Application of Time-Dependent Hartree-Fock Theory to Ne^{20}: Odd-Parity Bands

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The constraint that the O^{16} "core" be inert with respect to particle-hole excitations in Ne^{20}, imposed in a recent calculation, is relaxed. In this time-dependent Hartree-Fock treatment of Ne^{20}, excitations are considered in which a particle from the energetically highest level in the core is promoted to a level in the *s-d* shell. The wave function describing the core particle is assumed to be given by the shell model. The single-particle wave functions and energy spectra ascribed to the outer four particles are those obtained by a static Hartree-Fock calculation done previously. Such excitations give rise to excited "intrinsic" states of odd parity, the lowest lying of which correspond to the observed odd-parity rotational bands. The agreement between the observed and calculated band positions gives credence to the assumption, proposed in the earlier calculation, that the O^{16} core is nearly spherical in Ne^{20} despite the deformation of the orbitals of the outer particles.

INTRODUCTION

RECENTLY the results of a static Hartree-Fock (H.F.) calculation[1,2] for Ne^{20} and Mg^{24} have been used as the basis for a time-dependent Hartree-Fock (T.D.H.F.) calculation.[3] In the application of the H.F. method the variation of the single-particle wave functions was limited to the four (or eight) particles in the *s-d* shell. The underlying O^{16} core was assumed to be spherical. In the T.D.H.F. calculation it was furthermore assumed that the core was inert and thus, since particle-hole excitations were confined to the *s-d* shell, only the even-parity excited states were obtained. In this calculation the restriction that the O^{16} core be inert is removed, and single-particle excitations are allowed from the core to the *s-d* shell. The intrinsic states resulting from the application of the T.D.H.F. method will therefore be of negative parity.

It is still assumed that the single-particle wave functions for the particles within the core are as given by the shell model. Within the limitations of the present calculation this assumption will be tested by a comparison between the observed and predicted rotational bands of odd parity. The limitations, which will be discussed in detail in a following section, are the result of a lack of information concerning the moment of inertia of the nucleus in an excited state and a lack of a well-defined energy difference between the major shells.

SINGLE-PARTICLE WAVE FUNCTIONS AND ENERGY LEVELS

The matrix equation which one is lead to by the T.D.H.F. theory[4] is

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}\begin{pmatrix} X^i \\ Y^i \end{pmatrix}=\omega_i\begin{pmatrix} X^i \\ Y^i \end{pmatrix}, \tag{1}$$

where

$$A_{uo,u'o'}=(E_u-E_o)\delta_{oo'}\delta_{uu'}+V_{uo'ou'} \tag{2}$$

and

$$B_{uo,u'o'}=V_{uu'oo'}. \tag{3}$$

The two-body matrix elements and the single-particle energy differences are no longer solely determined by the H.F. calculation performed in Ref. 2. In order to calculate the matrix elements, it is here assumed that the single-particle excitations can originate only from the energetically highest level in the O^{16} core and that this single-particle level is a pure $p_{1/2}$ level. Thus, since the even-parity states have previously been considered, the summation in Eqs. (2) and (3) over occupied states reduces to a single term, i.e., "o"$=p_{1/2}$. The unoccupied levels are described by the H.F.-generated single-particle wave functions.

The determination of the single-particle energies to be used in Eq. (2) is not quite as straightforward. In order to determine the differences in energy, without doing a H.F. calculation in which the single-particle wave functions and energies of the particles in the *p* shell are also varied, one must first of all choose a value of $\hbar\omega$, the shell-model energy difference between the *p* and *s-d* shells. A survey of odd-even nuclei in the *p* shell gave an estimate of this quantity, though certainly no definite conclusion was possible. The value $\hbar\omega=7.5$ MeV was chosen because it is compatible with the experimental information. A deviation in this quantity of 30% is, of course, possible and such a deviation would strongly affect the results of this calculation. This will be discussed further.

