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ENERGY SPECTRUM OF ^{20}Ne USING HARTREE-FOCK
AND TAMM-DANCOFF WAVE FUNCTIONS[†]

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Abstract

The energy spectrum of the first excited 0^+ band has been calculated by projecting out good angular momentum states from a Tamm-Dancoff intrinsic state. The predicted spectrum is in good agreement with the experiment. The admixture of the Tamm-Dancoff and the Hartree-Fock states in the projected basis by the interaction Hamiltonian has also been calculated. The admixture improves the agreement with the experiment for some of the states.

[†]This work was done under the auspices of the U. S. Atomic Energy Commission.

The static Hartree-Fock (HF) theory together with the angular momentum projection technique has been successfully applied to explain the energy spectrum of the ground 0^+ band in ^{20}Ne [1,2]. The accuracy of the projected HF wavefunctions of ^{20}Ne and of many other nuclei in the 2s,1d shell has been studied in several recent publications [3,4,5,6], and it is clear from these works that the projected wavefunctions are, to a very good approximation, the eigenstates of the nucleus.

Attempts have been made to explain the first excited 0^+ band and its energy spectrum in the framework of the HF theory [7,8]. The energy spectrum of the excited 0^+ band, unlike the ground band, does not show very much of the rotational character. A natural approach in the framework of the HF theory for explaining the excited 0^+ band may consist of describing it by a superposition of configurations composed of hole-particle excitations out of the HF state describing the ground band. Because of the large energy gap (~ 10 MeV) between the occupied and the unoccupied states of the HF Hamiltonian of ^{20}Ne , one can safely assume that the configurations needed to describe the excited 0^+ band will consist of mainly one particle - one hole excitations. A strong support to this assumption is lent by the various calculations [9,10] performed to evaluate the pairing effects on the HF state of ^{20}Ne , since without exception all of them predict negligible pairing effects. The time-dependent HF formalism is the appropriate form of HF theory for treating such hole-particle excited states. This approach has been utilized by Bassichis et al. [7], to derive the excited bands of ^{20}Ne and ^{24}Mg . The energies of the different states in a given band were calculated by them by using the energy formula of the rotational model with some empirical value for the moment of inertia $\mathfrak{J}$.

Since the excited bands are not purely rotational in nature, there was some latitude in their choice of $\mathcal{J}$ and by choosing a suitable value they obtained a fair agreement with the experiment.

An interesting and significant conclusion of the work of Bassichis et al. [7], which served as a motivation for the work presented here, is the result that the effect of correlations in the ground state giving rise to the so-called backward going graph is negligible except for the spurious solutions. The result implies that one can safely use the Tamm-Dancoff approximation (TDA) instead of TDHF in the case of ^{20}Ne and ^{24}Mg . The starting point in the present work, therefore, is to assume that the TDA provides a satisfactory scheme for deriving the intrinsic state of the first excited 0^+ band. The energies of the different states within this band are, then, calculated using the angular momentum projection technique. The admixture of the projected TDA states and the projected HF states has been also calculated by diagonalizing (2×2) energy matrices for each of the $J = 0, 2, 4, 6$ states.

First, an HF calculation was performed for the ground 0^+ band in ^{20}Ne using the following experimental single-particle energies (ϵ_j):

$$\begin{aligned}\epsilon_{d_{5/2}} &= -4.142 \text{ MeV} \\ \epsilon_{2s_{1/2}} &= -3.271 \text{ MeV} \\ \epsilon_{d_{3/2}} &= +0.94 \text{ MeV}\end{aligned}\tag{1}$$

and a Gaussian two-body interaction with a Rosenfeld mixture given by,

$$V(r) = V_0 e^{-(r/\mu)^2} \frac{\vec{\tau}_1 \cdot \vec{\tau}_2}{3} [0.3 + 0.7 \vec{\sigma}_1 \cdot \vec{\sigma}_2]\tag{2}$$

The results of the HF calculation are given in table 1.

