

Time-Dependent Hartree-Fock Theory Applied to Ne²⁰ and Mg²⁴

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(Received 12 May 1964)

The time-dependent Hartree-Fock method is applied to the even-even nuclei Ne²⁰ and Mg²⁴. The starting point of the calculation is a static Hartree-Fock solution, with the assumptions that in both the ground and the excited state, the deformed nuclei are axially symmetric, that the self-consistent wave functions have the usual shell-model radial dependence, and that the two-body interaction is the Rosenfeld mixture proposed by Elliott and Flowers. Application of the method yields intrinsic excited states corresponding to the rotational bands of the nuclei being considered. The calculated differences in energy between the lowest lying members of these bands agree quite well with experiment. The spurious solutions or states, corresponding to the invariance of the system under rotation about the axis of symmetry, occur with zero excitation energy, as predicted, when correlation effects in the ground state are included. The effect of these correlations on the energy spectra for the nonspurious solutions is shown to be negligible.

INTRODUCTION

RECENTLY¹ the static Hartree-Fock (H.F.) theory has been applied to the nuclei in the first half of the *s-d* shell. The result of these calculations was a set of single-particle energy levels which gave the ground-state rotational spectra and moments of inertia. In the case of even-odd nuclei the excited states were also obtained, simply by promoting the valence nucleon into the unoccupied energy levels, taking into account the polarization effect of such a promotion on the even-even core. Again moments of inertia were calculated, using the cranking formula or the Skyrme formula and the agreement with experiment was quite good. The static Hartree-Fock theory was, however, inadequate for a treatment of the excited states in even-even nuclei. Here the low-lying excited states will be made up of superpositions of configurations in which a single particle is promoted from the core, leaving a hole. In these H.F. single-particle energy spectra, perhaps the most striking feature is the appearance of a large energy gap between the occupied and unoccupied states. This is in marked contrast with the level structure predicted by the Nilsson model where no such gap occurs. The existence of such a gap leads one to assume that configurations in which there are more than one particle-hole pair present are very improbable.

Moreover, since this gap mainly results from two-particle interactions in the $T=0$ state,¹ one is justified in neglecting pair correlations of the Hartree-Bogolyubov type, for the present calculation.

The formalism of time-dependent Hartree-Fock (T.D.H.F.) is well suited for treating such particle-hole excited states. The static Hartree-Fock orbitals or the corresponding density matrix can be used as the starting

point for such a time-dependent calculation. In this way no external self-consistency restraints need to be imposed since the calculation will be inherently self-consistent. This internal self-consistency should manifest itself in the appearance of spurious, zero-frequency "excited states" which result from the assumed symmetry of the nuclei under investigation.

The T.D.H.F. theory is well presented elsewhere² and the presentation of Baranger will be briefly summarized in the next section.

SUMMARY OF TIME-DEPENDENT HARTREE-FOCK THEORY

The Hamiltonian under consideration is of the standard form

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

with $V_{\alpha\beta\gamma\delta}$ antisymmetrized. Assuming a determinantal wave function, the Hartree-Fock factorization,

$$\langle \text{H.F.} | a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} | \text{H.F.} \rangle \equiv \langle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \rangle \\ = \langle a_{\alpha}^{\dagger} a_{\gamma} \rangle \langle a_{\beta}^{\dagger} a_{\delta} \rangle - \langle a_{\alpha}^{\dagger} a_{\delta} \rangle \langle a_{\beta}^{\dagger} a_{\gamma} \rangle, \quad (2)$$

is exact. The expectation value of the Hamiltonian in a Hartree-Fock determinantal state, is then given by

$$\langle H \rangle = \sum_{\alpha\gamma} T_{\alpha\gamma} \rho_{\gamma\alpha} + \frac{1}{2} \sum_{\alpha\gamma} \Gamma_{\alpha\gamma} \rho_{\gamma\alpha}, \quad (3)$$

where $\rho_{\alpha\beta} = \langle a_{\beta}^{\dagger} a_{\alpha} \rangle$ (the single-particle density matrix) and $\Gamma_{\alpha\beta} = \sum_{\gamma\delta} V_{\alpha\beta\gamma\delta} \rho_{\delta\gamma}$ (the Hartree-Fock potential).

