Four-Particle-Two-Hole Core-Excitation in Heavy Nuclei

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Abstract. Four-particle-two-hole core-excitation in heavy nuclei with two nucleons outside the closed shells is investigated by including the highest core orbits into the configuration space of a shell-model calculation. The core-excitation is supposed to be effected by an interaction between core nucleons and valence nucleons which is essentially the same as the well-known residual interaction between the valence nucleons. The nucleons in the core are assumed to be excited only in pairs coming from the same core orbit. Therefore, the angular momentum of the core is always even.

For the description of core-excited configurations in second quantization formalism an orthogonal system of four-fermion operators is constructed. Using a phenomenological interaction potential with appropriate spin-spin and tensor parts and restricting to excitations with core-spin 0 energy levels and transition probabilities of the nuclei Pb^{206}, Po^{210} and Hg^{206} are calculated.

1. Introduction

Low-lying energy levels and transition probabilities of many nuclei with two identical nucleons or holes outside or inside the closed shells can rather well be reproduced by assuming a phenomenological residual interaction between the valence nucleons, and by treating the completely filled closed shells as inert core. Thus the calculation of the energy levels of Pb^{206} by using a simple residual interaction with appropriate spin-spin and tensor parts yields the correct sequence of the lower nuclear states [2].

In the last years it has become clear from experimental and theoretical investigations that the core nucleons are not quite unaffected by the residual interactions and that the excitation of these nucleons to outer orbits can play an important role. Especially the effects of 4-particle-2-hole core-excitation can be so great that treatment as perturbations does not seem to be convincible [21].

In Reference [1] we presented a short review of a simple model which allows to account for 4-particle-2-hole core-excitation by direct extension of the configuration space. We are giving here a more detailed representation of this model together with the application to the nuclei Pb^{206}, Po^{210} and Hg^{206}. Although the core-excitation effects in these heavy nuclei are less pronounced than in light and medium heavy nuclei, Pb^{206}, Po^{210} and Hg^{206} offer the advantage that proton shells and neutron shells are well separated. Thus we need not deal with excitations of non-identical nuclei. Also the violation of translation invariance, which is a common feature of shell-model calculations, but can become even more important in a model where many core nucleons are considered, is less serious in these heavy nuclei.

In section two the physical model and its approximations are described. In sections three and four the Hamiltonian is introduced and the secular matrix and electromagnetic transition probabilities are calculated. The interaction potential and numerical results for the nuclei mentioned above are discussed in section five. Concluding remarks and a discussion of Ni^{58} can be found in section six.

In the appendix the most important relations of two- and four-fermion operators and some details about the construction of the base functions of four-fermion systems are stated. The notations and abbreviations which are used in the text are also quoted there.

2. Model for 4-particle-2-hole Core-Excitation

We extend the configuration space of the shell-model calculation by including the highest few orbits of the core, and permit to one pair of nucleons in any of these orbits to jump out from the core to the valence orbits.

For this excitation process we make the following approximations:
- The configuration space of the nucleus consists of three kinds of orbits,
  the outer orbits or valence orbits, which are considered in usual shell-model calculations,
  a number of core orbits whose nucleons may interact with the nucleons in the valence orbits
  and an inert core, not taking part in core-excitation.
- The core nucleons are excited only in pairs coming from the same core orbit, but they may occupy different outer orbits after excitation. Thus the excitation of single nucleons from the core is neglected.
- The nucleons remaining in the core are always coupled in pairs of total angular momentum 0, except for one pair which takes up the recoil angular momentum of the excited nucleon pair, i.e. the spin of the core.

An important consequence of the second approximation is that the angular momentum of the core must always be even, since Pauli's principle permits only even values of the total angular momentum of two identical nucleons in the same state. It is shown in [1] that at least for pure configurations the effects of excitations with core spin 4 are small compared to those of excitations with lower core spins.

The validity of the approximations is discussed further in the following sections. But we point out here that they are based mainly on physical arguments and are introduced in order to reach some mathematical simplicity, and therefore cannot be satisfactoring in all cases.

The total spin I of not core-excited configurations is the sum of the single-particle spins of the two outer nucleons (the angular momentum of the completely filled core is zero), whereas in core-excited configurations it is the sum of the core spin R and the total spin of the four nucleons in valence orbits, Λ:

$$I = R + \Lambda .$$

As in [1] we denote the quantum numbers of outer orbits by lower indices, those of core orbits by upper ones. A bar over the respective quantum numbers indicates both kinds of orbits.

3. The Base-States and the Hamiltonian

The base states of not core-excited configurations are given by

$$
\mid j_1' \, j_2' \, I' \, m', \sigma \rangle = B_{I'm'}^+(j_1' \, j_2') \, \Gamma^{-1/2} \prod_{i=1}^{\sigma} B_{00}^+(j^i \, j^i)^{\omega_i} \mid 0 \rangle ,
\tag{1}
$$

where ω_i denotes the number of nucleon-pairs that can be placed in an orbit of spin j^i,

$$
\omega_i = \frac{2 \, j^i + 1}{2} \equiv \frac{\hat{j}^{i\,2}}{2} ,
\tag{2}
$$

and σ indicates the number of core orbits considered. The operators $B_{I'm'}^+(j_1' \, j_2')$ create one pair of nucleons with single-particle spins j_1', j_2' and total spin I' with magnetic quantum number m' (see appendix).

Since the states $B_{I'm'}^+(j_1' \, j_2') \mid 0 \rangle$ form an orthonormal set and are orthogonal to the core functions, the normalization of the base states (1) is determined by the scalar product of the core functions, (A14):

$$
\Gamma = \prod_{i=1}^{\sigma} (\omega_i!) \prod_{k=1}^{\omega_i-1} \left(1 - \frac{k}{\omega_i} \right) .
\tag{3}
$$

The base states of core-excited configurations are chosen in direct relation to the core-excitation Hamiltonian described below. We construct them by applying the operator $B_{RM}(j^q \, j^q)$ on the states (1) for all possible values of q and all possible core-spins $\boldsymbol{R}$.

The correct orthogonal and normalized base functions can then be chosen as follows:

$$
\mid j_1 \, j_2 \, j_3 \, j_4 \, (\Lambda \, \alpha \, R \, q) \, I \, m, \sigma \rangle = \Omega^{-1/2} \sum_{\lambda M} \langle \Lambda \, \lambda \, R \, M \mid I \, m \rangle
$$

$$
\mathcal{D}_{\Lambda\lambda\alpha}^+ (j_1 \, j_2 \, j_3 \, j_4) \, B_{RM}^+ (j^q \, j^q) \, B_{00}^+(j^q \, j^q)^{\omega_q - 2} \prod_{i \neq q}^{\sigma} B_{00}^+(j^i \, j^i)^{\omega_i} \mid 0 \rangle .
\tag{4}
$$

The orthonormalized four-fermion operators $\mathcal{D}_{\Lambda\lambda\alpha}^+(j_1 \, j_2 \, j_3 \, j_4)$ are defined by

$$
\mathcal{D}_{\Lambda\lambda\alpha}^+(j_1 \, j_2 \, j_3 \, j_4) = \sum_{SS'} d_{\Lambda\alpha}^{SS'}(j_1 \, j_2 \, j_3 \, j_4) \, D_{\Lambda\lambda}^+ (j_1 \, j_2 \, S, \, j_3 \, j_4 \, S') ,
\tag{5}
$$

where

$$
D_{\Lambda\lambda}^+(j_1 \, j_2 \, S, \, j_3 \, j_4 \, S') = \sum_{\nu \nu'} \langle S \, \nu \, S' \, \nu' \mid \Lambda \, \lambda \rangle \, B_{S\nu}^+(j_1 \, j_2) \, B_{S'\nu'}^+(j_3 \, j_4)
\tag{6}
$$

and the $d_{\Lambda\alpha}^{SS'}(j_1 \, j_2 \, j_3 \, j_4)$ are orthogonalization coefficients (for further details see appendix).

Since we are not directly interested in the nuclear states which consist mainly of core-excited configurations, we could attempt to describe the four-fermion states by boson-pair operators (Boson approximation [22]) and thus reach greater mathematical simplicity in the following formulas. But an important advantage of the consequent

use of Pauli's principle is that it reduces the size of the secular matrix, since many 4-particle states which can be constructed in the boson approximation are not antisymmetric and are thus forbidden. We therefore prefer to construct a complete orthonormal system of antisymmetric base functions.

In (4) the spin $\boldsymbol{R}$ of the core is carried by a nucleon pair in the orbit q from which an other pair is excited to the valence orbits. It is combined with the total angular momentum $\boldsymbol{\Lambda}$ of the outer nucleons to form the spin $\boldsymbol{I}$ of the nucleus with magnetic quantum number m. The number σ is the same as in (1). The normalization, Ω, of these states results from (A16) and (A17):

$$
\Omega(q) = \prod_{i \neq q}^{\sigma} (\omega_i!) \prod_{k=1}^{\omega_i - 1} \left(1 - \frac{k}{\omega_i} \right)
\begin{cases}
(\omega_q - 1)! \displaystyle\prod_{l=1}^{\omega_q - 2} \left(1 - \frac{l}{\omega_q} \right), & \text{if } R = 0 \\[2ex]
(\omega_q - 2)! \displaystyle\prod_{l=2}^{\omega_q - 1} \left(1 - \frac{l}{\omega_q} \right), & \text{if } R \neq 0.
\end{cases}
\tag{7}
$$

The Hamiltonian is devided into five parts

$$
H = H_0 + H' = H_0 + H_{res}^{(val)} + H_{res}^{(core)} + H_{CE} + H'' .
\tag{8}
$$

H_0 represents the mean shell-model potential with single-particle energies $\varepsilon_{\bar{\jmath}}$, which is diagonal in the above system of base states,

$$
H_0 = \sum_{\bar{\jmath}} \hat{\bar{\jmath}} \, \varepsilon_{\bar{\jmath}} \, A_{00}^+(\bar{\jmath} \, \bar{\jmath}) .
\tag{9}
$$

The general residual interaction H' may be expressed as

$$
H' = \sum_{\substack{K\mu \\ \bar{\jmath}_a \geqslant \bar{\jmath}_b, \, \bar{\jmath}_{a'} \geqslant \bar{\jmath}_{b'}}} G_K (\bar{\jmath}_a \, \bar{\jmath}_b \, \bar{\jmath}_{a'} \, \bar{\jmath}_{b'}) \, B_{K\mu}^+(\bar{\jmath}_a \, \bar{\jmath}_b) \, B_{K\mu}(\bar{\jmath}_{a'} \, \bar{\jmath}_{b'}) \, 2 \, \Delta(\bar{\jmath}_a \, \bar{\jmath}_b \, \bar{\jmath}_{a'} \, \bar{\jmath}_{b'}) ,
\tag{10}
$$

where G_K is the antisymmetrized matrix element between the coupled states $|\bar{\jmath}_a \bar{\jmath}_b K\mu\rangle$ and $|\bar{\jmath}_{a'} \bar{\jmath}_{b'} K\mu\rangle$ [2].

