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Nuclear-Structure Calculations in ^{18}F

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The two intrinsic Hartree-Fock (HF) states, one characterized by isospin $T = T_z = \frac{1}{2}(N-Z)$ and the other containing an admixture of $T = T_z$ and $T = T_z + 1$, lie energetically very close in the case of light odd-Z–odd-N nuclei. As a result, the low-lying $T = T_z$ states of these nuclei have substantial "band mixing." The HF projection formalism is employed to investigate the effect of band mixing on the properties of nuclear states in ^{18}F by explicitly treating all the nucleons. The results of our calculations are in fair agreement with the experimental data.

1. INTRODUCTION

There are many shell-model calculations available in the literature[1] for simple odd-Z–odd-N nuclei such as ^{18}F and ^{14}N. With ^{16}O as a core, these nuclei provide the simplest system of a neutron-proton pair of particles or holes. The recent trend has been to employ, in these shell-model calculations, effective model interactions derived from the realistic nucleon-nucleon (NN) interactions.[2] The simplicity of these calculations is more than compensated for by difficulties and uncertainties involved in the derivation[3] of the model interaction. The first successful attempt to explain the two-nucleon (outside the ^{16}O core) energy spectra of ^{18}O and ^{18}F by employing the model interaction derived from the free NN interaction was by Kuo and Brown.[3] However, there were some errors[4] in calculating the contributions from the second-order tensor interaction and the core-polarization effects. When these are properly rectified in rather involved calculations, the computed energy spectrum of ^{18}F does not agree well with the experimental spectrum: The lowest state is predicted to have $J=3$, $T=0$ in contrast to the actual $J=1$, $T=0$ for the ground state. It is quite obvious[4] that the calculation of core-polarization effects is very laborious and it involves some approximations to take the core excitations into account. In view of this state of affairs in computing the renormalized effective NN interaction to incorporate the effect of core polarization, one cannot use the electromagnetic properties of the nuclear states to test the shell-model wave functions; rather one has to introduce an arbitrary "effective charge" for the "valence" nucleons. These undesirable features can be removed in the framework of Hartree-Fock (HF) projection formalism by explicitly treating all the nucleons in the system in a sufficiently large configuration space. The two intrinsic HF states, one characterized by $T = T_z$ and the other containing an admixture of $T = T_z$ and $T = T_z + 1$, lie very close in energy in the case of light odd-Z–odd-N nuclei. This necessitates a band-mixing calculation[5] which is rather involved. From the calculations reported in this paper, we find that the properties of the low-lying positive-parity levels of ^{18}F are quite sensitively dependent on the band-mixing matrix element between the good J and T states projected from the two intrinsic HF states.

2. METHOD OF CALCULATION

The HF method of solving for self-consistent single-particle wave functions and energies is well known and can be found, for example, in Ref. 6. The projection method for obtaining states

of good angular momentum J and isospin T from the intrinsic HF state is described in Ref. 7. Since the $K=1$ and $K'=0$ HF bands of ^{18}F are very close in energy, there is considerable band mixing in the wave functions for states with $T=0$. The formulation of the band-mixing calculation is given in Ref. 5. However, for completeness, we quote here the relevant formulas. The normalized wave function of the state $|JM\rangle$ with energy ϵ_J can be written in the form

$$\Psi_M^J = N_J(\psi_{MK}^J + \omega_J \psi_{MK'}^J), \tag{1}$$

where ψ_{MK}^J is the normalized wave function with energy E_{JK} from the intrinsic HF state Φ_K, and the band-mixing coefficient ω_J is given by

$$\omega_J = \left(\frac{E_{JK} - \epsilon_J}{E_{JK'} - \epsilon_J}\right)^{1/2}. \tag{2}$$

