EXCITED STATES OF ^{16}O IN THE HARTREE–FOCK (H F) APPROXIMATION[1]

R. MUTHUKRISHNAN
Department of Physics, University of Michigan, Ann Arbor, Michigan
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The intrinsic 4-particle – 4-hole state of ^{16}O is calculated in the Hartree–Fock approximation. The energy and single-particle levels are compared with previous calculations and some observations regarding the two-nucleon interaction are made.

The experiments of Carter *et al.* (1964) show that the excited 0^+(6.06 MeV), 2^+(6.92 MeV), 4^+(10.36 MeV), and 6^+(16.2 MeV) states of ^{16}O have a rotational structure. Shell model calculations (Wong 1966) based on all configurations of $2\hbar\omega$ excitation have failed to explain the 0^+ level at 6.06 MeV. It has been suggested (Brown 1965) that the above states can be described as a rotational band generated by a deformed intrinsic state of a 4-particle – 4-hole type. It is of interest, therefore, to calculate such states in a self-consistent Hartree–Fock approximation. Calculations in which only part of the nucleons are included (Bassichis and Ripka 1965), have been reported. In this paper the results of a H F calculation including all the nucleons is presented. The two-nucleon interaction used is a nonlocal separable potential which acts only in relative *s*-states (Muthukrishnan and Baranger). The form of the potential is

$$V(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}_1', \boldsymbol{r}_2') = -\delta(\boldsymbol{R} - \boldsymbol{R}')f(r)f(r'),$$

where $\boldsymbol{R} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$ and $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. The form of $f(r)$ is

$$f(r) = (4\pi\alpha^2)^{-1}(\gamma/m\alpha)^{1/2}e^{-r^2/4\alpha^2}.$$

The parameters γ and α are chosen to fit the binding energy and density of nuclear matter,

$$\alpha_S = \alpha_T = 1.175 \text{ fm},$$

$$\gamma_S + \gamma_T = 6.167$$

(S and T refer to singlet and triplet respectively). H F calculations for closed shell nuclei with the above interaction have been reported (Muthukrishnan and Baranger 1965).

The Hamiltonian for a many-particle system is (Baranger 1963)

$$H = \sum_{\alpha\beta} T_{\alpha\beta}C_\alpha^\dagger C_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}C_\alpha^\dagger C_\beta^\dagger C_\delta C_\gamma,$$

where T is the kinetic energy operator, $V_{\alpha\beta\gamma\delta}$ is the antisymmetrized two-body matrix element, and the C's are fermion creation and annihilation operators in an arbitrary representation. The H F wave function for an N fermion system is

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$$|\mathrm{H\ F}\rangle = a_1^\dagger a_2^\dagger \ldots a_N^\dagger |0\rangle,$$

where

$$a^\dagger{}_i = \sum_{\alpha=1}^{m} A_\alpha{}^i C_\alpha^\dagger \tag{1}$$

and m is the dimension of the truncated basis (see later). The coefficients A (which can be assumed to be real) are determined by minimizing $\langle \mathrm{H\ F}|H|\mathrm{H\ F}\rangle$ with respect to A. The H F equations are

$$\sum_\gamma W_{\alpha\gamma} A_\gamma{}^i = \epsilon_i A_\alpha{}^i, \tag{2a}$$

where

$$W_{\alpha\gamma} = T_{\alpha\gamma} + \sum_{\beta\delta} V_{\alpha\beta\gamma\delta}\rho_{\delta\beta} \tag{2b}$$

and

$$\rho_{\delta\beta} = \sum_{i=1}^{N} A_\beta{}^i A_\delta{}^i. \tag{3}$$

The one-body density matrix ρ satisfies the conditions

$$\begin{aligned} \rho^2 &= \rho, \\ \mathrm{Tr}\ \rho &= N. \end{aligned} \tag{4}$$

The total energy $E_0 = \langle \mathrm{H\ F}|H|\mathrm{H\ F}\rangle$ is given by

$$E_0 = \left[\sum_{i=1}^{N} \epsilon_i + Tr(T\rho)\right] \Big/ 2.$$

Since W is a function of ρ, an iterative method is used to solve eq. (2a). An initial ρ which satisfies eq. (4) is chosen, W is calculated and diagonalized. A modified ρ is calculated (eq. (3)), with the eigenfunctions of W and the iteration is continued until the A's and ϵ_i's converge to constant values.

The basis functions $|\alpha\rangle$ are chosen to be anisotropic harmonic oscillator wave functions, viz $|n_x n_y n_z\rangle$. The quantum numbers n_x, n_y, and n_z are the number of oscillator quanta in the x, y, and z directions respectively. If one uses a complete set in the expansion (1), the oscillator parameters $a_i = m\omega_i/\hbar (i = x, y \text{ or } z)$ are arbitrary. Owing to the fact that a truncation is made (for practical reasons), the a_i's are also varied to obtain minimum energy.

