

# Particle Number Dependence of Collective Properties of Nuclei in the Rare Earth Region \*

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Within the framework of the pairing plus quadrupole interaction model and by using the technique of quasi spin formalism it is possible to determine the collective potential and kinetic energy surfaces as analytic functions of the particle number in the limit that single particle splittings are neglected. Pushing the quasi spin model in an extended version up to the 4<sup>th</sup> order in perturbation theory the stiffness and mass parameters of harmonic and anharmonic terms for Dy, Er, Yb, and Hf-isotopes have been calculated. The theoretical particle dependence of collective quantities shows a good qualitative and even quantitative agreement with experimental data and former calculations.

## I. Introduction

During the last years there has been considerable success of the collective model in its most extended version by Gneuss and Greiner<sup>1</sup>. The ansatz for the Hamiltonian

$$H = T + V,$$

$$\begin{aligned} T = & \frac{5}{4B_2} [\pi \times \pi]^{[0]} + P_3 [\pi \times \alpha \times \pi]^{[0]} \\ & + \sum_j P_4^j ([\pi \times \pi]^{[j]} \times [\alpha \times \alpha]^{[j]})^{[0]} \\ & + [[\alpha \times \alpha]^{[j]} \times [\pi \times \pi]^{[j]})^{[0]} \\ & + \bar{P}_4 [[\pi \times \pi]^{[0]} \times [\pi \times \pi]^{[0]}] + \\ & + \text{higher order terms,} \\ V = & C_2 [\alpha \times \alpha]^{[0]} + C_3 [\alpha \times \alpha \times \alpha]^{[0]} \\ & + C_4 [[\alpha \times \alpha]^{[0]} \times [\alpha \times \alpha]^{[0]}] \\ & + \text{higher order terms} \end{aligned} \quad (1)$$

is dictated by principles of rotational and time invariance. It is ambiguous as far as one does not know where to stop with higher order terms. The answer is given practically by truncating the power series arbitrarily and fitting mass and stiffness parameters to energy spectra and transition probabilities. Up to now, most calculations stopped with the third or even second power in the kinetic surface and with the sixth power in the potential surface.

It is not clear whether this procedure is unique if one takes higher order terms into account and it is an open question how far the influence of kinetic terms can be simulated by potential terms and vice

versa. Moreover, it is a lengthy and difficult job to determine particle number dependences of potential and kinetic surfaces by means of the fitting procedure.

The great success of the collective model in reproducing spectra and transition probabilities justifies a microscopic approach to a solution of these questions. In this paper we attack the calculation of collective quantities in their dependence on particle number. Kerman<sup>2</sup> and later Greiner<sup>3</sup> have shown that one can determine explicitly the particle number dependence by treating the pairing plus quadrupole interaction in the quasi spin model. In Sect. II we give a short summary of the main ideas of the quasi spin model and show how all mass and stiffness parameters up to the 4<sup>th</sup> power occurring in Eq. (1) can be calculated. For the application of the model to practical cases some extensions have to be done. The quasi spin model has to be applied simultaneously for protons and neutrons and a contribution to the collective potential energy coming from the core and the Coulomb interaction has to be included. This is discussed in Section, III. Groundstate deformations, deformation energies, mass parameters and E(2<sup>+</sup>)-energies are calculated for several isotope sequences and compared with former calculations and experiments.

## II. The Quasi Spin Model

The quasi spin model<sup>2,3</sup> is based on three idealizations of the atomic nucleus:

1. There exists only one large *j*-shell above a closed spherical core.

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2. The interaction of particles from the  $j$ -shell with the core is negligible.
3. Only a pairing and quadrupole-quadrupole force is acting between the particles in the  $j$ -shell.

