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Core Excitation in Semi-Closed Nuclei

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Abstract. Four-particle-two-hole core excitation in nuclei with two nucleons outside the closed shells is treated by direct extension of the configuration space. Some applications to a simple two-level case are given.

1. Introduction

With the growing success which the shell-model had during the last years in the calculation of the energy levels of nuclei with two nucleons outside the closed shells, it has become more and more clear that the effects of core excitation are considerable and should be taken into account when energy levels are calculated [3]. A few authors have therefore considered the influence of 3-particle-1-hole $\{(3 p, 1 h)\}$ and 4-particle-2-hole $\{(4 p, 2 h)\}$ core excitation as perturbation.

It turned out that the smallness of the $(3 p, 1 h)$ corrections is consistent with the experiments and no indications have been found that states excited in this way mix strongly in low-lying states of two-particle systems.

However, the situation is quite different for $(4 p, 2 h)$ corrections. The admixture of such states, in which a pair of nucleons has jumped out from the core to the outer orbits, can be so great [1] that a perturbation treatment seems to be most doubtful. A direct extension of the model space which is to include at least those core-excited states with two holes in the upper core orbits bears already some aspects of a many particle problem, but in such restricted form that the difficulties which arise especially when the normal residual interaction in the core is to be calculated, can be overcome relatively easy in a simple model. One of the greatest problems of a direct diagonalization of the Hamiltonian is the size of the secular matrix, which grows considerably, because of the great number of spin coupling possibilities, even if only a few core orbits are considered. But since we are only interested in the lowest eigenvalues, the diagonalization can be made by approximation methods (an excellent new method can be found in [2]). Nevertheless, if we want to calculate an actual nucleus, it seems that further approximations must be made in order to reduce the size of the secular matrix, especially when not only a very small number of core orbits and outer orbits is to be considered.

2. Model for $(4 p, 2 h)$ Excitations

2.1. Physical Assumptions

To avoid the difficulties that arise in a perturbation treatment of the $(4 p, 2 h)$ core excitation we diagonalize directly the full Hamilton matrix of a restricted model. We assume that the configuration scheme of the nucleus consists of three kinds of orbits (Fig. 1), namely the orbits of the light nucleons, treated in usual shell-model

calculations, a number (σ) of completely filled core orbits, from which a pair of nucleons may jump to the outer orbits, and an inert core not taking part in core excitation.

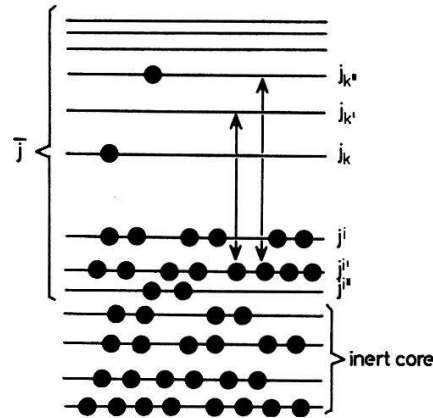


Figure 1

Configuration space for $(4p, 2h)$ excitation model.

We shall denote the quantum numbers of the outer orbits by lower indices, those of the core orbits by upper ones. If we do not want to distinguish between these two kinds of orbits, we shall put a bar over the respective quantum numbers. Single particle states are characterized by their angular momentum quantum numbers only. We shall neglect the excitation of a single nucleon from the core, because in most cases the effect is small and can be treated satisfactorily as perturbation. In addition, we assume that the nucleons are excited only in pairs coming from the same core orbit, but may occupy different outer orbits after excitation; for the excitation from different core orbits would implicate the breaking of two nucleon pairs. Moreover, the main effects are caused by core-spin- O excitations, as will be discussed in chapter 3.

We assume further that the nucleons which remain in the core are always coupled in pairs of total angular momentum O , except for one pair which takes up the recoil angular momentum from the two nucleons that have jumped out of the core to the outer orbits.