The normalization factor N_J in Eq. (1) is given in terms of the overlap $q_{KK'}^J$ of the wave functions ψ_{MK}^J and $\psi_{MK'}^J$ by the relation

$$N_J = (1 + \omega_J{}^2 + 2\omega_J q_{KK'}^J)^{-1/2}. \tag{3}$$

The energy ϵ_J can be expressed as

$$\epsilon_J = X_J \pm (X_J{}^2 + Y_J)^{1/2}, \tag{4}$$

where

$$X_J = \frac{\frac{1}{2}(E_{JK} + E_{JK'}) - q_{KK'}^J E_{KK'}^J}{1 - (q_{KK'}^J)^2},$$

$$Y_J = \frac{(E_{KK'}^J)^2 - E_{JK}E_{JK'}}{1 - (q_{KK'}^J)^2}.$$

Here $E_{KK'}^J$ is the band-mixing matrix element of the Hamiltonian between the states ψ_{MK}^J and $\psi_{MK'}^J$. The computation of static electromagnetic moments and the lifetimes of the nuclear states requires the evaluation of the matrix element of a tensor operator T^λ (of rank λ) between the initial and final states Ψ_M^J and $\Psi_{M'}^{J'}$, respectively. It is straightforward to obtain the following expressions:

$$\langle \Psi_J^J | T^\lambda | \Psi_J^J \rangle = N_J{}^2 (JJ, \lambda 0 | JJ) \times (T_{KK}^{JJ} + \omega_J{}^2 T_{K'K'}^{JJ} + 2\omega_J T_{KK'}^{JJ}), \tag{5}$$

$$B(\lambda; J \to J') = N_J N_{J'} \frac{2J'+1}{2J+1} \times (T_{KK}^{JJ'} + \omega_J \omega_{J'} T_{K'K'}^{JJ'} + \omega_{J'} T_{KK'}^{JJ'} + \omega_J T_{K'K}^{JJ'})^2, \tag{6}$$

where $(J_1M_1, J_2M_2 | J_3M_3)$ is the vector-coupling coefficient and $T_{KK'}^{JJ'}$ is the reduced matrix element $\langle \psi_K^J \| T^\lambda \| \psi_{K'}^{J'} \rangle$ for which the analytical expression is available.[8]

TABLE I. The HF energy E_{HF} (in MeV), intrinsic mass quadrupole moment Q_{HF} (in fm^2), and mass rms radius R_{HF} (in fm) for ^{18}F are tabulated.

NN interaction	Band	E_{HF}	Q_{HF}	R_{HF}
Modified Elliott	$K=1$	−134.01	24.96	2.861
	$K'=0$	−133.47	22.30	2.862
Elliott	$K=1$	−84.53	25.64	2.440
	$K'=0$	−84.47	24.73	2.441

3. CALCULATIONS AND RESULTS

The HF calculations for ^{18}F were performed in a configuration space of the first four major harmonic-oscillator shells with an appropriate value of 1.7 fm for the oscillator size parameter $b = (\hbar/M\omega)^{1/2}$. The effective *NN* interaction of Elliott *et al.*[9] was employed in these calculations. However, this interaction is inadequate to reproduce the binding energies and the excited-state spectra of the nucleus under consideration. The same conclusion was arrived at in our earlier investigations[5,10,11] in light and medium nuclei. The nuclear binding energies, sizes, and excited-state spectra are very sensitive to the $^3S_1$ matrix elements, which are precisely the matrix elements not accurately determined in all the available *NN* interactions, owing to the approximations involved in the derivation as well as the uncertainties in the experimental $T=0$ phase shifts. The diagonal $^3S_1$ matrix elements are underestimated, whereas the off-diagonal $^3S_1$ and $^1S_0$ matrix elements are overestimated in the *NN* interaction of Elliott *et al.*[9] as discussed in detail in Refs. 10 and 11. By increasing the diagonal $^3S_1$ matrix elements by 25% and reducing the off-diagonal S-state matrix elements by 40%, we have obtained a good fit[12] to the

TABLE II. The projected energy spectrum of ^{18}F with the modified Elliott interaction. The weight P_{JK} and energy E_{JK} of the state with good J and T in the intrinsic HF state are tabulated in the third and fourth columns, respectively. The energy ϵ_J after band mixing is shown in the fifth column.

