HOW GOOD IS THE HARTREE-FOCK APPROXIMATION FOR ¹⁶O?

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ABSTRACT

Hartree-Fock intrinsic states in ^{16}O are examined to find out the extent to which they are good approximations to the exact eigenstates of the system. For this purpose the notion of width of a state is introduced. In terms of the width we find that by itself the Hartree-Fock approximation is not good in ^{16}O , however it does provide a suitable basis to discuss the structure of the low-lying states. Our calculation of the 0^+ levels confirms earlier suggestions made regarding the nature of these levels and is also in agreement with exact calculations done in a small basis space.

Many Hartree-Fock (HF) calculations have been done to study the first excited 0^+ (6.05 MeV) level in ^{16}O and the rotational band based on it [1]. These have led to the conclusion that the four particle - four hole (4p-4h) intrinsic wave function plays an important role in the understanding of these states. It has however been emphasized by Krieger [2] that this intrinsic state lies at a very high excitation energy and hence a quantitative understanding of the ^{16}O levels in a HF picture is not available. On the other hand the model of Brown and Green [3] (BG) in which the low lying even parity eigenstates of ^{16}O have admixtures of (0p-0h), (2p-2h) and (4p-4h) configurations has been successful in describing the collective features of these states. Furthermore shell model calculations of Wong [4] and particularly that of Zuker, Buck and McGrory [5] (ZBM) have shown that the structure of wave functions assumed by BG is essentially correct.

In this note we describe the results of HF calculations for ^{16}O in the space of three major oscillator shells (1s, 1p and 2s-1d), using the bare Kuo [6] matrix elements with an oscillator frequency $\hbar\omega = 12.5$ MeV. The calculations were done with the aim of answering the following questions.

1) Do the HF intrinsic states provide a good approximation to the exact eigenstates of the Hamiltonian? For this purpose we need a suitable measure to test the wave functions, and therefore introduce the important concept of the width of a state.

This has been discussed earlier in the literature by Levinson [7], Banerjee et al. [8] and French and Ratcliffe [9].

2) How much admixture of states is implied by these widths? Can we obtain the energies and the structure of the lowest few levels in terms HF energies and widths?

3) What can we learn about the effective nuclear interaction from these energies and widths?

In our calculations we obtain two HF solutions. The lower one is spherical in nature, the intrinsic state being essentially the closed shell configuration $((1s)^4(1p)^{12})_{J=0, T=0}$. The solution corresponding to the second minimum is deformed (triaxial) having a 4p-4h structure relative to the closed shell. The HF energies, their breakup into kinetic and potential parts, and expectation values of some relevant operators for these solutions are shown in table 1.

We see that the (4p-4h) intrinsic state lies at a very high excitation energy as already noted by Krieger. This is due to the fact that the increase in K.E. is not compensated by additional attractive interaction of four particles in the 2s-1d shell amongst themselves and with the particles in p-shell. As can be seen from table 1 the potential energy of the (4p-4h) intrinsic state is in fact higher by about 10 MeV relative to that of the (0p-0h) solution. This leads to the very high excitation energy for the (4p-4h) state.

In order to find out whether our intrinsic states χ are close to being true eigenstates of the Hamiltonian H , we calculate a quantity called the total variance defined by

$$\sigma^2 = \langle \chi | H^2 | \chi \rangle - (\langle \chi | H | \chi \rangle)^2 \quad (1)$$

σ will be called the width of the state. It is clear that σ^2 will be zero if χ is an eigenstate of H . Thus σ^2 provides us with a measure of the goodness of our wavefunction χ . The width σ can in our case arise from a second source. In general the intrinsic wavefunction χ is deformed and hence is a linear combination of several angular momentum states

$$\chi = \sum_j C_j \Psi_j \quad (2)$$

The projected states Ψ_j are not in general degenerate in energy and therefore this energy spread will also contribute to the width of the underlying intrinsic state. We can make a correction for the second effect when the states Ψ_j have rotational ($J(J+1)$) or near rotational energy spacings. We replace H by H_α where

$$H_\alpha = H - \alpha \vec{J}^2 \quad (3)$$

and calculate

$$\sigma^2(\alpha) = \langle \chi | H_\alpha^2 | \chi \rangle - (\langle \chi | H_\alpha | \chi \rangle)^2 \quad (4)$$

as a function of the parameter α . It can be seen that for a suitable choice of α , obtained by minimizing $\sigma^2(\alpha)$ with respect to α , the states of different J projected from the intrinsic function will be essentially degenerate. Furthermore the value α will give the moment of inertia [7] for the band, which may be compared with the value obtained by other methods.

