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Higher Random-Phase-Approximation Studies of the Structure of O^{16} . I*

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The energy spectrum of O¹⁶ has been investigated theoretically using the basis functions of the nuclear (harmonic-oscillator) shell model. Random-phase-approximation (RPA) techniques are used to decouple the core state from the excited configurations, thereby overcoming the problem of the exaggerated ground-state depression found in standard shell-model calculations. The general equations of the higher RPA are reduced to a more restricted but tractable form which contains both the Tamm-Dancoff approximation and the standard (first) RPA as special cases. For the even-parity states, it is found that the resulting secular equation reduces in good approximation to that of a shell-model calculation with the core state removed. Interaction matrices between all one-hole one-particle and two-hole two-particle states at $1\hbar\omega$ and $2\hbar\omega$ excitation were diagonalized to obtain the level structure of O¹⁶ in the absence of spurious states of center-of-mass motion. A Gaussian central force with Rosenfeld exchange was employed, the strength being determined by a rough fit to the lowest J=0+ and 2+, T=0 levels. Despite the restricted nature of this fit, a remarkably good agreement between the calculated and observed energy spectrum is obtained. The T=0 spectrum is well represented apart from two states (with J=4+ and 6+) which are calculated below the lowest corresponding observed levels. Moreover, the T=1 states of both parities fall correctly in relation to each other and to the fitted states, and the T=2 states are well reproduced.

I. INTRODUCTION

IN recent years, many calculations have been per-formed in an attempt to determine the structure of O¹⁶. Although a measure of success has been achieved, as yet none of these investigations has been able to give a fully satisfactory account of the many experimental quantities now available. The early shell-model work of Elliott and Flowers¹ was directed towards an understanding of the low-lying odd-parity levels and appears to give an adequate description of all but a few of them. Agreement with the empirical data has subsequently been improved by the hole-particle calculations of Gillet,² Gillet and Vinh Mau,³ and of Green et al.,⁴ which were based on the random-phase approximation (RPA). Because of the importance of low-lying twohole two-particle (2h-2p) components, the even-parity

levels could not be successfully included within this framework.

Other models have also enjoyed a certain amount of success. The α -particle model has been used⁵ to predict T=0 levels of both parities. For the lower levels the results are quite satisfactory, but considerably less so at higher energies. Brink and Nash⁶ investigate the rotational bands of O^{16} using a force adapted to the SU_3 scheme. They include up to 2h-2p excitations out of the shell-model core but find their even-parity levels occurring at far too high an energy. A similar calculation⁷ using a more realistic force possesses the same defect but can be brought into reasonable agreement if the calculated energies are all arbitrarily reduced by 17 MeV. The rotational structure of O¹⁶ has also been investigated by Brown and Green,⁸ who include up to 4h-4p excitations from a deformed shell-model core. Taking the unperturbed energies of the configurations as free parameters allows them to fit the experimental energy levels and transition rates very well. The K=0+ and K=0rotational bands and some odd-parity levels have been

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¹ J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. (London) A242, 57 (1957).
² V. Gillet, Nucl. Phys. 51, 410 (1964).
³ V. Gillet and N. Vinh Mau, Nucl. Phys. 54, 321 (1964).
⁴ A. M. Green, A. Kallio, and K. Kolltveit, Phys. Letters 14, 142 (1965).</sup>

^{142 (1965).}

⁵ S. L. Kameny, Phys. Rev. **103**, 358 (1956). ⁶ D. M. Brink and G. F. Nash, Nucl. Phys. **40**, 608 (1963). ⁷ J. Borysowicz and R. K. Sheline, Phys. Letters **12**, 219 (1964).

⁸ G. E. Brown and A. M. Green, Nucl. Phys. 75, 401 (1966).

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described rather neatly by Kelson,⁹ using a deformed intrinsic state and hole-particle excitations arising from a simplified Hartree-Fock minimization technique. Here the agreement with experiment is again quite good. The specific problem of explaining the low energy and the lifetime of the J=0+ state at 6.06 MeV has also received considerable attention. In addition to the foregoing treatments, there have been a number of 1h-1pplus 2h-2p shell-model calculations, ^{10–13} none of which, however, has been entirely satisfactory.

Whereas all these efforts have been confined largely to some specific aspect of the structure of the O¹⁶ nucleus, the recent 1h-1p plus 2h-2p shell-model calculations of Eisenberg et al.,¹⁴ of Seaborn and Eisenberg,¹⁵ and of Wong¹⁶ suggest the possibility of achieving a simultaneous fit to a greater range of experimental results than has previously been practicable. The calculations of Ref. 14 omit the vacuum state and use a zero-range central interaction. In Ref. 15 the spurious states of center-of-mass motion are eliminated. Agreement with experiment is obtained for a few of the lower lying evenparity states, but the T=1 states lie too low in energy and there is a proliferation of even-parity states between 10 and 20 MeV which conflicts with the experimental picture. When the vacuum state is coupled in, the lowest excited 0+ level is shifted up into the region of 14 MeV. Since this shift is mainly due to the lowering of the O+ ground-state energy, the excited spectrum will now lie much higher than is observed. In a similar calculation, Wong¹⁶ couples in the vacuum state and finds that his best agreement with experiment occurs for a realistic Brueckner-Gammel-Thaler force. But in order to get this agreement, he is forced to include a special vacuum energy ϵ_0 which is nonzero only if no hole-particle excitations are present. The parameter ϵ_0 raises the vacuum state against the large depression produced by the matrix elements connecting the vacuum to the 2h-2p states. However, the arguments leading to the inclusion of a nonzero ϵ_0 appear obscure.

In this paper we intend to present some preliminary studies of the O¹⁶ problem based on a 1h-1p plus 2h-2pshell-model approach. For the results to be reliable, it is necessary to remove the spurious states of center-ofmass motion¹⁷ where they occur. This is done here in a way which involves a minimum of auxiliary computation.¹⁸ The problem of the vacuum state has received little attention in the past. If it is coupled in, one finds the large depression of the ground state noted earlier,

- ⁹ I. Kelson, Phys. Letters 16, 143 (1965).
 ¹⁰ Y. Abgrall, J. Phys. Radium 24, 1113 (1963).
 ¹¹ H. Nagai, Progr. Theoret. Phys. (Kyoto) 27, 619 (1962).
 ¹² N. Vinh Mau and G. E. Brown, Phys. Letters 1, 36 (1962).
 ¹³ N. Vinh Mau, Ann. Phys. (Paris) 8, 1 (1963).
 ¹⁴ I. M. Firsterberg, P. M. Science and M. E. Berge, Nucl. Phys.

- ¹⁴ J. M. Eisenberg, B. M. Spicer, and M. E. Rose, Nucl. Phys.
- **71**, 273 (1965). J. B. Scaborn and J. M. Eisenberg, Nucl. Phys. 82, 308 (1966).
 ¹⁶ S. S. M. Wong, Phys. Letters 20, 188 (1966).
 ¹⁷ J. P. Elliott and T. H. R. Skyrme, Proc. Roy. Soc. (London)
- A232, 561 (1955). ¹⁸ R. J. Philpott (to be published).

and if it is arbitrarily left out, one is in some doubt as to the significance of the calculation. We have attempted to solve this dilemma by making recourse to an RPA interpretation. The numerical calculation which is the initial result of this work proves to be identical to a 1h-1p plus 2h-2p shell-model calculation with the vacuum state uncoupled. From it we have obtained the energies of a large number of states of both parities. The extraction of other nuclear data, however, requires the full machinery of the RPA method and has not been attempted as yet. Instead, it is intended to make this the subject of continuing research, the results of which will be reported in due course.

II. THEORY

Derivation of the Random-Phase Formalism

In view of the above-mentioned difficulty associated with the inclusion of the core state in a normal shellmodel calculation, it appears necessary to find some valid alternative. We favor an approach based on the RPA theory. In the usual approximation¹⁹ (first RPA), equations of motion are obtained connecting the operators A^{\dagger} and A, where A^{\dagger} creates and A destroys a holeparticle pair. These can be manipulated into the form of a secular equation which is found to be an extension of the Tamm-Dancoff secular equation among the various 1h-1p states involved. We note that the core state does not appear in either of these methods. The first RPA, however, is too restrictive for our purposes, since we wish to have the 2h-2p states included as an integral part of our formalism. We shall therefore set up a specific formulation of the RPA theory in which these and other more complicated hole-particle excitations may be retained as required. If we choose to ignore all multiple hole-particle excitations beyond the 2h-2p states, we obtain a second RPA. For the sake of definiteness this will be done in the following description, although we may note that the criteria (4) below may be applied to any order of RPA. The equations of this section remain valid for all orders of RPA provided that criteria (4) are used.7 The theory of the second RPA has already been developed from a formal standpoint by Sawicki²⁰ and his co-workers.²¹ The method adopted here is more restrictive than Sawicki's treatment and leads to equations which are formally much simpler than those of the general theory. In spite of this, we nevertheless retain all the terms used by Sawicki in his numerical calculations. In addition, we may list the following important features of our method:

(i) The resulting secular equation reduces to the usual shell-model secular equation between 1h-1p and

¹⁹ M. Baranger, Phys. Rev. 120, 957 (1960), and references cited therein.

