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## A Tamm-Dancoff Calculation of Excited States of Ne<sup>20</sup>

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We use the Tamm-Dancoff approximation and the Peierls-Yoccoz projection method to obtain the states of the first excited  $0^+$  band of Ne<sup>20</sup>. We compute the energy spectrum and the *B*(*E*2) interband and intraband reduced transition probabilities using different types of two-body interactions. The results are not as good as the ones obtained previously for the ground state band. Only one *B*(*E*2) experimental measurement is available to compare with.

Usamos a aproximação de Tamm-Dancoff e o método de projeção de Peierls-Yoccoz para obter estados da primeira banda  $0^+$  excitada do  $Ne^{20}$ . Calculamos o espectro de energia e as probabilidades de transição B(E2) entre níveis desta banda e entre esta e a fundamental, usando diferentes tipos de interação de dois corpos. Os resultados não são tão bons quanto os obtidos anteriormente para a banda fundamental. Existe somente uma transição B(E2) medida experimentalmente com a qual podemos comparar nossos resultados.

In a previous paper<sup>1</sup>, one of us used the Hartree-Fock (HF) approximation and the angular momentum projection technique to calculate energy levels and E2 transitions within the ground state band of Ne<sup>20</sup>. We present here the same kind of information about low energy states of the first excited band described by a Tamm-Dancoff (TD) wave function. An intrinsic excited band can be a superposition of multiple particle-hole excitations built out of the HF ground state wave function. As the HF single particle spectrum of Ne<sup>20</sup> shows a large energy gap between occupied and unoccupied states, it is reasonable to assume that the first 0<sup>+</sup> excited band should be due mainly to the superposition of **lp-lh** excitations, because much more energy would be required to excite two or more particles from the ground state.

The nuclear wave function  $|\psi\rangle$  can be written as a sum of terms describing **lp-lh**, 2*p*-2*h*, ..., etc., excitations built out of the HF ground state  $|\psi_0\rangle$ ,

$$|\psi\rangle = X_0 |\psi_0\rangle + \sum_{mi} X_{mi} |\psi_{mi}\rangle + \sum_{\substack{mi\\nj}} X_{mi,nj} |\psi_{mi,nj}\rangle + \dots, \qquad (1)$$

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where

$$|\psi_{ni}\rangle = a_{m}^{\dagger}a_{i}|\psi_{0}\rangle,$$
  
$$|\psi_{mi,nj}\rangle = a_{m}^{\dagger}a_{i}a_{n}^{\dagger}a_{j}|\psi_{0}\rangle.$$
 (2)

Occupied states are labelled with letters i, j and unoccupied states with letters m, n; the operators'a' and a obey fermionic anticommutation relations. The more terms we add to (1) the more exact the wave functions will be; however the solution of the equation will become unpractical.

The first order TD approximation consists in keeping only terms up to **lp-lh** excitations,

$$\left|\psi^{(1)}\right\rangle = X_{0}\left|\psi_{0}\right\rangle + \sum_{mi} X_{mi}\left|\psi_{mi}\right\rangle.$$
(3)

In order to obtain the energy of the state  $|\psi^{(1)}\rangle$  we solve the equation

$$\delta \langle \psi^{(1)} | H - E^{(1)} | \psi^{(1)} \rangle = 0, \qquad (4)$$

where  $X_0$  and  $X_{mi}$  are variational parameters. The resulting equations are

$$(E^{(1)} - E_0) X_0 = 0 (5)$$

and

$$\sum_{nj} \mathscr{A}_{mi, \mathbf{y}}^* X_{nj} = (E^{\prime \prime \prime} - E_{,}) X_{mi}, \qquad (6)$$

*E*, being the *HF* ground state energy. The excited states will correspond to the solutions  $X_0 = 0$  and  $E^{(1)} - E$ ,  $= \hbar \omega = \text{excitation energy}$ , and they will be determined by solving the eigenvalue problem described by equation (6). The antisymmetrized matrix elements of the two-body interaction is contained in

$$\mathscr{A}_{mi,nj}^{*} = (\mathbf{E}, -\varepsilon_{i})\delta_{ij}\delta_{mn} + (\mathbf{mj} |v|in\rangle_{A}.$$
<sup>(7)</sup>

We use six types of interactions that enter in the calculation as different sets of the quantities  $G_{JT}(j_1j_2,j_3j)$ , which are known as the antisymmetrized and normalized particle-particle reduced matrix elements of the interaction. They are expressed in the basis of the harmonic oscillator single particle wave functions. These  $G_{JT}$  can be taken as the effective interactions determined from realistic two-body forces that fit the nucleon-nucleon scattering data. The truncation of the shell model space implies that renormalization corrections should be taken into account.