Though statements 1 and 2 are very severe idealizations, they are consistent with the schematic type of force used and lead to a simple Hamiltonian

$$H = H_S + H_{QQ}. \quad (2)$$

The seniority part  $H_S$  is given by

$$H_S = -G \sum_{\substack{m>0 \\ m'>0}} (-)^{2j+m+m'} a_{jm}^+ a_{j-m}^+ a_{j-m'} a_{jm'} \quad (3)$$

where the  $a_{jm}^+$  denote creation operators for a state with magnetic quantum number  $m$  in the  $j$ -shell ( $j$  will be omitted for convenience from now on). Instead of the quadrupole-quadrupole interaction

$$H_{QQ} = -\frac{1}{2} \kappa \sum_{\mu} Q_{\mu}^+ Q_{\mu} \quad (4)$$

we shall actually use the well deformed seniority operator  $H_{DS}$  [Equation (12)].

The pairing Hamiltonian can be written in the form

$$H_S = -G S_+ S_- \quad (5)$$

where  $S_+$  and  $S_-$  are the components of a vector

$$\mathbf{S} = \{S_+, S_-, S_0\} = \sum_{m>0} \{S_+^m, S_-^m, S_0^m\} \quad (6)$$

and  $S_+^m, S_-^m, S_0^m$  are defined by

$$S_+^m = (-)^{j+m} a_m^+ a_{-m}^+, \quad S_-^m = (S_+^m)^+, \quad S_0^m = \frac{1}{2} (a_m^+ a_m + a_{-m}^+ a_{-m} - 1). \quad (7)$$

The components of the so-called quasi spin  $\mathbf{S}$  obey the usual angular momentum commutator properties. Eigenstates of the square of the quasi spin and its projection to the  $z$ -axis are denoted by  $|S S_0\rangle$ . Now  $H_S$  can be expressed in the form

$$H_S = -G \{(\mathbf{S} \cdot \mathbf{S}) - S_0^2 + S_0\} \quad (8)$$

and is therefore diagonal in the states  $|S S_0\rangle$ . The projection  $S_0$  of quasi spin may be written in terms of the particle number  $N$  and the number of pos-

sible pairs  $\Omega = (2j+1)/2$  in the single  $j$ -shell

$$S_0 = \frac{1}{2} (N - \Omega). \quad (9)$$

Then the eigenvalues of  $H_S$  take the form

$$E(S) = -G \left\{ S(S+1) - \left( \frac{N-\Omega}{2} \right)^2 + \left( \frac{N-\Omega}{2} \right) \right\}. \quad (10)$$

Instead of the quasi spin  $S$  the seniority quantum number  $v$  is often used, where

$$S = \frac{1}{2} (\Omega - v). \quad (11)$$

Usually the pairing plus quadrupole Hamiltonian of Eq. (2) is substituted by the well deformed seniority operator<sup>4</sup>

$$H_{DS} = H_S - \kappa g \sum_{\mu} \alpha_{\mu}^+ Q_{\mu} \quad (12)$$

in which a collective deformation parameter  $\alpha_{\mu}$  is introduced and  $g$  is a constant with the dimension of a quadrupole moment. The eigenstates and energies of  $H_{DS}$ ,

$$H_{DS}(\alpha_{\mu}) \chi_n(\alpha_{\mu}) = \varepsilon_n(\alpha_{\mu}) \chi_n(\alpha_{\mu}), \quad (13)$$

will be determined by perturbation theory in the basis of quasi spin eigenfunctions with the perturbation term  $-\kappa g \sum_{\mu} \alpha_{\mu}^+ Q_{\mu}$  through 4<sup>th</sup> order. Then in a second step we get an eigenvalue problem containing the steady state classical parameters  $\alpha_{\mu}$  and their time derivatives  $\dot{\alpha}_{\mu}$

$$H'_{DS}(\dot{\alpha}_{\mu}, \alpha_{\mu}) \Psi(\dot{\alpha}_{\mu}, \alpha_{\mu}) = \varepsilon'(\dot{\alpha}_{\mu}, \alpha_{\mu}) \Psi(\dot{\alpha}_{\mu}, \alpha_{\mu}) \quad (14)$$

where

$$H'_{DS} = H_{DS} - i \hbar \sum_{\mu} \dot{\alpha}_{\mu} (\partial / \partial \alpha_{\mu}). \quad (15)$$

As usual the cranking problem is treated in the basis of eigenfunctions of  $H_{DS}$  (see Reference<sup>5</sup>).