²⁰ J. Sawicki, Phys. Rev. 126, 2231 (1962); Nucl. Phys. 23, 285 (1961).

²¹ G. Fano and J. Sawicki, Nuovo Cimento **25**, 586 (1962); J. Sawicki and T. Soda, Nucl. Phys. **28**, 270 (1961).

and

2h-2p states if all "backward-going" components are dropped.

(ii) As far as the energy determination is concerned, the core state is completely decoupled (although the core state is coupled through a subsidiary equation which affects the determination of the wave functions).

(iii) The spurious effects of excited center-of-mass motion are readily removed.

We start from the observation²² that the solutions Γ^{\dagger} of the equation

$$[\mathfrak{K},\Gamma^{\dagger}] = \omega \Gamma^{\dagger}, \qquad (1)$$

where \mathcal{K} is the Hamiltonian of the system and ω is a positive number, have the properties of energy-raising operators. Let us now seek an approximate solution of (1) in a second quantized representation, the vacuum state $|0\rangle$ of which corresponds to the unexcited closed shell core. Since we are interested in operators Γ^{\dagger} which conserve the total number of particles in the system, we may introduce fermion creation and destruction operators and write Γ^{\dagger} in the form

$$\Gamma^{\dagger} = c + \sum_{\alpha\beta} c_{\alpha\beta}(a_{\alpha}^{\dagger}a_{\beta}) + \sum_{\alpha\beta\gamma\delta} c_{\alpha\beta\gamma\delta}(a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\gamma}a_{\delta}) + \cdots, \quad (2)$$

where a_{α}^{\dagger} creates a particle in the state α if α refers to a state outside the core (particle state) or destroys a hole in the state α if α refers to a state inside the core (hole state) and $c, c_{\alpha\beta}, \cdots$ are a set of as yet undertermined constants. The round brackets enclosing each group of a operators indicate that the group is to be taken in normal order with respect to $|0\rangle$ (all creation operators standing to the left of all destruction operators together with an appropriate phase).

If the Hamiltonian 3C is written as

$$\Im C = \sum_{\alpha\beta} \epsilon_{\alpha\beta} (a_{\alpha}^{\dagger} a_{\beta}) + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} (a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}) , \quad (3)$$

where $\epsilon_{\alpha\beta}$ represents the contribution of all singleparticle operators together with the effective singleparticle contribution of the residual interaction V, the commutator of each term in (2) with 3C can be expressed as a sum of normal products of the *a* operators. Thus, we get an infinite sequence of coupled equations. These can be reduced to a closed soluble system if we break the sequence at some point by neglecting all normal products containing more than a certain definite number of *a* operators. The second RPA, which we shall be considering here, neglects all normal products beyond those containing four *a* operators.

At this point, it is advantageous to introduce another limiting assumption, the purpose of which is to formalize a further reduction in the number of terms retained.

We suppose that, among the operators \mathcal{O} resulting from the commutator of one of the components of Γ^{\dagger} with 3C, we may safely neglect all those which fail to obey both

$$\mathfrak{O}|0\rangle \neq 0$$
 (4a)

$$\mathfrak{O}^{\dagger}|\mathfrak{O} \neq 0.$$
 (4b)

The criteria (4a) and (4b) at once simplify the theory, because, apart from the unit operator 1, the only operators which survive are the state creation operators S_q^{\dagger} , which contain strings of *a* operators all of which create when operating on $|0\rangle$, and their Hermitian conjugates S_q . As introduced here, *q* is initially a label which describes the various modes of multiple hole-particle excitation in an uncoupled representation. By extension, we shall in general understand *q* to label any set of states orthogonal to $|0\rangle$. The interpretation of the theory is now much easier, and the removal of the spurious states can be readily accomplished by discarding the associated spurious state creation and destruction operators.

Although a full investigation of the acceptability of the criteria (4a) and (4b) has not been attempted as yet, we have seen that the surviving terms are sufficient to ensure consistency with the work of other authors. We may specifically note that if criterion (4a) alone is used, and either $\epsilon_{\alpha\beta}$ is diagonal or the states q are restricted to those of $2\hbar\omega$ excitation, a standard 1h-1pplus 2h-2p shell-model calculation results. The criteria (4a) and (4b) may also be used to set up the standard (first) RPA theory, in which case the excluded particlescattering and hole-scattering operators can be shown to be rigorously decoupled from the A^{\dagger} and A operators within the assumption that the Hamiltonian 3C contains no terms which create or destroy an odd number of hole-particle pairs. However, considerations of this kind cannot be applied to the second RPA, since such terms in 3°C are required by the matrix elements coupling the 1h-1p to the 2h-2p states.

The equations which arise from the present approximation are now easily obtained. We use the criteria (4) and reduce (2) to a form more suitable for our manipulations by writing

$$\Gamma_k^{\dagger} = c^k + \sum_q c^k_{\ q} S_q^{\dagger} + \sum_q \bar{c}^k_{\ q} S_q, \qquad (5)$$

where c^k , c^k_q , and \bar{c}^k_q are constants and the label k serves to distinguish the independent solutions of (1). The equations of motion for the operators S_q^{\dagger} and S_q become

$$[\mathfrak{IC}, S_q^{\dagger}] = r_q + \sum_{q'} S_{q'}^{\dagger} s_{q'q} + \sum_{q'} S_{q'} t_{q'q} \qquad (6)$$

together with its Hermitian conjugate, where r_q , $s_{q'q}$ and $t_{q'q}$ are known coefficients which are discussed below. Substitution of (5) into (1) then leads to the system of

²² P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, London 1958). See also A. M. Lane, *Nuclear Theory* (W. A. Benjamin, Inc., New York, 1964).

and

(9)

equations

$$\sum_{q'} s_{qq'} c^k{}_{q'} - \sum_{q'} t_{qq'} * \bar{c}^k{}_{q'} = \omega_k c^k{}_q, \qquad (7a)$$

$$\sum_{q'} t_{qq'} c^{k}{}_{q'} - \sum_{q'} s_{qq'} * \bar{c}^{k}{}_{q'} = \omega_{k} \bar{c}^{k}{}_{q}, \qquad (7b)$$

$$\sum_{q} r_{q} c^{k}{}_{q} - \sum_{q} r_{q}^{*} \bar{c}^{k}{}_{q} = \omega_{k} c^{k}.$$
(7c)

Equations (7a) and (7b) contain our second RPA eigenvalue problem for the determination of the excitation energies ω_k and the eigenvector components c^k_q and \bar{c}^k_q , while Eq. (7c) is an auxiliary equation which determines the amount of core component to be included in each energy-raising operator Γ_k^{\dagger} . Once the solutions to (7) have been obtained, we may define a ground-state $|g\rangle$ and excited states $|k\rangle$ in the usual way by

$$\Gamma_k |g\rangle = 0 \text{ for all } k$$
 (8)

$$|k\rangle = \Gamma_k^{\dagger} |g\rangle$$
,

where the state $|k\rangle$ lies at an energy ω_k above the ground-state energy. In this paper we shall use (7) to obtain the excitation energies ω_k , but not attempt to determine any other nuclear properties.