It is then easily shown that the static Hartree-Fock problem consists in finding the representation (or ρ

¹ I. Kelson, Phys. Rev. **132**, 2189 (1963); I. Kelson and C. A. Levinson, *ibid.* **134**, B269 (1964).

² M. Baranger, *Theory of Finite Nuclei, Cargese Lectures in Theoretical Physics* (W. A. Benjamin and Company, Inc., New York, 1963).

matrix) such that

$$[w, \rho] = 0, \tag{4}$$

where $w = T + \Gamma$, with the conditions that $\text{Tr} \rho = N$ and $\rho^2 = \rho$.

If we now assume a time variation in ρ caused by single-particle transitions we can write $i(d\rho/dt) = [\hat{w}, \rho]$, where the caret indicates that Γ is now a function of time. We make the standard approximation and write

$$\rho(t) = \rho^{(0)} + \rho^{(1)}(t), \tag{5}$$

where $\rho^{(0)}$ is a solution of (4) and $\rho^{(1)}(t)$ is assumed to be small. In the static Hartree-Fock representation, where both w and $\rho^{(0)}$ may be diagonal, $\rho^{(1)}$ can only connect an occupied (o) to an unoccupied (u) state and we find

$$i \frac{d}{dt} \rho_{uo}^{(1)} = (E_u - E_o) \rho_{uo}^{(1)} + \sum_{u'o'} V_{u'o'ou} \rho_{u'o'}^{(1)} + \sum_{u'o'} V_{uu'o'o'} \rho_{o'u'}^{(1)}, \tag{6}$$

where E_u and E_o are the appropriate eigenvalues of w .

The above linearization corresponds to assuming that the time-dependent wave function is given by

$$\Psi(t) = \Psi_0 e^{-i\omega_0 t} + \sum_i a_i \Psi_i e^{-i(\omega_0 + \omega_i)t}, \tag{7}$$

where Ψ_i is a determinant in which a single particle has been promoted ω_i in energy and a_i is small. We then have

$$\rho_{uo}^{(1)}(t) = \sum_i \{ a_i e^{-i\omega_i t} x_{uo}^i + a_i^* e^{i\omega_i t} y_{uo}^{i*} \}, \tag{8}$$

where

$$x_{uo}^i = \langle \Psi_0 | a_0^\dagger a_u | \Psi_i \rangle,$$

and

$$y_{uo}^{i*} = \langle \Psi_i | a_0^\dagger a_u | \Psi_0 \rangle. \tag{9}$$

Equation (8) and the corresponding equation for $\rho_{ou}^{(1)}$ now can be written in the form

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} x^i \\ y^i \end{pmatrix} = \omega_i \begin{pmatrix} x^i \\ y^i \end{pmatrix}, \tag{10}$$

where $A_{uo, u'o'} = (E_u - E_o) \delta_{oo'} \delta_{uu'} + V_{u'o'ou}$ and $B_{uo, u'o'} = V_{uu'o'o'}$. This is the T.D.H.F. equation.

If there is an operator Θ that commutes with the Hamiltonian, then (10) must have a $\omega = 0$ solution where the eigenvector is simply

$$\begin{aligned} x_{uo} &= \Theta_{uo}, \\ y_{uo}^* &= \Theta_{uo}. \end{aligned} \tag{11}$$

This solution corresponds to the spurious state.³

THE CALCULATION

For the details of the static Hartree-Fock calculation the reader is referred to Ref. 1. We only briefly remark

³ D. J. Thouless, Nucl. Phys. 22, 789 (1961).

