SINGLE-PARTICLE LEVELS IN O^{17} *AND* F^{17} *NUCLEI UNDER THE ASSUMPTION OF STRONG COUPLING OF NUCLEON AND TETRAHEDRALLY SYMMETRIC CORE*

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A method for calculating single-particle states in the α-particle model is proposed, based on the use of a nonspherical potential similar to the Nilsson potential but with different symmetry properties. The spectrum of low lying levels in O^{17} and F^{17} nuclei is calculated by taking into account the interaction between the particle motion and rotation. The results are in satisfactory agreement with the experiments.

As is known, the simplest shell-model description of the nuclei O^{17} and F^{17} (where the external nucleon moves in the field of the spherical core, the core being in the ground state 0^+) successfully explains the spin of the ground state, its magnetic moment, and in addition the relative position of the levels $1d_{5/2}$, $2s_{1/2}$, $1d_{3/2}$.[1,2] The inclusion of a weak interaction of the particle with a high-lying quadrupole vibrational state of the core enables one to explain both the magnitude of the quadrupole moment of O^{17} and also the observed intensity of the E2 transition $2s_{1/2} \to 1d_{5/2}$.[1,3] However, for O^{17} there exists, even at comparatively low excitation energies (starting at 3 MeV), a whole series of negative parity levels for which the reduced nucleon widths for elastic scattering lie within the limits from 1 to 5%. Until now, no satisfactory explanation of these facts had been found. The usual intermediate-coupling shell-theory calculations have not been carried out since, in the present case, they are very cumbersome. On the other hand, experimental results concerning the lower levels of C^{12} and O^{16}, representing an important verification of the α-particle model of the nucleus,[4,5] have recently been obtained. For O^{16} the value of $\hbar^2/2I$ (I is the moment of inertia) is, as indicated by the experimental data, comparatively small (~ 0.5 MeV),[5] but rotational states with small nuclear spin are forbidden by the symmetry properties of the system.

The experimental confirmation of the α-particle model raises the problem of calculating the levels of O^{17} and F^{17} in a scheme where the nucleon is strongly coupled to a core possessing tetrahedral symmetry. In this connection, the symmetry properties of the system already permit for O^{17} and F^{17} rotational excitation of a state with small nuclear spin, including negative parity. This gives hope that the experimental data can be explained. Actually the calculations, the results of which are stated below, indicate that the scheme of lower levels of the nuclei O^{17} and F^{17} agrees satisfactorily with experiment; moreover, owing to a mixing of α-model states, the lower levels $5/2^+$, $1/2^+$, and $3/2^+$ remain practically the same as the single-particle levels of shell theory.

1. CALCULATION METHOD

The Hamiltonian of the internal motion contains a nonspherical potential which, in analogy to the Nilsson potential,[6] we assume to have the form

$$V = \frac{m\omega^2(\delta)}{2} r^2 \left[1 - \delta \frac{i}{\sqrt{2}} (Y_{3,-2} - Y_{3,2})\right]. \tag{1}$$

V is an invariant, i.e., it has the type of symmetry A_1 with respect to transformations of the group T_d (see [7] for the theory of molecular symmetry and for the notation). The ratio $\omega(\delta)/\omega(0)$ equals 1.025, 1.08, 1.21 for $\delta = 0.6$, 1.1, and 1.45, respectively. We take the energy $\hbar\omega(0)$ equal to 14 MeV, [8] although this apparently overestimates the value somewhat, since the motion of the external nucleon is being considered, but $\hbar\omega = 14$ MeV is obtained from the proton density distribution in closed shells. As a consequence of the non-invariance of V with respect to inversion, the wave functions of the required nucleon states of the 1d-2s shell contain admixtures of states of the following 1f-2p shell.

We choose basis functions in the LS-coupling representation. In the calculation we shall take into account the nondiagonal matrix elements of the interaction of particle motion with rotation and the spin-orbit interaction, which play an important role.