K	$J(T)$	P_{JK}	E_{JK}	ϵ_J	ϵ_J (expt)
0	0(1)	0.1283	−133.04	−133.04	−136.33
0	1(0)	0.0407	−134.74	−135.62	−137.37
0	2(1)	0.2367	−132.67	−132.67	−134.31
0	3(0)	0.1741	−134.62	−135.00	−136.43
0	4(1)	0.1343	−131.90	−131.90	−132.72
0	5(0)	0.2659	−134.70	−134.70	−136.25
1	1(0)	0.2008	−134.12	−131.25	−135.67
1	2(0)	0.1364	−133.32	−133.32	−134.84
1	3(0)	0.3289	−134.33	−132.38	−134.02
1	4(0)	0.0650	−131.55	−131.55	
1	5(0)	0.2554	−134.70		

binding energies, sizes, and energy spectra of quite a number of p- and sd-shell nuclei. The results for ^{18}F obtained with this modified NN interaction are presented in this paper. It is found that ^{18}F has an axial prolate shape in the lowest intrinsic HF states which are characterized by band quantum numbers $K=1$ and $K'=0$. The HF energies, mass rms radii, and intrinsic mass quadrupole moments for both bands in ^{18}F are presented in Table I. The HF energy of ^{18}F is in good agreement with the experimental ground-state energy – 137.37 MeV. The rms radius is not known experimentally but nevertheless our calculated value seems to be reasonable for this mass region.

The computed energy spectrum of ^{18}F is shown in Table II and the relative level spacings are displayed in Fig. 1. The over-all agreement between the experimental and calculated energy spectra is quite satisfactory except in the case of the excited 1^+ ($T=0$) and 0^+ ($T=1$) states. Our result for the excited 1^+ ($T=0$) state is in conformity with that of shell-model calculations[1,3,4] in which this state comes out to be ~3 MeV too high as compared with the observed 1^+ state at 1.70 MeV. It has been stipulated[1] that this state probably arises because of 4p-2h configuration relative to ^{16}O core. However, the self-consistent HF calculations for this configuration place the corresponding intrinsic HF state 30 MeV too high. This seems to be the trend[13] for all the available effective NN interactions, which give the excited states corresponding to 2p-2h and 4p-2h excitations very high energies of this order. We fail to understand the structure of the excited 1^+ state at 1.70 MeV. The disagreement in the case of the excited 0^+ ($T=1$) state is probably due to the admixture of the higher 0^+ ($T=1$) state which is experimentally observed[14] at 4.74 MeV. There is no way to determine this admixture in the framework of the present projection calculations.

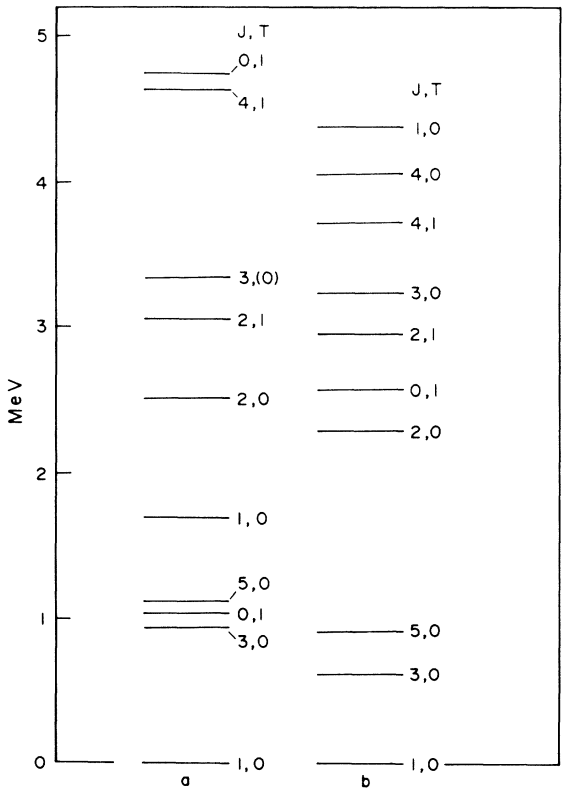

FIG. 1. The experimental energy spectrum of ^{18}F is shown in column a. The projected spectrum after band-mixing calculations is shown in column b.

