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Single-particle energies in enlarged shell-model spaces

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Abstract. For a standard nuclear shell-model calculation in an enlarged model-space different single-particle energies have to be used than in the original space. Here expressions are developed for the new single-particle energies and for the binding energy in the enlarged model space. The relation between the single-hole energy and the corresponding single-particle energy is given.

1. Introduction

The standard shell-model calculation is frequently used to compute energies of nuclear states and transition amplitudes of nuclear processes. A. De Shalit and I. Talmi [1] have described this method comprehensively and J. B. French et al. [2] have transformed it into a computer program usually called Oak Ridge–Rochester shell-model code which has been discussed by P. J. Brussaard and P. W. M. Glaudemans [3], too.

The model-space of a shell configuration is formed by the single-particle states (active orbits or shells) which lie out of the inert core and contribute to the basic states of the nucleus. The calculation bases on the effective two-body matrix elements describing the mutual interaction of two single-particle states. The effective interaction of one particle of an active shell with the inert core is represented by the single-particle energy. The effective two-body matrix elements and the single-particle energies are often determined empirically by regarding them as parameters. Their values are then obtained from a fit of calculated energies to experimental data on energy levels (empirical approach). [4], [5], and [6] report on successful approaches of this kind.

Large, modern computers are able to perform shell-model calculations with many active shells. However, it is advisable to start with few shells or to use old computations first. Then one enlarges the model-space of the old calculation to treat more states of the nuclei in question adequately, i.e. one introduces new shells which were empty originally or fully occupied if they were a part of the old core. By applying the empirical approach mentioned above on the extended model-space one has to adjust not only the new single-particle energies and two-body matrix-elements but the elements of the old model-space, too.

The present paper treats a commendable step suited to open this method as follows. By enlarging the model-space the old two-body matrix elements are kept unchanged and the single-particle energies are transformed in such a manner that the calculations reproduce the level energies gained in the original model-space provided that the following conditions are fulfilled

(a) new shells loosened from the core are still filled completely
(b) originally empty shells remain unoccupied.

S. T. Hsieh et al. [7] have transformed single-particle (single-hole) energies for a special case of this kind. In the present paper the transformation of single-particle energies is described more generally. Moreover, shell-model configurations with hole-states are treated. Further, the relative binding energy is calculated which relates the level energies of one model-space to the levels of the other.

2. Single-particle energies, energy scale

First, one considers a model-space with only one active shell. Its single-particle state is usually characterized with the letter ρ covering the radial quantum number, the angular momentum, the spin j_ρ, and the isospin $t_\rho = \frac{1}{2}$. n particles of this shell constitute the single-shell state $\rho^n_{JT\alpha}$ with spin J and isospin T. The quantity α stands there for the other quantum numbers of the state. The total binding energy of the nucleus in this state is called E_b (old core + $\rho^n_\alpha)_{JT}$. Next one separates a shell from the core which is named λ analogously as before. This shell is closed and contains $m=(2j_\lambda+1)\cdot 2$ particles. Within the scope of the spin–isospin formalism this number is also denoted by $2\lambda+1$. Both shells form the state $(\rho^n_\alpha\lambda^m)_{JT}$ which is coupled with the new core. The binding energy of the nucleus in this state is named E_b (new core $+\rho^n_\alpha\lambda^m)_{JT}$. Since both representations describe the same physical situation one equates their binding energies. Then either is expressed in terms of the shell-model formalism. It will be shown that both expressions formally are identical apart from two details discussed below.

Thus one states

$$E_b(\text{old core}+\rho^n_\alpha)_{JT} = E_b(\text{new core}+\rho^n_\alpha\lambda^m)_{JT} \tag{1}$$

with $m=2\lambda+1$. Both sides are rewritten by means of the shell-model formalism (see e.g. Brussaard, Glaudemans [3], equation 3.34)

$$E^o_{\text{core}}+ne^o_\rho+E(\rho^n)_{JT\alpha} = E_{\text{core}}+ne_\rho+me_\lambda+E(\rho^n_\alpha\lambda^m)_{JT} \tag{2}$$

with

E_{core} : binding energy of the particles in the core
e : single-particle energy
$E(\ldots)_{JT}$: interaction energy between the particles out of the core

The superscript o characterizes the original situation comprising the old core.