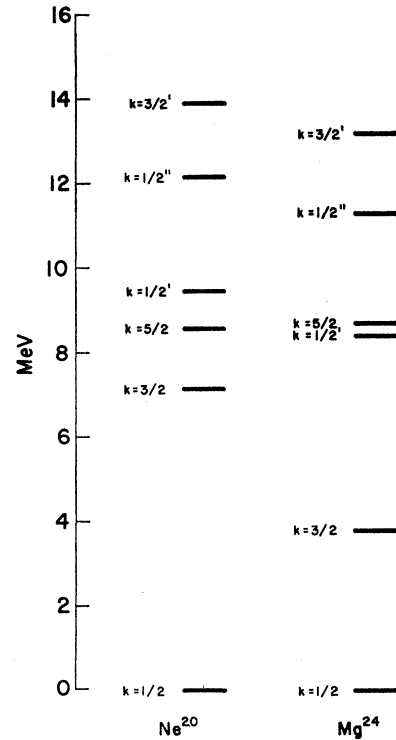


FIG. 1. Self-consistent single-particle spectra for Ne^{20} and Mg^{24} . The parameters employed are $V_0 = 42.5$ MeV, $\alpha_{L,S} = 2.48$ MeV.

here that the trial wave functions were assumed to retain axial symmetry. The λ th trial wave function was thus characterized by a quantum number k corresponding to the angular momentum along the body fixed axis of symmetry and

$$|\lambda; k\rangle = \sum_j C_{\lambda k}^j |j k\rangle, \tag{12}$$

where the sum was restricted to the s - d shell, i.e., to the states $d^{5/2}$, $d^{3/2}$, and $s^{1/2}$. The $C_{\lambda k}^j$'s were the variational parameters. In this way the underlying O^{16} core was taken to be spherical and inert. This assumption will be discussed in a following section.

For the purpose of the T.D.H.F. calculation we reproduce the relevant single-particle energy levels resulting from the static H.F. calculation (Fig. 1).

The necessary truncation of the sums in Eq. (6) is now obvious. For Ne^{20} we limit the sum over occupied states to the $k = \frac{1}{2}$ level and for Mg^{24} to the $k = \frac{1}{2}$ and $\frac{3}{2}$ levels. The sum over unoccupied states is restricted to the five and four levels shown in Fig. 1 for the corresponding nuclei. Consider, for example, an excited state of Ne^{20} with an assumed quantum designation $k = 1$. Such a state would be a superposition of configurations each with one of the following transitions:

$$\begin{aligned} k = \frac{1}{2} \quad m_k = \frac{1}{2} &\rightarrow k = \frac{3}{2} \quad m_k = \frac{3}{2}, \\ k = \frac{1}{2} \quad m_k = \frac{1}{2} &\rightarrow k = \frac{3}{2}' \quad m_k = \frac{3}{2}, \\ k = \frac{1}{2} \quad m_k = -\frac{1}{2} &\rightarrow k = \frac{1}{2}' \quad m_k = \frac{1}{2}, \\ k = \frac{1}{2} \quad m_k = -\frac{1}{2} &\rightarrow k = \frac{1}{2}'' \quad m_k = \frac{1}{2}. \end{aligned}$$

TABLE I. Single-particle self-consistent energies and wave functions for Ne^{20} and Mg^{24} . The italicized numbers are the self-energies in MeV, followed by the components of the eigenfunctions, in the $|jm\rangle$ representation, starting with $C_k^{j\text{max}}$. $V_0=42.5$ MeV.

	Ne^{20}	Mg^{24}
$k=\frac{1}{2}$	0	0
	0.829	0.816
	-0.397	-0.294
$k=\frac{3}{2}$	0.394	0.498
	<i>7.142</i>	<i>3.799</i>
	0.995	0.974
$k=\frac{5}{2}$	-0.098	-0.226
	<i>8.587</i>	<i>8.690</i>
	1.000	1.000
$k=\frac{1}{2}'$	<i>9.435</i>	<i>8.412</i>
	0.528	0.518
	0.321	0.755
$k=\frac{1}{2}''$	-0.787	-0.403
	<i>12.161</i>	<i>11.290</i>
	0.186	-0.257
$k=\frac{3}{2}'$	0.860	0.586
	0.475	0.768
	<i>13.888</i>	<i>13.186</i>
	0.098	0.226
	0.995	0.974

In order to calculate the desired matrix elements for Eq. (10), we need simply express them via Eq. (12) in terms of the $C_{\lambda k}^j$'s and matrix elements in the j representation which are tabulated.⁴ Thus, for completeness we list the relevant $C_{\lambda k}^j$'s (Table I).