The groundstate expectation value  $\varepsilon'(\dot{\alpha}_{\mu}, \alpha_{\mu})$  is identified with the collective potential and kinetic energy surface whose form is predetermined by rotational and time invariance. Taking historical notations we have

$$\begin{aligned} \varepsilon'(\dot{\alpha}_{\mu}, \alpha_{\mu}) = & \varepsilon(0) + \sqrt{5} B [\dot{\alpha} \times \dot{\alpha}]^{[0]} + B' [\dot{\alpha} \times \alpha \times \dot{\alpha}]^{[0]} \\ & + B'' [\alpha \times \alpha]^{[0]} [\dot{\alpha} \times \dot{\alpha}]^{[0]} - 5 \bar{B} [\dot{\alpha} \times \dot{\alpha}]^{[0]} [\dot{\alpha} \times \dot{\alpha}]^{[0]} \\ & - \frac{\sqrt{5}}{2} C [\alpha \times \alpha]^{[0]} - \frac{1}{3} D [\alpha \times \alpha \times \alpha]^{[0]} + \frac{5}{4} F [\alpha \times \alpha]^{[0]} [\alpha \times \alpha]^{[0]}. \end{aligned} \quad (16)$$

The coefficients are obtained by perturbation theory in the basis of quasi spin eigenfunctions as described above

$$C = (\kappa g)^2 2 \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2}{E(S-1) - E(S)}, \quad (17 a)$$

$$D = -(\kappa g)^3 3 \sqrt{\frac{2}{35}} \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2 \langle S-1 S_0 | Q_0 | S-1 S_0 \rangle}{[E(S-1) - E(S)]^2}, \quad (17 b)$$

$$F = (\kappa g)^4 4 \left\{ \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2}{[E(S-1) - E(S)]^2} \left[ \frac{|\langle S-1 S_0 | Q_0 | S-1 S_0 \rangle|^2}{E(S-1) - E(S)} + \frac{|\langle S-1 S_0 | Q_0 | S-2 S_0 \rangle|^2}{E(S-2) - E(S)} - \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2}{E(S-1) - E(S)} \right] \right\}, \quad (17 c)$$

$$B = 2 \hbar^2 (\kappa g)^2 \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2}{[E(S-1) - E(S)]^3}, \quad (18 a)$$

$$B' = 4 \sqrt{\frac{35}{2}} \hbar^2 (\kappa g)^3 \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2}{[E(S-1) - E(S)]^4} \langle S-1 S_0 | Q_0 | S-1 S_0 \rangle, \quad (18 b)$$

$$B'' = 2 \hbar^2 (\kappa g)^4 \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2}{[E(S-1) - E(S)]^4} \left[ \frac{|\langle S-1 S_0 | Q_0 | S-1 S_0 \rangle|^2}{E(S-1) - E(S)} + 2 \frac{|\langle S-1 S_0 | Q_0 | S-2 S_0 \rangle|^2}{E(S-2) - E(S)} - 2 \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2}{E(S-1) - E(S)} \right], \quad (18 c)$$

$$\bar{B} = \hbar^4 (\kappa g)^4 \left\{ \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2}{[E(S-1) - E(S)]^6} \left[ \frac{|\langle S-1 S_0 | Q_0 | S-1 S_0 \rangle|^2}{E(S-1) - E(S)} - \frac{|\langle S-1 S_0 | Q_0 | S-2 S_0 \rangle|^2}{E(S-2) - E(S)} + \frac{|\langle S S_0 | Q_0 | S-1 S_0 \rangle|^2}{E(S-1) - E(S)} \right] \right\}. \quad (18 d)$$

In these relations only the component  $Q_0$  enters since the expansion (16) is a unique one. Furthermore there exist terms with parameters  $B''^{[J]}$  belonging to intermediate angular momenta  $J$  similar to the term with  $B''$  in (16).