In reference [3], chapter 5, it is shown

$$E(\rho^n_\alpha\lambda^m)_{JT} = E(\rho^n)_{JT\alpha}+E(\lambda^m)_{oo}+\langle V_{\rho\lambda}\rangle \tag{3}$$

$\langle V_{\rho\lambda}\rangle$ contains only two-particle interactions between different shells. Using the normalization of the coefficients of fractional parentage and the fact that λ is a closed shell one finds

$$\langle V_{\rho\lambda}\rangle = \frac{n}{2\rho+1}\cdot\sum_\vartheta (2\vartheta+1)\cdot\langle\rho\lambda|V|\rho\lambda\rangle_\vartheta \tag{4}$$

$\langle\rho\lambda|V|\rho\lambda\rangle_\vartheta$ is a diagonal two-body matrix element for the effective interaction.

The sum runs over J_ϑ and T_ϑ which are included in ϑ. The interaction between the particles of the closed shell λ is given by

$$E(\lambda^m)_{oo} = \tfrac{1}{2} \cdot m \cdot (m-1) \cdot \sum_\delta \langle \lambda^m(oo)\{|\lambda^{m-2}, \lambda^2(\delta)\rangle \langle \lambda^2| V |\lambda^2\rangle_\delta \tag{5}$$

The coefficients of fractional parentage can be written as

$$\langle \lambda^m(oo)\{|\lambda^{m-2}, \lambda^2(\delta)\rangle = \frac{2(2\delta+1)}{m \cdot (m-1)}$$

One obtains

$$E(\lambda^m)_{oo} = \sum_\delta (2\delta+1) \cdot \langle \lambda^2|V|\lambda^2\rangle_\delta \tag{6}$$

The formulas (3), (4), and (6) are inserted in (2)

$$\begin{aligned} E^o_{\text{core}} + ne^o_\rho + E(\rho^n)_{JT\alpha} = E_{\text{core}} &+ ne_\rho + me_\lambda + E(\rho^n)_{JT\alpha} \\ &+ \sum_\delta (2\delta+1) \cdot \langle \lambda^2|V|\lambda^2\rangle_\delta \\ &+ \frac{n}{2\rho+1} \cdot \sum_\vartheta (2\vartheta+1) \cdot \langle \rho\lambda|V|\rho\lambda\rangle_\vartheta \end{aligned} \tag{7}$$

This equation is divided in two parts. One contains the arbitrary factor n and yields

$$e_\rho = e^o_\rho - \frac{1}{2\rho+1} \cdot \sum_\vartheta (2\vartheta+1) \cdot \langle \rho\lambda|V|\rho\lambda\rangle_\vartheta. \tag{8}$$

The other part is

$$E_{\text{core}} = E^o_{\text{core}} - (2\lambda+1) \cdot e_\lambda - \sum_\delta (2\delta+1) \cdot \langle \lambda^2|V|\lambda^2\rangle_\delta \tag{9}$$

These results have the following meaning. By using the single-particle energy of (8) for a calculation in the enlarged model-space one produces a level scheme which agrees energetically with the corresponding scheme of the original space except for the constant energy difference $E_{\text{core}} - E^o_{\text{core}}$ according to (9).

Now several active shells in the original model-space are considered. They are labeled with i and the states are denoted by $\rho(i)$. Their single-particle energies are named $e_{\rho(i)}$. It can be shown that (8) holds generally

$$e_{\rho(i)} = e^o_{\rho(i)} - \frac{1}{2\rho(i)+1} \cdot \sum_\vartheta (2\vartheta+1) \cdot \langle \rho(i)\lambda|V|\rho(i)\lambda\rangle_\vartheta \tag{10}$$

(9) does not change here.

In case several shells, $\lambda(1), \lambda(2), \ldots, \lambda(K)$, are separated from the core (9) and (10) can be generalized as follows

$$e_{\rho(i)} = e^o_{\rho(i)} - \frac{1}{2\rho(i)+1} \cdot \sum_{k=1}^{K} \sum_\vartheta (2\vartheta+1) \cdot \langle \rho(i)\lambda(k)|V|\rho(i)\lambda(k)\rangle_\vartheta \tag{11}$$

$$\begin{aligned} E_{\text{core}} = E^o_{\text{core}} &- \sum_{k=1}^{K} \left[(2\lambda(k)+1) \cdot e_{\lambda(k)} + \sum_\delta (2\delta+1) \cdot \langle \lambda^2(k)|V|\lambda^2(k)\rangle_\delta\right] \\ &- \sum_{\substack{l=q=1 \\ l<q}}^{K} \sum_\vartheta (2\vartheta+1) \cdot \langle \lambda(l)\lambda(q)|V|\lambda(l)\lambda(q)\rangle_\vartheta \end{aligned} \tag{12}$$

The last term in (12) describes the interaction energy between particles of different shells separated from the core.