The total widths for our HF states are shown in table 2. For the (4p-4h) intrinsic state we also give the width after minimizing with respect to α , and the value of the parameter α . We see that the widths are quite large for both the HF solutions indicating that these intrinsic states by themselves do not provide a good approximation to the lowest few eigenstates of H . Also the contribution of the $\vec{J}^2$ -like term in H to the width of the (4p-4h) state is quite small. This should be compared with the situation for nuclei in the 2s-1d shell (see ref. (8)) where the HF solutions have a very small width after removing the width arising out of the term proportional to $\vec{J}^2$. Thus the existence of such large widths implies that the low lying states in ^{16}O cannot be described in terms of single HF determinants. This is also evident from the calculations of BG, Wong and ZBM.

We now make use of these HF energies and widths to estimate the structure and energies of the lowest few 0^+ levels in ^{16}O , within the space of (0p-0h), (2p-2h) and (4p-4h) configurations.

For the (0p-0h) and (4p-4h) states we take the HF intrinsic wave functions. The nature of the (2p-2h) state is discussed below. In order to diagonalize the 3 x 3 matrix in this basis space we should know the three unperturbed energies,

$$E_0(np-nh) = \langle (np-nh)J=0, T=0 | H | (np-nh)J=0, T=0 \rangle$$

and the three off-diagonal matrix elements

$$M_1 = \langle (0p-0h)J=0, T=0 | H | (2p-2h)J=0, T=0 \rangle$$

$$M_2 = \langle (2p-2h)J=0, T=0 | H | (4p-4h)J=0, T=0 \rangle$$

$$M_3 = \langle (0p-0h)J=0, T=0 | H | (4p-4h)J=0, T=0 \rangle$$

$M_3 = 0$ since H is a (1+2)-body operator. $E_0(0p-0h)$ is just the intrinsic HF energy for the spherical solution of table 1.

$E_0(4p-4h)$ can be obtained from $E_{HF}(4p-4h)$, using $\langle \vec{J}^2 \rangle_{4p-4h}$ and the moment of inertia parameter α . From the numbers given in tables 1 and 2 we get $E_0(4p-4h) = -92.0$ MeV. The width $\sigma(0p-0h)$ gives us the matrix element which connects the (0p-0h) state with all possible $J=0, T=0(2p-2h)$ states. This is because for the HF solution the one-body part of H does not contribute to the width and moreover H is an angular momentum and isospin scalar. Thus $M_1 = \sigma(0p-0h)$. Since this matrix element describes mixing with all possible $(2p-2h)J=0, T=0$ states, it is clear that for $E_0(2p-2h)$ we must take some average position of the $(2p-2h)J=0$ states.

Therefore, for $E_0(2p-2h)$ we take a set of values ranging from a few MeV below $E_0(4p-4h)$ to a few MeV above it. The width $\sigma(4p-4h)$ gives the mixing matrix element of the (4p-4h) state with all possible (2p-2h) and (6p-6h) states. Assuming that the contribu-

tions to $\sigma^2(4p-4h)$ coming from $(2p-2h)$ and $(6p-6h)$ intermediate states are equal, and further that the width comes largely from the $J=0$ projection* of the deformed states we take $M_2 \approx \frac{1}{2}\sigma(4p-4h)$. We can now diagonalize the 3×3 matrix.

We find that the overall structure of the wave functions is very insensitive to both the $E_0(2p-2h)$ and the matrix element M_2 . For substantial variation of these quantities we obtain essentially the same results. To be specific we show in table 3 the eigenvalues and the intensities of the three configurations in the eigenvectors for $E_0(2p-2h) = E_0(0p-0h) + 36.0$ MeV and $M_2 = 11.43$ MeV. These eigenstates have zero width, in the sense of eq.(1). This is to be expected, to the extent that $(6p-6h)$ and higher configurations can be neglected in these states.