It is further assumed that the excited states being computed are characterized by good isotopic spin and possess symmetry with respect to reflections about the xy plane.¹

We introduce the notation for a determinant of single-particle orbitals.

$$\text{Det}(\alpha p \uparrow, \alpha p \downarrow, \alpha n \uparrow, \alpha n \downarrow),$$

where greek letters stand for the quantum numbers of the orbitals, and an up or down arrow designates a positive or negative k value. n and p designate neutron or proton. A particle-hole determinant, corresponding to the ground-state determinant for Ne^{20} , written above, will be written as

$$\Phi_{\alpha n \uparrow}^{\beta n \downarrow} = \text{Det}(\alpha p \uparrow, \alpha p \downarrow, \beta n \downarrow, \alpha n \downarrow).$$

This corresponds to the excitation of the occupied orbital $\alpha n \uparrow$ to the excited orbital $\beta n \downarrow$. In order to construct a state with good isospin, we must take linear combinations of proton and neutron particle-hole states. For example, in order to construct the particle-hole wave functions $\Phi_{\alpha \uparrow}^{\beta \uparrow}(T)$, corresponding to the excitation of the particle from the occupied state $\alpha \downarrow$ to the unoccupied state $\beta \uparrow$, with given T , we take

$$\begin{aligned} \Phi_{\alpha \uparrow}^{\beta \uparrow}(0) &= (1/\sqrt{2})[\Phi_{\alpha p \downarrow}^{\beta p \uparrow} + \Phi_{\alpha n \downarrow}^{\beta n \uparrow}], \\ \Phi_{\alpha \uparrow}^{\beta \uparrow}(1) &= (1/\sqrt{2})[\Phi_{\alpha p \downarrow}^{\beta p \uparrow} - \Phi_{\alpha n \downarrow}^{\beta n \uparrow}]. \end{aligned} \quad (13)$$

⁴ R. Thieberger, Nucl. Phys. 2, 533 (1956/57).

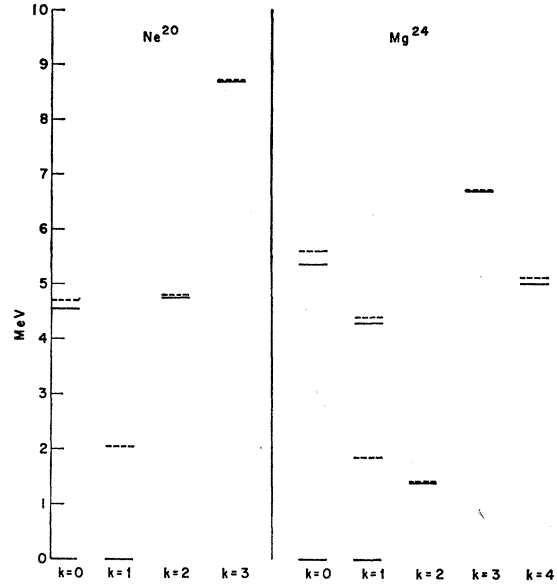


FIG. 2. The intrinsic states resulting from the T.D.H.F. calculation. The dashed lines represent the positions of the states when the backward-going graphs are neglected; the solid lines the results of the complete calculation. Only the lowest lying state for each k is shown.