As a consequence of these assumptions, to every state of angular momentum I of the original non-excited nucleus ("excited" refers here and in the following always to core excitation) a number of states of much higher energy is added, whereby the total angular momentum Λ of the four outer nucleons is coupled with the recoil angular momentum R of the core, so that the same total angular momentum I as in the original state results:

$$\Lambda + R = I.$$

2.2. Hamiltonian

According to our model, the base functions of the not excited states may be chosen to be

$$|j'_1 j'_2 J' M', \sigma\rangle = \Gamma^{-1/2} B_{J' M'}^+(j'_1 j'_2) \prod_{i=1}^{\sigma} B_{00}^+(j^i j^i)^{(2j^i+1)/2} |0\rangle, \quad (1)$$

where $B_{J' M'}^+(j'_1 j'_2)$ is a creation operator for one pair of nucleons with single particle spins j'_1 and j'_2 ($j'_1 \geq j'_2$) and the total spin $(J' M')$ [6], and the third term is the core function. The normalization, Γ , of these states can be calculated by recursion.

As base functions of the excited states, we chose

$$|j_1 j_2 j_3 j_4 (A \alpha R q) I m, \sigma\rangle = \Omega^{-1/2} \sum_{\lambda M} \langle A \lambda R M | I m \rangle \mathcal{D}_{A \lambda \alpha}^+(j_1 j_2 j_3 j_4) \\ \times B_{R M}^+(j^q j^q) B_{00}^+(j^q j^q)^{(2j^q-3)/2} \prod_{i \neq q} B_{00}^+(j^i j^i)^{(2j^i+1)/2} |0\rangle. \quad (2)$$

Here, $\mathcal{D}_{A \lambda \alpha}^+(j_1 j_2 j_3 j_4)$ is an orthogonalized, antisymmetrized operator which creates four nucleons in single particle states j_1, j_2, j_3, j_4 , coupled so that a total angular momentum $(A \lambda)$ results [4]. The index α denotes the different orthogonal coupling possibilities.

The four-particle creation operators are defined as

$$\mathcal{D}_{A \lambda \alpha}^+(j_1 j_2 j_3 j_4) = \sum_{S S'} d_{A \alpha}^{S S'}(j_1 j_2 j_3 j_4) D_{A \lambda}^+(j_1 j_2 S, j_3 j_4 S'), \quad (3)$$

where

$$D_{A \lambda}^+(j_1 j_2 S, j_3 j_4 S') = \sum_{\nu \nu'} \langle S \nu S' \nu' | A \lambda \rangle B_{S \nu}^+(j_1 j_2) B_{S' \nu'}^+(j_3 j_4), \\ (j_1 \geq j_2 \geq j_3 \geq j_4), \quad (4)$$

and the $d_{A \alpha}^{S S'}(j_1 j_2 j_3 j_4)$ are orthogonalization coefficients [4].

In (2), one core orbit, which is labeled by q , is not completely filled and a nucleon pair of this orbit carries the angular momentum \mathbf{R} of the core. The normalization of the excited states, Ω , may again be calculated by recursion.

The Hamiltonian is divided into two parts:

$$H = H_0 + H'. \quad (5)$$

The single particle or diagonal term, H_0 , which originates in the mean shell-model potential, can be written as

$$H_0 = \sum_{\bar{j} \bar{m}} \varepsilon_{\bar{j}} a_{\bar{j} \bar{m}}^+ a_{\bar{j} \bar{m}}, \quad (6)$$

where the $\varepsilon_{\bar{j}}$ are the single particle energies and $a_{\bar{j} \bar{m}}^+$ is a creation operator for one nucleon in the state $(\bar{j} \bar{m})$. From this we have for not excited states

$$\langle j'_1 j'_2 J' M', \sigma | H_0 | j''_1 j''_2 J'' M'', \sigma \rangle \\ = \delta_{J' J''} \delta_{M' M''} \delta_{j'_1 j''_1} \delta_{j'_2 j''_2} \left(\varepsilon_{j'_1} + \varepsilon_{j'_2} + \sum_{i=1}^{\sigma} (2j^i + 1) \varepsilon_{j^i} \right), \quad (7)$$

while for excited states we get

$$\langle j'_1 j'_2 j'_3 j'_4 (A' \alpha' R' q') I' m', \sigma | H_0 | j''_1 j''_2 j''_3 j''_4 (A'' \alpha'' R'' q'') I'' m'', \sigma \rangle \\ = \delta_{j'_1 j''_1} \delta_{j'_2 j''_2} \delta_{j'_3 j''_3} \delta_{j'_4 j''_4} \delta_{I' I''} \delta_{m' m''} \delta_{A' A''} \delta_{\alpha' \alpha''} \delta_{q' q''} \delta_{R' R''} \\ \times \left(\varepsilon_{j'_1} + \varepsilon_{j'_2} + \varepsilon_{j'_3} + \varepsilon_{j'_4} + (2j^{q'} - 1) \varepsilon_{j^{q'}} + \sum_{i \neq q'}^{\sigma} (2j^i + 1) \varepsilon_{j^i} \right). \quad (8)$$

