

$$= \frac{\delta_{j_h, j_{p'}}}{\hat{j}_{p'} \sqrt{2}} [\langle p || F || p' \rangle \delta_{hh'} - \langle h' || F || h \rangle \delta_{pp'}]. \qquad (B6)$$

$$M_{21}(j,k) = \langle (p_1 p_2) J_P T_P (h_1 h_2) J_H T_H ; JT, j | \hat{F} | p'h'\, 00, k \rangle$$

$$= n(p_1, p_2) n(h_1, h_2) \frac{\hat{J}_P \hat{J}_H \hat{T}_P \hat{T}_H}{\hat{j}_{p'} \sqrt{2}} \times \qquad (B7)$$

$$\times W(\tfrac{1}{2}\, \tfrac{1}{2}\, T T_H ; T_P \tfrac{1}{2}) \delta_{j_{p'} j_{h'}} P(p_1 p_2 J_P T_P) P(h_1 h_2 J_H T_H) \times$$

$$\times [-\delta_{p' p_2}\, \delta_{h' h_2} W(j_{p_1} j_{p'}\, J J_H ; J_P j_{h_1}) \langle p_1 || F || h_1 \rangle],$$

$$M_{12}(i,\ell) = \langle phJT, i | \hat{F} | (p_1' p_2') J_P' T_P' (h_1' h_1') J_H' T_H', \ell \rangle$$

$$= n(p_1', p_2') n(h_1', h_2') \delta_{J_P' J_H'} \delta_{T_P' T_H'} \hat{J}_P' \hat{T}_P'$$

$$\times W(\tfrac{1}{2}\, \tfrac{1}{2}\, T_P' T ; \tfrac{1}{2}\, \tfrac{1}{2}) (-)^{J_P' + T_P' + J + T} \times \qquad (B8)$$

$$\times P(p_1' p_2' J_P' T_P') P(h_1 h_2' J_H' T_H') [-\delta_{p p_2'}\, \delta_{h h_2'} \times$$

$$\times W(j_p J_P' J j_{h_1'} ; j_{p_1'}\, j_h) \langle p_1' || F || h_1' \rangle],$$

$$M_{22}(j,\ell) = \langle (p_1 p_2) J_P T_P (h_1 h_2) J_H T_H ; JT, j | \hat{F} |$$

$$(p_1' p_2') J_P' T_P' (h_1' h_2') J_H' T_H' ; 00, \ell \rangle =$$

$$= n(p_1, p_2) n(h_1, h_2) n(p_1', p_2') n(h_1', h_2') \delta_{J_P' J_H'} \delta_{T_P' T_H'} \times$$

$$\times W(\tfrac{1}{2}\, \tfrac{1}{2}\, T T_H ; T_P \tfrac{1}{2}) \times$$

$$\times\{\delta_{J_H J'_H}\,\delta_{T_H T'_H}\,\hat{J}_P\hat{T}_P\,P(h_1h_2J_HT_H)\,\delta_{h_1h'_1}\,\delta_{h_2h'_2}\times$$

$$\times P(p_1p_2J_PT_P)\,P(p'_1p'_2J'_PT'_P)\times$$

$$\times[\delta_{p_2p'_2}\,W(j_{p_1}j_{p_2}JJ'_P;J_Pj_{p'_1})\langle p_1||F||p'_1\rangle]- \qquad (B9)$$

$$-\delta_{J_PJ'_P}\,\delta_{T_PT'_P}\,\hat{J}_H\hat{T}_H\,P(p_1p_2J_PT_P)\,\delta_{p_1p'_1}\,\delta_{p_2p'_2}\times$$

$$\times P(h_1h_2J_HT_H)\,P(h'_1h'_2J'_HT'_H)\times$$

$$\times[\delta_{h_2h'_2}\,W(j_{h'_1}j_{h_2}JJ_H;J_{H'}j_{h_1})\langle h'_1||F||h_1\rangle]\}.$$

Indeed a sum over fully occupied orbitals appears if the expectation values in the correlated g.s. are calculated,

$$M_{00}=\langle C|F|C\rangle=\sum_a^{occ}\sqrt{2(2j_a+1)}\,\langle a||F||a\rangle. \qquad (B10)$$

Our reduced matrix elements are defined by the following form of the Wigner-Eckart theorem

$$\langle\alpha||\hat{F}^{k\kappa}_{tr}||\beta]=\frac{1}{\hat{j}_a\sqrt{2}}\begin{bmatrix} b & k & a \\ m_b & \kappa & m_a\end{bmatrix}\begin{bmatrix} \frac{1}{2} & t & \frac{1}{2} \\ q_b & \tau & q_a\end{bmatrix}\langle a||F||b\rangle. \qquad (B11)$$

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