Now the particle dependence of the matrix elements can be extracted by repeated use of Wigner-Eckart Theorem in quasi spin space

$$\langle S S_0 | Q_0 | S-1 S_0 \rangle = \sqrt{\frac{N(2\Omega - N)}{2(2\Omega - 2)}} \cdot \left\langle S \frac{2-\Omega}{2} \middle| Q_0 \middle| S-1 \frac{2-\Omega}{2} \right\rangle \quad (19 a)$$

$$\langle S-1 S_0 | Q_0 | S-1 S_0 \rangle = \frac{N-\Omega}{2-\Omega} \cdot \left\langle S-1 \frac{2-\Omega}{2} \middle| Q_0 \middle| S-1 \frac{2-\Omega}{2} \right\rangle \quad (19 b)$$

$$\langle S-1 S_0 | Q_0 | S-2 S_0 \rangle = \sqrt{\frac{(2\Omega - N - 2)(N-2)}{2(2\Omega - 6)}} \cdot \left\langle S-1 \frac{4-\Omega}{2} \middle| Q_0 \middle| S-2 \frac{4-\Omega}{2} \right\rangle. \quad (19 c)$$

In these formulas  $S$  is the quasi spin of the ground-state of even-even nuclei, namely  $S = \Omega/2$ . We are left with matrix-elements belonging to particle number 2 and 4 which can be calculated only in configuration space using many-particle functions with good angular momentum and seniority. This was done in the case of matrix elements for particle number 2. Matrix elements for particle number 4 were calculated with states which had not been projected to good seniority states. This gives a fairly good estimation of their value and is sufficient since the present model does not justify extensive configuration space calculations. The four particle matrix element was adjusted in the near of its estimated value to one nucleus (it is the same for all nuclei of the treated isotope sequences).

### III. Extensions of the Quasi Spin Model

To obtain a more realistic model some extensions of the quasi spin model have to be done. This can be easily achieved by three more assumptions in addition to those state in Sect. II:

4. The quasi spin model is simultaneously applied to a  $j$ -shell filled up with neutrons and a  $j'$ -shell which accommodates protons.
5. Assumptions 2. and 3. in Sect. II are separately fulfilled by the neutron and the proton shell.
6. Like in most BCS-calculations interactions between neutrons and protons are neglected.

To get more realistic potential energy surfaces we include contributions from the core and from Coulomb energy. In selfexplaining notation we then have

$$H_{np} = H_{\text{core}} + H_{\text{DS}}^{(n)} + H_{\text{DS}}^{(p)} + H_{\text{coul}} \quad (20)$$

For the calculation in the region of rare earth isotopes a  $Z=50$ ,  $N=82$  core has to be taken into account. The potential energy surface for the (50, 82)-core was calculated by Mosel<sup>6</sup> and can be very well approximated by a harmonic oscillator  $H_{\text{core}} = C_{\text{core}} \alpha_0^2$  with  $C_{\text{core}} = 90$  [MeV]. Because of this strong spherical contribution the potential energy surface is pushed to smaller values of deformation and the deformation energy is decreased. This influence is shown in Figure 1.

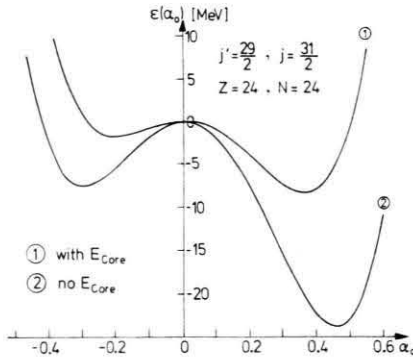


Fig. 1. The influence of core contributions on the potential energy surface.