According to our model, we decompose the second term in (5) again into two parts:

$$H' = H_{res} + H_{CE}. \quad (9)$$

H_{res} is the residual interaction of usual shell-model calculations, taken separately for excited and not excited states. It can be put into the form [5] [6]

$$H_{res} = \sum_{\substack{K\mu \\ \bar{j}_1 \geq \bar{j}_2 \\ \bar{j}_3 \geq \bar{j}_4}} G_K(\bar{j}_1 \bar{j}_2 \bar{j}_3 \bar{j}_4) B_{K\mu}^+(\bar{j}_1 \bar{j}_2) B_{K\mu}(\bar{j}_3 \bar{j}_4) 2 \sqrt{(2 - \delta_{\bar{j}_1 \bar{j}_2})(2 - \delta_{\bar{j}_3 \bar{j}_4})}, \quad (10)$$

where G_K is the antisymmetrized coupling function. The second part, H_{CE} , which effects the interaction between the core and the light nucleons, must contain an operator, which annihilates a pair of nucleons in the core orbit labeled by q and re-create it in the outer orbits. Therefore we write

$$H_{CE} = \sum_{\substack{K\mu \\ j_3 \geq j_4 \\ j^q}} G_K(j_3' j_4' j^q j^q) B_{K\mu}^+(j_3' j_4') B_{K\mu}(j^q j^q) 2 \sqrt{2 - \delta_{j_3' j_4'}} + h.c., \quad (11)$$

similar to (10).

2.3. General Results

In the following the ordering of the single particle states in the orthogonalization coefficients $d_{A\alpha}^{JJ'}$ is always to be preserved, even if the other quantum numbers are interchanged.

The matrix elements can be simplified considerably by introducing the "recoupled" orthogonalization coefficients

$$f_{A\alpha}^{JJ'}(j_i j_k j_l j_m) = \sum_{SS'} t_{j_l j_m}^{j_i j_k} \sqrt{(2S+1)(2S'+1)} d_{A\alpha}^{SS'}(j_1 j_2 j_3 j_4) \begin{Bmatrix} j_i j_k S \\ j_l j_m S' \\ J J' A \end{Bmatrix}, \quad (12)$$

where the phase factor is defined as

$$t_{j_l j_m}^{j_i j_k} = \begin{cases} 1 & , \quad \text{if } j_i = j_1, j_k = j_2, j_l = j_3, j_m = j_4 \\ -(-)^{j_1+j_2+S} & , \quad \text{if } j_i = j_2, j_k = j_1, j_l = j_3, j_m = j_4 \\ -(-)^{j_3+j_4+S'} & , \quad \text{if } j_i = j_1, j_k = j_2, j_l = j_4, j_m = j_3 \\ (-)^{j_1+j_2+S+j_3+j_4+S'} & , \quad \text{if } j_i = j_2, j_k = j_1, j_l = j_4, j_m = j_3. \end{cases} \quad (13)$$

The core exciting part of the Hamilton matrix can now be calculated from (1), (2) and (11). The result is

$$\begin{aligned} \langle j_1 j_2 j_3 j_4 (A \alpha R q) I m, \sigma | H_{CE} | j_1' j_2' J' M', \sigma \rangle = & (-)^{\delta_{R0}} \delta_{IJ'} \delta_{mM'} \\ & \times 2 \left\{ \left(\delta_{j_1' j_2'} \delta_{j_2' j_4} \frac{\Delta_{j_1' j_2'} \Delta_{j_1 j_3}}{\Delta_{j_1 j_2} \Delta_{j_3 j_4}} \sqrt{2 - \delta_{j_1 j_3}} \hat{A} \hat{R} f_{A\alpha}^{R J'}(j_1 j_2 j_3 j_4) G_R(j_1 j_3 j^q j^q) \right. \right. \\ & + \{j_1 \leftrightarrow j_2\} + \{j_3 \leftrightarrow j_4\} + \left. \left. \begin{Bmatrix} j_1 \leftrightarrow j_2 \\ j_3 \leftrightarrow j_4 \end{Bmatrix} \right) \right. \\ & - \frac{\hat{A}}{\hat{J}'} \left(\delta_{j_1' j_3} \delta_{j_2' j_4} \sqrt{2 - \delta_{j_1 j_2}} d_{A\alpha}^{R J'} G_R(j_1 j_2 j^q j^q) \right. \\ & \left. \left. + (-)^{J'+A} \delta_{j_1' j_1} \delta_{j_2' j_2} \sqrt{2 - \delta_{j_3 j_4}} d_{A\alpha}^{J' R} G_R(j_3 j_4 j^q j^q) \right) \right\}, \quad (14) \end{aligned}$$