The coefficients r_q , $s_{qq'}$, $t_{qq'}$ may be evaluated from (6) by taking appropriate matrix elements. We assume that the state creation operators S_q^{\dagger} have been chosen to be orthonormal in the sense that

$$\langle 0 | S_q S_{q'}^{\dagger} | 0 \rangle = \delta_{qq'}. \tag{10}$$

Then r_q is given by

$$\boldsymbol{r}_{\boldsymbol{q}} = \langle 0 | [\mathfrak{K}, \boldsymbol{S}_{\boldsymbol{q}}^{\dagger}] | 0 \rangle = \langle 0 | \mathfrak{K} | \boldsymbol{q} \rangle, \qquad (11)$$

where $|q\rangle$ is the state obtained when S_q^{\dagger} operates on the vacuum $|0\rangle$. The r_q coefficients are standard matrix elements connecting the core to the 1h-1p and 2h-2p states. From Eqs. (7) it is seen that these matrix elements have no effect on the excitation energies ω_k which are determined by (7a) and (7b) alone. In a similar way, we have

$$s_{qq'} = \langle q | \mathfrak{K} | q' \rangle - \langle 0 | S_q S_{q'}^{\dagger} \mathfrak{K} | 0 \rangle \tag{12}$$

and

$$t_{qq'} = \langle 0 | \Im C S_{q'}^{\dagger} S_q^{\dagger} | 0 \rangle.$$
(13)

The first term in the formula for $s_{qq'}$ is a standard matrix element and is symmetric in q and q'. The second term is not symmetric; but its action is very limited. To demonstrate this, we note that the only components of 3 \mathcal{C} which can contribute to this term are those containing no destruction operators. If we write n(h) for the number of a operators in one of these components [from Eq. (3) we see that n(h) can take on the values 2 and 4 only] and similarly n(q) for the number of a operators in S_q^{\dagger} , we find that the contribution is nonzero only if

$$n(q) = n(q') + n(h).$$
 (14)

Remembering that $s_{qq'}$ results from the evaluation of

a commutator, it may also be seen that for any component of 3C satisfying (14) the total contribution to $s_{qq'}$ must be zero. It is thus sufficient to evaluate $s_{qq'}$ from the first term of Eq. (12) alone, provided only that we omit the contribution of any component of 3C for which (14) holds. Among the $2\hbar\omega$ states used in the present application of this theory to O¹⁶ the coefficient $s_{qq'}$ is always equal to the standard shell-model matrix element $\langle q | 3C | q' \rangle$.

Because of the form (13) of the matrix element for $t_{qq'}$, in which 3C can contain at most four destruction operators, it can be seen that $t_{qq'}$ is nonzero only if both q and q' refer to 1h-1p states. In view of this, it may happen that the shell-model calculation which results from a complete neglect of the matrix elements $t_{qq'}$ is actually rather a good approximation of the second RPA from which it was derived. (For the T=2 states the two calculations become identical, since in this case there can be no 1h-1p contributions.) If the states of interest obtained from the corresponding shell-model calculation consist mainly of 2h-2p states, a perturbative treatment of $t_{qq'}$ shows that the energies ω_k and the amplitudes c^{k}_{q} remain largely unchanged. The numerical calculations reported below make use of this fact: they have been performed with the specific neglect of all matrix elements $t_{qq'}$.

Formulas for the coefficients r_q , $s_{qq'}$, and $r_{qq'}$ when the states $|q\rangle$ involve angular-momentum couplings can be found in Appendix A.

III. NUMERICAL CALCULATION

Specific Formulation

We now outline the method by which the numerical work was approached. Broadly speaking, the calculation was performed in three stages. Firstly, all the required antisymmetric two-particle matrix elements $_a\langle j_1j_2JT | v | j_3j_4JT \rangle_a$ were evaluated and tabulated. Here, j refers to a single-particle harmonic-oscillator state with quantum numbers nlj and v is the residual pair interaction

$$v = V_0 \exp(-r^2/r_0^2)(W + MP^r + BP^{\sigma} + HP^rP^{\sigma}),$$
 (15)

where P^r , P^σ cause the interchange of the spatial and spin coordinates, respectively, in the two-particle wave function on which they operate. Then, working within the $O^{16} 2\hbar\omega$ states corresponding to a given $J\pi T$ combination, the Hamiltonian matrix $s_{qq'}$ was set up. Finally, this matrix was diagonalized. The last two stages were repeated for all the $J\pi T$ combinations of interest.

This procedure enabled a number of over-all checks to be made on the program. These are described in Appendix B. In addition, we were able to use an especially simple technique¹⁸ for the elimination of the spurious states of center-of-mass motion.

Within the harmonic-oscillator shell-model states, the center-of-mass Hamiltonian \mathcal{H}_{o} has eigenvalues

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 $(n+\frac{3}{2})\hbar\omega$ where $\hbar\omega$ is the oscillator spacing. It can also be shown that \mathcal{K}_c is diagonal between model states in which the total oscillator energy of the contributing single-particle states is different. Thus \mathcal{K}_c can be exactly diagonalized among our set of all $2\hbar\omega$ (or all $1\hbar\omega$) model states. By subtracting the constant term and eliminating unnecessary factors, one can construct from \mathcal{K}_c an operator $\alpha \mathcal{R}_{sp}$ with eigenvalues αn , where n takes on the value of zero for a good state or some positive integer for a spurious state. When this operator is added to the original Hamiltonian *K*, the spurious states are weighted by an additional positive energy αn . If α is taken large enough, the spurious states become effectively decoupled and no longer affect the composition of the low-energy eigenstates. For ease of calculation, the addition was made by modifying the tabulated twoparticle matrix elements and the single-particle energies. In the present work, we arbitrarily took $\alpha = 2400$ to achieve an effective separation of the spurious states without introducing unwanted roundoff errors.

The Energy Parameters

The energy parameters are those entering into the definition of the Hamiltonian 3C. Values for the singleparticle energies ϵ_i are listed in Table I.

The energies for the particles in the 2s-1d shell were obtained from levels observed in O^{17} and the 1p hole energies from the ground state and first excited states of O¹⁵. The 1s hole energy is that used by Spicer and Eisenberg²³ and was derived from (p,2p) scattering experiments and shell-model calculations in N¹⁵. The energies of particles in the 2p-1f shell are not as well known. Jolly,²⁴ analyzing $O^{16}(p,p)O^{16}$ data,²⁵ puts an $f_{7/2}$ resonance at about 15 MeV. He then obtains the energies of the remaining single-particle states from estimates of the spin-orbit energy. These single-particle energies are considerably larger than those of Spicer and Eisenberg. Neither set of 1 f - 2p single-particle energies can be considered particularly reliable. However, the Spicer and Eisenberg 1f-2p energies lie much too close to the 2s-1d shell. If their values are used in an ordinary shell-model calculation of O^{16} , there are such strong 1h-1p components in the first excited state that its lifetime for pair emission is a factor of 3 too short. The present calculation uses Jolly's results for the 1f-2p energies which seem to be more realistic.26

TABLE I. The single-particle spectrum (MeV).

181/2	1\$\$3/2	1/21/2	$1d_{5/2}$	251/2	1 <i>d</i> 3/2	1 <i>f</i> 7/2	2\$3/2	$1f_{5/2}$	2\$p_1/2
-47.7	-21.82	-15.67	-4.15	-3.28	0.93	15	20	22	23

 ²² B. M. Spicer and J. M. Eisenberg, Nucl. Phys. 63, 520 (1965).
 ²⁴ H. P. Jolly, Jr., Phys. Letters 5, 289 (1963).
 ²⁵ G. Hardie, R. L. Dangle, and L. D. Oppliger, Phys. Rev. 129,

TABLE II. The force parameters.

Name	V ₀ (MeV)	<i>r</i> ₀ (F)	W	М	В	H
True's force Rosenfeld force	-48.75 -51	1.85 1.85	$0.42 \\ -0.13$	0.42 0.93	$\begin{array}{c} 0.08\\ 0.46\end{array}$	$0.08 \\ -0.26$

The two-particle matrix elements which make up the remainder of the Hamiltonian are determined by the force parameters appearing in (15) and the oscillator parameter $\nu = m\omega/\hbar$. Here we have taken $\nu = 0.323$ F⁻² as determined from the results of electron scattering experiments on O¹⁶.27

Unfortunately, there is no way of determining a priori the best set of force parameters for our purpose. Because of the magnitude of the present calculation it was not possible to do an extensive force survey. Rather, we assumed a specific exchange mixture and range at the outset and allowed the over-all depth V_0 to vary. V_0 was then chosen to fit the energies of the J=0+, T=0 states supposed to be at 6.06, 11.26, and 14.81 MeV and the J=2+, T=0 states at 6.92, 9.85, and 11.52 MeV. After using these figures it was noticed that the evidence for the 0+ state at 11.26 MeV is not very strong. In a recent paper, Larson and Tombrello²⁸ fail to confirm the existence of this level. Instead they make a 0+ assignment to the level observed at 12.05 MeV. The fitted value of V_0 remains practically unchanged whether we use 11.26 or 12.05 MeV for the energy of the second excited 0+ level. Moreover, the extent to which the present calculation is able to reproduce the observed O¹⁶ spectrum is an indication that any ambiguities associated with the fitting method were relatively unimportant.

