CALCULATION OF PARTICLE-HOLE STATES IN THE 2s-1d SHELL *

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A method is developed for calculating the positions of the particle-hole states in the sd-shell. Configurations with up to 4-holes have been included. Results are presented for the nuclei ^{16}O to ^{20}Ne.

The presence of low-lying particle-hole states in the spectra of the sd-shell nuclei is well established. In a shell model description of such states one is confronted with two major problems. First, the number of possible excitations is very large and it is at present not clear which type of correlations are energetically favoured [1, 2]. Second, the energy positions have to be calculated rather accurately since the final aim is to make a comparison with the particle states and analyze the interference between the two types of configurations. In the method used here we have tried to minimize these difficulties. A similar approach has recently been used by Arima et al. [3].

The total Hamiltonian is expressed in the form

$$H = H_p + H_h + V_{ph} \qquad (1)$$

where H_p refers to the coordinates of the sd-shell particles H_h the coordinates of the p-shell particles (or holes) and V_{ph} the residual particle-hole interaction. The basic form of the wave functions is chosen to be

$$|\Phi_{\nu JT}\rangle = \{\,|(sd)^{n_p}\,\alpha J_p T_p\rangle |p^{-n_h}\,\beta J_h T_h\rangle\}_{JT} \qquad (2)$$

where n_p is the number of particles in the sd-shell, J_p and T_p the spin and isospin of the particles, n_h the number of holes in the p-shell with spin and isospin J_h and T_h. Finally, the wave function is coupled to total spin J and isospin T.

As a good physical starting point we choose the wave function in eq. (2) to be a solution of the two first terms in the Hamiltonian (1). The particle wave function is taken to be an eigenstate of H_p corresponding to the shell model problem for n_p particles in the sd-shell. Similarly, the hole wave function represents the shell model problem for n_h holes in the p-shell. The structure of such eigenstates are rather well known. Furthermore, to the extent that the two or three lowest eigenstates correspond to particles or holes outside a closed ^{16}O core the energy eigenvalues can be obtained from the experimental binding energies [4]. The eigenstates with fixed numbers of particles and holes for the total Hamiltonian are in general a linear combination of states of the form given in eq. (2). However, our main purpose is to calculate the energy position of the different particle-hole configurations and the energy expression is given by

$$E_{\nu JT} = E_{\alpha J_p T_p} + E_{\beta J_h T_h} + \langle \Phi_{\nu JT} | V_{ph} | \Phi_{\nu JT} \qquad (3)$$

The two first terms are taken from experiment and only the last term has to be evaluated explicity. When necessary, off-diagonal matrix elements which are due to V_{ph} only, can be calculated in a similar way. The calculation of the particle-hole matrix elements is performed in the SU_3 coupling scheme where the particle and hole wave functions take a particularly simple form. The elements which enter the calculation are the coefficients of fractional parentage for $SU_6 \rightarrow SU_3$ [5] together with the Wigner and Racah coefficients for the SU_3 group in the chain $SU_3 \rightarrow R_3$ [6]. The details of the calculation will be given elsewhere. For the twobody interaction we have chosen Gillet's potential [7], the Coulomb interaction is also included. As a basis for the wave functions we have used the calculation of Inoue et al. [8] for the sd-shell part and that of Cohen and Kurath [9] for the p-shell part. So far

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Table 1
Positions of negative parity particle-hole configurations. The excitation energies are referred to the ground state of the respective nuclei.