The single-particle wave functions $|i\rangle$ are assumed to be eigenstates of parity. As a consequence, the matrices W and ρ do not connect states of different parity as shown in Fig. 1(a), (b). Further, each single-particle level is assumed to be occupied by two neutrons (spins up and down) and two protons.

For the even parity levels, 7 basic states are included (all $n_x + n_y + n_z = 0$ and 2) and for the odd parity states, 13 states are included (all $n_x + n_y + n_z = 1$ and 3). The ground state of ^{16}O is calculated by starting with a ρ as shown in

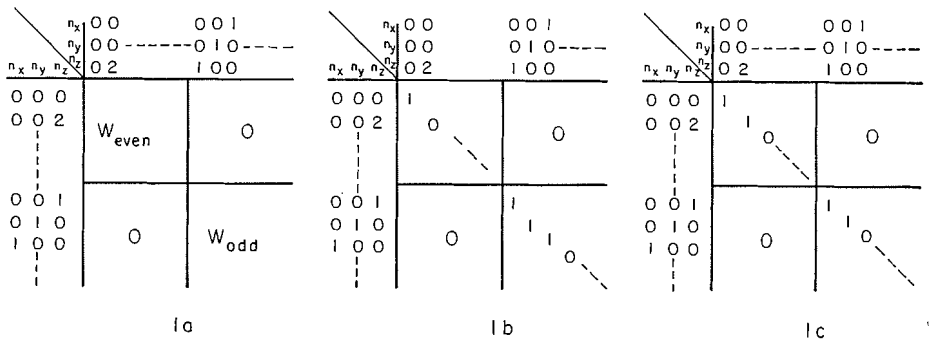

FIG. 1. The form of the matrices W and ρ under the assumption that parity is a good quantum number for the single-particle wave functions. The initial choices of ρ for the ground state and the 4p–4h state of ^{16}O are shown in (b) and (c).

Fig. 1(b). For the 4-particle – 4-hole state, depending on the initial choice of ρ, one obtains different solutions (corresponding to different kinds of deformation). The initial choice of ρ giving minimum energy is that shown in Fig. 1(c).

As is seen from Fig. 2 and Table I, the lowest occupied single-particle state (which is neglected in Bassichis and Ripka (1965)) has gone up in energy by 8 MeV. Thus it is important to include all the particles in any H F calculation

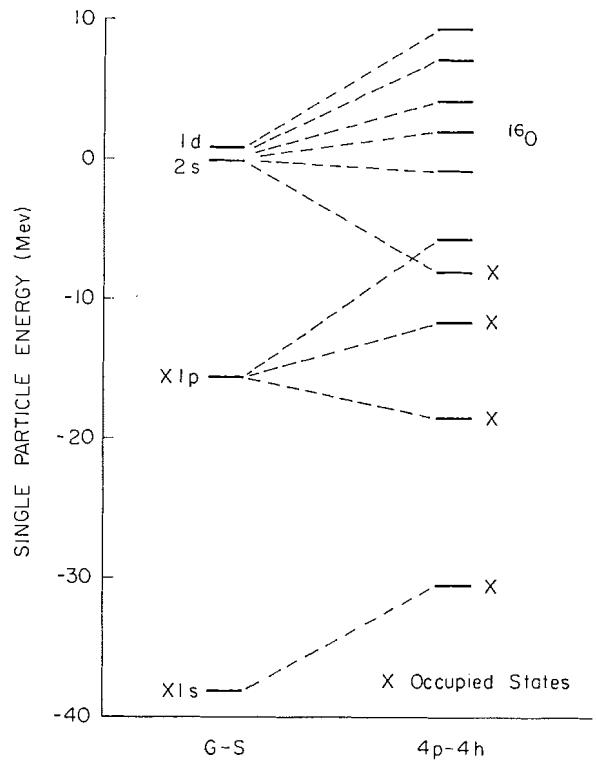

FIG. 2. The single-particle energies for the ground state and the 4p–4h state of ^{16}O.

TABLE I

The single-particle energies and wave functions for the ground state and 4p–4h state of ^{16}O (Each state is occupied by two neutrons and two protons)