At first we tried a singlet even plus triplet even force,²⁹ the parameters of which are given in Table II (True's force). This force is consistent with the low-energy twobody scattering data and has worked well for shell-model calculations in various mass regions.^{29,30} However, it was found that the strength of this potential had to be increased by 40% in order to obtain reasonable correspondence between the lowest even-parity levels observed in O¹⁶ and those calculated by our model. Moreover, the positions of the odd-parity levels, notably the quartet of T=1 levels at about 13 MeV, conflicted with the experimental picture. We then used a Rosenfeld force which, within the freedom allowed by the variation of V_{0} , was found to give generally better results. The energies of the first three excited 0+ levels and the first three 2+ levels of O^{16} were reproduced with an rms deviation of 0.8 MeV. This force also places the quartet of odd-parity T=1 levels at approximately the correct energies, although the prediction of the odd-parity T=0

³⁵³ (1963). ²⁶ A. M. Green (private communication).

²⁷ L. R. B. Elton, *Nuclear Sizes* (Oxford University Press, London, 1961).

 ²⁸ J. D. Larson and T. A. Tombrello, Phys. Rev. 147, 760 (1966).
 ²⁹ J. C. Carter, W. T. Pinkston, and W. W. True, Phys. Rev.

^{120, 504 (1960).} ³⁰ W. W. True, Phys. Rev. 130, 1530 (1963).



FIG. 1. Even-parity T=0 energy levels of O¹⁶. For each spin, the left-hand column shows the calculated energy levels while the right-hand column shows the experimental levels. Levels with uncertain spin assignments are enclosed in parentheses. A level which may have one of several spins is shown for each of the possible spins and the entries are connected with a looped line. Levels whose existence is uncertain are indicated by dashed lines.

levels still leaves much to be desired. The numerical results discussed in the next section are based on the parameters of the Rosenfeld force given in Table II. We note that this force is somewhat stronger than that used by Elliott and Flowers,¹ but is comparable with the force used in Hartree-Fock deformed-core calculations in the same mass region.³¹

IV. COMPARISON WITH EXPERIMENT

General Comparison

The strength of the force was essentially the only free parameter in the calculation, and this was fitted by comparison with the observed energies of just six even-parity T=0 states. In spite of this, there is a remarkable agreement with experiment³² for a wide range of energy levels (more than 30) of both parities and of isobaric spins from 0 to 2. With few exceptions, notably a 4+ level at 7.54 MeV and 6+ state at 10.10 MeV, neither of which has been observed in experiments to date, most even-parity T=0 states (Fig. 1) are properly represented in this calculation. The majority of those odd-parity levels consisting predominantly of 1h-1p configurations is also accurately described (Figs. 2 and 3), though the quality of the fit to these levels is generally less satisfactory than that to the even-parity levels. More complex configura

tions than 1h-1p appear to be necessary³³ and for consistency the odd-parity states should be treated in the usual RPA and also included in the force fit. Nevertheless, our success here can be compared favorably to that of Gillet,³ who performed an extensive force survey² in conjunction with his description of the odd-parity states of O¹⁶. Though the theoretical predictions of the energies for the T=1 even-parity states (Fig. 4) are low, they are still within 1-1.5 MeV of their experimental counterparts. Furthermore, a 3-MeV energy gap observed between the low-lying quartet of odd-parity levels in N¹⁶ and the next excited state is almost fully reproduced in the calculated T=1 states. The energies predicted for the lowest T=2 levels, which have spins and parities of 0+ and 2+, are close to the experimental measurements (Fig. 5). In the sections to follow the calculated and experimental energy levels will be compared in more detail.

T=0 Levels

Levels below 11-MeV Excitation (Experimental)

Definite spin and parity assignments have been made to the nine excited states in O¹⁶ below 11 MeV. These are all T=0 levels. The three levels in this region which were included in the force fit and the 4+ state at 10.36 MeV are reproduced on the average to within 0.5 MeV of corresponding experimental levels.



FIG. 2. Odd-parity T=0 energy levels of O¹⁶. For each spin, the left-hand column shows the calculated energy levels while the right-hand column shows the experimental levels. Levels with uncertain spin assignments are enclosed in parentheses. A level which may have one of several spins is shown for each of the possible spins and the entries are connected with a looped line.

³³ G. E. Brown and A. M. Green, Phys. Letters **15**, 168 (1965); E. Boeker, Physica **32**, 669 (1966).

³¹ W. H. Bassichis, B. Giraud, and G. Ripka, Phys. Rev. Letters 15, 25 (1965).

³² Where experimental energies, spin and parity assignments, or widths are quoted without explicit reference to the literature, the information has been taken from: T. Lauritsen and F. Ajzenberg-Selove, *Energy Levels of Light Nuclei* (National Academy of Sciences—National Research Council, Washington, D. C., 1962); F. Ajzenberg-Selove and T. Lauritsen, Nucl. Phys. **11**, 1 (1959), and references cited in these two publications.



FIG. 3. Odd-parity T=1 energy levels of O¹⁶. For each spin, the left-hand column shows the calculated energy levels while the right-hand column shows the experimental levels. Levels with uncertain spin assignments are enclosed in parentheses. For J = 1, the experimental column shows only the broader levels, since these have a greater probability of being 1h-1p states.

The energy of the lowest 1- state and that of the 2- level are also in good agreement with the observed values. For reasons cited earlier, one of the 1- states observed in this region is absent from the calculation and the lowest 0- state is predicted at about 2 MeV above the single-particle energy of the dominant configuration rather than below. Possibly a weakening of the nucleonnucleon force or varying the exchange mixture would improve the fit to the first 3- state whose predicted energy is already about 2 MeV too low.

Neither the theoretical 4+ level at 7.54 MeV nor the 6+ state at 10.10 MeV can be associated with experimental levels below 11 MeV. The shell-model investigation of O¹⁶ performed by Wong¹⁶ led to a similar result when a strictly central potential with a Rosenfeld mixture was used; there is a 4+ state below the lowest 2+, and the first 6+ level is lower than is indicated in experiments.^{34,35} However, the energies of the 4+ and 6+ states resulting from that calculation are not nearly as low as in ours. These states were obtained at more nearly the correct energies and bore the proper relationsip to the lowest 2+ state when the calculation was repeated with a more realistic force containing tensor and twobody spin-orbit components.



FIG. 4. Even-parity T=1 energy levels of O¹⁶. For each spin, the left-hand column shows the calculated energy levels while the right-hand column shows the experimental levels. Levels with uncertain spin assignments are enclosed in parentheses. A level which may have one of several spins is shown for each of the possible spins and the entries are connected with a looped line.

Many levels in O¹⁶ have even-parity and high-spin assignments (though some of these are only tentative). These high-spin levels are important in determining the validity of the present treatment of the O¹⁶ nucleus and warrant a separate section. Further comments on the low-lying 4+ and 6+ levels will be postponed until the discussion of the high-spin levels is taken up.



FIG. 5. The T=2 energy levels of O¹⁶. Spins and parities are indicated on the diagram.

³⁴ B. G. Harvey, J. Cerny, R. H. Pehl, and E. Rivet, Nucl. Phys.

 <sup>39, 160 (1962).
 &</sup>lt;sup>85</sup> E. B. Carter, G. E. Mitchell, and R. H. Davis, Phys. Rev. 133, B1421 (1964).

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Levels between 11 and 12.6 MeV

Because of limitations on the odd-parity configurations, the three odd-parity states in the region 11-12.6 MeV are not accounted for in our calculation. On the other hand, the theory does indicate 0+, 2+, and 3+states which can be related to experimental levels observed in this region.

The narrow energy range under discussion is of considerable interest because of the existence of experimental ambiguities concerning the levels at 11.1 MeV and at 12.05 MeV. At one time, a level at 11.1 MeV had been variously described as having natural parity (since it was observed in $C^{12}+\alpha$ scattering experiments³⁶), and having unnatural parity [since it was also excited in the N¹⁴(He³, $p\gamma$)O¹⁶ reaction used specifically to search for unnatural parity states³⁷]. A high-resolution $N^{14}(\text{He}^3, p)O^{16}$ experiment³⁸ has demonstrated that there are in fact two levels at 11.1 MeV separated by only 16 keV. The state of unnatural parity, which is probably the lower of the two levels has spin and parity 3+; only very recently²⁸ has a 4+ assignment been made to the other member of this pair. While our model does predict a 3+ level at 9.46 MeV, it does not explain the existence of two 4+ states separated by less than 1 MeV. Within the uncertainties of the calculations, either of the observed 4+ states (at 10.36 and at 11.096 MeV) could correspond to the calculated level at 10.15 MeV. These two levels differ considerably in their α particle widths, the level at 10.36 MeV being much broader than the other. The overlap of the wave function for the calculated 4+ level with that for $C^{12}+\alpha$ clusters moving in a relative g state would be helpful in making the proper association to the experimental levels.