Nucleus	Number of holes	Particle structure $(\lambda_p \mu_p)$	L_p	J_p^{μ}	T_p	Hole structure $(\lambda_h \mu_h)$	L_h	J_h^{μ}	T_h	J^{μ}	T	$E_{\nu JT}$ (MeV)
^{16}O	3	(60)	0	$1/2^+$	1/2	(03)	1	$1/2^-$	1/2	1^-	0	14.0
		(60)	2	$5/2^-$	1/2	(03)	1	$1/2^-$	1/2	3^-	0	14.0
		(60)	0	$1/2^+$	1/2	(03)	1	$1/2^-$	1/2	0^-	0	15.8
		(60)	2	$5/2^+$	1/2	(03)	1	$1/2^-$	1/2	2^-	0	16.0
^{17}O	1	(40)	0	0^+	1	(01)	1	$1/2^-$	1/2	$1/2^-$	1/2	4.6
		(02)	2	2^+	1	(01)	1	$1/2^-$	1/2	$5/2^-$	1/2	6.8
		(40)	0	1^+	0	(01)	1	$1/2^-$	1/2	$3/2^-$	1/2	6.8
	3	(80)	0	0^-	0	(03)	1	$1/2^-$	1/2	$1/2^-$	1/2	6.1
		(80)	2	2^+	0	(03)	1	$1/2^-$	1/2	$5/2^-$	1/2	7.6
		(80)	2	2^+	0	(03)	1	$1/2^-$	1/2	$3/2^-$	1/2	8.3
^{18}O	1	(60)	0	$1/2^+$	1/2	(01)	1	$1/2^-$	1/2	1^-	1	5.9
		(60)	2	$5/2^+$	1/2	(01)	1	$1/2^-$	1/2	3^-	1	5.8
		(60)	0	$1/2^+$	1/2	(01)	1	$1/2^-$	1/2	0^-	1	6.8
		(60)	2	$5/2^+$	1/2	(01)	1	$1/2^-$	1/2	2^-	1	7.2
	3	(81)	1	$3/2^+$	1/2	(03)	1	$1/2^-$	1/2	2^-	1	10.1
^{18}F	1	(60)	0	$1/2^+$	1/2	(01)	1	$1/2^-$	1/2	0^-	0	3.0
		(60)	2	$5/2^+$	1/2	(01)	1	$1/2^-$	1/2	3^-	0	4.0
		(60)	2	$5/2^+$	1/2	(01)	1	$1/2^-$	1/2	2^-	0	3.8
		(60)	0	$1/2^+$	1/2	(01)	1	$1/2^-$	1/2	1^-	0	4.0
	3	(81)	1	$3/2^+$	1/2	(03)	1	$1/2^-$	1/2	1^-	0	7.9
^{19}F	1	(80)	0	0^+	0	(01)	1	$1/2^-$	1/2	$1/2^-$	1/2	0.5
		(80)	2	2^+	0	(01)	1	$1/2^-$	1/2	$5/2^-$	1/2	1.9
		(80)	2	2^+	0	(01)	1	$1/2^-$	1/2	$3/2^-$	1/2	2.6
	3	(82)	0	0^+	1	(03)	1	$1/2^-$	1/2	$1/2^-$	1/2	9.4
^{19}O	1	(61)	1	2^+	1	(01)	1	$1/2^-$	1/2	$5/2^-$	3/2	4.8
		(42)	0	0^+	2	(01)	1	$1/2^-$	1/2	$1/2^-$	3/2	4.9
	3	(82)	0	0^+	1	(03)	1	$1/2^-$	1/2	$1/2^-$	3/2	7.1
^{20}Ne	1	(81)	2	$5/2^+$	1/2	(01)	1	$1/2^-$	1/2	3^-	0	8.1
		(81)	1	$3/2^+$	1/2	(01)	1	$1/2^-$	1/2	2^-	0	8.3
		(81)	1	$3/2^+$	1/2	(01)	1	$1/2^-$	1/2	1^-	0	9.5

only the major SU_3 components for the particle and hole wave functions have been included which represent at least 70% of the wave functions.

The results in tables 1 and 2 show that the particle-hole interaction depends rather weakly on the spin and isospin quantum numbers. The main contribution is proportional to the product of the number of particles and holes and is due to that part of the force which is a SU_3 scalar in the particle and hole coordinates separately. Thus the spacings between the different particle-hole states are mainly determined by the two first terms in eq. (3). Furthermore, the particle-hole interaction shows large off-diagonal matrix elements between different particle-hole states with the same space structure. This can in some cases give rise to a significant mixing which is the case for the 2-hole states in ^{16}O and ^{20}Ne (see footnote in table 2). Another feature which shows up in the results is that the particle-hole interaction favours high intermediate T_p and T_h, an effect discussed in refs. 1 and 2. However, this is usually compensated by a preference of low T-values for the particle and hole energies. A total SU_3 classification of the particle-hole states has earlier been suggested [10]. We have found clear indications that such a coupling scheme is not favoured by the particle-hole interaction. For example in ^{16}O, the $(\lambda\,\mu) = (84)$ $J = 0$ state with 4-particle excitations lies approximately 3 MeV above the results obtained here. This also seems to be the case in the other nuclei studied so far.