We retain only three parts of H', namely the residual interaction of the valence nucleons between themselves

$$
H_{res}^{(val)} = 2 \sum_{\substack{K\mu \\ \jmath_a \geqslant \jmath_b, \jmath_{a'} \geqslant \jmath_{b'}}} G_K (\jmath_a \, \jmath_b \, \jmath_{a'} \, \jmath_{b'}) \, B_{K\mu}^+ (\jmath_a \, \jmath_b) \, B_{K\mu} (\jmath_{a'} \, \jmath_{b'}) \, \Delta(\jmath_a \, \jmath_b \, \jmath_{a'} \, \jmath_{b'}) ,
\tag{11}
$$

the interaction of nucleon pairs in the core

$$
H_{res}^{(core)} = 2 \sum_{\substack{K\mu \\ \jmath^{q'}, \jmath^{q''}}} G_K (\jmath^{q'} \, \jmath^{q'} \, \jmath^{q''} \, \jmath^{q''}) \, B_{K\mu}^+(\jmath^{q'} \, \jmath^{q'}) \, B_{K\mu}(\jmath^{q''} \, \jmath^{q''}) ,
\tag{12}
$$

and the core-excitation interaction

$$
H_{CE} = 2 \sum_{\substack{K\mu \\ \jmath_{a'} \geqslant \jmath_{b'}, \jmath^q}} G_K (\jmath_{a'} \, \jmath_{b'} \, \jmath^q \, \jmath^q) \, B_{K\mu}^+(\jmath_{a'} \, \jmath_{b'}) \, B_{K\mu}(\jmath^q \, \jmath^q) \, \sqrt{2 - \delta_{\jmath_{a'} \jmath_{b'}}} + \text{h.c.} .
\tag{13}
$$

The term H'' summarizes the various other processes that are neglected in our model. These restrictions are in accordance to the choice of the base states. In the following (11) and (12) shall be designated as residual interaction, not including core-excitation (13).

We consider first the term H_{CE}. Since the orthogonalization procedure of the base states cannot be inverted, the matrix elements of H_{CE} must be calculated by decomposing the base states of core-excited configurations into their non-orthogonal constituents

$$|j_1' \, j_2' \, j_3' \, j_4' \, (\Lambda' \, \lambda' \, S \, S') \, R' \, M' \, q', \sigma\rangle = \Omega^{-1/2} \, D^+_{\Lambda' \lambda'}(j_1' \, j_2' \, S, \, j_3' \, j_4' \, S')$$

$$B^+_{R'M'}(j^{q'} \, j^{q'}) \, B^+_{00}(j^{q'} \, j^{q'})^{\omega_{q'}-2} \prod_{i \neq q'}^{\sigma} B^+_{00}(j^i \, j^i)^{\omega_i} \, |0\rangle \,, \tag{14}$$

(cf. equation (4)) and by calculating the following expressions from (A13) and (A24):

$$B_{K\mu}(j^q \, j^q) \, |j_1'' \, j_2'' \, I'' \, m'', \sigma\rangle \tag{15}$$

and

$$B_{K\mu}(j_a' \, j_b') \, |j_1' \, j_2' \, j_3' \, j_4' \, (\Lambda' \, \lambda' \, S \, S') \, R' \, M' \, q', \sigma\rangle \,. \tag{16}$$

The further evaluation can be made with help of equations (A11)–(A17). Then reintroducing the orthogonalization and the coupling of the spins of the valence nucleons and the core, we get

$$\langle j_1' \, j_2' \, j_3' \, j_4' \, (\Lambda' \, \alpha' \, R' \, q') \, I' \, m', \sigma \, |H_{CE}| \, j_1'' \, j_2'' \, I'' \, m'', \sigma\rangle = (-)^{\delta_{R'0}} \, \delta_{I'I''} \, \delta_{m'm''}$$

$$\times \, 2 \, \frac{\hat{\Lambda}'}{\hat{I}''} \left\{ \left(\delta_{j_2'j_1''} \, \delta_{j_4'j_2''} \, \frac{\Delta_{j_1'j_4'} \Delta_{j_1'j_3'}}{\Delta_{j_1'j_2'} \Delta_{j_3'j_4'}} \, \sqrt{2 - \delta_{j_1'j_3'}} \, f^{R'I''}_{\Lambda'\alpha'} \, (j_1' \, j_2' \, j_3' \, j_4') \, G_{R'} \, (j_1' \, j_3' \, j^{q'} \, j^{q'}) \right. \right.$$

$$\left. + \{j_1' \leftrightarrow j_2'\} + \{j_3' \leftrightarrow j_4'\} + \begin{Bmatrix} j_1' \leftrightarrow j_2' \\ j_3' \leftrightarrow j_4' \end{Bmatrix} \right)$$

$$- \, \delta_{j_3'j_1''} \, \delta_{j_4'j_2''} \, \sqrt{2 - \delta_{j_1'j_2'}} \, d^{R'I''}_{\Lambda'\alpha'} \, G_{R'}(j_1' \, j_2' \, j^{q'} \, j^{q'})$$

$$\left. - \, (-)^{I''+\Lambda'} \, \delta_{j_1'j_1''} \, \delta_{j_2'j_2''} \, \sqrt{2 - \delta_{j_3'j_4'}} \, d^{I''R'}_{\Lambda'\alpha'} \, G_{R'} \, (j_3' \, j_4' \, j^{q'} \, j^{q'}) \right\} \,. \tag{17}$$

The 'recoupled' orthogonalization coefficients $f^{R'I''}_{\Lambda'\alpha'}(j_1' \, j_2' \, j_3' \, j_4')$ are defined in (A32).

The residual interaction matrix elements of not core-excited configurations are well known. We have

$$\langle j_1' \, j_2' \, I' \, m', \sigma \, |H^{(val)}_{res} + H^{(core)}_{res}| \, j_1'' \, j_2'' \, I'' \, m'', \sigma\rangle$$

$$= \delta_{I'I''} \, \delta_{m'm''} \, (2 \, \Delta(j_1' \, j_2' \, j_1'' \, j_2'') \, G_{I'}(j_1' \, j_2' \, j_1'' \, j_2'') + \delta_{j_1'j_1''} \, \delta_{j_2'j_2''} \, \tilde{E}) \,, \tag{18}$$

where the contribution of the completely filled core,

$$\tilde{E} = 2 \sum_{i=1}^{\sigma} \sum_{\substack{L \\ even}} \hat{L}^2 \, G_L \, (j^i \, j^i \, j^i \, j^i) \,, \tag{19}$$

is only a renormalization of the total energy and may be omitted together with a similar term in the matrix elements between core-excited configurations.

In order to calculate the contribution of the outer nucleons to the residual interaction matrix elements of core-excited configurations we must first determine by

(A26) the scalar products between non-orthogonal states of the type (16). Then, by introducing the orthogonalization coefficients (A28) and (A32) and the coupling of the spins of the valence nucleons and the core, we get

$$\langle j_1'' \, j_2'' \, j_3'' \, j_4'' \, (\Lambda'' \, \alpha'' \, R'' \, q'') \, I'' \, m'', \sigma \, | H_{res}^{(val)} | \, j_1' \, j_2' \, j_3' \, j_4' \, (\Lambda' \, \alpha' \, R' \, q') \, I' \, m', \sigma \rangle$$

$$= 2 \, \delta_{I'I''} \, \delta_{m'm''} \, \delta_{\Lambda'\Lambda''} \, \delta_{R'R''} \, \delta_{q'q''} \, (T_1 + T_2 + T_3) \,, \tag{20}$$

where

$$T_1 = \sum_{SL} \left(\delta_{j_1'j_1''} \, \delta_{j_2'j_2''} \, \Delta(j_3' \, j_4' \, j_3'' \, j_4'') \, G_L(j_3' \, j_4' \, j_3'' \, j_4'') \, d_{\Lambda'\alpha'}^{SL} \, d_{\Lambda'\alpha''}^{SL} \right.$$

$$+ (-)^{L+S+\Lambda'} \begin{Bmatrix} j_1' \leftrightarrow j_3' \\ j_2' \leftrightarrow j_4' \end{Bmatrix} d_{\Lambda'\alpha'}^{LS} \, d_{\Lambda'\alpha''}^{SL} + (-)^{L+S+\Lambda'} \begin{Bmatrix} j_1'' \leftrightarrow j_3'' \\ j_2'' \leftrightarrow j_4'' \end{Bmatrix} d_{\Lambda'\alpha'}^{SL} \, d_{\Lambda'\alpha''}^{LS}$$

$$+ \begin{Bmatrix} j_1' \leftrightarrow j_3' \\ j_2' \leftrightarrow j_4' \\ j_1'' \leftrightarrow j_3'' \\ j_2'' \leftrightarrow j_4'' \end{Bmatrix} d_{\Lambda'\alpha'}^{LS} \, d_{\Lambda'\alpha''}^{LS} \right) \,, \tag{21}$$

$$T_2 = \frac{\Delta_{j_1'j_3'} \Delta_{j_2'j_4'} \Delta_{j_1''j_3''} \Delta_{j_2''j_4''}}{\Delta_{j_1'j_2'} \Delta_{j_3'j_4'} \Delta_{j_1''j_2''} \Delta_{j_3''j_4''}} \, \delta_{j_1'j_1''} \, \delta_{j_3'j_3''} \, \Delta(j_2' \, j_4' \, j_2'' \, j_4'') \sum_L G_L(j_2' \, j_4'' \, j_2' \, j_4')$$

$$\times \sum_K f_{\Lambda'\alpha'}^{KL} (j_1' \, j_2' \, j_3' \, j_4') \, f_{\Lambda'\alpha''}^{KL} (j_1'' \, j_2'' \, j_3'' \, j_4'') \left(1 + \{j_1' \leftrightarrow j_2'\} + \{j_3' \leftrightarrow j_4'\} \right.$$