where

$$\Delta_{j_1 j_2} = (1 + \delta_{j_1 j_2})^{1/2} \quad \text{and} \quad \hat{J} = (2J + 1)^{1/2}.$$

The residual interaction matrix elements can be found to be for the not excited states

$$\begin{aligned} & \langle j_1'' j_2'' J'' M'', \sigma | H_{res} | j_1' j_2' J' M', \sigma \rangle \\ &= \delta_{J' J''} \delta_{M' M''} \left(2 \sqrt{(2 - \delta_{j_1' j_2'}) (2 - \delta_{j_1'' j_2''})} G_{J'}(j_1'' j_2'' j_1' j_2') + \delta_{j_1' j_1''} \delta_{j_2' j_2''} \tilde{E} \right), \end{aligned} \quad (15)$$

where the core contribution,

$$\tilde{E} = 2 \sum_{i=1}^{\sigma} \sum_{\substack{L \\ \text{even}}} (2L + 1) G_L(j^i j^i j^i j^i), \quad (16)$$

is equivalent to a scattering with angular momentum O and causes only a renormalization of the total energy. For the residual interaction matrix elements of excited states we find after a rather lengthy calculation

$$\begin{aligned} & \langle j_1'' j_2'' j_3'' j_4'' (\Lambda'' \alpha'' R'' q'') I'' m'', \sigma | H_{res} | j_1' j_2' j_3' j_4' (\Lambda' \alpha' R' q') I' m', \sigma \rangle \\ &= 2 \delta_{I' I''} \delta_{m' m''} \delta_{\Lambda' \Lambda''} \delta_{R' R''} \{ \delta_{q' q''} (T_1 + T_2 + T_3) + \delta_{\alpha' \alpha''} \delta_{j_1' j_1''} \delta_{j_2' j_2''} \delta_{j_3' j_3''} \delta_{j_4' j_4''} T_{\text{CORE}} \}, \end{aligned} \quad (17)$$

where

$$\begin{aligned} T_1 = \sum_{SL} & \left(\delta_{j_1' j_1''} \delta_{j_2' j_2''} \Delta(j_3' j_4' j_3'' j_4'') G_L(j_3'' j_4'' j_3' j_4') d_{\Lambda' \alpha'}^{SL} d_{\Lambda' \alpha''}^{SL} + (-)^{L+S+\Lambda'} \begin{Bmatrix} j_1' \leftrightarrow j_3' \\ j_2' \leftrightarrow j_4' \end{Bmatrix} \right. \\ & \times d_{\Lambda' \alpha'}^{LS} d_{\Lambda' \alpha''}^{LS} + (-)^{L+S+\Lambda'} \begin{Bmatrix} j_1'' \leftrightarrow j_3'' \\ j_2'' \leftrightarrow j_4'' \end{Bmatrix} d_{\Lambda' \alpha'}^{SL} d_{\Lambda' \alpha''}^{LS} + \left. \begin{Bmatrix} j_1' \leftrightarrow j_3' \\ j_2' \leftrightarrow j_4' \end{Bmatrix} d_{\Lambda' \alpha'}^{LS} d_{\Lambda' \alpha''}^{LS} \right), \end{aligned} \quad (18)$$