The low-lying negative parity states are well reproduced in nearly all cases. It is especially encouraging to find a $1/2^-$ state in ^{19}F already at 0.5 MeV. In all nuclei the 1-hole states lie lowest. It has been suggested [11] that the 3-hole states in ^{16}O should start at approximately 10 MeV in order to resolve the difficulties in the

Table 2
Positions of positive parity particle-hole configurations. The excitation energies are referred to the ground state of the respective nuclei

Nucleus	Number of holes	Particle structure $(\lambda_p\mu_p)$	L_p	J_p^μ	T_p	Hole structure $(\lambda_h\mu_h)$	L_h	J_h^μ	T_h	J^μ	T	$E_{\nu JT}$ (MeV)
^{16}O	4	(80)	0	0^-	0	(04)	0	0^+	0	0^+	0	8.9
	2	(40)	0[a]			(02)	0[a]			0^+	0	9.5
^{17}O	2	(60)	0	$1/2^+$	1/2	(02)	0	0^+	1	$1/2^+$	1/2	7.9
		(60)	2	$5/2^-$	1/2	(02)	0	0^+	1	$5/2^-$	1/2	8.2
		(60)	2	$5/2^+$	1/2	(02)	2	1^+	0	$7/2^-$	1/2	9.0
		(60)	0	$1/2^+$	1/2	(02)	2	1^-	0	$3/2^+$	1/2	9.2
	4	(81)	1	$3/2^+$	1/2	(04)	0	0^+	0	$3/2^+$	1/2	9.2
^{18}O	2	(80)	0	0^+	0	(02)	0	0^+	1	0^+	1	3.9
		(80)	2	2^+	0	(02)	0	0^+	1	2^+	1	5.6
		(80)	4	4^+	0	(02)	0	0^-	1	4^+	1	8.5
	4	(82)	0	0^+	1	(04)	0	0^+	0	0^+	1	9.7
^{18}F	2	(80)	0	0^+	0	(02)	2	1^+	0	1^+	0	2.7
		(80)	2	2^+	0	(02)	2	1^+	0	3^+	0	4.3
		(80)	2	2^+	0	(02)	2	1^-	0	2^+	0	4.0
	4	(82)	2	3^+	0	(04)	0	0^+	0	3^+	0	11.1
^{19}F	2	(81)	1	$3/2^+$	1/2	(02)	0	0^+	1	$3/2^+$	1/2	6.5
^{19}O	2	(81)	1	$3/2^+$	1/2	(02)	0	0^+	1	$3/2^+$	3/2	4.4
		(81)	2	$5/2^-$	1/2	(02)	0	0^+	1	$5/2^+$	3/2	4.7
^{20}Ne	2	(82)	0[a]			(02)	0[a]			0^+	0	8.9

a. These states are mixtures of intermediate T_p and T_h with the same space structure

$$|^{16}O\rangle = 0.888\,|T_p \text{ and } T_h = 1\rangle - 0.459\,|T_p \text{ and } T_h = 0\rangle$$

$$|^{20}Ne\rangle = 0.908\,|T_p \text{ and } T_h = 1\rangle - 0.419\,|T_p \text{ and } T_h = 0\rangle$$

For comparison. states with total maximum space symmetry [f] = [4444] and [f] = [44444] respectively. the magnitude of the coefficients is $2^{-1/2}$ with the same signs as above.

1-particle 1-hole model. However, we do not find any such states below 14 MeV. This may mean that the interaction has to changed somewhat, although the results for the other nuclei do not seem to support such a solution. In ^{20}Ne the odd parity states are somewhat too high. Here the 3-hole states could make up the difference, but their positions have not yet been calculated.

