HARTREE-FOCK CALCULATIONS IN ^{16}O USING A CARTESIAN BASIS

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ABSTRACT

A comparison is made of different variational calculations using cartesian basis wave functions. Preliminary results obtained for the 4p - 4h state in ^{16}O using the modified Sussex matrix elements indicate that a reasonable description of the first excited O^+ state of ^{16}O may be possible with an interaction which has no adjustable parameters and is used self-consistently for both ground and excited states.

Some years ago Brink and Boeker[1,2] using phenomenological interactions carried out a series of variational calculations for light nuclei with atomic number A = 4n. We are in the process of repeating and extending some of these calculations using the modified Sussex matrix elements[3] which are derived from the two nucleon phase shifts and which give a fairly good description of nuclei near to closed shells[4,3,5].

In the cartesian harmonic oscillator basis $(n_x\ n_y\ n_z)$ the simplest description of the 4p - 4h state in ^{16}O is the configuration

$$(000)^4\ (001)^4\ (100)^4\ (002)^4 \qquad (1)$$

The first three variational calculations considered make use of the oscillator length parameters b_x, b_y, b_z as variational parameters where as usual $b^2 = \hbar/mw$, relates b to the corresponding oscillator energy $\hbar w$.

Type 1	$b_x = b_y = b_z$	spherical
Type 2	$b_x = b_y \neq b_z$	axially symmetric
Type 3	$b_x \neq b_y \neq b_z$	asymmetric
Type 4	Restricted Hartree-Fock calculation	

In the last method we allow the single particle configurations given in (1) to mix with configurations of the same cartesian parity up to two oscillator shells away. In this case the variational parameters are in effect the expansion coefficients (for a fixed oscillator length b) of the eigenvectors determined from the self-consistent HF interaction procedure.

The results of our calculations show that whereas there is a gain of 12 MeV binding energy by allowing an axially symmetric deformation only a further 1.5 MeV is gained by relaxing the condition $b_x = b_y$. In contrast a further 9 MeV is gained by allowing individual orbits to deform independently as occurs in the HF calculation. This result is very similar to that found by Boeker[2].

The ground state of ^{16}O being spherically symmetric gains only 4 MeV binding energy in the HF calculation[6] using the same interaction with the result that the excitation energy of the 4p - 4h intrinsic state is 21.5 MeV. Angular momentum projection of the O^+ level from this is estimated[7] to gain a further 9 MeV giving approximately 12 MeV to be compared with the experimental value of 6 MeV. A less restricted HF calculation allowing mixing over four oscillator shells is in progress.

REFERENCES

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