Our results are presented under the following labels: (K<sub>R</sub>), (K), (KLS), (KLS), (S<sub>R</sub>) and (Y) where the index R was written in order to point out matrix elements including renormalization corrections. (K) refers to the effective interaction derived by T. T. S. Kuo<sup>2</sup> using the Hamada-Johnston potential; (KLS) are the effective matrix elements obtained by S. Kahana, H. C. Lee and C. K. Scott<sup>3</sup> from a non-local potential; (S) refers to the Sussex matrix elements derived by Elliott *et al.*<sup>4</sup>. Finally, a Yukawa (Y) central force with a range of 1.4 fm was used, with an exchange mixture having the following parameters: triplet-even, -43.0 MeV; singlet-even, -31.5 MeV; triplet-odd, 17.8 MeV; singlet-odd, 37.4 MeV

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| Т | K   | s  | κ <sub>r</sub> | K     | Y     | KLS   | KLS <sub>R</sub> | s <sub>r</sub> |
|---|-----|----|----------------|-------|-------|-------|------------------|----------------|
| 0 | 0   | 1  | 6.71           | 4.92  | 4.41  | 5.81  | 5.23             | 5.10           |
| 0 | 0   | 1  | 12.71          | 11.16 | 12.62 | 13.18 | 11.66            | 11.81          |
| 0 | 0   | -1 | 10.13          | 7.78  | 10.58 | 9.19  | 8.98             | 9.48           |
| 0 | 0   | -1 | 12.26          | 10.13 | 13.83 | 11.65 | 10.97            | 10.72          |
| 0 | 1   |    | 2.55           | 1.56  | 2.44  | 2.25  | 2.42             | 2.14           |
| 0 | 1   |    | 9.84           | 7.68  | 10.31 | 9.09  | 8.88             | 9.53           |
| 0 | 1   |    | 12.17          | 10.39 | 12.66 | 11.80 | 9.90             | 10.35          |
| 0 | 1   |    | 15.66          | 13.38 | 15.44 | 15.21 | 14.26            | 14.95          |
| 0 | 2   |    | 8,33           | 6.48  | 7.58  | 8.03  | 6.55             | 6.72           |
| 0 | 2   | ÷  | 8.97           | 7.06  | 9.41  | 8,69  | 8.16             | 8.36           |
| 0 | 2   |    | 13.51          | 11.43 | 13.45 | 13.01 | 12.50            | 12.69          |
| 0 | 3   |    | 11.08          | 8.54  | 10.68 | 10.22 | 9.03             | 9.55           |
| 1 | 0   | 1  | 11.31          | 8.81  | 11.13 | 10.56 | 10.55            | 10.83          |
| 1 | 0   | 1  | 13.61          | 11.30 | 14.14 | 13.02 | 12.42            | 12.41          |
| 1 | 0   | -1 | 10.66          | 8.14  | 10.59 | 9.62  | 9.07             | 9.82           |
| 1 | 0   | -1 | 13.10          | 10.90 | 13.98 | 12.40 | 11.84            | 12.13          |
| 1 | 1   |    | 9.14           | 7.09  | 10.03 | 8.65  | 8.18             | 8.23           |
| 1 | 1   |    | 10.91          | 8.38  | 10.79 | 9.97  | 9.57             | 9.93           |
| 1 | 1   |    | 13.63          | 11.37 | 14.27 | 12.98 | 12.31            | 12.47          |
| 1 | 1   |    | 15.90          | 13.16 | 15.65 | 14.93 | 14.55            | 15.08          |
| 1 | 2   |    | 8.60           | 6.52  | 9.71  | 7.90  | 7.58             | 7.65           |
| 1 | 2   |    | 11.30          | 8.57  | 11.04 | 10.32 | 9.60             | 10.05          |
| 1 | 2   |    | 16.31          | 13.41 | 15.87 | 15.14 | 14.80            | 15.54          |
| 1 | 3 . |    | 10.84          | 8.10  | 10.69 | 9.76  | 9.10             | 9.59           |

**Table I - Ne<sup>20</sup>** Tamm-Dancoff excitation energies in MeV. In the third column there is the eigenvalue of the operator  $e^{-i\pi J_y}$ . Only the first state with K = 0 and T = 0 was studied.

We first performed the HF calculation for the ground state band of Ne<sup>20</sup>, assuming the nucleus of 0<sup>16</sup> to behave as an inert core. Time reversal and charge symmetry were also assumed. With the axially symmetric HF solution we constructed the matrix elements (mj | v | in), for fixed values of the third component of the angular momentum  $K = m_m - m_i = m_n - m_j$ , and total isospin T = 0 or T = 1.

We reproduce in Table I the Tamm-Dancoff excitation energies, in MeV, measured from the  $0^{16}$  binding energy. These are the solutions of Eq. (6). We believe that one of the experimental  $0^+$  energy levels of Ne<sup>20</sup> at 6.72 and 7.20 MeV could possibly belong to the first K=0, T=0 intrinsic excited state.