Next, the intrinsic state for the excited 0^+ band was derived by doing a Tamm-Dancoff calculation which consists in diagonalizing the matrix $A_{(\sigma\lambda),(\tau\mu)}$ defined by [7,8],

$$A_{(\sigma\lambda),(\tau\mu)} \equiv (\epsilon_{\sigma}^{(0)} - \epsilon_{\lambda}^{(0)}) \delta_{\sigma\tau} \delta_{\lambda\mu} + \langle \sigma\mu | V | \lambda\tau \rangle \quad (3)$$

where λ, μ and σ, τ are pairs of occupied and unoccupied states respectively, $\epsilon_{\sigma}^{(0)}$ and $\epsilon_{\lambda}^{(0)}$ are HF single-particle energies as given in table 1, and V is the two-body interaction defined by eq. (2).

The intrinsic state of the excited 0^+ band has $T = 0$ and therefore the basis wave functions ϕ_{λ}^{σ} for matrix A are constructed by taking a linear combination of neutron and proton states. Clearly the appropriate linear combination is

$$\phi_{\lambda}^{\sigma}(T=0) = \frac{(a_{\sigma P}^{+} a_{\lambda P} + a_{\sigma N}^{+} a_{\lambda N}) \phi_{HF}}{\sqrt{2}} \quad (4)$$

with the limitation $k_{\sigma} - k_{\lambda} = 0$.

Using the basis wave functions given in eq. (4) one can easily show that the matrix A is given by

$$A_{(\sigma\lambda),(\tau\mu)} = (\epsilon_{\sigma}^{(0)} - \epsilon_{\lambda}^{(0)}) \delta_{\sigma\tau} \delta_{\lambda\mu} + \frac{3}{2} \langle \sigma\mu | V_A^{T=1} | \lambda\mu \rangle + \frac{1}{2} \langle \sigma\mu | V_A^{T=0} | \lambda\mu \rangle \quad (5)$$

Because of the restriction $k_{\sigma} - k_{\lambda} = 0$, A is only a (4×4) matrix. The lowest eigenvalue and the corresponding eigenfunction of A give the band-head

energy and the intrinsic wave function of the first excited 0^+ band. Table 2 lists the various eigenvalues and eigenfunctions of the matrix A.

The physical states of the ground 0^+ band[†] and the excited 0^+ band

[†]The HF and the projection calculation with the interaction described by eq. (1) and eq. (2) has already been done by Ripka [3] for the ground 0^+ band in ^{20}Ne . The purpose of redoing this calculation was to seek a higher accuracy on the HF and the projection results. However our results are only slightly different from those of Ripka.

are constructed by projecting out good angular states from their respective intrinsic wave functions using the method of Hill-Wheeler Integral [11]. The energies of the physical states are then calculated using the following expression

$$E_J = \frac{\langle \phi | P_{MK}^J H | \phi \rangle}{\langle \phi | P_{MK}^J | \phi \rangle} \quad (6)$$

P_{MK}^J in eq. (6) is the angular momentum projection operator defined as

$$P_{MK}^J = \frac{2J+1}{1} \int_0^\pi d_{MK}^J(\theta) \exp(-i\theta J_y) \sin\theta d\theta \quad (7)$$

where $d_{MK}^J(\theta)$ is the reduced rotation matrix.

In evaluating the energy E_J one can set $M = K$ in the projection operator without any loss of generality. In the present context we have $M = K = 0$.

For the HF state, the projected energies E_J given by eq. (6) were evaluated using the techniques discussed in refs. [1,12]. For the TDA state, the corresponding calculation is more involved since the TDA state is a linear combination of determinants which are not of the HF type and therefore H operating on them can excite two-particle as well as one-particle states. Techniques have been developed to carry out the projection calculation using arbitrary intrinsic state and will be presented in a separate paper [13]. The results on the projected energies are given in table 3.

The possibility that the interaction Hamiltonian can mix the same J -states projected from the HF and TDA intrinsic states and thereby modify the energy spectrum has also been investigated. If the mixing is significant one can diagonalize a (2×2) energy matrix for each of the $J = 0, 2, 4$, etc., states. To perform this calculation one needs a knowledge of the overlap functions $\langle \phi_{HF} | P_{00}^J | \phi_{TDA} \rangle$ and the matrix elements $\langle \phi_{HF} | P_{00}^J H | \phi_{TDA} \rangle / N_J$ for the various J states, where N_J is the product of the normalization constants $(\langle \phi_{HF} | P_{00}^J | \phi_{HF} \rangle)^{1/2}$ and $(\langle \phi_{TDA} | P_{00}^J | \phi_{TDA} \rangle)^{1/2}$. These quantities were calculated by the techniques discussed in refs. [1,12,13]. The non-orthogonality of the projected states was properly taken into account in setting up the energy matrices. Table 4 gives the values of the overlap functions and the modified energies obtained from the diagonalization. The comparison between the experiment and the predicted results are shown in fig. 1 and table 5.