The force strength was fitted with a 0+ level observed at 11.26 MeV ³⁶ which has not been confirmed in later experiments. However, the state at 12.05 MeV is now believed to be 0+.²⁸ The results of the calculation would not change appreciably if this state rather than that at 11.26 MeV were included in the force fit. Bishop et al.,³⁹ using the reaction $O^{16}(e,e')O^{16*}$, describe the state at 12.05 MeV as 2+ as a result of fitting $|\langle 1 \rho | j_2(kr) | 1 f \rangle|^2$ to the electron inelastic-scattering form factor. The fit assumes the existence of large 1h-1p components in the wave functions of the even-parity states. This seems unlikely because of the large single-particle energies of the 1h-1p even-parity configurations. However, the resolution of the experiment was low and effects attribued to the 12.05-MeV state could have been modified by contributions from other nearby levels.

While there is some evidence for another 0+ state in this region at 12.6 MeV,⁴⁰ the existence of the state has

53, 366 (1964). ⁴⁰ D. F. Hebbard, Nucl. Phys. 15, 289 (1960).

not been verified experimentally nor is such a level indicated by our theory.

Levels above 13 MeV with Spins ≤ 3

This part of the discussion concerns reasonably welldocumented levels with spins of 3 or less. Even-parity states with spins of 4 and larger are treated in the following section.

With the discovery of a 3-T=0 level at 13.13 MeV⁴¹ and a 3- assignment³⁵ to a very broad state at 15.7 MeV (listed also as 15.79 MeV^{42,43}), five odd-parity T=0 levels are now known to exist in the region 13-16 MeV. The theory predicts only two such levels, a 2and a 3- (Fig. 2), in the vicinity of these experimental states. This does not imply that these calculated oddparity levels necessarily correspond to the nearest observed odd-parity state with the same spin. Rather, one might expect that the 1h-1p configurations contributing to these calculated states are actually distributed over several observed states of the same spin in conjunction with admixtures of more complex configurations.

The 0- level observed at 16.3 MeV probably has T=0 and is not the analog of a possible 0- state in N¹⁶ at 3.52 MeV 44 (16.35 MeV in O¹⁶) which is at least an order of magnitude narrower. As has already been observed, the present calculation cannot accurately predict the energies of the 0-, T=0 states.

The model successfully reproduces four even-parity T=0 states (with spins <3) between 13 and 16 MeV including the 2+ level now confirmed to exist at 13.15 MeV.^{40,41,45} However, a 1- assignment^{35,42} cannot be completely excluded for the level at 14.81 MeV listed in Fig. 1 as a $0+.^{32}$ Among the even-parity states in this region, only a broad level, at 14.7 MeV (believed to have even parity and spin³⁵), is not compatible with the results of the calculation.

The paper of Carter *et al.*³⁵ contains an extensive list of 2+ assignments to levels above 15 MeV, though the isobaric spin of the states is not indicated. If these 2+ levels are accepted as correct, they cannot all be described by the present theory even if the calculated T=0 and T=1 states are combined; however, most of the 2+ assignments are only tentative. It is possible that some of these levels cannot be obtained within a calculation limited to configurations of $2\hbar\omega$ excitation.

High-Spin, Even-Parity States

With the exception of the two 4+ levels at 10.36 and 11.096 MeV, all the observed levels with spins 4 and

³⁶ J. W. Bittner and R. D. Moffatt, Phys. Rev. 96, 374 (1954).
⁸⁷ D. A. Bromley, H. E. Gove, J. A. Kuehner, E. A. Litherland, and E. Almqvist, Phys. Rev. 114, 758 (1959).
⁸⁸ C. P. Browne and I. Michael, Phys. Rev. 134, B133 (1964).
⁸⁹ G. R. Bishop, C. Betourne, and D. B. Isabelle, Nucl. Phys. 52, 266 (1964).

⁴¹ I. V. Mitchell and T. R. Ophel, Nucl. Phys. 58, 529 (1964); 66, 553 (1965). ⁴² G. E. Mitchell, E. B. Carter, and R. H. Davis, Phys. Rev.

^{133.} B1434 (1964).

It is not clear that this level is the same as the level observed in $N^{15}(p,\alpha)$ reactions, the latter of which was much narrower. See Ref. 25

⁴⁴ P. V. Hewka, C. H. Holbrow, and R. Middleton, Nucl. Phys. 88, 561 (1966).
 ⁴⁵ J. D. Larson and R. H. Spear, Nucl. Phys. 56, 497 (1964).

higher occur above 13 MeV. The agreement between the calculated levels and known high-spin experimental levels (Fig. 1) is rather impressive, although it must be remembered that a large number of the experimental spin assignments are only tentative.³⁵ The exceptions to this good fit are the low 4+ level calculated at 7.54 MeV and the 6+ level at 10.10 MeV, both of which were mentioned earlier. The existence of an unobserved 4+ level below 10 MeV is extremely unlikely since this energy region has been thoroughly explored. It is more probable that the 4+ state has just been calculated low and could be associated with one of the observed 4+levels at 10.36 or 11.096 MeV. The problem of the low 6+ level remains unsolved since there are no known 6+levels near 10 MeV. Levels at 14.94 MeV (4+) and at 14.72 MeV (described in the previous section as being of even spin) are unaccounted for by the theory.

Recent $N^{14}(\alpha, d)O^{16}$ experiments⁴⁶ have been interpreted as being the excitation of high-spin, even-parity levels in which a pair of particles in the state $|(d_{5/2})^2 J = 5\rangle$ (a neutron and proton with their maximum) total angular momentum) is coupled to the ground state of N¹⁴. Three states are observed very strongly in O¹⁶ at 14.33, 14.74, and 16.16 MeV to which spins of 4, 6, and 5, respectively, are assigned. A possible 5+ state previously thought to exist at about 17 MeV ³⁴ does not appear in these experiments. Since the level at 16.16 MeV has been assigned 6+ from the results of $C^{12}+\alpha$ elastic scattering experiments³⁵ (a 5+ state cannot be excited in this reaction) and the same experiments indicate that the state at 14.74 MeV has even spin and parity, it would appear that the most likely candidate for the 5+ member of the "triplet" is the level at 14.33 MeV and this is so indicated in Fig. 1.

The spins are assigned in the $N^{14}(\alpha, d)O^{16}$ experiment by comparing the ratios of the total cross sections for each of the three levels with (2J+1) statistical factors. In other words, it is assumed that the three states arising from the configuration

$$|N^{14}(g.s.)J_h=1, T_h=0 (d_{5/2})^2 J_p=5, T_p=0\rangle$$

(where h refers to holes and p to particles) remain pure so that the spin assignments can be determined solely on angular-momentum arguments. Configuration mixing and other nuclear effects are ignored. The 1+, T=0ground state of N¹⁴ consists mainly of the $(p_{1/2})^{-2}$ configuration but with a very strong $(p_{3/2})^{-1}(p_{1/2})^{-1}$ admixture.47 Thus if the assumptions made above are correct, then states with large components of $|(p_{1/2})^{-2}$ $J_{h}=1, T_{h}=0 (d_{5/2})^{2}J_{p}=5, T_{p}=0$ (configuration 1) and $|(p_{1/2})^{-1}(p_{3/2})^{-1}J_h=1, T_h=0 \ (d_{5/2})^2J_p=5, T_p=0\rangle$ (configuration 2) should be excited strongly by the (α, d) reactions on N14.