$$+ \left. \begin{Bmatrix} j_1' \leftrightarrow j_2' \\ j_3' \leftrightarrow j_4' \end{Bmatrix} \right) \left(1 + \{j_1'' \leftrightarrow j_2''\} + \{j_2'' \leftrightarrow j_4''\} + \begin{Bmatrix} j_1'' \leftrightarrow j_2'' \\ j_3'' \leftrightarrow j_4'' \end{Bmatrix} \right) \,, \tag{22}$$

$$T_3 = \left\{ \left[\left(- \frac{\Delta_{j_1''j_3''} \Delta_{j_2''j_4''}}{\Delta_{j_1''j_2''} \Delta_{j_3''j_4''}} \, \delta_{j_3'j_1''} \, \delta_{j_4'j_3''} \, \Delta(j_1' \, j_2' \, j_2'' \, j_4'') \sum_{LS} (-)^{L+S+\Lambda'} \, d_{\Lambda'\alpha'}^{LS} \right. \right. \right.$$

$$\times f_{\Lambda'\alpha''}^{SL}(j_1'' \, j_2'' \, j_3'' \, j_4'') \, G_L (j_2'' \, j_4'' \, j_1'' \, j_2') + \{j_1'' \leftrightarrow j_2''\} + \{j_3'' \leftrightarrow j_4''\}$$

$$+ \left. \begin{Bmatrix} j_1'' \leftrightarrow j_2'' \\ j_3'' \leftrightarrow j_4'' \end{Bmatrix} \right) + (-)^{L+S+\Lambda'} \begin{Bmatrix} j_1' \leftrightarrow j_3' \\ j_2' \leftrightarrow j_4' \\ L \leftrightarrow S \ \text{in} \ d \end{Bmatrix} \right] + \begin{Bmatrix} j_1' \leftrightarrow j_1'', \ j_2' \leftrightarrow j_2'' \\ j_3' \leftrightarrow j_3'', \ j_4' \leftrightarrow j_4'' \\ \alpha' \leftrightarrow \alpha'' \end{Bmatrix} \right\}. \tag{23}$$

In T_1 and T_3 the ordering of the single-particle spins in the arguments of the orthogonalization coefficients $d_{\Lambda\alpha}^{JJ'}$ must always be preserved, even if the arguments of the other functions are interchanged, because the ordering of the states is determined from the beginning by the base functions. We point out that the recoupled exchange terms T_2 and T_3, which involve 9-j-symbols or products of these through the definition of the recoupled orthogonalization coefficients $f_{\Lambda\alpha}^{JJ'}$, are in general not much smaller than the 'direct' term T_1. In many cases they may even cancel it.

The contribution of the core orbits to the residual interaction matrix elements of core-excited configurations,

$$\langle j_1'' \, j_2'' \, j_3'' \, j_4'' \, (\Lambda'' \, \alpha'' \, R'' \, q'') \, I'' \, m'', \sigma \, | H_{res}^{(core)} | \, j_1' \, j_2' \, j_3' \, j_4' \, (\Lambda' \, \alpha' \, R' \, q') \, I' \, m', \sigma \rangle, \tag{24}$$

is most easily calculated by introducing the state of the completely filled core, $|\tilde{0}\rangle$, as new reference state. If we define this state by

$$|\tilde{0}\rangle = \prod_{i=1}^{\sigma} \left[\left(\omega_i! \prod_{s=1}^{\omega_i-1} \left(1 - \frac{s}{\omega_i}\right) \right)^{-1/2} B_{00}^+(j^i\, j^i)^{\omega_i} \right] |0\rangle, \tag{25}$$

we have from (A14) and (A15) and according to Pauli's principle the equations

$$\langle \tilde{0} \mid \tilde{0} \rangle = 1, \tag{26}$$

$$B_{RM}^+(j^1\, j^2)\, |\tilde{0}\rangle = 0, \quad \text{if } j^1 \text{ or } j^2 \text{ in } |\tilde{0}\rangle, \tag{27}$$

and

$$A_{K\varkappa}^+(j^1\, j^2)\, |\tilde{0}\rangle = \begin{cases} \delta_{K0}\, \delta_{j^1 j^2}\, \hat{j}^1\, |\tilde{0}\rangle, & \text{if } j^1 \text{ and } j^2 \text{ in } |\tilde{0}\rangle. \\ 0, & \text{otherwise.} \end{cases} \tag{28}$$

Moreover, the states $B_{RM}(j^1\, j^2)\, |\tilde{0}\rangle$ form an orthonormal set, as may easily be verified. With help of (25) and (A13) the matrix elements (24) can be written in the form

$$\delta_{\Lambda'\Lambda''}\, \delta_{\alpha'\alpha''}\, \delta_{j_1'j_1''}\, \delta_{j_2'j_2''}\, \delta_{j_3'j_3''}\, \delta_{j_4'j_4''}\, 2 \sum_{\lambda' M' M''} \langle \Lambda'\, \lambda'\, R'\, M' \mid I'\, m' \rangle$$

$$\times\, \langle \Lambda'\, \lambda'\, R''\, M'' \mid I''\, m'' \rangle \sum_{\substack{L\mu \\ j^a j^{a'}}} G_L\,(j^a\, j^a\, j^{a'}\, j^{a'})\,(-)^{M'+M''}$$

$$\times\, \langle \tilde{0} \mid B_{R''-M''}^+(j^{q''}\, j^{q''})\, B_{L\mu}^+(j^a\, j^a)\, B_{L\mu}(j^{a'}\, j^{a'})\, B_{R'-M'}(j^{q'}\, j^{q'}) \mid \tilde{0} \rangle. \tag{29}$$

Using (27), (28), (A10) and (A11) the core contribution can now easily be calculated. We get the result

$$\langle j_1''\, j_2''\, j_3''\, j_4''\,(\Lambda''\, \alpha''\, R''\, q'')\, I''\, m'', \sigma| H_{res}^{(core)}| j_1'\, j_2'\, j_3'\, j_4'\,(\Lambda'\, \alpha'\, R'\, q')\, I'\, m', \sigma\rangle$$

$$= 2\, \delta_{I'I''}\, \delta_{m'm''}\, \delta_{\Lambda'\Lambda''}\, \delta_{\alpha'\alpha''}\, \delta_{R'R''}\, \delta_{j_1'j_1''}\, \delta_{j_2'j_2''}\, \delta_{j_3'j_3''}\, \delta_{j_4'j_4''}$$

$$\times \left[G_{R'}\,(j^{q''}\, j^{q''}\, j^{q'}\, j^{q'}) - \delta_{q'q''}\, \frac{2}{\omega_{q'}} \sum_L \hat{L}\, G_L\,(j^{q'}\, j^{q'}\, j^{q'}\, j^{q'}) + \delta_{q'q''}\, \tilde{E} \right], \tag{30}$$

where $\tilde{E}$ is defined by (19) and may again be omitted.

The nuclear states are defined as

$$|\, I\, m\, k\rangle = \sum_{j_1 \geqslant j_2} c^{Ik}(j_1\, j_2)\, |\, j_1\, j_2\, I\, m, \sigma\rangle$$

$$+ \sum_{j_1 \geqslant j_2 \geqslant j_3 \geqslant j_4} \sum_{Rq\, \Lambda\alpha} c^{Ik}_{\Lambda\alpha\, Rq}(j_1\, j_2\, j_3\, j_4)\, |j_1\, j_2\, j_3\, j_4\,(\Lambda\, \alpha\, R\, q)\, I\, m, \sigma\rangle. \tag{31}$$

The coefficients $c^{Ik}(j_1\, j_2)$ and $c^{Ik}_{\Lambda\alpha\, Rq}(j_1\, j_2\, j_3\, j_4)$ are the amplitudes of not core-excited and core-excited configurations respectively. The index k numbers the states of spin I.

4. Electromagnetic Transition Probabilities

Using the definition (A6) of the particle-hole operators and the Wigner-Eckart theorem [4], multipole operators can be expressed by the formula

$$T_{L\mu} = \frac{1}{\hat{L}} \sum_{jj'} \langle j \parallel T_L \parallel j' \rangle\, A_{L\mu}^+(j\, j'). \tag{32}$$

The reduced matrix elements $\langle j \parallel T_L \parallel j' \rangle$ for electromagnetic M1- and E2-transitions may be found in [3]. The reduced transition probabilities are calculated by the same methods as the secular matrix. We therefore state only the final results.

It is convenient to define the function

$$T_L^{SS'}(j_a\, j_b\, j_{a'}\, j_{b'}) = \delta_{aa'} \begin{Bmatrix} L & S & S' \\ j_{a'} & j_b & j_{b'} \end{Bmatrix} \langle j_b \parallel T_L \parallel j_{b'} \rangle - (-)^{j_a + j_b + S'} \{j_a \leftrightarrow j_b\}. \qquad (33)$$

The reduced matrix elements between nuclear states $\langle I\, m\, k \mid$ and $\mid I'\, m'\, k' \rangle$ can be expressed as

$$\langle I\, m\, k \parallel T_L \parallel I'\, m'\, k' \rangle = U_{neV} + U_{eV} + U_{eC}, \qquad (34)$$

where U_{neV} is the contribution of not core-excited configurations

$$U_{neV} = (-)^{L+I}\, \hat{I}\, \hat{I}' \sum_{\substack{j_a \geqslant j_b \\ j_{a'} \geqslant j_{b'}}} \frac{1}{\Delta_{j_a j_b} \Delta_{j_{a'} j_b}} (-)^{j_{a'} + j_{b'}}\, c^{Ik}(j_a\, j_b)\, c^{I'k'}(j_{a'}\, j_{b'})$$

$$\times \left(T_L^{I'I}(j_a\, j_b\, j_{a'}\, j_{b'}) - (-)^{j_{a'} j_{b'} + I'} \{j_{a'} \leftrightarrow j_{b'}\} \right) \qquad (35)$$

and U_{eC} is the contribution of the core orbits in core-excited configurations

$$U_{eC} = 2\, (-)^{L+I}\, \hat{I}\, \hat{I}' \sum_{\substack{j_1 \geqslant j_2 \geqslant j_3 \geqslant j_4 \\ \Lambda\, \alpha\, q\, R\, R'}} (-)^{\Lambda}\, c^{Ik}_{\Lambda\alpha\, Rq}(j_1\, j_2\, j_3\, j_4)$$

$$\times c^{I'k'}_{\Lambda\alpha\, R'q}(j_1\, j_2\, j_3\, j_4)\, \hat{R}\, \hat{R}' \langle j^q \parallel T_L \parallel j^q \rangle \begin{Bmatrix} I & I' & L \\ R' & R & \Lambda \end{Bmatrix}. \qquad (36)$$