It may be noted here that the band-mixing overlap $q^J_{KK'}$ for the $J=5$, $T=0$ state is unity. This indicates that one is obtaining the same $J=5$ state from the two bands $K=1$ and $K'=0$. This conclusion is also substantiated by the fact that the numerical values of E_{JK} and $E_{JK'}$ for the $J=5$ state from the two bands are the same, as seen in Table II. We should also stress one more point regarding the band-mixing calculations in ^{18}F. The results for the $T=0$ states are found to be quite sensitive to the band-mixing matrix element $E^J_{KK'}$. We have evaluated $E^J_{KK'}$ quite accurately to obtain the results presented in Table II and Fig. 1. We have, however, seen that a slight variation in the value of $E^J_{KK'}$ significantly affects the positions of the 1^+ ($T=0$) and 3^+ ($T=0$) states. This means that the computed energies of these $T=0$ states will critically depend on the effective NN interaction employed in the calculations. The NN interaction employed in our calculations seems to be reasonable in view of the agreement obtained in the binding energies, rms radii, and excited-state spectra of the nuclei in this mass region.[12]

The experimental data on the static electromagnetic moments are not available for the states in ^{18}F with the exception of the magnetic dipole moment of the $J=5$ ($T=0$) state. The computed value of $2.90\mu_N$ is in good agreement with the observed magnetic moment ($2.83\mu_N$). It should be mentioned

TABLE III. The computed quadrupole moment Q (in $e\times10^{-24}$ cm^2), magnetic moment μ (in μ_N), and mean lifetime τ (in psec) for the states in ^{18}F are tabulated.

$J(T)$	ϵ_J (expt)	μ	Q	τ	τ (expt)
1(0)	0	1.14	−0.005		
3(0)	0.94	2.25	−0.048	120.0	68 ± 7
0(1)	1.04	···	···	0.02	<0.30
5(0)	1.12	2.90	−0.068	63.0×10^4	$(21\pm1)\times10^4$
2(0)	2.53			3.0	0.90 ± 0.20
2(1)	3.06			0.01	<0.17

here that the simple shell-model calculation gives $\mu = 2.88\mu_N$ corresponding to the configuration $(d_{5/2})^2_{J=5}$. We have tabulated (Table III) the static moments for the lowest $J = 1, 3, 5$ states with the expectation that experimental data will be available in the near future. The lifetimes of various excited states computed with $e_p = e$, $e_n = 0$ are shown in Table III. The calculated lifetimes in the case of $E2$ transitions are a factor of 2 to 3 larger than the experimental values.[14] This could be due to the truncation of the model space, since the effect of the *sdg* shell on the two "valence nucleons" in the *sd* shell is expected to be quite significant. We find from the HF calculations that the intrinsic charge quadrupole moment $Q^p_{\rm HF}$ increases by a factor of 1.2 when the *sdg* shell is included in the model space. This means that the inclusion of the *sdg* shell would increase the $B(E2)$ values and correspondingly reduce the lifetimes of the nuclear states. The projection calculations, however, become too lengthy and were therefore not carried out. The computed large lifetimes may also be due to the fact that we have considered only the two lowest bands in our calculations. The band mixing from higher bands neglected in our calculation may also lead to improved values for the lifetimes. However, band-mixing calculations for the 18-nucleon system are too lengthy to be carried out for more than two bands. Due to these practical difficulties, one has to assign an effective charge in order to obtain correct lifetimes. We find that by assigning $e_p = 1.25e$ and $e_n = 0.25e$, the experimental lifetimes can be reproduced. It should be stated here that the spectroscopic factors can also be computed from the projected wave functions as shown in Ref. 8. We have computed the spectroscopic factors for the $J = 1$, $T = 0$ (ground); $J = 3$, $T = 0$; and $J = 0$, $T = 1$ states of ^{18}F. The relative spectroscopic factors are 1.0, 1.6, and 1.25, respectively. These values are in fair agreement with the experimental results.

4. CONCLUSIONS

The HF projection formalism has been applied to investigate the effect of band mixing on the properties of $T = 0$ states in ^{18}F by explicitly treating all the nucleons in the configuration space of the *s*, *p*, *sd*, and *pf* shells. The over-all satisfactory agreement between the calculated and experimental energy spectrum is obtained by employing the effective *NN* interaction of Elliott *et al.*[8] with the *S*-state matrix elements reasonably modified so as to obtain the proper binding energy and size. The static electromagnetic moments are also predicted. The computed lifetimes are a factor of 2 to 3 larger than the experimental values in the case of $E2$ transitions. This is most probably due to configuration truncation. The probable effects of configuration truncation are under investigation.

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