Matrix elements for a two-body operator between such states, are given generally by

$$\begin{aligned} \langle \Phi_A^B(0) | V | \Phi_{A'}^{B'}(0) \rangle &= \frac{1}{2} \langle AB'(T=0) | V | A'B(T=0) \rangle \\ &\quad - \frac{3}{2} \langle AB'(T=1) | V | A'B(T=1) \rangle, \\ \langle \Phi_A^B(1) | V | \Phi_{A'}^{B'}(1) \rangle &= -\frac{1}{2} \langle AB'(T=0) | V | A'B(T=0) \rangle \\ &\quad - \frac{1}{2} \langle AB'(T=1) | V | A'B(T=1) \rangle. \end{aligned} \quad (14)$$

H is invariant under the operation $R = e^{i\pi J_x}$, a rotation of π radians about the x axis. $k=0$ states can be taken to be odd or even under R . (If $k \neq 0$, then R changes the sign of k as well as introducing a phase factor.) H has no matrix elements joining even states to odd states, hence we can introduce a quantum number S , which is zero for even states, and unity for odd states. Under the operation R , we have for single-particle orbitals

$$\begin{aligned} R | \uparrow \rangle &= | \downarrow \rangle, \\ R | \downarrow \rangle &= - | \uparrow \rangle. \end{aligned}$$

Even states can be produced by operation of $(1+R)/\sqrt{2}$, and odd states by $(1-R)/\sqrt{2}$. For example, we can construct states $\Phi_{\alpha}^{\beta}(T, S)$ for $k=0$ states (note that $k_{\alpha} = k_{\beta}$ since the total k vanishes):

$$\begin{aligned} \Phi_{\alpha}^{\beta}(0,0) &= (1/\sqrt{2})[\Phi_{\alpha \uparrow}^{\beta \uparrow}(0) + \Phi_{\alpha \downarrow}^{\beta \downarrow}(0)], \\ \Phi_{\alpha}^{\beta}(0,1) &= (1/\sqrt{2})[\Phi_{\alpha \uparrow}^{\beta \uparrow}(0) - \Phi_{\alpha \downarrow}^{\beta \downarrow}(0)], \\ \Phi_{\alpha}^{\beta}(1,0) &= (1/\sqrt{2})[\Phi_{\alpha \uparrow}^{\beta \uparrow}(1) + \Phi_{\alpha \downarrow}^{\beta \downarrow}(1)], \\ \Phi_{\alpha}^{\beta}(1,1) &= (1/\sqrt{2})[\Phi_{\alpha \uparrow}^{\beta \uparrow}(1) - \Phi_{\alpha \downarrow}^{\beta \downarrow}(1)]. \end{aligned} \quad (13A)$$

The result of diagonalizing the matrix (10) will be a set of "intrinsic" excited states. Each intrinsic state

will be a linear combination of the rotational levels in the band being considered, i.e.,

$$\Psi = \sum_J A^J \Psi^J \quad \text{where} \quad \sum_J |A^J|^2 = 1. \quad (15)$$

This follows from the ansatz, as formulated in the Hill-Wheeler analysis of rotational spectra,⁵ that the result of operating on the intrinsic state by an angular momentum projection operator p^J yields a member of the rotational band Ψ^J , i.e.,

$$p^J \Psi_{\text{intrinsic}} = \Psi^J. \quad (16)$$

In order to compare the positions, in energy, of the calculated states with the empirical findings, one can simply use the empirical moment of inertia as follows:

$$\begin{aligned} \omega &= \langle \Psi_I | H | \Psi_I \rangle = \sum_J E_J |A^J|^2 \\ &\cong \sum_J \left(E_0 + \frac{\hbar^2}{2\mathcal{J}} J(J+1) |A^J|^2 \right) \\ &= E_0 + \langle J^2 \rangle \frac{\hbar^2}{2\mathcal{J}}. \end{aligned} \quad (17)$$

Here E_0 will be the energy of the lowest member of the rotational band. It is assumed, in the above, that the band is purely rotational in order to obtain the third equality. In principle the quantity \mathcal{J} , the moment of inertia, could be calculated theoretically. At present, however, there exists no method for calculating the moment of inertia of an excited nucleus so we used the empirical value.⁶ This value is not completely specified by experiment, partially because the bands are not purely rotational. There was thus some latitude in our choice of \mathcal{J} ; the values decided upon were those most

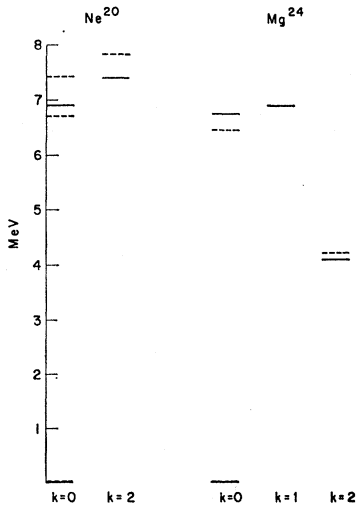


FIG. 3. Comparison of the empirical (dashed lines) and calculated positions (solid lines) of the rotational band heads. Again only the lowest bands are considered because of the lack of data.