It is clear from our results shown in table 5 and fig. 1 that the projected TDA states provide a good description for the energy spectrum of the first excited 0^+ band in ^{20}Ne . The effect of admixing the projected HF

and the projected TDA states is not quite unimportant. It helps to improve the agreement with the experiment for the 0^+ and 4^+ states of the excited band.

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Table Captions

Table 1. HF single-particle energies (ϵ_{μ}^0) and wave functions of ^{20}Ne . The orbit $k_{\mu} = 1/2$ at -16.600 MeV is filled with four nucleons.
 $E_{\text{HF}} = -39.278$ MeV.

Table 2. Eigenvalues and eigenfunctions of the Tamm-Dancoff matrix A defined in eq. (5). Eigenvalues are labelled by E_{TDA} and the eigenfunctions are expressed in the basis wave functions ϕ_{λ}^{σ} defined in eq. (4).

Table 3. Normalization constants and energies of the projected states derived from the HF and TDA intrinsic wave functions using eq. (6).

Table 4. Normalized overlap of the projected HF and TDA wave functions and the modified energies calculated using their admixture.

Table 5. Comparison between the experimental and the predicted spectrum.

Theory (a) and theory (b) correspond to results without and with admixture of projected states. (* After the preparation of this article the author came across a similar calculation by Satpathy [14] published very recently. His results are quite poor compared to the results presented here.)

Table 1

k_μ	$\epsilon_\mu^{(0)}$ (MeV)	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2	-16.600	-0.7149	0.5728	0.4011
3/2	- 6.295	-0.9917	0.0	0.1285
1/2'	- 5.025	-0.6874	-0.6807	-0.2531
5/2	- 4.652	1.0000	0.0	0.0
1/2''	- 2.095	-0.1281	0.4566	-0.8804
3/2	0.112	0.1285	0.0	0.9917

Table 2

E_{TDA} (MeV)	Wave Function			
	$\phi_{1/2}^{1/2'}$	$\phi_{1/2}^{-1/2'}$	$\phi_{1/2}^{1/2''}$	$\phi_{1/2}^{-1/2''}$
5.653	-0.6038	-0.6038	0.3681	0.3681
12.881	0.7060	-0.7060	-0.0389	0.0389
14.729	0.3681	0.3681	0.6038	0.6038
15.909	0.0389	-0.0389	0.7060	-0.7060

Table 3

J	$\langle \Phi_{\text{HF}} P^J \Phi_{\text{HF}} \rangle$	$\langle \Phi_{\text{TDA}} P^J \Phi_{\text{TDA}} \rangle$	E_J^{HF} (MeV)	E_J^{TDA} (MeV)
0	0.1148	0.1467	-3.015	3.158
2	0.4124	0.4628	-1.761	4.932
4	0.3327	0.2864	0.996	7.450
6	0.1224	0.0873	4.793	8.256

Table 4

J	$\langle \Phi_{\text{HF}} P^J \Phi_{\text{TDA}} \rangle N_J$	Modified energy (MeV)	
		Ground 0^+ band	Excited 0^+ band
0	0.2308	-3.043	3.334
2	0.1525	-1.878	4.953
4	-0.0789	0.878	7.750
6	-0.5320	4.765	10.134

Table 5*

J	Experiment	Theory	
		(a)	(b)
0^+	0.0 MeV	0.0 MeV	0.0 MeV
2^+	1.63 MeV	1.25 MeV	1.22 MeV
4^+	4.25 MeV	4.01 MeV	3.92 MeV
0^+	6.72 MeV	6.17 MeV	6.38 MeV
2^+	7.84 MeV	7.95 MeV	7.99 MeV
6^+	8.79 MeV	7.81 MeV	7.82 MeV
4^+	11.07 MeV	10.46 MeV	10.79 MeV

Figure Caption

Fig. 1. Comparison between the experimental and theoretical spectrum of the ground 0^+ and first excited 0^+ band in ^{20}Ne . Theory (a) and theory (b) imply the same as in table 5. For the facility of comparison only the relevant experimental energies are shown.

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Fig. 1

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