The contribution of the valence orbits in core-excited configurations may be written as follows:

$$U_{eV} = (-)^{I'+L}\, \hat{I}\, \hat{I}' \sum_{\substack{j_1 \geqslant j_2 \geqslant j_3 \geqslant j_4 \\ j'_1 \geqslant j'_2 \geqslant j'_3 \geqslant j'_4 \\ \Lambda\, \alpha\, R\, q\, \Lambda'\, \alpha'}} c^{Ik}_{\Lambda\alpha\, Rq}(j_1\, j_2\, j_3\, j_4)\, c^{I'k'}_{\Lambda'\alpha'\, Rq}(j'_1\, j'_2\, j'_3\, j'_4)$$

$$\times (-)^{\Lambda + \Lambda' + R}\, \hat{\Lambda}\, \hat{\Lambda}' \begin{Bmatrix} I & I' & L \\ \Lambda' & \Lambda & R \end{Bmatrix} \frac{1}{\Delta_{j_1 j_2} \Delta_{j_3 j_4} \Delta_{j'_1 j'_2} \Delta_{j'_3 j'_4}} (U_1 + U_2), \qquad (37)$$

where

$$U_1 = \sum_{Q'S'} d^{Q'S'}_{\Lambda'\alpha'} \sum_{QS} d^{QS}_{\Lambda\alpha} \left\{ (-)^{j'_1 + j'_2 + S'} \left(\delta_{SS'}\, \hat{Q}\, \hat{Q}' \begin{Bmatrix} L & Q' & Q \\ S' & \Lambda & \Lambda' \end{Bmatrix} \delta_S (j_3\, j_4\, j'_3\, j'_4) \right. \right.$$

$$\times T_L^{Q'Q}(j_1\, j_2\, j'_1\, j'_2) + (-)^{Q+S+\Lambda} \begin{Bmatrix} j_1 \leftrightarrow j_3 \\ j_2 \leftrightarrow j_4 \\ Q \leftrightarrow S \end{Bmatrix} \right) - (-)^{j'_1 + j'_2 + Q'} \{j'_1 \leftrightarrow j'_2\}$$

$$+ (-)^{Q'+S'+\Lambda'} \begin{Bmatrix} j'_1 \leftrightarrow j'_3 \\ j'_2 \leftrightarrow j'_4 \\ Q' \leftrightarrow S' \end{Bmatrix} + (-)^{j'_1 + j'_2 + j'_3 + j'_4 + \Lambda'} \begin{Bmatrix} j'_1 \leftrightarrow j'_4 \\ j'_2 \leftrightarrow j'_3 \\ Q' \leftrightarrow S' \end{Bmatrix} \right\} \qquad (38)$$

and

$$
U_2 = -\sum_{Q'S'} d_{\Lambda'\alpha'}^{Q'S'} \hat{Q}' \left\{ (-)^{j_1'+j_2'+S'} \sum_U \hat{U} \begin{Bmatrix} L & Q' & U \\ S' & \Lambda & \Lambda' \end{Bmatrix} \left[\delta_{S'} (j_2\,j_4\,j_3'\,j_4')\, T_L^{Q'U} (j_1\,j_3\,j_1'\,j_2') \right. \right.
$$

$$
\times f_{\Lambda\alpha}^{US'} (j_1\,j_2\,j_3\,j_4) + \{j_1 \leftrightarrow j_2\} + \{j_3 \leftrightarrow j_4\} + \begin{Bmatrix} j_1 \leftrightarrow j_2 \\ j_3 \leftrightarrow j_4 \end{Bmatrix} \bigg] - (-)^{j_1'+j_2'+Q'}
$$

$$
\times \{j_1' \leftrightarrow j_2'\} + (-)^{Q'+S'+\Lambda'} \begin{Bmatrix} j_1' \leftrightarrow j_3' \\ j_2' \leftrightarrow j_4' \\ Q' \leftrightarrow S' \end{Bmatrix} + (-)^{j_1'+j_2'+j_3'+j_4'+\Lambda'} \begin{Bmatrix} j_1' \leftrightarrow j_4' \\ j_2' \leftrightarrow j_3' \\ Q' \leftrightarrow S' \end{Bmatrix} \left.\left.\vphantom{\begin{Bmatrix} j_1' \\ j_2' \\ Q' \end{Bmatrix}}\right\}\right\}. \quad (39)
$$

For the same reason as in (21) and (23) the ordering of the single-particle states in the orthogonalization coefficients $d_{\Lambda\alpha}^{JJ'}$ must always be preserved. The reduced transition probabilities are obtained by substituting the expression (34) into

$$
B(\sigma\,\lambda,\, I'\,k' \to I\,k) = \frac{1}{2\,I'+1}\, |\langle I\,m\,k \parallel T_\lambda \parallel I'\,m'\,k' \rangle|^2 . \quad (40)
$$

5. Numerical Calculations

5.1. *The interaction potential*

Since we assume that core-excitation is produced by an interaction between the core nucleons and the valence nucleons which is essentially the same as the residual interaction of the valence nucleons between themselves, we employ the same form of potential for both interactions, namely [2]

$$
V(r_1,\, r_2) = V_0(r_1,\, r_2) \left[1 + a\,\sigma_1\sigma_2 + b \left(\frac{3\,(\sigma_1\,r_{12})\,(\sigma_2\,r_{12})}{r_{12}^2} - \sigma_1\sigma_2 \right) \right] \quad (41)
$$

with the scalar part

$$
V_0(r_1,\, r_2) = V_0 \frac{1}{r_1\,r_2}\, e^{-\alpha\,r_{12}^2}\, \delta(\Omega_{12}) . \quad (42)
$$

This interaction, especially its angular dependence is not realistic at all, but it yields a good accordance between calculated and experimental energy levels for the nuclei Pb^{206}, Pb^{210} and Po^{210}, when core-excitation is neglected; and it is rather easy to handle. For this potential the antisymmetric two-particle matrix element $G_k(\bar{j}_a\,\bar{j}_b\,\bar{j}_{a'}\,\bar{j}_{b'})$ has been given in [2].

Although the same general shape for both interactions is assumed, the values of the parameters which fit best to the experimental level schemes are not necessarily the same, for the approximations in the treatment of the interactions are different. Thus the neglection of some low-lying core orbits may cause a change in the core-excitation coupling constant V_{0CE}.

The relative strength of the spin-spin and the tensor part have been fixed in all calculations as the values given in [2], i.e. $a = 0.1$, $b = 0.776$. These values yield results which agree best to experimental level schemes when core-excitation is neglected, and they are very close to those determined by the deuteron properties.

In the potential of the residual interaction the range parameter α was as well fixed as the value of [2], namely $\alpha = 2.0$ for Pb^{206}, Po^{210} and Hg^{206}, and $\alpha = 3.6$ for Ni^{58}. This corresponds to about one quarter of the nuclear radius. On the other hand the range of the core-excitation interaction has been varied in order to test if a longer range could be more appropriate. However, we got the best results with equal ranges for both interactions.

5.2. *Determination of nuclear states*

Since the secular matrix of core-excited configurations with core-spin 0 is already very large, we have restricted ourselves to core-spin 0 excitations in all numerical calculations. It is shown in [1] that at least for one pure configuration the influence of core-spin-2 excitations on level positions is much smaller. In actual nuclei, however, where various types of configurations occur, the contributions of core-spin-2 excitations may become more important, because selection rules let a great number of matrix elements vanish between the not core-excited configurations and those excited with core-spin 0. On the other hand, as a consequence of these selection rules only a few core-excited configurations contribute essentially to the wave functions of nuclear states of low energy. Therefore, it will be possible to neglect the other core-excited configurations from the beginning. This enables to include higher core-spins. An investigation of this problem will be the subject of further work.

The single-particle energies ε_j in (9) have been extracted from experimental level schemes of neighbouring nuclei. The levels that are considered for Pb^{206}, Po^{210} and Hg^{206} are shown in Figure 1.

The energy difference ΔE between the lowest outer level and the first core orbit has been determined from reaction data [10]. A small change in this energy gap causes essentially only a renormalization of the core-excitation coupling constant V_{0CE}.

All calculations were performed on the UNIVAC 1108 computer at the SANDOZ Computing Center at Basel. For the computation of the energy eigenvalues the variation method described in [20] has been used, which is excellently adapted to the determination of the lowest few eigenvalues of large matrices. Thus the entire level
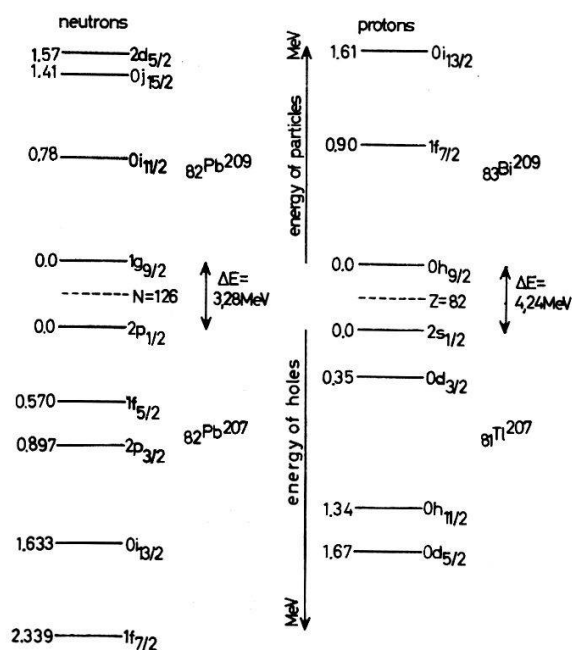

Figure 1

Single-particle states of neighbouring nuclei which are considered in the calculations of Pb^{206}, Po^{210} and Hg^{206}.

scheme of Pb[206] up to 5 MeV could be calculated in a few minutes. The main amount of computer time is however necessary for the construction of the secular matrix, for it implies a computation of an enormous number of 9-j-symbols to great accuracy.