$$\begin{aligned} T_2 = & \frac{\Delta_{j_1' j_3'} \Delta_{j_2' j_4'} \Delta_{j_1'' j_3''} \Delta_{j_2'' j_4''}}{\Delta_{j_1' j_2'} \Delta_{j_3' j_4'} \Delta_{j_1'' j_2''} \Delta_{j_3'' j_4''}} \delta_{j_1' j_1''} \delta_{j_3' j_3''} \Delta(j_2' j_4' j_2'' j_4'') \\ & \times \sum_L (2L + 1) G_L(j_2'' j_4'' j_2' j_4') \sum_K (2K + 1) f_{\Lambda' \alpha'}^{KL}(j_1' j_2' j_3' j_4') f_{\Lambda' \alpha''}^{KL}(j_1'' j_2'' j_3'' j_4'') \\ & \times \left(1 + \{j_1' \leftrightarrow j_2'\} + \{j_3' \leftrightarrow j_4'\} + \begin{Bmatrix} j_1' \leftrightarrow j_2' \\ j_3' \leftrightarrow j_4' \end{Bmatrix} \right) \\ & \times \left(1 + \{j_1'' \leftrightarrow j_2''\} + \{j_3'' \leftrightarrow j_4''\} + \begin{Bmatrix} j_1'' \leftrightarrow j_2'' \\ j_3'' \leftrightarrow j_4'' \end{Bmatrix} \right), \end{aligned} \quad (19)$$

$$\begin{aligned} T_3 = & \left\{ \left(- \frac{\Delta_{j_1'' j_3''} \Delta_{j_2'' j_4''}}{\Delta_{j_1' j_2'} \Delta_{j_3' j_4'}} \delta_{j_3' j_1''} \delta_{j_4' j_3''} \Delta(j_1' j_2' j_2'' j_4'') \right. \right. \\ & \times \sum_{LS} \hat{L} \hat{S} (-)^{L+S+\Lambda'} d_{\Lambda' \alpha'}^{LS} f_{\Lambda' \alpha''}^{SL}(j_1'' j_2'' j_3'' j_4'') G_L(j_2'' j_4'' j_1' j_2') \\ & + \{j_1'' \leftrightarrow j_2''\} + \{j_3'' \leftrightarrow j_4''\} + \begin{Bmatrix} j_1'' \leftrightarrow j_2'' \\ j_3'' \leftrightarrow j_4'' \end{Bmatrix} \Bigg) \\ & \left. + (-)^{L+S+\Lambda'} \begin{Bmatrix} j_1' \leftrightarrow j_3' \\ j_2' \leftrightarrow j_4' \\ L \leftrightarrow S \text{ in } d \end{Bmatrix} \right\} + \left\{ \begin{Bmatrix} j_1' \leftrightarrow j_1'', j_2' \leftrightarrow j_2'' \\ j_3' \leftrightarrow j_3'', j_4' \leftrightarrow j_4'' \\ \alpha' \leftrightarrow \alpha'' \end{Bmatrix} \right\}. \end{aligned} \quad (20)$$

In (18), (19) and (20) we have used the notation

$$\Delta(j_1 j_2 j_3 j_4) \equiv \sqrt{(2 - \delta_{j_1 j_2})(2 - \delta_{j_3 j_4})}.$$

According to the assumption that the excitation of nucleons from the core occurs only in pairs, inside the core only scattering of nucleon pairs (j^b, j^b) is taken into consideration. The contribution of the core orbits is then given by

$$\begin{aligned} T_{\text{CORE}} = & G_{R'}(j^{q'} j^{q'} j^{q''} j^{q''}) - \delta_{q' q''} \frac{4}{2 j^{q'} + 1} \sum_{\substack{L \\ \text{even}}} \hat{L}^2 G_L(j^{q'} j^{q'} j^{q'} j^{q'}) \\ & + \delta_{q' q''} \sum_{i=1}^{\sigma} \sum_{\substack{L \\ \text{even}}} \hat{L}^2 G_L(j^i j^i j^i j^i). \end{aligned} \quad (21)$$

3. Two-level Case

To get an idea of the effect which is caused by the core-exciting part (11) of the Hamiltonian, we consider the most simple case that the configuration scheme consists of only two orbits, i.e. one orbit of spin j and energy 1.5 MeV, occupied by the outer two nucleons, and one completely filled core orbit of spin j' and energy 0.5 MeV. The two single particle states are assumed to have the same parity.

Since for every total spin only one not core-excited state exists in this two-level case, the secular matrix has a simple form and its dimension is so small that it can be diagonalized with help of the computer by standard methods.