With the value of $\hbar\omega$ thus (somewhat arbitrarily) fixed, one can now establish the single-particle energy

[1] I. Kelson, Phys. Rev. **132**, 2189 (1963).
[2] I. Kelson and C. A. Levinson, Phys. Rev. **134**, B269 (1964).
[3] W. H. Bassichis, I. Kelson, and C. A. Levinson, preceding article, Phys. Rev. **136**, B380 (1964).
[4] For details of the calculations and references the reader is referred to Ref. 3.

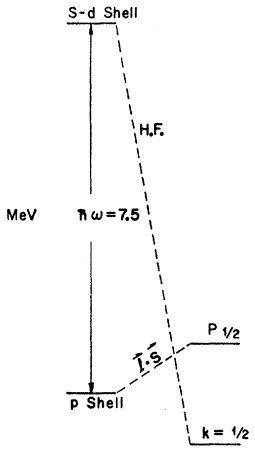

FIG. 1. The proposed shifting of the energy levels. The levels on the left indicate the separation of the major shells. On the right the $k=\frac{1}{2}$ level has been displaced downward such that the set of H.F. level retain the original "center of mass" and the $p_{1/2}$ level has been raised by the $\mathbf{l}\cdot\mathbf{s}$ force.

spectrum. Since the core is still inert with respect to the determination of the relative positions of the levels in the *s-d* shell, these levels split only because of their mutual interaction. Thus, the "center of mass" or the position of the average value of the energy of these levels must remain stationary. The result, using the single-particle energies obtained by H.F.,[2] is that the lowest level of the *s-d* shell, that level which contains the four outer particles, is shifted downwards from the "center of mass" by 8.53 MeV. In order to complete the determination of the spectra one needs also the magnitude of the $\mathbf{l}\cdot\mathbf{s}$ splitting in the *p* shell. Using the $\mathbf{l}\cdot\mathbf{s}$ parameter which was used throughout the H.F., this splitting is found to be such that the $p_{1/2}$ level is raised by 1 MeV. This shifting of the $p_{1/2}$ and $k=\frac{1}{2}$ (the lowest *s-d* level) levels is illustrated in Fig. 1. Thus, the single-particle energy spectra is as shown in Fig. 2. It is perhaps at first surprising that the $k=\frac{1}{2}$ level lies lower than the $p_{1/2}$ level. This apparent contradiction of an important, verified feature of the shell model can be resolved by the following argument. The Hartree-Fock results have shown that the positions of the single-particle energy levels depend strongly to what extent they are filled. It is therefore plausible that the $k=\frac{1}{2}$ level will lie above the $p_{1/2}$ level (as it must) when it is empty but that as the $k=\frac{1}{2}$ level becomes filled it drops in energy to such an extent that when completely filled it lies below the $p_{1/2}$.

RESULTS OF THE CALCULATION

The application of the T.D.H.F. method carried out here exactly parallels that discussed in Ref. 3. Here there are no spurious solutions because there is no operator which commutes with the Hamiltonian in the truncated space and changes the parity of the ground state. In the even parity calculation the backward-going graphs [B in Eq. (1)] were only appreciable for the spurious solution and similarly here, the backward-going graphs were in every case negligible.

The results of the calculation are shown in Table I. The first column is the quantum designation of the bands. The second is the energy position of the intrinsic states, i.e., the eigenvalue of Eq. (1). The third column is the observed value[5] of the moment of inertia parameter used to extract the position of the band heads from the intrinsic states. (This procedure is discussed in Ref. 3.) No definite value of this parameter could be obtained from the data so the values chosen were those most compatible with the observed bands. In the case of the second 0^- band, where little experimental information exists, two values of this parameter are given and the effect of a deviation of this magnitude is shown in the resulting computed band head position. For the 1^- state an even greater freedom of choice existed but just one value, perhaps reasonable, was used. Next are listed the computed average values of J^2, also needed in the extraction process. In the column of the computed band head positions, the two energy positions of the 0^- state correspond to the two listed moment of inertia parameters. In the last column is shown the experimental positions[5] of the band heads. Only the two lowest are definitely known to be rotational bands and thus a question mark was included with the upper states. The positions of the band heads, computed and experimentally observed, are shown also in Fig. 3.