In the light of the present theory, the eigenstates resulting from the diagonalization of the interaction Hamiltonian matrix can be interpreted as the actual state functions only insofar as the O¹⁶ ground state contains a very large amplitude of the closed-core configuration. While this is a reasonable expectation, it has not been confirmed by actually generating the wave function of the ground state. Subject to this reservation, the amount of configurations 1 and 2 in the wave functions for the J=4, 5, and 6 states can be determined and estimates made of the strength with which the levels will be excited in (α, d) reactions on N¹⁴. The first two 6+ states predicted by the theory have large amplitudes of configuration 1, while the third state consists mainly of the second configuration. The yield of these three 6+levels should be appreciable. The 5+ state calculated at 13.10 MeV has a significant fraction of the first configuration. It is not inconceivable that this 5+ state could be associated with the experimental level occuring at 14.33 MeV. The next two 5+ levels have nearly equally large amplitudes of the two configurations. However, the effects of interference between these components on the $N^{14}(\alpha, d)O^{16}$ cross section are not known. It does not appear that the 4+ levels should be excited as strongly as those of 5+ and 6+ by the (α,d) reactions. The configurations with the largest amplitudes in the 4+ states are $|N^{14}(g.s.)J_h=1, T_h=0 \quad (d_{5/2})^2 J_p=3, T_p=0 \rangle$ and those formed by coupling particles to the excited configurations of N14.

T=1 Levels

Odd-Parity States

The T=1 quartet of levels observed in the region of 13 MeV in O^{16} is fitted well in our calculation. The holeparticle matrix elements of the $|(1p_{1/2})^{-1}2s_{1/2}\rangle$ and $|(1p_{1/2})^{-1}1d_{5/2}\rangle$ configurations for the Rosenfeld force used in the calculation are small, so that states arising from these configurations appear close to their singleparticle energies. On the other hand, the singlet-even plus triplet-even force (True's force, see Table II) acting between these same states is strongly repulsive.

Some of the gross structure observed in the giant dipole resonance⁴⁸⁻⁵¹ can be explained by the calculated 1-, T=1 levels. A comparison is made in Table III.

There is considerably more structure in the yield curves of photonucleon production from O¹⁶ 49,50 and the inverse reaction⁵¹ than would be implied from Table III. This cannot be interpreted on the basis of our simple particle-hole description. States with more complex configurations are certainly a possible source of some of the fine structure, but this is not the entire explanation. A complete interpretation of the experimental picture is rather difficult. Additional peaks in the vicinity of 17 MeV (at 17.15 and 17.55 MeV) are thought to arise

⁴⁶ E. Rivet, R. Pehl, J. Cerny, and B. G. Harvey, Phys. Rev. 141, 1021 (1966). ⁴⁷ D. Amit and A. Katz, Nucl. Phys. 58, 388 (1964).

 ⁴⁸ S. Fujii, Nucl. Phys. 67, 592 (1965).
 ⁴⁹ K. N. Geller and E. G. Muirhead, Phys. Rev. Letters 11, 371 (1963).

 ⁵⁰ F. W. K. Firk, Nucl. Phys. 52, 437 (1964).
 ⁵¹ N. N. Tanner, G. C. Thomas, and E. D. Earle, Nucl. Phys. 52, 45 (1964).

TABLE III. Electric dipole states of O¹⁶.

7	Observed energy (MeV) ^a	Calculated energy (MeV)
	13.1 17.55 ^b	13.18 17.67
	20.8 22.5°	21.20 24.66
	24.1 25.2	26.88

^a The experimental levels consist of those gross features of the giant resonance for which there is no evidence for assignments conflicting with 1-, T=1. See Ref. 48 and the modified experimental curve in Ref. 51. ^b The broad level seen at this energy (Ref. 49) has more likelihood of being a 1h-1p state than the prominent but much narrower peak at 17.3 MeV. ^c See Ref. 49. This is also a broad level and probably a 1h-1p state.

from these higher configurations.⁴⁹ Another possibility is the mixing of states of isobaric spin 0 and 1 which can explain some of the structure at the lower end of the giant resonance using the particle-hole model.⁵² This mechanism could account for the additional levels around 17 MeV as well as the others observed in the region of 22 and 24 MeV. The prediction of 1-, T=0states in the vicinity of 17 and 24 MeV (Fig. 2) lends support to this idea. The situation is further complicated by the assignment of 1+ to a state in N¹⁶ at 4.32 MeV,⁴⁴ which corresponds to an energy of 17.15 MeV in O¹⁶, the same as that of an alleged electric dipole state.⁵¹ There is also evidence that states near 19 and 23 MeV, normally attributed to the electric dipole absorption of γ rays, may in fact result from excitation by M1 radiations.⁵⁰ Other experiments⁵³ suggest that the latter level may be excited by E2 radiation.

Several broad states observed⁴⁴ in N¹⁶ are believed to originate from 1h-1p configurations and are assigned spins and configurations on the basis of shell-model calculations.^{3,54} The results of the present theory are compatible with the assignment of the configuration $(1p_{1/2})^{-1}1d_{3/2}$ with J=1- and 2-, respectively, to levels existing at 4.725 and 5.305 MeV in N¹⁶ (17.56 and 18.14 MeV in O¹⁶; note that there is a broad peak in the giant resonance of O¹⁶ at 17.55 MeV).⁴⁹ Similarly, our calculation reproduces a 3- level observed at 6.009 MeV (18.84 MeV in O¹⁶) and agrees with the assignment of the configuration $|(1p_{3/2})^{-1}1d_{5/2}\rangle$ to that level. However, the calculation does not support the assignment of $|(1p_{3/2})^{-1}1d_{5/2}\rangle$ to a level at 6.422 MeV (19.25 MeV in O¹⁶). Previous calculations^{3,54} find considerable mixing of the $|(1p_{3/2})^{-1}1d_{5/2}\rangle$ and $|(1p_{3/2})^{-1}$ $2s_{1/2}$ configurations. The present calculation supports a 2- spin assignment (which is a possible spin and parity of the state) but suggests that the level is a rather pure $|(1p_{3/2})^{-1}2s_{1/2}\rangle$ state. A singlet-even plus triplet-even force results in more mixing in the state in question but the $|(1p_{3/2})^{-1}2s_{1/2}\rangle$ component still has the larger amplitude.

Other T=1 Levels

The discussion here will relate to states of uncertain parity as well as to the few states in the mass-16 nuclei known to have even parity. Energy levels in N¹⁶ at 3.36 and 4.32 MeV (16.19 and 17.15 MeV) have $J = 1 + .^{44,55}$ The uncertainty of the parity assignment to the analogue in O¹⁶ of the latter state has already been indicated in the treatment of the giant dipole resonance. These states are reproduced to within about 1 MeV by the calculation. The theory favors an even-parity assignment to a J=0 level at 3.52 MeV in N¹⁶ (16.35 MeV in O¹⁶) because of the 0+, T=1 level predicted at 15.52 MeV in O¹⁶. No calculated 0-, T=1 states appear in this region. The experimental results for the total neutron cross section⁵⁶ in $(N^{15}+n)$ lean towards the evenparity assignment, whereas the data resulting from the $N^{14}(t,p)N^{16}$ reaction indicate that the level should have odd parity.⁴⁴ Levels arising at 3.96 and 4.77 MeV (16.79 and 17.60 MeV in O¹⁶) from the capture of an L=2dineutron in the same $N^{14}(t,p)N^{16}$ reaction have even parity. The former level may have any spin between 1 and 3, whereas the latter level most likely has spin 2. Other even-parity T=1 levels are predicted by the theory in this energy region including some of high spin which have not been observed in experiments to date.

T=2 States

Energy levels with T=2 are observed at 22.9 MeV (0+), and at 24.7 MeV (2+).⁵⁷ The present calculation predicts T=2 states at 22.12 MeV (0+) and at 23.75 MeV (2+) in good agreement with the experimental results. Other T=2 levels predicted by the theory below 30 MeV are shown in Fig. 5. Recent 2h-2p shell-model calculations have been performed to account for these T = 2 states.^{58,59} The calculation of Covello and Sartoris⁵⁸ obtains the first 2+, T=2 state at too high an energy for all the potentials used and for a Yukawa potential with a Rosenfeld mixture obtains two 0+ levels below the first 2+. After considering a wide variety of exchange mixtures, Leonardi et al.59 obtain excellent agreement with experiment for the two T=2 levels using a Serber mixture. Their 0+ and 2+, T=2 levels occur with the same relative ordering and at very nearly the same energies as ours.