It turns out that depending upon the values chosen for $E_0(2p-2h)$ and M_2 the lowest 0^+ level comes at an energy 15-20 MeV below $E_0(0p-0h)$. With this correlation energy the ground state of ^{16}O has the energy -136 MeV to -141 MeV to be compared with the value -139.6 MeV obtained from the binding energy table after including a Coulomb repulsion of 0.430 MeV per proton pair. Furthermore the intensities of the $(0p-0h)$ and $(2p-2h)$ configurations in the ground state range from $0.66 \rightarrow 0.75$ and $0.23 \rightarrow 0.33$ respectively with 1 to 2% going to the $(4p-4h)$ configuration.

* Experience with projection from HF intrinsic states in the $2s-1d$ shell indicates that the $J=0$ component of the wave function dominates in the intrinsic state.

Thus the agreement with previous calculations and experiment is quite impressive. For the first excited 0^+ state the structure is again in good agreement with earlier calculations. One has essentially a dominant (4p-4h) configuration with only a few per cent each in (0p-0h) and (2p-2h) configurations. Of course the fact that this state lies at a 40 MeV excitation energy is a serious matter, which requires further study. We will briefly discuss this aspect later. It should perhaps be emphasized again that the (2p-2h) component in the above discussion refers to the contribution coming from all possible $J=0^+(2p-2h)$ states whereas the (0p-0h) and (4p-4h) components refer to projection from definite HF states. Thus it is meaningful only to compare the structure of our lowest two 0^+ levels with those of other calculations.

As regards the nature of the interaction we find that it seems to correctly reproduce the binding energy and the gross structure of the ground state wave functions in ^{16}O . Secondly the large value of $\sigma^2(0p-0h)$ indicates that, either there will be important renormalization correction for the effective interaction of two valence particles in the 2s-1d shell due to a (4p-2h) intermediate state, or a (4p-2h) state should be explicitly introduced in the basis space to account for the experiments. There is evidence [10] that the 0^+ levels in ^{18}O at a low enough excitation energy have admixtures of (4p-2h) configurations in them, so that the latter possibility seems more likely.

In common with other, similar calculations [1,2] our work puts the 4p-4h state at too high an excitation above the ground state. To try to understand where this feature comes from, we changed the strength of some selected matrix elements, to see how sharply this influences the location of the 4p-4h state. We find that multiplying all matrix elements of the type $\langle p,d|V|p,d \rangle_{JT}$ by a factor 1.25 brings $E_0(4p-4h)$ down to -96.8 MeV, 10 MeV down from the value given in table 1*. No particular matrix elements of this set seem to dominate in the lowering of the value of E_0 . Other things also improve with these modified matrix elements: (i) in the ground state the p-sd shell gap is decreased to 11.3 MeV (from 16.0 for the unmodified matrix elements), a more reasonable value; (ii) in the 4p-4h solution the Hartree-Fock gap between occupied and unoccupied shells is increased to 3.5 MeV (from 2.0). Finally, it is perhaps not unreasonable that the Kuo matrix elements should be changed from those in ref.6 when dealing with 4 particles in the (s-d) shell. This would affect both the Pauli operator and the energy denominator in Kuo's calculation of the G-matrix.

* The 0p-0h energy is not affected by this change.

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TABLE CAPTIONS

- Table 1 The results of HF calculations for ^{16}O .
(Q_{20} denotes the expectation value of the quadrupole operator in units of $b^2 = \hbar/m\omega$).
- Table 2 Widths for the HF solutions.
- Table 3 The energies and intensities of the three configurations for the lowest two 0^+ levels in ^{16}O . The absolute energy of the 0_1^+ level is -135.6 MeV.

Table 1

HF Solutions χ	$E_{HF}(\text{MeV})$	K.E.	1/2(P.E.)	$\langle Q_{20} \rangle$	$\langle J^2 \rangle$
(0p-0h) Spherical	-121.08	227.30	-348.38	0	0
(4p-4h) deformed	- 86.67	252.98	-339.65	10.56	22.33

Table 2

HF Solution	$\sigma^2(\text{MeV}^2)$	$\sigma^2_{\text{min}}(\text{MeV}^2)$	Inertial parameter α
(0p-0h) Spherical	690.17	-	-
(4p-4h) deformed	477.58	459.39	0.237

Table 3

Level	$E_{\text{ex}}(\text{MeV})$	(0p-0h)	(2p-2h)	(4p-4h)
0_1^+	0.0	0.75	0.23	0.02
0_2^+	40.12	0.08	0.08	0.84