TABLE I. Comparison of computed and observed rotational band heads. ω is the energy of the intrinsic state, A_{ob} the observed moment of inertia parameter, and $\langle J^2\rangle$ the calculated average value of J_{op}^2 in the intrinsic state. The question marks in the last column indicate that these bands are only suggested by the available experimental data.

Band	ω	A_{ob}	$\langle J^2\rangle$	Level computed	Positions observed
$0^-(T=0)$	5.5	0.14	22.0	6.60	5.80
$2^-(T=0)$	3.3	0.15	24.5	4.63	4.97
$0^-(T=0)$	7.2	0.12–0.14	22.2	8.88–8.47	8.71(?)
$1^-(T=0)$	9.1	0.14	21.6	10.45	8.87(?)

DISCUSSION

The agreement between the calculated and observed positions of the rotational band heads is quite gratify-

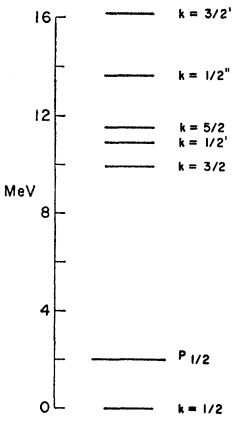

FIG. 2. The single-particle energy spectra. The states labeled by k are placed according to a H.F. calculation. Plausibility arguments led to placing the $p_{1/2}$ in the position shown, relative to the H. F. levels.

[5] J. D. Pearson, E. Almqvist, and J. A. Kuehner, Can. J. Phys. 42, 489 (1964).

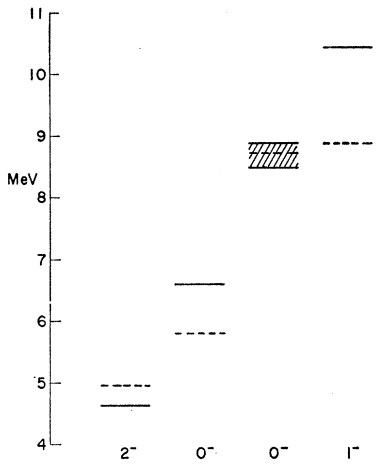

FIG. 3. Comparison of observed (dashed lines) and computed positions of rotational band heads. The two higher lying levels are only suggested by the experimental data to be band heads. The crosshatched area for the higher 0^- level indicates the degree of uncertainty in the computed position because of lack of information concerning the moment of inertia parameter.

ing. It would, however, be imprudent to conclude from this agreement that the assumption of a spherical O^{16} core in the H.F. calculation is indeed valid. The strong dependence of the results on the major shell energy difference, a quantity for which no exact value can be given, renders the calculation suspect in this respect. The following conclusion can, however, be drawn: The odd-parity, excited, rotational bands in Ne^{20} can be obtained with the T.D.H.F. method, assuming that the O^{16} core is well described by pure shell-model wave functions, with what appears to be a reasonable choice of the parameter $\hbar\omega$. With this reservation one sees that transitions from the p shell to this s-d shell give rise to not only the well-established two low-lying odd-parity bands but also to two possible, higher lying bands.

One may also adopt an alternate approach. The success of the calculation of the even-parity levels[3] may be considered as a justification of the spherical core assumption. The quantity $\hbar\omega$ may then be considered a parameter which is to be determined by a comparison of the computed band head energies, which depend on $\hbar\omega$, and the observed spectra. For example, suppose it were decided to choose $\hbar\omega$ such that the lowest observed level (2^-) is fitted exactly. From Table I it seen that such a choice would lead to an $\hbar\omega$ not appreciably different from the value used. The test of the calculation would then be the comparison of the observed and computed 0^- level and perhaps the higher lying 0^- and 1^- levels. It is seen that the results are also satisfactory when viewed from this approach and that the reversal of the order of the filled $p_{1/2}$ and $k=\frac{1}{2}$ levels would still be found.

The results of this calculation suggest that it would be worthwhile to perform a H.F. calculation in which the wave functions for the particles in the p shell are also treated variationally.