V. CONCLUDING REMARKS

The main approximations made in the above treatment of O¹⁶ are the use of the criteria (4) to restrict the number of terms contributing to the general RPA equa-

- ⁵⁵ C. P. Sikkema, Nucl. Phys. 32, 470 (1962).
 ⁵⁶ D. B. Fossan, R. A. Chalmers, L. F. Chase, Jr., and S. R. Salisbury, Phys. Rev. 135, B1347 (1964).
 ⁵⁷ J. Cerny, R. H. Pehl, and G. T. Garvey, Phys. Letters 12, 254 (1964).
- 234 (1964).
 - A. Covello and G. Sartoris, Nucl. Phys. 75, 297 (1965).
- 59 R. Leonardi, P. Loneke, and J. Pradal, Phys. Rev. 146, 615 (1966).

⁵² W. Greiner, Universitty of Maryland Technical Report No. 311 (unpublished). See Ref. 50 for further details.

⁵⁴ R. H. Lemmer and C. M. Shakin, Ann. Phys. (N. Y.) 27, 13 (1964).

tions discussed in Sec. II and the truncation of the states q to those of $2\hbar\omega$ excitation above the closed-shell core. These, together with the simplicity of form chosen for the Hamiltonian and the additional approximation inherent in our neglect of the coefficients $t_{qq'}$, serve to characterize the level of our present calculation. With these limitations in mind, the extent of the agreement

trum is at once rather surprising and most encouraging. There is still, of course, much that remains to be done before the value of this approach can be properly assessed. Certain improvements can be readily envisaged. One could redo the calculation using a more "realistic" residual interaction and one could retain the coefficients $t_{qq'}$. But modifications such as these represent refinements of detail rather than significant advances in our understanding of this approach. More importantly, it will be necessary to obtain a better idea of the nature and limitations of the criteria (4). It will also be necessary to calculate transition rates and other nuclear properties for comparison with experiment, since such comparison will be important in evaluating the success of this approach. The requisite formulas may be developed from the wave functions defined by Eqs. (8) and (9) using methods similar to those employed in the usual (first) RPA calculations.

obtained between the calculated and observed O¹⁶ spec-

With these and other uncertainties still to be resolved, it is too early for us to forecast the final outcome of such investigations. But the success of this preliminary calculation suggests that further work along these lines may eventually lead to a valid description of many of the states of O^{16} .

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APPENDIX A: FORMULAS FOR THE MATRIX ELEMENTS

The matrix elements for the present work are those denoted by $s_{qq'}$ in Sec. II, where q and q' are 1h-1p or 2h-2p states. For completeness, we also list the matrix elements r_q and $t_{qq'}$ since the formulas for these are rather simple. In the following, we show the Racah

algebra appropriate to the angular-momentum couplings only. When the isobaric spin is included, there will be additional factors due to the isobaric spin recouplings which exactly parallel those introduced by the angular momenta. Where an explicit minus sign is shown not raised to any power, this arises from the antisymmetrization and should not be repeated in the isobaric spin factors.

We define the antisymmetric 1h-1p and 2h-2p states in second quantization by

$$|\dot{j}_1 j_2 JM\rangle_a = S^{\dagger}(\dot{j}_1 j_2 JM)|0\rangle$$
 (A1)

and

$$|j_1 j_2 J_h j_3 j_4 J_p J M\rangle_a = S^{\dagger} (j_1 j_2 J_h j_3 j_4 J_p J M) |0\rangle,$$
 (A2)

where

$$S^{\dagger}(j_1 j_2 JM) = \sum_{m_1 m_2} (j_1 m_1 j_2 m_2 | JM) S_{j_1 m_1} a_{j_2 m_2}^{\dagger} a_{j_1, -m_1},$$
(A3)

and

and

and

$$\dot{S}^{\dagger}(ar{j}_1ar{j}_2 J_h j_3 j_4 J_p JM)$$

$$=\sigma_{12}\sigma_{34}\sum_{m_1m_2m_3m_4M_hM_p}(j_1m_1j_2m_2|J_hM_h)$$
$$\times(j_3m_3j_4m_4|J_pM_p)(J_hM_hJ_pM_p|JM)$$
$$\times s_{j_1m_1}s_{j_2m_2}a_{j_4m_4}^{\dagger}a_{j_3m_3}^{\dagger}a_{j_2,-m_2}a_{j_1,-m_1}.$$
 (A4)

In these equations the notation $(j_1m_1j_2m_2|JM)$ refers to a Clebsch-Gordan coefficient. Also, s_{jm} and σ_{12} are defined by

$$s_{jm} = (-)^{j+m} \tag{A5}$$

$$\sigma_{12} = (1 + \delta_{j_1 j_2})^{-1/2}, \qquad (A6)$$

where $\delta_{j_1j_2}$ is zero unless state j_1 (defined by $n_1l_1j_1$) is equal to state j_2 .

Formulas for r_q [Eq. (11)] are then

$$\langle 0|\mathfrak{K}|\,\hat{j}_1j_2JM\rangle_a = (-)^{2j_1}\hat{j}_1\langle j_1|\,\epsilon|\,j_2\rangle\delta_{JO}\delta_{MO} \quad (A7)$$

 $\langle 0|30|\overline{j_1}\overline{j_2}J_k\overline{j_2}J_k\overline{j_1}J_mIM \rangle$

$$= -\hat{J}_{p \ a} \langle j_1 j_2 J_p | v | j_3 j_4 J_p \rangle_a \delta_{JO} \delta_{MO}, \quad (A8)$$

where the single-particle matrix element $\langle j_1 | \epsilon | j_2 \rangle$ is another notation for $\epsilon_{j_1m_1j_2m_2}$, which is diagonal with respect to and otherwise independent of the *m*'s , and \hat{J} is defined by

$$\hat{J} = (2J+1)^{1/2}.$$
 (A9)

Frequently, Brillouin's theorem⁶⁰ is invoked to allow one to equate the matrix element $\langle j_1 | \epsilon | j_2 \rangle$ to zero when, as in Eq. (A7), j_1 refers to a hole state and j_2 to a particle state.

⁶⁰ The Hartree-Fock minimization condition may be written $\langle 0|3C|j_1j_2JM \rangle = 0$. See G. E. Brown, Unified Theory of Nuclear Models (John Wiley & Sons, Inc., New York, 1964). The matrix element $\langle j_1|\epsilon|j_2 \rangle$ is zero if the single-particle states are sufficiently close to Hartree-Fock orbitals.

We note that the off-diagonal components of $\epsilon_{\alpha\beta}$ are also off diagonal in the total oscillator energy because in each oscillator shell there is only one level with a given *jm*. Since apart from the core state itself our model states will be confined to those at $2\hbar\omega$ excitation above the closed shell, the off-diagonal matrix elements of $\epsilon_{\alpha\beta}$ cannot contribute except through (A7). Consequently we have disregarded them in the following. Formulas for $s_{qq'}$ [Eq. (12)] are given below:

(a) If q and q' both refer to 1h-1p states, we have

$${}_{a}\langle j_{1}j_{2}JM | \mathfrak{SC} | j_{1}'j_{2}'JM \rangle_{a} = (\epsilon_{j_{2}} - \epsilon_{j_{1}})$$

$$\times_{a}\langle j_{1}j_{2}JM | j_{1}'j_{2}'JM \rangle_{a} - \sum_{J'} (2J'+1)W(j_{1}j_{2}j_{2}'j_{1}';JJ')$$

 $\times_{a} \langle j_{2} j_{1}' J' | v | j_{2}' j_{1} J' \rangle_{a}, \quad (A10)$

where the first term gives the (diagonal) single-particle contribution and the second is the usual hole-particle interaction involving a sum over a Racah coefficient.

(b) If q and q' are different, one referring to a 1h-1p state and the other to a 2h-2p state, we get

$$a \langle \hat{j}_1 \hat{j}_2 J_h j_3 j_4 J_p J M | 5 c | \hat{j}_1' j_2' J M \rangle_a = \left[(-)^{2j_3} \sigma_{34} (\hat{J}_h \hat{J}_p) W (J_h j_3 J j_2'; j_1' J_p) a \langle j_1 j_2 J_h | v | j_3 j_1' J_h \rangle_a \delta_{j_2' j_4} \right]_{A(j_3 j_4)} \\ - \left[(-)^{2j_2} \sigma_{12} (\hat{J}_h \hat{J}_p) W (J_p j_2 J j_1'; j_2' J_h) a \langle j_2' j_2 J_p | v | j_3 j_4 J_p \rangle_a \delta_{j_1 j_1'} \right]_{A(j_1 j_2)},$$
(A11)

where $A(j_3j_4)$ means that the contents of the preceding square bracket must be antisymmetrized with respect to states j_3 and j_4 . For example, the first square bracket must be calculated as it stands and then recalculated with j_3 and j_4 interchanged, the latter result being multiplied by an additional phase $-(-)^{j_3+j_4+J_p}$. The total contribution of the first square bracket is then taken as the sum of the two results so obtained. Similar remarks refer to the second square bracket.