5.3. *The lead isotope Pb[206]*

The level scheme of Pb[206] is very well known [11, 12] and it therefore offers an excellent opportunity to test the changes in the positions of energy levels which are caused by core-excitation.

In our calculations only four states of Pb[207] were considered, namely the $p_{1/2}$, the $f_{5/2}$, the $p_{3/2}$ and the $i_{13/2}$ levels [7]. As a consequence of this restriction some of the experimental nuclear states are missing entirely in the calculated scheme, e.g. the 4+-state at 2,9 MeV whose main configuration is $(p_{1/2} f_{7/2})$. The influence of the $f_{7/2}$ level on the lower states can nearly be absorbed in the potential strength.

The energy gap ΔE between the lowest valence orbit and the first core orbit was determined from reaction data [10] to be 3,28 MeV. The level scheme is not sensitive to small deviations from ΔE, but only the exact value yields the best fit with *equal* coupling constants V_{0res} and V_{0CE} of residual interaction and core-excitation interaction respectively.

Calculations have been performed with two and with four core orbits. It turned out that the effect of the $j_{15/2}$ and the $d_{5/2}$ core orbit is very small since the excitation of nucleon pairs from these orbits requires an energy of at least 6 MeV.

If the coupling constants of both interactions are equal ($\Delta E = 3.28$ MeV) the value $V_{0res} = V_{0CE} = -6.4$ MeV fits best to the experimental scheme; it is about ten percent less than the value determined without core-excitation. (Note that the definition of coupling strength is not the same as in [2].)

The interaction energy of a nucleon pair in the ground state is -1.2 MeV. This energy may be compared to the Q-value of the reaction Pb[208](d, t)Pb[207], which is -1.13 ± 0.01 MeV [13].

In Figure 2 the theoretical level scheme, calculated with two core orbits, is compared to the experimental one and to the scheme of [2]. It is obvious that the positions of the second 0+-state and of the first 3+- and 1+-states agree better with the experiment. We conclude that core-excitation with core-spin 0 is important for these lower states of Pb[206]. Nevertheless, the second 0+-state is always too low.

A second problem is the energy gap between 2.2 and 2.5 MeV, which is even slightly enlarged by core-excitation. The region where higher single-particle states become important begins somewhat above this gap, so that it cannot be explained satisfactorily by the neglection of those states.

The states consisting mainly of core-excited configurations are not shown in Figure 2. The first one appears at about 8 MeV. It has spin 0 and positive parity and consists mainly of the configurations $(f_{5/2})^2 (p_{1/2})^2 (g_{9/2})^{-2}$ [60%], $(f_{5/2})^2 (p_{3/2})^2 (g_{9/2})^{-2}$ [10%] and $(f_{5/2})^2 p_{3/2} p_{1/2} (g_{9/2})^{-2}$ [7%].

The 3−-state at 2.53 MeV is known to be an octupole vibration of the core and therefore cannot be reproduced in our simple model.

In the calculations of transition probabilities the gyromagnetic ratios of orbital angular momentum have been supposed to equal one for neutrons and protons, and the effective charge of the nucleons has been assumed to be one electron charge.
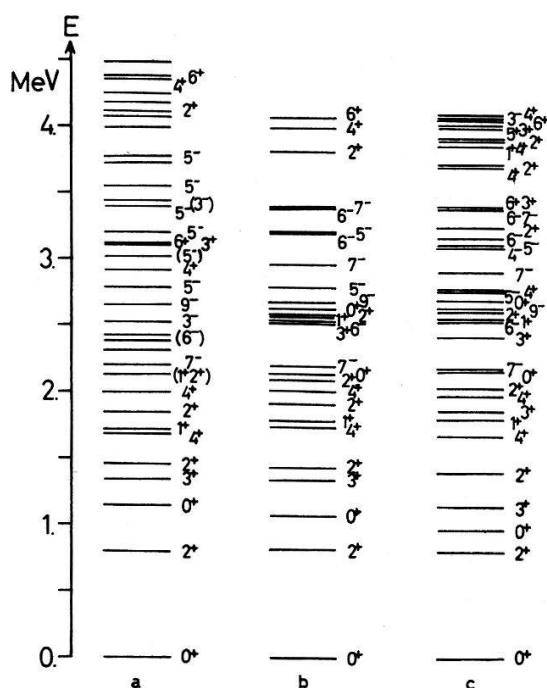
Figure 2
Level schemes of Pb^{206}. a: experiment, b: theoretical level scheme with core-spin-0 excitation, V_{ores} = V_{oCE} = -6.4 MeV, c: theoretical level scheme without core-excitation [2].

Table 1

Some reduced transition probabilities in Pb^{206}, calculated with two and with four core-orbits, are compared. Units are (barns)^2 and (nuclear magnetons)^2 for E2- and M1-transitions respectively.

Transition	$\sigma\lambda$	$B(\sigma\lambda)$	
		2 core orbits	4 core orbits
$0_1^+ \to 1_0^+$	M1	$.280 \cdot 10^{+1}$	$.293 \cdot 10^{+1}$
$0_3^+ \to 2_0^+$	E2	$.330 \cdot 10^{-2}$	$.327 \cdot 10^{-2}$
$1_0^+ \to 0_0^+$	M1	$.671$	$.688$
$1_1^+ \to 2_0^+$	M1	$.360 \cdot 10^{+1}$	$.349 \cdot 10^{+1}$
$2_0^+ \to 0_0^+$	E2	$.890 \cdot 10^{-2}$	$.943 \cdot 10^{-2}$ [a]
$2_1^+ \to 0_0^+$	E2	$.170 \cdot 10^{-1}$	$.167 \cdot 10^{-1}$
$2_1^+ \to 2_0^+$	E2	$.400 \cdot 10^{-2}$	$.405 \cdot 10^{-2}$
	M1	$.771 \cdot 10^{-6}$	$.104 \cdot 10^{-3}$
$2_2^+ \to 2_0^+$	E2	$.170 \cdot 10^{-1}$	$.170 \cdot 10^{-1}$
	M1	$.460 \cdot 10^{-2}$	$.310 \cdot 10^{-2}$
$2_2^+ \to 2_1^+$	E2	$.189 \cdot 10^{-3}$	$.217 \cdot 10^{-3}$
	M1	$.102$	$.104$
$3_1^+ \to 2_0^+$	M1	$.925 \cdot 10^{-1}$	$.115$
$3_1^+ \to 3_0^+$	M1	$.124 \cdot 10^{+1}$	$.123 \cdot 10^{+1}$
$4_0^+ \to 2_0^+$	E2	$.654 \cdot 10^{-2}$	$.611 \cdot 10^{-2}$
$4_0^+ \to 2_1^+$	E2	$.125 \cdot 10^{-1}$	$.118 \cdot 10^{-1}$
$5_0^- \to 6_0^-$	E2	$.845 \cdot 10^{-2}$	$.874 \cdot 10^{-2}$
	M1	$.808$	$.716$

[a] The experimental value is $(.270^{+0.05}_{-0.09}) \cdot 10^{-1}$ [19].

As was already mentioned only a few core excited configurations contribute appreciably to the wave functions of low-lying states. Therefore, the changes of the transition probabilities which are caused by core-spin-0 excitations take place mainly because of the changes in the amplitudes of not core-excited configurations. The contribution U_{eV} (equation (37)) of core-excited configurations is much smaller and U_{eC} (equation (36)) vanishes.

In Table 1 some reduced transition probabilities, calculated with two and four core orbits, are compared. It can be seen that the influence of the $j_{15/2}$ and the $d_{5/2}$ core orbit is rather small, except for the M1-transition from the second 2^+- to the first 2^+-state. This transition also depends strongly on the choice of the spin-spin and tensor part of the residual interaction [2].

The calculated probability for the E2-transition from the first 2^+-state to the ground state is rather independent of the parameters of the interaction [2], but still to small compared to the experimental value. It must be expected that for transition probabilities higher core-spins, at least core-spin 2, must be taken into account, even if the core-spin-0 excitations are more important for level positions.

5.4. *The polonium isotope Po²¹⁰*

Although energy levels and transition probabilities of Pb^{210} have been mesured recently [14] only little information on spins and parities is available.

In [2] it is pointed out that the level scheme at low energies is rather insensitive to the choice of the parameters of the residual interaction. The same is true for the influence of excitations with core-spin 0.

In all our calculations the $s_{1/2}$, the $d_{3/2}$ and the $h_{11/2}$ core orbits were taken into account. The energy difference between the ground states of Bi^{209} and Tl^{207} is 4.24 MeV [10]. As for Pb^{206} the level scheme is not sensitive to small deviations from this value.

For a coupling constant $V_{0res} = V_{0CE} = -4.0$ MeV, which matches the energy difference between the ground state and the first excited state, the ground state is lowered by 1,63 MeV with respect to the pure single-particle picture. Core-spin-0 excitation makes up 0.17 MeV of this value.

In Figure 3 the calculated scheme is compared to the experimental one and to the scheme which is obtained without core-excitation. It can be seen that the changes induced are very small especially for the lower states. Therefore core-spin 0 excitation alone cannot account for the large gap between the first 2^+- and the first 4^+-state.
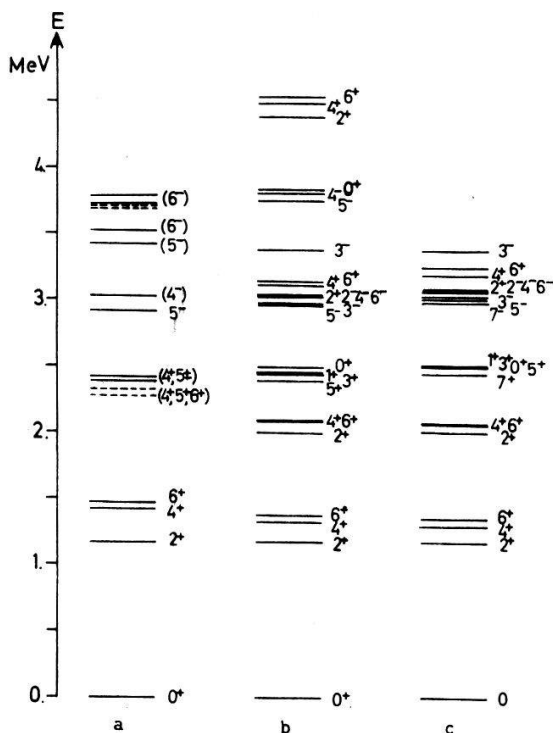

Figure 3

The theoretical level scheme (b) of Po^{210}, calculated with core-spin-O excialtion, is compared to the experimental one (a) and to the scheme obtained without core-excitation (c) [2].