The Coulomb energy can be treated as a function of proton and neutron number of the core and the outer shells and as a function of the collective coordinates<sup>6</sup>

$$H_{\text{coul}}(\alpha_0) = 0.7242 \frac{(Z_{\text{core}} + Z)^2}{(Z_{\text{core}} + Z + N_{\text{core}} + N)^{1/2}} \cdot \left[ 1 - \frac{1}{4\pi} \alpha_0^2 + \frac{19}{1680} \left( \frac{5}{\pi} \right)^{3/2} \alpha_0^3 - \frac{39}{8960} \left( \frac{5}{\pi} \right)^2 \alpha_0^4 + \dots \right] \quad (21)$$

Its influence increases the groundstate deformation and the deformation energy as can be seen from Figure 2.

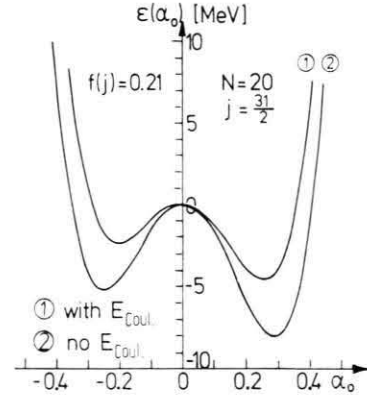


Fig. 2. The influence of Coulomb energy on the potential energy surface.

Naively one is tempted to associate the values  $j$  and  $j'$  for the single shells with the realistic outer shells in the considered isotope sequences. But it was already stated in Ref.<sup>3</sup> that deformations start to built up only for  $j > 19/2$  in the middle of the shells. From this it is clear that we need large  $j$ -values to describe the strongly deformed rare earths and that there is no connection with the  $j$ -value of subshells occurring outside the core. On the other hand, one could be tempted to identify  $j$  and  $j'$  with  $43/2$  and  $31/2$  such that the shells can accommodate the 44 neutrons between neutron numbers 82 and 126 and the 32 protons between 50 and 82. Doing so most of the rare earth nuclei fall into the first half of the shells with  $N < \Omega$  which generate only oblate nuclei whereas in nature the prolate ones dominate.

We can overcome this shortcoming of the quasi spin model by assuming that there are already some core nucleons in the single shells when we start filling up with outer nucleons. This is justified by the fact that the outer shells polarize the core and consequently their single particle levels start crossing with levels from the core. The number of core nucleons occupying places in the outer shells as well as the values of  $j$  and  $j'$  are arbitrary within certain limits. The results presented below could be also obtained with other  $j$  and  $j'$ -values but consequently different numbers of core nucleons in the  $j$ -shells. These values serve only to fix the basis we are working in. The calculation for all isotope se-

quences were done with  $j' = 29/2$  for the proton shell and  $j = 31/2$  for the neutron shell. We assumed six core protons and two core neutrons in the outer shells. The four particle matrix element of Eq. (19c) was estimated as described above. Using the reduced single particle matrix element  $q_{00}$  of the quadrupole operator we split up in the following form

$$\left\langle S-1 \frac{4-\Omega}{2} \left| Q_0 \right| S-2 \frac{4-\Omega}{2} \right\rangle = f(j) q_{(j)}. \quad (22)$$

Then  $f(j)$  has a value of approximately 0.22 for  $j$  around  $31/2$ . We assumed  $f(j) = f(j') = 0.22$ . In formulas (17) and (18) the quantity  $P = \kappa \cdot g \cdot q$  for protons and neutrons enters. They were fitted to reproduce the potential energy surface of one Yb-isotope calculated by Mosel<sup>6</sup> within the Nilsson model. This gives values  $P_n = 56$  MeV and  $P_p = 37$  MeV.