⁵ D. L. Hill and J. A. Wheeler, Phys. Rev. **89**, 1102 (1953).

⁶ See I. M. Pavlichenkov, Zh. Eksperim i Teor. Fiz. **44**, 2001 (1963) [English transl.: Soviet Phys.—JETP **17**, 1345 (1963)].

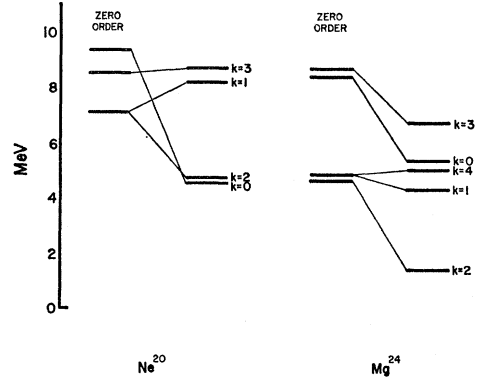


FIG. 4. Comparison between zero-order intrinsic states (only single-particle energy taken into account) and rigorously computed intrinsic states for Ne^{20} and Mg^{24} . The lowest intrinsic state for each k -value is given.

compatible with the observed spectra. The test of our calculation will then be comparison of the relative positions of these levels for the various k bands with the empirical positions.

There should be a spurious solution to Eq. (10) even though the summations are truncated. This is a result of the fact that the angular momentum operator along the axis of symmetry J_k commutes with the Hamiltonian in the truncated space as well as in the complete space.

RESULTS

In Fig. 2 one sees the positions in energy of the intrinsic states, for various k values, for Ne^{20} and Mg^{24} . The solid lines indicate the calculated positions when Eq. (10) is solved, in the relevant subspace, without ignoring any terms. The dashed lines indicate the energy positions when the last term, the so-called backward going graphs, are neglected. This corresponds to the Tamm-Dancoff approximation. Note that the effect of the correlations in the ground state giving rise to the backward going graph is negligible except for the spurious solutions.

In Fig. 3 the empirical spectra⁷ (dashed lines) are compared with the calculated bands (solid lines), extracted from the intrinsic states via Eq. (17).

It is also interesting to note the important role played by the two-body interaction in shifting the intrinsic states from their zero-order position to their actual position. The zero-order intrinsic energy is obtained by simply promoting the particle and taking into account only the single-particle energy change. Figure 4 illustrates this shifting for lowest k bands in Ne^{20} and Mg^{24} .

The agreement of the predicted and observed levels is gratifying. There are, evidently, two characteristics of the observed spectra not predicted by the calculation. First, the odd-parity levels were not predicted because we had limited ourselves to the s - d shell. Secondly,

⁷ A. E. Litherland, J. A. Kuehner, H. E. Gove, M. A. Clark, and E. Almquist, Phys. Rev. Letters **7**, 5537 (1961). P. M. Endt and C. Van Der Leun, Nucl. Phys. **34**, 1 (1962).

TABLE II. All of the calculated intrinsic states with (column labeled T.D.H.F.) and without (labeled T.D.) backward graphs. At present, there is insufficient data (moments of inertia) to fully analyze these states. Those of the above states, not appearing in Figs. 2 and 3, lie in an energy region where rotational bands have not yet been identified.