The orbital functions of the particle have the following types of symmetry: A_1 (mixes 2s and 1f states), E(1d), and F_2(1d, 2p, and 1f).

The energy levels $\epsilon(\alpha)$ (α is the index of the irreducible representation, $\alpha = A_1, E, F_2$) of a particle in the potential (1) without spin-orbit interaction are as follows: the level A_1 is lowest, for $\delta = 0.6$ the separation $\epsilon(F_2) - \epsilon(A_1)$ equals 0.1 MeV and $\epsilon(E) - \epsilon(A_1)$ amounts to 1.4 MeV; for $\delta = 0.8$ these separations equal 0.8 and 3.2 MeV respectively. The remaining levels are higher by approximately $\hbar\omega$ (the following 2p-1f shell) and so forth.

Each state of the particle has its own corresponding rotational band. For a state with given orbital momentum L and parity π, the orbital part of the total wave function has the form

$$|L\pi(\alpha)M_L\rangle = \frac{1}{\sqrt{f_\alpha}}\sum_r D_{Mr}^{L\pi\alpha *}\varphi_r^\alpha, \qquad (2)$$

since it must be invariant with respect to all transformations of the nuclear axes belonging to the group T_d.

Here $D_{Mr}^{L\pi\alpha *}$ is the r-th basis function of the irreducible representation α, and is represented by a linear combination of the functions $D_{MK}^{L\pi *}$ (the functions D_{MK}^{J} are the same as given by Edmonds [9]; the additional index π denotes the parity of the total wave function); φ_r^α is the wave function describing the motion of the nucleon in the field of the core and is a linear combination of functions $\varphi_r^{l\alpha}$ with given orbital momentum (of the nucleon) l, found by diagonalizing the single-particle Hamiltonian $H_{s.p.} = V + (p^2/2m)$. The Melvin projection operators [10] were used to construct the functions $D_{Mr}^{L\pi\alpha *}$ and $\varphi_r^{l\alpha}$. Matrix representations needed for the calculation are also given in the article by Melvin. We cite the angular part of the functions $\varphi_r^{l\alpha}$:

$$l = 0: \quad \varphi_{r=1}^{l,A_1} = Y_{0,0};$$

$$l = 1: \quad \varphi_{r=1}^{l,F_2} = (Y_{1,-1} - Y_{1,1})/\sqrt{2},$$

$$\varphi_{r=2}^{l,F_2} = i(Y_{1,-1} + Y_{1,1})/\sqrt{2}, \qquad \varphi_{r=3}^{l,F_2} = Y_{1,0};$$

$$l = 2: \quad \varphi_{r=1}^{l,F_2} = i(Y_{2,-1} + Y_{2,1})\ \sqrt{2},$$

$$\varphi_{r=2}^{l,F_2} = (Y_{2,-1} - Y_{2,1})\ \sqrt{2}, \quad \varphi_{r=3}^{l,F_2} = i(Y_{2,-2} - Y_{2,2})\ \sqrt{2},$$

$$\varphi_{r=1}^{l,E} = (Y_{2,-2} + Y_{2,2})/\sqrt{2}, \qquad \varphi_{r=2}^{l,E} = Y_{2,0};$$

$$l = 3: \quad \varphi_{r=1}^{l,F_2} = -(\sqrt{5}Y_{3,-3} - \sqrt{3}Y_{3,-1} + \sqrt{3}Y_{3,1} - \sqrt{5}Y_{3,3}$$

$$\varphi_{r=2}^{l,F_2} = i(\sqrt{5}Y_{3,-3} + \sqrt{3}Y_{3,-1} + \sqrt{3}Y_{3,1} + \sqrt{5}Y_{3,3})/4$$

$$\varphi_{r=3}^{l,F_2} = -Y_{3,0}, \qquad \varphi_{r=1}^{l,A_1} = (Y_{3,-2} - Y_{3,2})/\sqrt{2}.$$

The coefficients of the expansion of the functions $D_{Mr}^{L\pi\alpha *}$ with respect to the functions $D_{MK}^{L\pi *}$ are obtained from the above by complex conjugation.