The results for the positive parity states show that the 4-hole excitations are of little importance for the low-lying states, except for the ^{16}O case. Here the two lowest 0^+ states come at 8.9 and 9.5 MeV with the 4-hole state lowest. This indicates an appreciable admixture of 2-particle excitation in the 6.06 MeV state. In ^{17}O the positive parity states above 5 MeV are found to be primarily 2-hole states with spin values in good agreement with experiment. The ^{18}O case shows only four states below 10 MeV. The 2-hole configuration with $T_p = 2$ as suggested by Zamick [2] is clearly too high (~ 12 MeV). Also in ^{18}F low-lying particle-hole states are important. As earlier suggested [3], the 1^+ state at 1.7 MeV seems to be dominantly a 4-particle 2-hole state. The ^{19}O spectrum provides some difficulties. The state at 3.22 MeV with $J = 1/2^+$ which does not arise from a 3-particle configuration is not obtained in this calculation. However, two low-lying states with $J = 3/2^+$ and $5/2^+$ have been found which could modify the usual 3-particle description somewhat. The calculation of ^{20}Ne shows a $J = 0^+$ state at 8.9 MeV which indicated that one of the two 0^+ states around 7 MeV could be a 6-particle 2-hole state.

The results obtained so far will be modified somewhat by using better particle and hole wave functions. However, preliminary calculations show only minor changes in the energy positions are to be expected. Far more important is the mixing between configurations with different numbers of holes. Such calculations are now in progress. In the method used here spurious states due to center-of-mass motion can occur. For the selection of states used so far the calculations indicate an admixture of the order of 10%

in some cases and it is at present not clear how this will affect the energies.

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A NOTE ON RE-ARRANGEMENT ENERGY

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The Brueckner re-arrangement energy in light closed shell nuclei is estimated using wavefunctions in a Saxon-Woods well. that fit electron scattering and proton separation energies. In contrast with previous work. the energy is approximately constant at 5-6 MeV per particle.

Köhler [1] has pointed out that an estimate of the Brueckner re-arrangement energy can be obtained from our knowledge of (a) the total energy E of a nucleus, as obtained from mass data and (b) the separation energies E_i of individual nucleons, as obtained from the (p, 2p) and (e, e'p) reactions, together with a calculated value of the average kinetic energy of nucleons in nuclei. In fact, the average re-arrangement energy per nucleon is then given by

$$E_R = (2/A)\left[\tfrac{1}{2}\sum(E_i + \langle T_i\rangle) - E\right]. \qquad (1)$$

From a study of ^{12}C, ^{16}O and ^{27}Al he concludes that E_R decreases as A increases.

We first apply the method used by Köhler to the data for ^{32}S and ^{40}Ca, i.e. we use harmonic oscillator wavefunction with the appropriate spring constant in order to calculate $\langle T_i\rangle$, and we put the neutron separation energies equal to the proton ones, allowing for the Coulomb repulsion by means of the mass formula. Results are given in table 1. The major uncertainties do not lie, as might be thought, in the experimental values for E_i, but in the values of $\langle T_i\rangle$, which are based for nuclei beyond $A > 16$ on the simple formula $\hbar\omega = 41A^{-1/3}$ MeV, and in the validity of the simple Coulomb correction.

In order to test these uncertainties, we have calculated E_i for neutrons and $\langle T_i\rangle$ for both protons and neutrons, for ^{12}C, ^{16}O, ^{28}Si, ^{32}S and ^{40}Ca, using single particle wavefunctions in an energy-dependent Saxon-Woods well, the parameters of which have been adjusted so that the proton wavefunctions yield the correct charge density for elastic electron scattering, and the proton eigenenergies are those found from the (p, 2p) and (e, e'p) reaction [6, 7]. The corresponding neutron well was obtained by taking into account the energy and i-spin dependence of the potential [7]. Results are given in table 2. These are substantially in agreement with those in table 1 and thus confirm the simple estimates [1]. (It should be noted that $\sum E_i$ in table 2 includes the Coulomb repulsion, while in table 1 it does not, so that we must compare $\sum E_i - 2E_c$ in table 1 with $\sum E_i$ in table 2. The agreement is then excellent.) The accuracy of