(c) If q and q' refer to 2h-2p states, we obtain the more cumbersome formula

$$\begin{split} {}_{a}\langle \hat{j}_{1}\hat{j}_{2}J_{h}j_{3}j_{4}J_{p}JM | \mathbf{5}\mathbf{C} | \hat{j}_{1}'\hat{j}_{2}'J_{h}'j_{3}'j_{4}'J_{p}'JM \rangle_{a} \\ = (\epsilon_{j_{3}} + \epsilon_{j_{4}} - \epsilon_{j_{1}} - \epsilon_{j_{2}}) {}_{a}\langle j_{1}j_{2}J_{h}j_{3}j_{4}J_{p}JM | j_{1}'j_{2}'J_{h}'j_{3}'j_{4}'J_{p}'JM \rangle_{a} + {}_{a}\langle j_{1}j_{2}J_{h} | v | j_{1}'j_{2}'J_{h} \rangle_{a} {}_{a}\langle j_{3}j_{4}J_{p} | v | j_{3}'j_{4}'J_{p} \rangle_{a} {}_{a}\langle j_{1}j_{2}J_{h} | j_{1}'j_{2}'J_{h} \rangle_{a} {}_{b}\delta_{J_{p}J_{p}'} - \left[(-)^{j_{1} - j_{1}' + J_{h} - J_{h}'}\sigma_{12}\sigma_{34}\sigma_{1'2'}\sigma_{3'4'}(\hat{J}_{h}\hat{J}_{p}\hat{J}_{h}'\hat{J}_{p}') \right] \\ \times \sum_{K} (2K+1) \begin{cases} K & j_{3}' & j_{1} & J_{h} \\ j_{3}' & j_{4}' & J_{p} & J_{h}' \end{cases} {}_{a}\langle j_{3}j_{1}'K | v | j_{3}'j_{1}K \rangle_{a}\delta_{j_{2}j_{2}'}\delta_{j_{4}j_{4}'} \end{bmatrix}_{A(j_{1}j_{2})A(j_{3}j_{4})A(j_{1}'j_{2}')A(j_{3}'j_{4}')}, \end{split}$$

where the expression in braces is the $12 \cdot j$ coefficient of Jahn and Hope.⁶¹ When the square-bracket term is evaluated in accordance with the prescription given above, we get a total of sixteen separate components. However, some of these components may vanish because of the delta functions and others may be equal among themselves. In general, the maximum number of independent terms arising from the square-bracket expression is four, which situation occurs only for a configuration-diagonal matrix element when neither the holes nor the particles are in equivalent orbits.

Before giving the formula for $t_{qq'}$ [Eq. (13)] it is necessary to introduce a slight change in the representation employed. When the angular momenta are coupled, it is found that S(qJM), where q refers now to the state quantum numbers other than JM, does not have the same rotational properties as $S^{\dagger}(qJM)$. Thus, Eqs. (5) and (6) should be reformulated in terms of

$$\bar{S}(qJM) \equiv (-)^{J+M}S(qJ-M) \tag{A13}$$

rather than S(qJM) so that the coefficients are independent of M. When this has been done the formula for

 $t_{qq'}$ will be modified by the substitution of $\bar{\mathbf{S}}_q$ for S_q , and we find

$$\langle 0| \Im CS^{\dagger}(j_{1}j_{2}JM)S^{\dagger}(j_{1}'j_{2}'JM)|0\rangle = \sum_{J'} (2J'+1)W(j_{1}'J'Jj_{2}; j_{1}j_{2}')(\sigma_{11'}\sigma_{22'})^{-1} a\langle j_{1}j_{1}'J'|v|j_{2}j_{2}'J'\rangle_{a}, \quad (A14)$$

which has a form similar to (A10) but uses the same two-particle matrix elements as (A8).

APPENDIX B: TESTS OF THE PROGRAM

In the course of setting up a computational problem of any reasonable complexity, it is possible that certain errors may develop. Even after detailed checks have been made on all the individual stages of the problem, one cannot be absolutely sure that all such errors have been eliminated. It is the purpose of this appendix to describe certain over-all checks on our calculations which serve to indicate the accuracy of their execution.

1. Orthonormality

The program was run for various $J\pi T$ combinations with all two-particle matrix elements replaced by the overlap integral $_a\langle j_1j_2JT | j_3j_4JT \rangle_a$ and the single-

⁶¹ H. A. Jahn and J. Hope, Phys. Rev. 93, 318 (1954); M. Rotenberg, R. Bivins, N. Metropolis, and J. K. Wooten, Jr., *The 3-j* and 6-j Symobls (The Technology Press, Massachusetts Institute of Technology, Cambridge, Massachusetts, 1959).

particle energies set to zero. The resultant matrix was then diagonal with eigenvalues of -1 for a 1h-1p state and -2 for a 2h-2p state. In view of the fact that the constant core contribution and the single-particle contributions have been neglected, this is the expected result.

2. LS Check

Two-particle matrix elements for the operator

$$\mathcal{O}_{12} = \mathbf{l}_1 \cdot \mathbf{l}_2 + \gamma_1 (\mathbf{l}_1 \cdot \mathbf{l}_2)_p + \gamma_2 (\mathbf{s}_1 \cdot \mathbf{s}_2)_p \tag{B1}$$

were introduced, where the subscript p appended to a particular component means that that component is effective among particle states only (hole-state contributions ignored). The resultant matrix was set up and diagonalized for the J=0+, T=0 states, taking $\gamma_1=0.1$, $\gamma_2=0.04$. Among the states of a 2h-2p LS configuration, the eigenvalues of this operator are

$$\begin{aligned} & \epsilon_{LS} = \frac{1}{2}L(L+1) + \gamma_{1\frac{1}{2}}L_{p}(L_{p}+1) \\ & + \gamma_{2\frac{1}{2}}S_{p}(S_{p}+1) + \text{const.}, \end{aligned} \tag{B2}$$

where L is the total-orbital-angular-momentum quantum number and $L_p S_p$ are the intermediate LS quantum numbers associated with the particle orbits. Thus, the result of the diagonalization enabled the LS states for L=0 to be completely distinguished. Using the resultant eigenvectors as transformation amplitudes, the J=0+, T=0 interaction matrices of certain central potentials were transformed into the LS coupling scheme. It was found that the L=0 mainfold was completely decoupled from the L=1 manifold, provided that the single-particle energies ϵ_j were functions of n and l but not of j. This expresses the well-known result that L and S are good quantum numbers in this case.

The above procedures allow detailed comparison to be made with the LS coupled calculations¹⁰⁻¹³ of the 0+states of O¹⁶. When this was done, we found that we were unable to obtain complete agreement with any of these papers. Vinh-Mau,¹³ however, gives a complete set of eigenvalues and eigenvectors from which we were able to reconstruct her 12×12 interaction matrix. The discrepancies between this and our equivalent matrix consisted almost entirely of factors of 2 and $\sqrt{2}$, suggesting some differences in the normalizations. On the other hand, using $\alpha \mathcal{H}_{sp}$ instead of \mathcal{H}_{c} , the structure of the *LS* coupled spurious states as listed by Abgrall¹⁰ was completely verified. As an additional check on our work, we adapted the formulas (A10), (A11), and (A12) to an *LS* coupled representation and evaluated a few of the *LS* interaction matrix elements directly. These were in agreement with those obtained by numerical transformation from the *j j* coupled scheme.

3. Center-of-Mass Check

The operator $\alpha \mathcal{K}_{sp}$ described in Sec. II was diagonalized independently of the Hamiltonian \mathcal{K} for a number of $J\pi T$ combinations. The eigenvalues were correctly obtained as αn , where the number of nonzero eigenvalues gives the number of spurious states for that particular $J\pi T$. This number was correct in all cases checked. For the J=0+, T=0 combination, the amplitudes of the 2S spurious state agreed with those published by Giraud.⁶²

As a check on the approximate method of removing the spurious states which was adopted in our final numerical work (see Sec. III), some calculations were done in which the interaction matrix was transformed into a new representation having no spurious states. After diagonalization within this representation, the eigenvectors were rotated back for comparison with the ones generated by the approximate method. With our value of α , the discrepancies were less than a few parts in a thousand in all cases.

⁶² B. Giraud, Nucl. Phys. 71, 373 (1965).