The complete Hamiltonian, which is subject to diagonalization, has the form

$$H_{s.p.} + C\mathbf{ls} + B(\mathbf{L} - \mathbf{l})^2 \qquad (3)$$

where C = −2 MeV, [1] and $B = \hbar^2/2I = 0.5$ MeV as mentioned above. The nondiagonal matrix elements, as already mentioned, play a rather significant role. For example,

$$\langle 2^-(E), 1/2 : 3/2^- \mid \mathbf{ls} \mid 1^-(F_2), 1/2 : 3/2^- \rangle = 3/\sqrt{5},$$

$$\langle 2^+(F_2) \mid \mathbf{Ll} \mid 2^+(E) \rangle = 2\sqrt{6},$$

Here a function such as $|L\pi(\alpha), 1/2: J\pi, M_J\rangle$ represents the vector sum of an orbital function (2) and a nucleon spin function, and φ_r^α is taken in the form $\varphi_r^{1d,\alpha}$.

2. RESULTS OF THE CALCULATION AND COMPARISON WITH EXPERIMENT

The best agreement between the calculated level spectrum and experiment is obtained for $\delta = 0.8$ to 0.9. For $\delta = 0.8$ the wave functions of the levels have the following form (the order of the levels is the same as that given in the table, see below):

1) $5/2^+$: $\Psi = 0.82\,|2^+(F_2), 1/2 : 5/2^+\rangle + 0.57\,|2^+(E), 1/2 : 5/2^+\rangle$.

Here the nucleon wave function is given by

$$\varphi_r^{F_2} = 0.94\,\varphi_r^{1d,F_2} - 0.28\,\varphi_r^{2p,F_2} - 0.17\,\varphi_r^{1f,F_2};$$

2) $1/2^+$: $\Psi = |0^+(A_1), 1/2 : 1/2^+\rangle$,

$$\varphi^{A_1} = 0.88\,\varphi^{2s} - 0.45\,\varphi^{1f,A_1};$$

3) $1/2^-$: $\Psi = |1^-(F_2), 1/2 : 1/2^-\rangle$;

4) $7/2^-$: $\Psi = 0.99\,|3^-(F_2), 1/2 : 7/2^-\rangle - 0.10\,|4^-(E), 1/2 : 7/2^-\rangle$;

5) $3/2^-$: $\Psi = 0.80\,|1^-(F_2), 1/2 : 3/2^-\rangle + 0.60\,|2^-(E), 1/2 : 3/2^-\rangle$;

6) $3/2^+$: $\Psi = 0.87\,|2^+(F_2), 1/2 : 3/2^+\rangle + 0.49\,|2^+(E), 1/2 : 3/2^+\rangle$;

7) $7/2^-$: $\Psi = |3^-(A_1), 1/2 : 7/2^-\rangle$.

It is assumed, for all of these levels, that the vibrational part of the wave function describes the zero-point oscillations of the O^{16} core.

8) The wave function of the second level $1/2^+$ differs from the wave function of the first level $1/2^+$ by the excitation of one vibrational quantum of the core of type A_1.

The basic results, which are to be compared with experiment, are presented in the table, which includes all the experimentally observed levels