With these parameters fixed we calculated the potential and kinetic energy surfaces of the Dy, Er, Yb and Hf-isotopes. Figure 3 gives a general view of the potential energy surfaces and their dependence on particle number. From here we can extract important collective quantities like groundstate deformations and deformation energies. Groundstate deformations were transformed to quadrupole moments using<sup>5</sup>

$$Q_0 \sim \frac{3}{4} \frac{A R_0^2}{\pi} \beta_0 \quad (23)$$

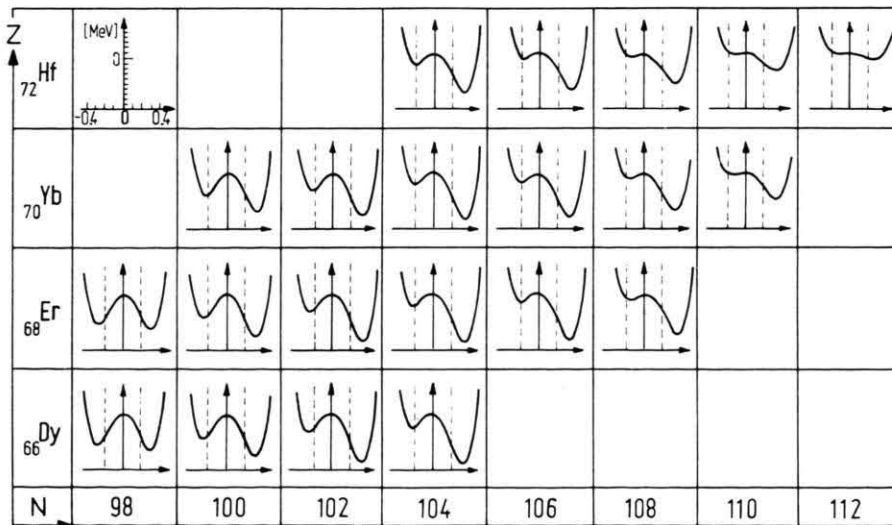


Fig. 3. Particle number dependence of the potential energy surface. The dotted lines mark points of deformation  $\pm 0.2$ .

and are compared with experimental values in Figure 4. The magnitude as well as the overall trend is very well reproduced. Finally we compare the deformation energies of the calculated isotope se-

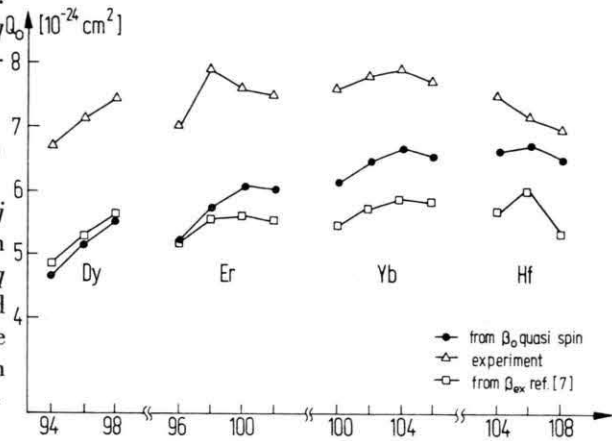


Fig. 4. Comparison of quadrupole moments calculated with the extended quasi spin model and from experiment.

quences with the semi-empirical analysis of Myers and Swiatecki<sup>8</sup> and the calculations of Sobiczewski<sup>9</sup> in Figure 5. Again there is a strikingly good agreement with them.

With respect to the kinetic energy surface one is not able to extract quantities which have such an obvious meaning like groundstate deformations or deformation energies. In Fig. 6 we show mass parameters calculated only with one  $j$ -shell. It is impos-



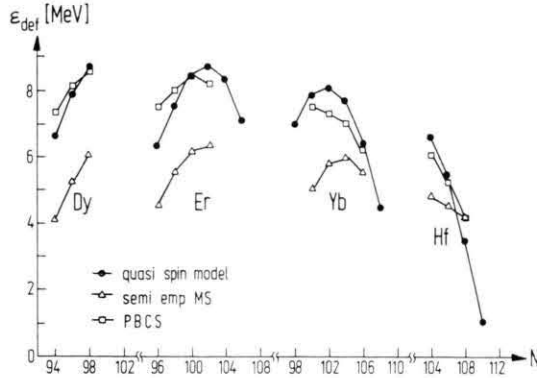


Fig. 5. Comparison of deformation energies with values from Myers and Swiatecki<sup>8</sup> and calculations of Sobczewski<sup>9</sup>.