			Ne ²⁰					Mg ²⁴	
K	T	S	T.D.H.F.	T.D.	K	T	S	T.D.H.F.	T.D.
0	0	0	0(G.S.)	0	0	0		0(G.S.)	0
0	0	0	4.56	4.70	0	0	0	9.68	9.77
0	0	0	11.67	11.81	0	0	0	8.81	8.86
0	0	1	10.47	10.46	0	0	0	5.38	5.60
0	0	1	12.95	13.01	0	0	1	12.33	12.39
0	1	0	10.51	10.79	0	0	1	9.64	9.65
0	1	0	13.56	13.59	0	0	1	8.79	8.84
0	1	1	9.71	9.77	0	1	0	13.14	13.17
0	1	1	12.86	12.92	0	1	0	9.38	9.38
					0	1	0	7.16	7.18
1	0		14.50	14.52	0	1	1	11.94	11.97
1	0		12.04	12.07	0	1	1	11.45	11.53
1	0		9.38	9.87	0	1	1	8.93	8.97
1	0		0	2.05					
1	1		13.39	13.41	1	0		13.70	13.74
1	1		14.31	14.36	1	0		11.91	11.97
1	1		9.97	10.06	1	0		6.03	6.40
1	1		8.26	8.27	1	0		6.14	6.22
					1	0		4.30	4.41
2	0		8.53	8.55	1	0		0	1.85
2	0		4.75	4.81	1	1		13.37	13.38
2	0		13.30	13.34	1	1		11.74	11.77
2	1		9.38	9.42	1	1		10.56	10.59
2	1		7.49	7.53	1	1		8.60	8.65
2	1		14.85	14.88	1	1		6.99	7.03
					1	1		6.20	6.21
3	0		9.22	9.26	2	0		12.61	12.64
3	1		8.71	8.71	2	0		8.26	8.29
					2	0		5.97	5.98
					2	0		1.42	1.44
					2	1		14.19	14.19
					2	1		9.40	9.42
					2	1		7.88	7.89
					2	1		6.19	6.23
					3	0		9.51	9.59
					3	0		6.72	6.72
					3	1		8.72	8.74
					3	1		10.72	10.80
					4	0		5.66	5.68
					4	1		5.04	5.14

there is a 0^+ state in Ne²⁰ that is not predicted. It is believed that this state may be the result of multiple particle-hole excitations, and thus cannot be obtained

by the simple random-phase approximation (R.P.A.). Credence to this hypothesis is given by the existence of a 0^+ level at approximately the same energy in the O¹⁶ spectra, indicating that it is a result of the promotion of two or four particles from an odd-parity state in the O¹⁶ core to the s - d levels.

For completeness, all of the intrinsic states resulting from the T.D.H.F. calculation are shown in Table II. The results in column labeled "time-dependent Hartree-Fock" (T.D.H.F.) take into account ground-state correlations, or backward going graphs, while those in the column labeled Tamm-Dancoff (T.D.) ignore such correlations. Since a moment of inertia parameter is needed in order to analyze these states, the analysis was only carried out for these bands which have been identified experimentally.

CONCLUSIONS

In the past, several approaches have been followed in order to make use of the powerful T.D.H.F. or random-phase approximation theories. Generally, these calculations were based on the guess that the static Hartree-Fock solution is the same, or nearly the same, as the result of a Nilsson calculation. That such a guess is unreasonable in the s - d shell is immediately evident from an examination of experimental evidence. In Fig. 3 we see that an energy gap of approximately 6 MeV is observed between the first two 0^+ levels of Ne²⁰. The occurrence of such a gap cannot be explained on the basis of a Nilsson single-particle energy level scheme, where no such gaps occur. Obviously, to achieve such a gap in a calculation one must start with a single-particle basis in which a gap also occurs. As is seen from Fig. 1, such a gap indeed appears in the H.F. level scheme. Thus, even if the T.D.H.F. or R.P.A. theories did not demand the use of a static H.F. basis, one would be lead to believe that such a scheme is more capable of explaining the observed spectra than a Nilsson basis.

The results quoted here are the result of a preliminary calculation. Consideration of transition probabilities, odd-parity states, multiple particle-hole excitations, and pairing effects is presently being undertaken.