J^{π}	E^*, MeV		$\gamma^2 MR/\hbar^2$		J^{π}	E^*, MeV		$\gamma^2 MR/\hbar^2$	
	theory	exp	theory	exp [11]		theory	exp	theory	exp [11]
5/2+	0	0	0.9	0.4	3/2−	6.1	4.6	0.05	0.06
1/2+	1.6	0.9	0.8	1	3/2+	4.9	5.1	0.9	0.4
1/2−	4.9	3.1	0.05	0.01	7/2−	7.6	5.7	0.2	—
7/2−	6.5	3.9	0.01	0.02	1/2+	7.0	6.4	—	0.02

with excitation less than 5.1 MeV, as well as those levels between 5.1 and 7 MeV which can apparently be unambiguously interpreted. The reduced widths were calculated according to the formula

$$\gamma^2 = \frac{\hbar^2}{MR}\left|\sum_{\alpha} a_\alpha b_{l,\alpha} \sqrt{f_\alpha/(2l+1)}\right|^2,$$

where a_α is the coefficient of the basis function α (e.g., for the $3/2^-$ level we have $a_{F_2} = 0.80$ and $a_E = 0.60$), and $b_{l,\alpha}$ is the coefficient of the function $\varphi^l_{\alpha,r}$ as a function of $\varphi_{\alpha,r}$ (for the same level $3/2^-$, $b_{2p,F_2} = -0.28$ and $b_{2p,E} = 0$).

In addition to the quantities shown in the table, the magnetic moment of the ground state was calculated. The core contribution is

$$\mu_R = \frac{Z}{A}\frac{\langle \mathbf{LJ} - \mathbf{lJ}\rangle}{J+1} = \frac{Z}{A}\frac{J(J+1)+L(L+1)-3/4-2\langle \mathbf{lL}\rangle-2\langle \mathbf{ls}\rangle}{2(J+1)},$$

and a calculation with the foregoing wave functions yields $\mu_R = 0$, so that $\mu_{theor} = -1.91$ nuclear magnetons, i.e., the shell-theory value.

The results with regard to reduced nucleon widths and the magnetic moment indicate that the lower levels $5/2^+$, $1/2^+$, and $3/2^+$ are extremely close to the single-particle $1d_{5/2}$, $2s_{1/2}$, and $1d_{3/2}$ states of the shell model. It is possible that the discrepancy between γ^2_{expt} and γ^2_{theor} for the levels $1d_{5/2}$ and $1d_{3/2}$ is related simply to the choice of scale for the single-particle reduced width.

The results of our calculation confirm the preliminary conclusions reached in the article by one of the present authors and Orlin,[12] but the latter work refers to a situation close to the weak coupling limit. The not very exact agreement between the theoretical and experimental values of the energy levels is apparently due to simplifications made in the calculation: We did not take into account the interaction of the particle with oscillations of the core and the deviation of the shape of the potential well from that of an oscillator; fourth-order harmonics may appear in the potential V [formula (1)], and so forth.

Intermediate-coupling shell-theory calculations for O^{16} yield the same good description of the lower levels as the α-particle model.[13] It appears that they should also give an excellent description of the levels in the nuclei O^{17} and F^{17}. But these complicated calculations, as the example of p-shell nuclei shows, are equivalent to a simple description within the framework of the unified model.[14] In our case it appears that there will be an analogous situation: The intermediate coupling description will be equivalent to our description, only more complicated.

In principle we can also apply our proposed method of describing single-particle states in the α model to nuclei such as C^{13}, Ne^{21}, and others, each of which will have its own particular form of the potential V. Wherever the core has rotational states 2^+, 4^+, ..., the description of many levels will apparently be close to the description within the framework of the unified model (this fact was mentioned in [15] for Be^9). We note that Be^9, C^{13}, and Ne^{21} are nuclei of the latter type, but O^{17} is not.

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Note added in proof (January 17, 1962). In connection with the recent work of D. H. Wilkinson ("Open Questions in Nuclear Structure", BNL 5013, 1961), we remark that the α-particle model of the nucleus gives a quadrupole sum rule distribution (for T=0) over many levels, but the effective charge of a neutron in O^{17} depends, in practice, on the lowest of these levels; moreover, an account of the coupling between the external neutron and E and F_2 vibrations of the core also improves the agreement between theory and experiment with respect to the position of the odd parity levels of O^{17} (the difference in energy values does not exceed 0.3 MeV).

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