Physical states having good total angular momentum were obtained from the intrinsic HF state and from the first K=0, T=0, TD intrinsic excited state, using the angular momentum projection technique. The Hill-Wheeler integrals give us the wave functions belonging to the ground state and to the first excited bands:

$$\left\{ \begin{vmatrix} \psi_{MK}^{J} \rangle_{g \cdot s} \\ \psi_{MK}^{J} \rangle_{1 \, st \, exc.} \end{matrix} \right\} = \frac{2J+1}{8\pi^2} \frac{1}{C_{JK}} \int d\Omega \, D_{MK}^{J*}(\Omega) R(\Omega) \left\{ \begin{vmatrix} \psi_{0} \rangle_{HF} \\ \psi^{(1)} \rangle_{TD} \end{matrix} \right\}.$$
(8)

We calculate the expectation value of the Hamiltonian operator in these states as well as the intranband and interband matrix elements of the electric quadrupole moment operator. The energy levels of Ne<sup>20</sup> are shown in Fig. 1



**Fig. 1** • Projected HF (full lines) and TD (dashed lines) energies of Ne<sup>20</sup> using different types of two-body interactions. The spin value is on the right of each level. The number in the bottom is the energy of the lowest  $J^{\pi} = 0^+$  level relative to the  $0^{16}$  binding energy. a) Ref. (9); Yukawa interaction with Rosenfeld mixture (TD). b) Ref. (10); Gaussian interaction with Rosenfeld mixture (TD). c) Ref. (6);  $K_R$  interaction (Shell Model).

for each type of two-body interaction. Dotted lines belong to the first excited band. The experimental spectrum for T = 0 is also shown. All energies are in MeV. The agreement is quite good for the ground state band, and it seems to be even better if we use renormalized two-body interactions. A simple Yukawa force also works extremely well. However, the situation is not the same for the excited states. The calculation produces one  $0^+$  state and one  $2^+$  state but experimentaly we have two  $0^+$  states in 6.72 MeV and 7.20 MeV plus two  $2^+$  states in 7.42 MeV and 7.83 MeV. In 1967, Litherland<sup>5</sup> suggested that these levels would form two pairs of  $0^+ - 2^+$  states belonging to different bands, namely, one pair in 6.72 and 7.42 MeV respectively, and the remaining pair in 7.20 and 7.83 MeV. A shell model calculation performed by E. C. Halpert et al.<sup>6</sup> also found only one pair of  $0^+ - 2^+$  states in this energy region. They also calculated spectroscopic factors that were compared with known experimental values, indicating that the shell model energy levels correspond to the  $0^+ - 2^+$ pair in 6.72 and 7.42 MeV.

A. Arima *et al.*<sup>7</sup> suggested that the other pair of  $0^+ - 2^+$  levels in 7.20 and 7.83 MeV could be related to a quartet structure of these excited states of Ne<sup>20</sup>. Experimental investigations by R. Middleton et al.<sup>8</sup> lead these authors to propose that the Ne<sup>20</sup> configurations in the states  $0^+ - 2^+$ at 7.20 and 7.83 MeV, respectively, should be that of two a-particles bound to  $C^{12}$ . Therefore, we can assume that the standard shell model or the Tamm-Dancoff calculation we performed are reproducing the other pair of  $0^+ - 2^+$  levels at 6.72 and 7.42 MeV. However, even using the various types of two-body interactions, we were not able to fit both of these  $0^+ - 2^+$ levels simultaneously. No comparison is intended between states with higher angular momenta. We show in Fig. 1 the results of similar TD calculations found in the literature<sup>9,10</sup>. We also display the shell model spectrum obtained in Ref. (6), using Kuo's renormalized effective interaction, and assuming  $0^{16}$  as an inert core. In the TD approximation, the Hamiltonian was diagonalized in the lp-lh sub-space while in the shell model calculation a much larger sub-space was considered, but the results concerning energy levels are practically the same. In both attempts only the ground state band is reasonably well reproduced.

We also used the wave functions (8) to calculate the electric quadrupole transition probability between two states of the first excited band or between one of these states and another belonging to the ground state band. Transitions between energy levels in the ground state band were reported in Ref. (1), and they were found in very good agreement with experiment, assuming the usual effective charges of  $e_1 = 1.5 e$  and  $e_2 = 0.5 e$ .