For the normal residual interaction a surface- δ -force is assumed. Its antisymmetric coupling function can be found to be in this simple case [7]

$$G_J^{res}(j j j j) = \frac{1}{2} (1 + (-)^J) V_{0res} (2j + 1)^2 \begin{pmatrix} j & j & J \\ -1/2 & 1/2 & 0 \end{pmatrix}^2, \quad (22)$$

where

$$V_{0res} = \frac{1}{32\pi} g_{res} \mathcal{R} = \text{const.} \quad (23)$$

In (22), g_{res} is the coupling constant of the residual interaction; the radial matrix element \mathcal{R} has been considered constant.

Although it may be expected that in an actual nucleus core excitation is partially effected by the long-range part of the residual interaction and then, a quadrupole coupling function would be well adapted in this simple two level-case, we have restricted ourselves in most calculations to a surface- δ -force also for core excitation because of the spin selection rules of the quadrupole interaction, which let the coupling function vanish if the single particle spins j and j' differ by more than 2. Moreover, it will be easier to compare the coupling constants of core excitation and residual interaction, if the same coupling potential is used for both. The spin selection rules of the quadrupole interaction may be useful, however, to explain the variable effects of core excitation in actual nuclei. For a surface- δ -interaction, the core excitation coupling function is

$$G_J^{CE}(j j j' j') = \frac{1}{2} (1 + (-)^J) V_{0CE} (2j + 1) (2j' + 1) \begin{pmatrix} j & j & J \\ -1/2 & 1/2 & 0 \end{pmatrix} \begin{pmatrix} j' & j' & J \\ -1/2 & 1/2 & 0 \end{pmatrix}, \quad (24)$$

where V_{0CE} is the analogue of V_{0res} in (23). For a quadrupole interaction we get [5]

$$G_j^Q(j j j' j') = \frac{1}{2} (1 + (-)^J) V_Q (2j + 1) (2j' + 1) (-)^{j+j'} \begin{Bmatrix} j & j' & 2 \\ j' & j & J \end{Bmatrix} \begin{pmatrix} j & 2 & j' \\ 1/2 & 0 & -1/2 \end{pmatrix}, \quad (25)$$

with

$$V_Q = \frac{5}{4\pi} g_Q \mathcal{R} = \text{const.} \quad (26)$$

In Figure 2 the core excitation corrections for both surface- δ -force and quadrupole force are compared in the case of $j = 5/2$, $j' = 3/2$. It can be seen that the change of level positions is significant only for the 2^+ -state.

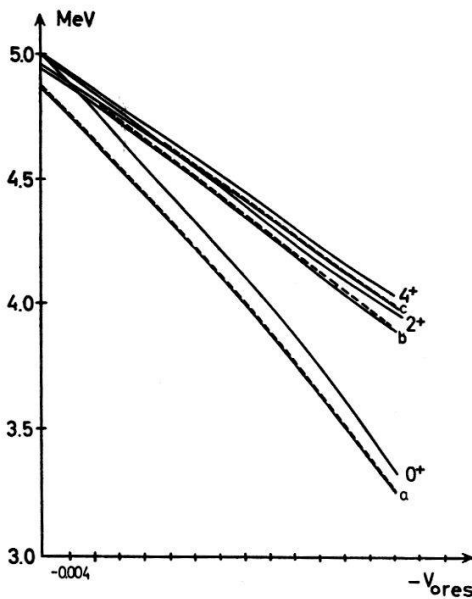


Figure 2

$j = 5/2$, $j' = 3/2$. a, b, c: quadrupole force and surface- δ -force (dashed lines) corrections for $V_{0CE} = -0.040$. Core-spin 0 and 2.

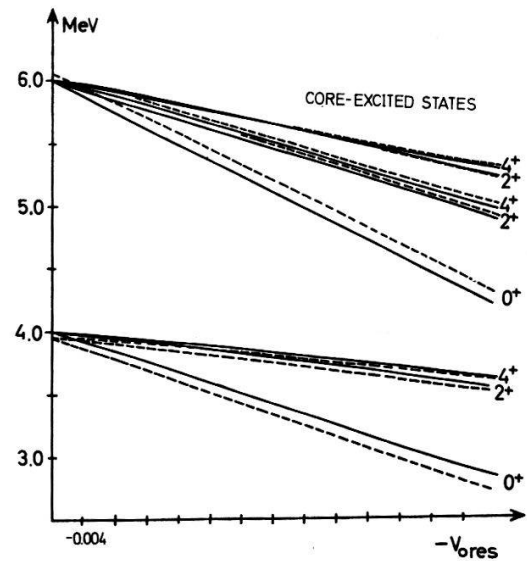


Figure 3

$j = 7/2$, $j' = 1/2$. The dashed lines show the corrections for $V_{0CE} = -0.040$.