In Table 2 some reduced transition probabilities are given and compared to experimental values, as far as they are known, and to the values of [2]. The calculated transition probabilities agree rather well with the mesured values, but it is obvious that they are practically not changed at all by excitations with core-spin 0.

Table 2

Some reduced E2-transition probabilities in Po^{210} are compared to the values of Ref. 2 and to experiment. Units are (barns)^2

Transition	B (E2)		
	This work	Ref. 2	Experiment
$2_0^+ \rightarrow 0_0^+$	$.107 \cdot 10^{-1}$	$.107 \cdot 10^{-1}$	–
$4_0^+ \rightarrow 2_0^+$	$.132 \cdot 10^{-1}$	$.134 \cdot 10^{-1}$	$(.192 \pm 0.025) \cdot 10^{-1}$ [10]
$4_1^+ \rightarrow 4_0^+$	$.188 \cdot 10^{-3}$	$.186 \cdot 10^{-3}$	–
$4_0^- \rightarrow 5_0^-$	$.795 \cdot 10^{-2}$	$.826 \cdot 10^{-2}$	–
$5_0^+ \rightarrow 6_0^+$	$.123 \cdot 10^{-4}$	$.121 \cdot 10^{-4}$	–
$6_0^+ \rightarrow 4_0^+$	$.923 \cdot 10^{-2}$	$.933 \cdot 10^{-2}$	$(.128 \pm 0.016) \cdot 10^{-1}$ [10]

5.5. The mercury isotope Hg^{206}

No experimental information is available about the excited states of Hg^{206}. This nucleus is however of theoretical interest since its configuration space is the same as the one of Po^{210}, but with the roles of outer orbits and core orbits interchanged (Fig. 1).

In our calculation we considered the $s_{1/2}$, the $d_{3/2}$, the $h_{11/2}$ and the $d_{5/2}$ states of Tl^{207} and the $h_{9/2}$, the $f_{7/2}$ and the $i_{13/2}$ states of Bi^{209}. For the approximate determination of the coupling constants of core excitation and residual interaction the energy gap between the ground state and the first 2$^+$-state was assumed to be about the
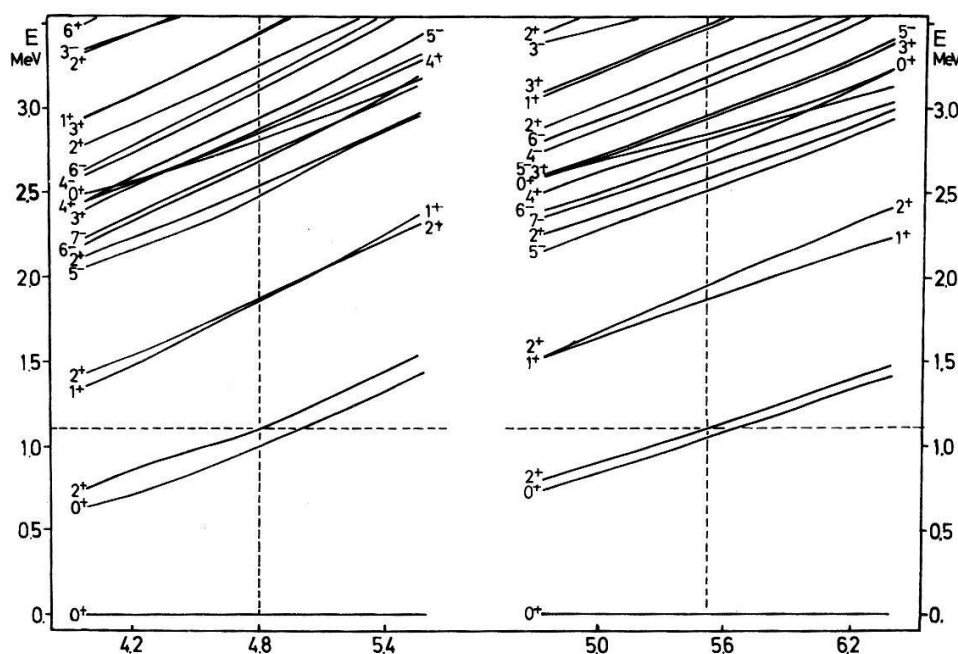

Figure 4

The dependency of theoretical energy levels in Hg^{206} to coupling constants. Left: With core-excitation, near $V_{ores} = V_{oCE} = -4.8$ MeV. Right: Without core-excitation, near $V_{ores} = -5.6$ MeV.

same as in Po²¹⁰, i.e. about 1.1 MeV. The coupling constants of core-excitation and residual interaction were assumed to be equal.

A gap of 1.1 MeV corresponds to the coupling constants $V_{0res} = V_{0CE} = -4.8$ MeV. If core-excitation is neglected, the coupling constant of residual interaction alone is $V_{ores} = -5.6$ MeV. The interaction energy of a nucleon pair in the ground state equals -1.81 MeV with, and -1.49 MeV without core-excitation.

The dependency of the calculated energy levels to coupling constants near the values mentioned above is illustrated in Figure 4. One sees that the level scheme is sensitive to core-excitation with core-spin 0 in contrast to that of Po²¹⁰. We recall that a similar phenomenon is observed in the pair of nuclei Pb²⁰⁶ and Pb²¹⁰, where only in Pb²⁰⁶ the lower part of the level scheme is sensitive to the parameters of the residual interaction [2].

6. Conclusion

The calculated level schemes show that core-excitation may substantially affect the low-lying states of nuclei in the lead region. But excitations with core-spin 0 are important for those nuclei only whose general properties are determined by single-hole states of small spins. On the contrary for Po²¹⁰, which has two protons with large single-particle spins more than the magic numbers, the admixture of configurations excited with core-spin 0 is small in the lower states, and the transition probabilities are practically unaffected. We expect that the same will be true for Pb²¹⁰, since the single-particle spins of this nucleus are also very large and [2] shows that the properties of the low-lying states are also rather independent of the parameters of the residual interaction.

This difference in behaviour is a consequence of the different magnitude of the single-particle spins of the valence nucleons. In Po²¹⁰ all the low states 0_0^+, 2_0^+, 4_0^+ and 6_0^+ have the same main configuration $(h_{9/2})^2$ and are influenced in about the same way by residual interaction and core-excitation. On the other hand the single-particle spins in Hg²⁰⁶ and Pb²⁰⁶ are small and therefore various different main configurations are necessary to build up the sequence of low-lying states.

We have already mentioned that electric dipole transitions are strongly forbidden in our model, since the reduced matrix elements between all considered single-particle states vanish. Based on the assumption that core nucleons are excited only in pairs from the same core orbit, the term U_{eC} (equation (36)) contains only diagonal matrix elements, which are zero for electric dipole transitions because of parity selection rules. Consequently the contribution of the core orbits in excited configurations vanishes too. On the other hand, electric dipole transitions have been found [15] in the decay of the first 4⁻-state in Po²¹⁰. Because these transitions are weak, they can be explained by the admixture of further single-particle states not included in our calculations. Core-excited configurations may also bring about finite electric dipole transition probabilities, but only if the scattering of single nucleons from one core orbit to the other is permitted.

Since the term U_{eC} (equation (36)) contains directly the influence of transitions between different core-spins, we expect that this term contributes appreciably to E2-transitions [23]. But if only excitations with core-spin 0 are considered, U_{eC} vanishes

identically for E2-transitions. Therefore, from this point of view the restriction to core-spin 0 is certainly very crude and it is desirable to consider at least also excitations with core-spin 2.

We have made the attempt to calculate the level scheme of Ni[58] [16]. As was to be expected, the level positions are changed considerably by the admixture of core-excited configurations. However, no reasonable correspondence between the calculated and the mesured levels could be achieved. The large gap between the first 2[+]- and the first 4[+]-state cannot be explained by excitations with core-spin 0 nor at all by four-particle-two-hole excitation alone.

Since the level scheme of Ni[57] [17] contains states of low energy which consist mainly of two-particle-one-hole configurations, we conclude that the approximations made in our model cannot yield satisfactoring results for Ni[58]. Furthermore, beyond the excitation of single protons excitation of neutrons and neutron pairs from the Ni[56] core should also be considered.

Acknowledgments

7. Appendix

We give here the definitions and the most important relations of the two- and four-fermion operators and some details about the orthogonalization of four-fermion operators. Some of these relations may also be found in [18].

In this paper the following abbreviations are used:

$$\hat{j} \equiv 2j + 1, \tag{A1}$$

$$\delta_J(j_1 j_2 j_3 j_4) \equiv \delta_{j_1 j_3} \delta_{j_2 j_4} - (-)^{j_1 + j_2 + J} \delta_{j_1 j_4} \delta_{j_2 j_3}, \tag{A2}$$

$$\Delta_{j_1 j_2} \equiv (1 + \delta_{j_1 j_2})^{1/2}, \tag{A3}$$

$$\Delta(j_1 j_2 j_3 j_4) \equiv [(2 - \delta_{j_1 j_2})(2 - \delta_{j_3 j_4})]^{1/2}. \tag{A4}$$

Exchange terms of the form $A(j_1 j_2) + c\, A(j_2 j_1)$, where A is any expression in j_1 and j_2 and c is independent of j_1 and j_2, are generally denoted by

$$[A(j_1 j_2) + c\,\{j_1 \leftrightarrow j_2\}].$$

In all definitions of angular momentum algebra the notation of [4] has been adopted.

Single-particle states are characterized by their angular momentum quantum numbers j only. Thus, $\delta_{j_a j_b}$ requires the equality of the states a and b. From the single-particle creation operators a_{jm}^+, which obey the anticommutation relation

$$\{a_{jm}, a_{j'm'}^+\} = \delta_{jj'}\,\delta_{mm'},$$

the pair-creation operator

$$B_{JM}^+(j_1 j_2) = \frac{1}{\varDelta_{j_1 j_2}} \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 \mid J M \rangle a_{j_1 m_1}^+ a_{j_2 m_2}^+ \qquad (j_1 \geqslant j_2) \qquad (A5)$$

and the particle-hole operator

$$A_{JM}^+(j_1 j_2) = \sum_{m_1 m_2} (-)^{j_2-m_2} \langle j_1 m_1 j_2 -m_2 \mid J M \rangle a_{j_1 m_1}^+ a_{j_2 m_2} \qquad (A6)$$

are constructed. The convention

$$j_1 \geqslant j_2 \qquad (A7)$$

and the factor $1/\varDelta_{j_1 j_2}$ have been introduced in (A5) in order to get an orthogonal and normalized system of base functions for two-fermion states.