Unfortunately, due to the lack of experimental data we could not check our present **B**(E2) values for transitions involving states of the first excited band. We display our results in Table II together with the shell model transition probabilities calculated by E. C. Halpert et *al.*. They also used several interactions so that we just show their smallest and largest values for a given transition. We also display their results for Kuo's renorma-

| $J_i^+$ | $J_f^+$ | K <sub>R</sub>     | K       | Y     | KLS   | KLS,  | S     | $\mathbf{K}_{R}^{a)}$ | Shell Model <sup>a</sup> | Exp. <sup>b)</sup> |
|---------|---------|--------------------|---------|-------|-------|-------|-------|-----------------------|--------------------------|--------------------|
| 0'      | 2       | 28.86              | 28.37   | 23.86 | 25.16 | 24.84 | 24.73 | 9.8                   | 1.9 → 13.7               | 12.34±?            |
| 2'      | 0       | 3.18               | 2.93    | 2.23  | 2.52  | 2.47  | 2.43  | 0.1                   | $0 \rightarrow 0.1$      |                    |
| 2′      | 2       | 5.35               | 4.72    | 3.33  | 3.92  | 3.93  | 3.87  | 2.6                   | $1.8 \rightarrow 4.9$    |                    |
| 2′      | 4       | 10.19              | 8.63    | 5.26  | 6.85  | 7.05  | 6.93  | 0.7                   | $0 \rightarrow 0.9$      |                    |
| 4′      | 2       | $2 \times 10^{-1}$ | 4 0.076 | 1.00  | 0.24  | 0.20  | 0.25  | 2.8                   | $2.8 \rightarrow 3.9$    |                    |
| 4′      | 4       | 0.06               | 0.006   | 0.96  | 0.13  | 0.09  | 0.13  | 0.                    | $0 \rightarrow 4.3$      |                    |
| 4′      | 6       | 0.58               | 0.043   | 1.15  | 0.05  | 0.012 | 0.03  | 8.1                   | $0.1 \rightarrow 10.3$   |                    |
| 6'      | 4       | 21.30              | 27.18   | 33.54 | 27.62 | 26.55 | 26.96 |                       |                          |                    |
| 6′      | 6       | 21.18              | 29.22   | 39.73 | 31.29 | 29.59 | 30.18 |                       |                          |                    |
| 6'      | 8       | 12.60              | 17.86   | 24.81 | 19.21 | 18.30 | 18.70 |                       |                          |                    |
| 2′      | 0′      | 49.54              | 50.11   | 49.36 | 46.11 | 42.94 | 42.45 | 16.2                  | $7.8 \rightarrow 16.2$   |                    |
| 4′      | 2′      | 34.65              | 38.73   | 34.80 | 35.26 | 32.40 | 31.86 | 0.1                   | 0.1 → 5.6                |                    |
| 6′      | 4′      | 0.38               | 0.87    | 14.73 | 5.33  | 2.42  | 2.35  |                       |                          |                    |

**Table II -** Electric quadrupole transition probabilities in units of  $(e^{Z} \text{ fm}^{4})$ , for different types of two-body interactions. Initial or final excited levels are marked. [a) Ref. (6);Shell Model calculation. b) Ref. (11); Experimental result.]

lized two-body interaction. All transitions probabilities in Table II are in units of  $e^2$  fm<sup>4</sup> with effective charges e, = 1.5 e and e, = 0.5 e.

We found that the excited states energies of  $Ne^{20}$  are equally well reproduced with the shell model calculation of Halpert and with our Tamm-Dancoff wave functions. The B(E2) transition probabilities were calculated in order to verify the goodness of the TD wave function when compared with the results of a better approximation, namely the shell model. However, our B(E2) results are very much different from their values.

It would be interesting to calculate the overlapping between the shell model wave functions and the ones projected from the first excited Tamm-Dancoff state to know how they depart from the shell model ones and where they do fail.

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## References

1. D. R. de Oliveira, Rev. Brasil. Fis. 1,403 (1971). Part of the formalism and other references can be found in this paper.

- 2. T. T. S. Kuo, Nucl. Phys. A103, 71 (1967).
- 3. S. Kahana, H. C. Lee and C. K. Scott, Phys. Rev. 185, 1378 (1969).
- 4. J. P. Elliott, H. A. Mavromatis and E. A. Sanderson, Phys. Letters 24B, 358 (1967).
- 5. A. E. Litherland, J. A. Kuehner, H. E. Gove, M. A. Clark and E. Almqvist, Phys. Rev. Letters 7, 98 (1961).
- 6. E. C. Halpert, J. B. McGrory, B. H. Wildenthal and S. P. Pandya, Advances in Nucl. Physics, Vol. 4, Plenum Press, 1971.
- 7. A. Arima, V. Gillet and J. Ginocchio, Phys. Rev. Letters 25, 1043 (1970).
- 8. R. Middleton, J. D. Garrett, H. T. Fortune, Phys. Rev. Letters 27, 950 (1971).
- 9. L. Satpathy, Phys. Rev. 174, 1324 (1968).
- 10. S. N. Tewari and G. L. Struble, Phys. Rev. C1, 1156 (1970).
- 11. C. Van der Leun, D. M. Sheppard, P. J. M. Smulders, Phys. Letters 18. 134 (1965).