sible to compare them with quantities which can directly be related to experiments. In the middle of the shell  $B/\hbar^2$  is about  $40 \text{ MeV}^{-1}$  and  $B'$  vanishes. Leaving the middle of the shell  $B$  decreases and  $B'$  increases. This is in agreement with observations in the dynamical model where  $B$  has to be reduced as soon as  $B'$  is turned on<sup>1, 10</sup>. The authors of Ref. <sup>10</sup> use a value of  $B/\hbar^2 = 60 \text{ MeV}^{-1}$ .

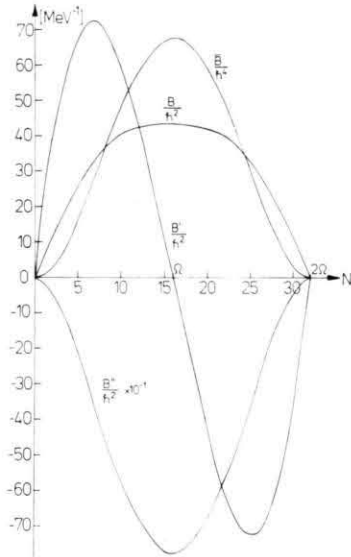


Fig. 6. Mass parameters in the simple quasi spin model.

The very interesting parameter  $\bar{B}$  of the  $\alpha^4$ -term has been used very seldom. Reference <sup>11</sup> contains an intensive study of its effect on the collective energy spectra. Turning on this parameter the whole energy spectrum spreads and a slow reordering of the levels occurs. The effect is similar to the influence of  $B$  on energy spectra. In order to get a realistic

energy of the first  $2^+$ -level in deformed nuclei the value of  $B/\hbar^4$  must be smaller than  $100 \text{ MeV}^{-1}$ . Our values are in agreement with this upper limit.

With the mass parameters  $B$  and groundstate deformations of the extended quasi spin model we estimated moments of inertia by  $I = 3B\beta_0^2$  and from this  $E(2^+)$ -energies. Of course, we cannot expect to get the right order of magnitude using only mass parameter  $B$ . At the average the  $E(2^+)$ -energies turned out to be 2.3 times too large. Adjusted by a factor 0.44 they are compared with experimental values in Figure 7. The trend of the variation with neutron number is very well reproduced.

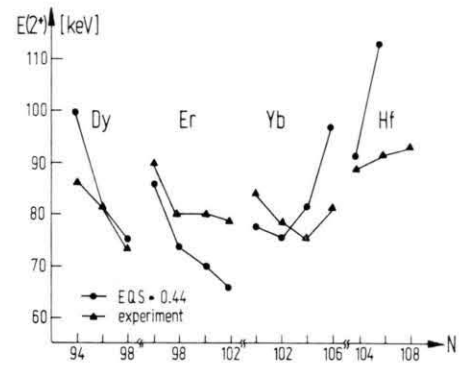


Fig. 7. Comparison of the  $E(2^+)$ -energies in the extended quasi spin model adjusted by a factor 0.44 with experimental values.

#### IV. Conclusions

We have extended the schematic quasi spin model to include both protons and neutrons. Taking into account a contribution from the core and the Coulomb energy and assuming that some core nucleons occupy places in the outer shells it is possible to describe collective properties of four rare earth isotope sequences with one set of parameters. The extended quasi spin model yields explicitly the correct particle number dependence for different collective quantities of interest like groundstate deformations, deformation energies and  $E(2^+)$ -energies. Therefore the particle number dependence of mass and stiffness parameters can be used as a guideline in the time-consuming search for best parameters in the dynamical model. The mass parameter of the  $\alpha^4$ -term turns out to be of a magnitude where this term has similar influence on collective energy spectra like the  $\alpha^2$ -term. Therefore it seems to be justified that the  $\alpha^4$ -term is usually dropped.

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