The operators satisfy the symmetry-relations

$$B_{JM}^+(j_1 j_2) = -(-)^{j_1+j_2+J} B_{JM}^+(j_2 j_1) , \qquad (A8)$$

$$A_{JM}^+(j_1 j_2) = -(-)^{j_1+j_2+M} A_{J-M}(j_2 j_1) \qquad (A9)$$

and the commutation relation

$$[A_{JM}^+(j_1 j_2) , \; B_{J'M'}^+(j_1' j_2')]$$
$$= \frac{(-)^{j_1+j_2+J'}}{\varDelta_{j_1' j_2'}} \left(\delta_{j_2 j_2'} \varDelta_{j_1 j_1'} \hat{J} \hat{J}' \sum_{L\varLambda} (-)^L \langle JM J'M' \mid L\varLambda \rangle \begin{Bmatrix} J & J' & L \\ j_1' & j_1 & j_2 \end{Bmatrix} \right.$$
$$\times \left. B_{L\varLambda}^+(j_1 j_1') - (-)^{j_1'+j_2'+J'} \{j_1' \leftrightarrow j_2'\} \right). \qquad (A10)$$

If the convention (A7) cannot be applied, the commutator between pair-creation and pair-annihilation operators is

$$[B_{JM}(j_1 j_2), B_{J'M'}^+(j_1' j_2')] = \frac{\delta_{JJ'} \delta_{MM'} \delta_J(j_1 j_2 j_1' j_2')}{\varDelta_{j_1 j_2} \varDelta_{j_1' j_2'}}$$
$$+ \frac{(-)^{J'+M'}}{\varDelta_{j_1 j_2} \varDelta_{j_1' j_2'}} \left(\delta_{j_2 j_1'} \hat{J} \hat{J}' \sum_{L\varLambda} (-)^{L-\varLambda} \langle JM J' -M' \mid L -\varLambda \rangle \begin{Bmatrix} J & J' & L \\ j_2' & j_1 & j_2 \end{Bmatrix} A_{L\varLambda}^+(j_2' j_1) \right.$$
$$\left. - (-)^{j_1+j_2+J} \{j_1 \leftrightarrow j_2\} - (-)^{j_1'+j_2'+J'} \{j_1' \leftrightarrow j_2'\} + (-)^{j_1+j_2+J+j_1'+j_2'+J'} \begin{vmatrix} j_1 \leftrightarrow j_2 \\ j_1' \leftrightarrow j_2' \end{vmatrix} \right). \qquad (A11)$$

From (A11) we get immediately

$$\langle 0 \mid B_{JM}(j_1 j_2) B_{J'M'}^+(j_1' j_2') \mid 0 \rangle = \delta_{JJ'} \delta_{MM'} \delta_{j_1 j_1'} \delta_{j_2 j_2'} , \qquad (A12)$$

if $j_1 \geqslant j_2$ and $j_1' \geqslant j_2'$ hold. (A11) and (A12) are both necessary since in many intermediate calculations the single-particle spins are arbitrary.

From (A10), (A11) and the operator relation

$$[A^m, B^n] = \sum_{\nu=0}^{n-1} \sum_{\mu=0}^{m-1} B^\nu A^\mu [A, B] A^{m-\mu-1} B^{n-\nu-1}$$

the following equations can be derived (in most cases by recursion), which are used to calculate the normalizations of the core-parts of base functions:

$$[B_{RM}(j_1 \, j_2), \, B_{00}^+(j \, j)^n] \, |0\rangle = \delta_{j_1 j_2} \, \delta_{j_1 j}$$

$$\times \left\{ \delta_{RO} \, \delta_{MO} \, n \, B_{00}^+(j \, j)^{n-1} - \frac{2}{2 \, j + 1} \, (-)^M \, n \, (n - 1) \, B_{R-M}^+(j \, j) \, B_{00}^+(j \, j)^{n-2} \right\} |0\rangle, \quad \text{(A13)}$$

$$\langle 0 | \, B_{00}(j \, j)^n \, B_{00}^+(j \, j)^n \, |0\rangle = n! \prod_{k=1}^{n-1} \left(1 - \frac{2 \, k}{\hat{j}^2} \right), \quad \text{(A14)}$$

$$[A_{JM}^+(j_1 \, j_2), \, B_{00}^+(j \, j)^n] = \delta_{j_2 j} \, \Delta_{j_1 j_2} \, \frac{\sqrt{2}}{\hat{j}} \, n \, B_{JM}^+(j_1 \, j) \, B_{00}^+(j \, j)^{n-1}, \quad \text{(A15)}$$

$$\langle 0 | \, B_{00}(j \, j)^n \, B_{RM}(j \, j) \, B_{R'M'}^+(j \, j) \, B_{00}^+(j \, j)^n \, |0\rangle = \delta_{RR'} \, \delta_{MM'} \, \gamma_n, \quad \text{(A16)}$$

where

$$\gamma_n = \begin{cases} (n + 1)! \displaystyle\prod_{k=1}^{n} \left(1 - \frac{2 \, k}{\hat{j}^2} \right), & \text{if } R = 0 \\[2ex] n! \displaystyle\prod_{k=2}^{n+1} \left(1 - \frac{2 \, k}{\hat{j}^2} \right), & \text{if } R \neq 0. \end{cases} \quad \text{(A17)}$$

Four-fermion operators are built up by coupling two pair operators to a total angular momentum Λ with projection λ:

$$D_{\Lambda\lambda}^+(j_1 \, j_2 \, J, \, j_3 \, j_4 \, J') = \sum_{\nu \, \nu'} \langle J \, \nu \, J' \, \nu' \, | \, \Lambda \, \lambda \rangle \, B_{J\nu}^+(j_1 \, j_2) \, B_{J'\nu'}^+(j_3 \, j_4). \quad \text{(A18)}$$

If base function of four-particle systems are to be described by (A18) a convention similar to (A7) must be made, namely

$$j_1 \geqslant j_2 \geqslant j_3 \geqslant j_4. \quad \text{(A19)}$$

The four-particle creation operators defined in this way are however not orthogonal. They have to be orthogonalized later (see below).

They satisfy the symmetry-relations

$$D_{\Lambda\lambda}^+(j_1 \, j_2 \, J, \, j_3 \, j_4 \, J') = (-)^{J+J'+\Lambda} \, D_{\Lambda\lambda}^+(j_3 \, j_4 \, J', \, j_1 \, j_2 \, J), \quad \text{(A20)}$$

$$D_{\Lambda\lambda}^+(j_1 \, j_2 \, J, \, j_3 \, j_4 \, J') = - \, (-)^{j_1+j_2+J} \, D_{\Lambda\lambda}^+(j_2 \, j_1 \, J, \, j_3 \, j_4 \, J') \quad \text{(A21)}$$

and

$$D_{\Lambda\lambda}^+(j_1 \, j_4 \, J, \, j_3 \, j_2 \, J') = (-)^{j_2+j_4+J'} \, \hat{J} \, \hat{J'} \, \frac{\Delta_{j_1 j_2} \Delta_{j_3 j_4}}{\Delta_{j_1 j_4} \Delta_{j_2 j_3}}$$

$$\times \sum_{LL'} (-)^{L'} \, \hat{L} \, \hat{L'} \begin{Bmatrix} j_1 & j_4 & J \\ j_2 & j_3 & J' \\ L & L' & \Lambda \end{Bmatrix} D_{\Lambda\lambda}^+(j_1 \, j_2 \, L, \, j_3 \, j_4 \, L'). \quad \text{(A22)}$$

Without the convention (A19) the commutators between two-particle and four-particle operators are

$$[A^+_{K\mu}(j_3\,j_4),\, D^+_{\Lambda\lambda}(j_1\,j_2\,J,\,j'_1\,j'_2\,J')] =$$

$$= \left(\frac{\Delta_{j_3 j_1}}{\Delta_{j_1 j_2}}\, \delta_{j_2 j_4}\, (-)^{j_1+j_4+K+J'}\, \hat{\Lambda}\, \hat{K}\, \hat{J} \sum_{L L'} \hat{L}\, (-)^{L'} \langle K\mu\,\Lambda\,\lambda \mid L'\,\lambda+\mu \rangle \begin{Bmatrix} K & J & L \\ j_1 & j_3 & j_2 \end{Bmatrix} \right.$$

$$\times \begin{Bmatrix} K & J & L \\ J' & L' & \Lambda \end{Bmatrix} D^+_{L'\lambda+\mu}(j_1\,j_3\,L,\,j'_1\,j'_2\,J') - (-)^{j_1+j_2+J}\,\{j_1 \leftrightarrow j_2\} + (-)^{J+J'+\Lambda}$$

$$\times \begin{Bmatrix} j_1 \leftrightarrow j'_1 \\ j_2 \leftrightarrow j'_2 \\ J \leftrightarrow J' \end{Bmatrix} + (-)^{j_1+j_2+j'_1+j'_2+\Lambda} \left. \begin{Bmatrix} j_1 \leftrightarrow j'_2 \\ j_2 \leftrightarrow j'_1 \\ J \leftrightarrow J' \end{Bmatrix} \right) \tag{A23}$$

and

$$[B_{K\mu}(j_3\,j_4),\, D^+_{\Lambda\lambda}(j_1\,j_2\,J,\,j'_1\,j'_2\,J')] =$$

$$= \frac{\delta_{JK}}{\Delta_{j_1 j_2}\,\Delta_{j_3 j_4}}\, \delta_K(j_1\,j_2\,j_3\,j_4)\, \langle J\mu\,J'\,\lambda-\mu \mid \Lambda\,\lambda \rangle\, B^+_{J'\lambda-\mu}(j'_1\,j'_2)$$

$$+ \frac{\delta_{J'K}}{\Delta_{j'_1 j'_2}\,\Delta_{j_3 j_4}}\, \delta_K(j'_1\,j'_2\,j_3\,j_4)\, \langle J\,\lambda-\mu\,J'\mu \mid \Lambda\,\lambda \rangle\, B^+_{J\,\lambda-\mu}(j_1\,j_2)$$

$$- \frac{\hat{K}\,\hat{J}\,\hat{J}'}{\Delta_{j_1 j_2}\,\Delta_{j_3 j_4}\,\Delta_{j'_1 j'_2}} \left(\Delta_{j_1 j'_1}\, \delta_K(j_3\,j_4\,j_2\,j'_2) \sum_L \hat{L}\, \langle L\,\lambda-\mu\,K\,\mu \mid \Lambda\,\lambda \rangle \right.$$

$$\times \begin{Bmatrix} j_1 & j_2 & J \\ j'_1 & j'_2 & J' \\ L & K & \Lambda \end{Bmatrix} B^+_{L\lambda-\mu}(j_1\,j'_1) - (-)^{j_1+j_2+J}\,\{j_1 \leftrightarrow j_2\} - (-)^{j'_1+j'_2+J'}\{j'_1 \leftrightarrow j'_2\}$$

$$+ (-)^{j_1+j_2+J+j'_1+j'_2+J'} \left. \begin{Bmatrix} j_1 \leftrightarrow j_2 \\ j'_1 \leftrightarrow j'_2 \end{Bmatrix} \right) + \text{terms in } B^+ A^+. \tag{A24}$$

Equation (A24) can be slightly simplified by introducing the conventions (A7) and (A19).