Figure 3 shows the level scheme of both excited and not excited states for $j = 7/2$, $j' = 1/2$, in which case only core-spin-0 excitation is possible. It can be seen that a dependence of the energy levels on the residual interaction coupling constant is obtained, which is familiar from the "degenerate case" of usual shell-model calculations. The dashed lines show the corrections for core-spin-0 excitation calculated with a coupling constant $V_{0CE} = -0.040$, and it can be seen that for a residual interaction coupling constant $V_{0res} = -0.040$ (which fits good to the experimental values of the energy levels of the Pb-region), the corrections are rather small, but have the right direction even in our simple two level case.

In Figures 4 and 5 the corrections for core-spin 0 and core-spin 2 are shown separately, both for $j = 7/2$, $j' = 11/2$. It is remarkable that the core-spin-2 corrections are small compared with those for core-spin 0, at least for states of total spin 0, 2 and 4. Therefore, in the calculation of actual nuclei, it will be a good approximation to neglect the contributions from core spins higher than 2.

Secondly, the approximation made in chapter 2, namely to consider only the excitation of nucleon pairs coming from the same core orbit, seems not to be very crude, for the spins of two particles, which jump out of different core orbits, cannot be coupled to give a total spin of 0.

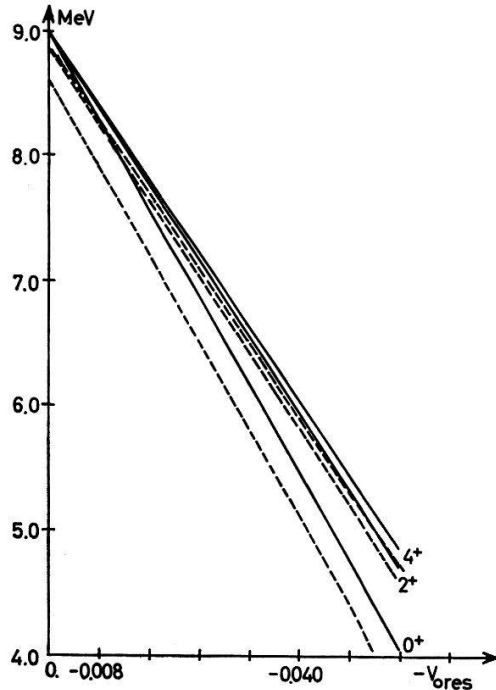


Figure 4

$j = 7/2$, $j' = 11/2$. Core-spin-0 corrections for $V_{0CE} = -0.040$. Energy renormalization (eq. 16) subtracted.

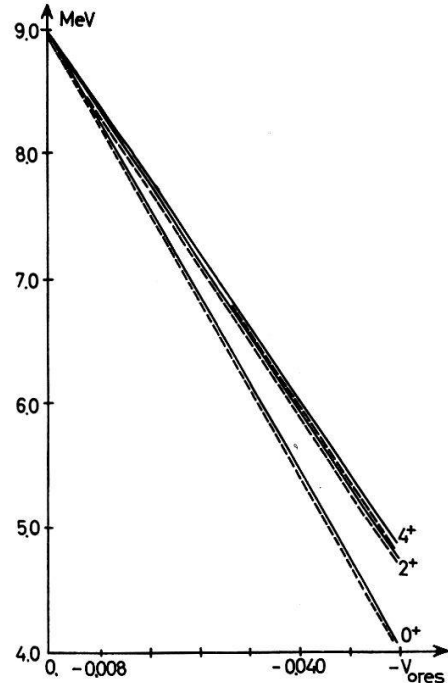


Figure 5

$j = 7/2$, $j' = 11/2$. Core-spin-2 corrections for $V_{0CE} = -0.040$. Energy renormalization (eq. 16) subtracted.

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