State	Binding* energy (MeV)	Single-particle energy (MeV)	Single-particle wave function expanded on the basis $\|n_x n_y n_z\rangle$
^{16}O ground	87	$-38.4(1s)$	$0.998\,0\ \|000\rangle - 0.036\,8\ \|002\rangle - 0.036\,8\ \|020\rangle - 0.036\,8\ \|200\rangle$
state		-15.7	$0.999\,9\ \|001\rangle + 0.009\,9\ \|003\rangle + 0.005\,7\ \|021\rangle + 0.005\,7\ \|201\rangle$
$a_x=a_y=a_z$		$-15.7(1p)$	$0.999\,9\ \|010\rangle + 0.009\,9\ \|030\rangle + 0.005\,7\ \|210\rangle + 0.005\,7\ \|012\rangle$
$=0.245$ fm^{-2}		-15.7	$0.999\,9\ \|100\rangle + 0.009\,9\ \|300\rangle + 0.005\,7\ \|120\rangle + 0.005\,7\ \|102\rangle$
^{16}O 4p–4h	60	-30.4	$0.997\,1\ \|000\rangle - 0.031\ \|002\rangle + 0.055\,3\ \|200\rangle - 0.041\,4\ \|020\rangle$
state		-8.3	$0.998\,8\ \|002\rangle + 0.033\,5\ \|000\rangle - 0.026\,6\ \|200\rangle + 0.023\,2\ \|020\rangle$
$a_x=a_y=0.29$ fm^{-2}		-18.5	$0.998\,3\ \|001\rangle - 0.026\,2\ \|003\rangle - 0.005\,7\ \|021\rangle + 0.052\,2\ \|201\rangle$
$a_z=0.14$fm^{-2}		-11.7	$0.987\,5\ \|100\rangle + 0.152\,1\ \|300\rangle + 0.017\,0\ \|120\rangle - 0.036\,3\ \|102\rangle$

*Center-of-mass kinetic energy is subtracted.

of this kind. The 4-particle – 4-hole state is highly deformed ($a_x = a_y = 0.29$ fm^{-2}, $a_z = 0.14$ fm^{-2}) and asymmetric. The energy of the 4-particle – 4-hole state is 27 MeV above the ground state of ^{16}O. The head of the band corresponding to the O^+ state can be obtained approximately by subtracting the rotational energy,

$$E_{\text{rot}} = \frac{\hbar^2\langle L_x^2\rangle}{2I_x} + \frac{\hbar^2\langle L_y^2\rangle}{2I_y} + \frac{\hbar^2\langle L_z^2\rangle}{2I_z},$$

where $\boldsymbol{L}$ is the total orbital angular momentum. The moments of inertia I are calculated in the rigid body approximation (Mottelson 1958). After subtracting E_{rot}, the energy of the 4-particle – 4-hole state is still 21.2 MeV above the ground state.* This may be due to the fact that the interaction only acts in relative s-states as shown below. Let us assume that the ground state of ^{16}O is $|000\rangle^4$, $|100\rangle^4$, $|010\rangle^4$, $|001\rangle^4$, and the 4-particle – 4-hole state is $|000\rangle^4$, $|010\rangle^4$, $|001\rangle^4$, $|002\rangle^4$. For the present discussion the oscillator parameters a will be assumed to be the same for the ground state and the 4-particle – 4-hole state ($a_x = a_y = a_z$). In practice, because of the deformation of the 4-particle – 4-hole state, there will be a gain in energy. The energy above the ground state of the 4-particle – 4-hole state, under the above assumptions, is

$$\Delta E = 2\hbar\omega + \frac{15}{8} I_{000} + \left(6I_{100} + \frac{3}{4} I_{010} - \frac{15}{4} I_{001}\right) + \left(\frac{3}{2} I_{200} + \frac{3}{2} I_{101} + \frac{3}{2} I_{110} - \frac{15}{4} I_{002} - \frac{3}{2} I_{011}\right) - \frac{3}{4} I_{003} - \frac{3}{8} I_{004},$$

*The author learned that calculations by D. M. Brink and E. Boecker (to be published) for various interactions that fit nuclear matter give similar results for the energy of the 4p–4h state of ^{16}O as the present calculation.

where $I_{n_1 n_2 n_3} = \langle n_1 n_2 n_3 | V_{\text{singlet}} + V_{\text{triplet}} | n_1 n_2 n_3 \rangle$ and the wave functions $|n_1 n_2 n_3\rangle$ are in relative coordinates, $x = x_1 - x_2$, $y = y_1 - y_2$, and $z = z_1 - z_2$. The terms are grouped together according to the total quantum number $N = n_1 + n_2 + n_3$. For interactions which act only in relative even parity states, terms with odd N vanish. In particular, for an s-state interaction of the type used here and for other realistic interactions (Kallio and Kollveit 1964), the term with $N = 0$ is much larger than others. So from eq. (5) we see that with an s-state interaction the only energy gain is due to deformation. On the other hand, if we have a p-state repulsion, the term with $N = 1$ helps to bring down the energy of the 4-particle – 4-hole state, even without deformation (Hayward 1966). But if one includes a p-state repulsive interaction, the s-state attraction has to be increased in order to fit the binding energy of nuclear matter. Thus the only conclusion that can be drawn from the above discussion is that it is unlikely that an s-state interaction (which gives saturation) alone will lower the 4-particle – 4-hole state sufficiently to explain the 0^+ state at 6.06 MeV.

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