The vacuum-expectation value of the commutator between two four-particle operators can be expressed in the formula

$$\langle 0 \mid [D_{\Lambda\lambda}(j_1\,j_2\,J,\,j_3\,j_4\,J'),\, D^+_{\Lambda'\lambda'}(j'_1\,j'_2\,K,\,j'_3\,j'_4\,K')] \mid 0 \rangle$$

$$= \delta_{\Lambda\Lambda'}\,\delta_{\lambda\lambda'}\, \frac{1}{\Delta_{j_1 j_2}\,\Delta_{j_3 j_4}\,\Delta_{j'_1 j'_2}\,\Delta_{j'_3 j'_4}} \left\{ \delta_{JK}\,\delta_{J'K'}\,\delta_J(j_1\,j_2\,j'_1\,j'_2)\,\delta_{J'}(j_3\,j_4\,j'_3\,j'_4) \right.$$

$$+ (-)^{J+J'+\Lambda}\,\delta_{JK'}\,\delta_{J'K}\,\delta_J(j_1\,j_2\,j'_3\,j'_4)\,\delta_{J'}(j_3\,j_4\,j'_1\,j'_2) +$$

$$- \hat{J}\,\hat{J}'\hat{K}\hat{K}' \left(\delta_J(j_1\,j_2\,j'_1\,j'_3)\,\delta_{J'}(j_3\,j_4\,j'_2\,j'_4) \begin{Bmatrix} j'_1 & j'_2 & K \\ j'_3 & j'_4 & K' \\ J & J' & \Lambda \end{Bmatrix} - (-)^{j'_1+j'_2+K}\{j'_1 \leftrightarrow j'_2\} + \right.$$

$$- (-)^{j_3' + j_4' + K'} \{j_3' \leftrightarrow j_4'\} + (-)^{j_1' + j_2' + K + j_3' + j_4' + K'} \left. \left. \begin{Bmatrix} j_1' \leftrightarrow j_2' \\ j_3' \leftrightarrow j_4' \end{Bmatrix} \right) \right\} . \tag{A25}$$

If the convention (A19) can be used, (A25) is simplified to the form

$$\langle 0 \mid [D_{\Lambda \lambda}(j_1 \, j_2 \, J, \, j_3 \, j_4 \, J'), \quad D_{\Lambda' \lambda'}^+(j_1' \, j_2' \, K, \, j_3' \, j_4' \, K')] \mid 0 \rangle$$

$$= \delta_{\Lambda \Lambda'} \, \delta_{\lambda \lambda'} \, \delta_{j_1 j_1'} \, \delta_{j_2 j_2'} \, \delta_{j_3 j_3'} \, \delta_{j_4 j_4'} \left(\delta_{JK} \, \delta_{J'K'} + (-)^{J + J' + \Lambda} \, \delta_{J'K} \, \delta_{JK'} \, \delta_{j_1 j_3} \, \delta_{j_2 j_4} \right.$$

$$\left. - \Delta_{j_1 j_2} \Delta_{j_3 j_4} \Delta_{j_1' j_2'} \Delta_{j_3' j_4'} \, \hat{J} \, \hat{J}' \, \hat{K} \, \hat{K}' \begin{Bmatrix} j_1 \, j_2 \, K \\ j_3 \, j_4 \, K' \\ J \, J' \, \Lambda \end{Bmatrix} \delta_{j_2 j_3} \right),$$

$$(j_1 \geqslant j_2 \geqslant j_3 \geqslant j_4, \, j_1' \geqslant j_2' \geqslant j_3' \geqslant j_4'), \tag{A26}$$

which is to be used for the description of base states. It can be seen from (A26) that by the convention (A19) the four-particle operators become orthogonal with respect to the total angular momentum and the single-particle spins. Therefore, only the orthogonality of operators with the same single-particle spins and the same total spin must be investigated further. First we consider two special cases:

If all single particle states are different or if $j_2 \neq j_3$, the operators are indeed orthogonal. If only the middle single-particle spins are equal, the operators can be orthogonalized by recoupling the spins with help of (A22), so that the states which are equal are coupled first. Then Pauli's principle can be satisfied by allowing only even values of the intermediate angular momentum. We thus define orthogonal four-particle operators in this case as follows:

$$\mathcal{D}_{\Lambda \lambda (JJ')}^+(j_1 \, j \, j \, j_4) = \frac{1}{\sqrt{2}} \sum_{SS'} (-)^{S'} \, \hat{J} \, \hat{J}' \, \hat{S} \, \hat{S}' \begin{Bmatrix} j_1 \, j_4 \, J \\ j \, j \, J' \\ S \, S' \, \Lambda \end{Bmatrix} D_{\Lambda \lambda}^+(j_1 \, j \, S, \, j \, j_4 \, S') . \tag{A27}$$
$$\scriptstyle J' even$$

In the case that three or four single-particle states are equal the operators with different intermediate coupling modes create a non-orthogonal and redundant set of states. Then an orthogonal set of states is constructed numerically by Schmidt's procedure, starting with the state of lowest seniority. We thus define the general four-particle creation operators by

$$\mathcal{D}_{\Lambda \lambda \alpha}^+(j_1 \, j_2 \, j_3 \, j_4) = \sum_{JJ'} d_{\Lambda \alpha}^{JJ'} (j_1 \, j_2 \, j_3 \, j_4) \, D_{\Lambda \lambda}^+(j_1 \, j_2 \, J, \, j_3 \, j_4 \, J') , \tag{A28}$$

where $d_{\Lambda \alpha}^{JJ'}(j_1 \, j_2 \, j_3 \, j_4)$ are the coefficients of numerical orthogonalization or the coefficients in (A27) and α denotes the different orthogonal coupling possibilities.

It is easy to show that the general orthogonalization coefficient $d_{\Lambda \alpha}^\beta$ (we denote here the pairs of intermediate angular momenta symbolically by small greek letters) can be expressed by the recursion formula

$$d^{\beta}_{\Lambda\alpha} = \begin{cases} -\dfrac{1}{N}\sum_{\varkappa=\beta}^{\alpha-1}\sum_{\sigma=1}^{\varkappa} d^{\sigma}_{\Lambda\varkappa}\, d^{\beta}_{\Lambda\varkappa}\,\langle 0\,|\,D_{\Lambda\lambda}(\alpha),\,D^{+}_{\Lambda\lambda}(\sigma)\,|\,0\rangle \\ \qquad\qquad\quad \text{if } \beta = 1,\ldots,(\alpha-1) \\[4pt] \dfrac{1}{N}, \qquad\qquad \text{if } \beta = \alpha \end{cases}, \text{ if } N > 0 \qquad (A29)$$

and

$$d^{\beta}_{\Lambda\alpha} = 0, \quad \text{if } N = 0, \tag{A30}$$

where N is the norm of the constructed orthogonal states

$$N = \sum_{\mu\nu}^{\alpha} d^{\mu}_{\Lambda\alpha}\, d^{\nu}_{\Lambda\alpha}\,\langle 0\,|\,D_{\Lambda\lambda}(\mu),\,D^{+}_{\Lambda\lambda}(\nu)\,|\,0\rangle. \tag{A31}$$

For the description of 'recoupled' exchange terms it is convenient to define the 'recoupled' orthogonalization coefficients

$$f^{LL'}_{\Lambda\alpha}(j_i\, j_k\, j_l\, j_m) = \sum_{JJ'} \hat{J}\,\hat{J}'\,\hat{L}\,\hat{L}'\, t^{j_i j_k}_{j_l j_m} \begin{Bmatrix} j_i & j_k & J \\ j_l & j_m & J' \\ L & L' & \Lambda \end{Bmatrix} d^{JJ'}_{\Lambda\alpha}(j_1\, j_2\, j_3\, j_4), \tag{A32}$$

where the phase factor is given by

$$t^{j_i j_k}_{j_l j_m} = \frac{(1 + (-)^L\delta_{il})\,(1 + (-)^{L'}\delta_{km})}{(1 + \delta_{il})\,(1 + \delta_{km})}$$

$$\times \begin{cases} 1, & \text{if } j_i = j_1, j_k = j_2, j_l = j_3, j_m = j_4 \\ -(-)^{j_1+j_2+J}, & \text{if } j_i = j_2, j_k = j_1, j_l = j_3, j_m = j_4 \\ -(-)^{j_3+j_4+J'}, & \text{if } j_i = j_1, j_k = j_2, j_l = j_4, j_m = j_3 \\ (-)^{j_1+j_2+J+j_3+j_4+J'}, & \text{if } j_i = j_2, j_k = j_1, j_l = j_4, j_m = j_3. \end{cases} \tag{A33}$$

It should be noted that the transformation (A32) is in general not equivalent to (A22), for the orthogonalization procedure is not unitary and cannot be inverted. However, if only the middle single-particle spins are equal, we get by (A22)

$$f^{LL'}_{\Lambda(SS')}(j_2\, j_1\, j_2\, j_4) = -\frac{1}{\sqrt{2}}\,(-)^{j_2+j_4+L+L'+\Lambda}\,\delta_{L'S}\,\delta_{LS'}. \tag{A34}$$

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