Finally one considers a model enlarged by shells not populated in the original space. For the time being they are kept empty in the enlarged model-space. Naturally here the single-particle energies of the active shells are not to be modified so that shell-model calculations yield the same results in both model-spaces.

3. Relation between the single-particle energy e_λ and the single-hole energy $\bar{e}_\lambda$

Certain shell-model codes (e.g. [2]) are not able to treat model-spaces covering particle states and hole states simultaneously. In order to handle such problems with these codes the hole states have to be transformed into particle states by separating their shells from the core.

One considers a nucleus with one sole hole. The corresponding shell is loosened from the core by keeping the number of particles unchanged. As before, one demands that the binding energy of the nucleus is not altered. i.e.

$$E_b(\text{old core} + \lambda^{-1})_\lambda = E_b(\text{new core} + \lambda^{m-1})_\lambda \tag{13}$$

with $m = 2\lambda + 1$.

The left hand side has a simple form, the right one is expressed like in chapter 2

$$E^{\text{o}}_{\text{core}} + \bar{e}_\lambda = E_{\text{core}} + (m-1) \cdot e_\lambda + E(\lambda^{m-1})_\lambda. \tag{14}$$

It can be shown that $E(\lambda^{m-1})_\lambda = \dfrac{m-2}{m} \cdot E(\lambda^m)_{oo}$. E_{core} is replaced by (9). From (14) one obtains

$$e_\lambda = -\bar{e}_\lambda - \frac{2}{2\lambda+1} \cdot \sum_\vartheta (2\vartheta+1) \cdot \langle \lambda^2 | V | \lambda^2 \rangle_\vartheta. \tag{15}$$

(15) holds likewise if there are several holes in the shell λ and if there exist active shells in the original model-space. The single-particle energies of the active shells have to be calculated by means of (10). If several shells containing holes are separated from the core each single-particle energy is influenced by the other shells of this kind according to (11) as follows

$$e_{\lambda(i)} = -\bar{e}_{\lambda(i)} - \frac{1}{2\lambda(i)+1} \cdot \sum_{k=1}^{K} (1+\delta_{ik}) \cdot \sum_\vartheta (2\vartheta+1) \cdot \langle \lambda(i)\lambda(k) | V | \lambda(i)\lambda(k) \rangle_\vartheta \tag{16}$$

with $\delta_{ik} = 1$ for $i = k$, $\delta_{ik} = 0$ else.

Even if part of the shells $\lambda(k)$ with $k \neq i$ does not contain holes in the original space, equation (16) still holds. In order to calculate $e_{\rho(i)}$ for originally active shells through (11) all shells $\lambda(k)$ have to be put in irrespective of the existence of holes. The same holds for E_{core} in (12).

4. Discussion

I have verified the formulas (11), (12), and (16) with the Oak Ridge–Rochester shell-model code [2]. The calculations yield the same level scheme in the original as in the expanded model-space provided that the activated shells are equally occupied in both spaces as mentioned above. Both level schemes differ by the constant $E_{\text{core}} - E^{\text{o}}_{\text{core}}$ according to (12).

The results of the present paper may be applied to the following situations

(i) If one has to enlarge the model-space to treat more states adequately the first approximative shell-model calculation may be performed with the new single-particle energies according to (11).
(ii) This calculation is a good starting-point for the empirical approach mentioned in chapter 1 producing a set of fitted single-particle energies and two-body matrix elements.
(iii) The present theory may be used to procure the single-particle energy of a shell scarcely occupied and lying energetically high. One starts with a nucleus which contains only one particle in this shell and whose other shells are regarded as closed and forming a large core. The measured binding energy of the particle referred to is its single-particle energy in this simple model-space. With (11) and (12) it can be transformed to the space of the original nucleus containing a smaller core and some active shells poorly occupied.
(iv) In chapter 3 it is shown how shell-model calculations originally performed in the particle-hole representation can be reproduced with codes written only for particle representation.

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