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A. Sobiczewski

EQUILIBRIUM DEFORMATIONS CALCULATED WITH PROJECTED WAVE FUNCTIONS FOR RARE EARTH NUCLEI

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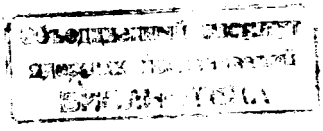

[x] Institute for Nuclear Research, Warsaw, Poland.

1. Introduction

The first microscopic calculation of the equilibrium deformation of nuclei, based on the Nilsson model[1] was performed by Mottelson and Nilsson[2]. They calculated the energy of a nucleus for a given deformation by summing up the Nilsson single-particle energies corresponding to this deformation. For every configuration the dependence of the energy on the deformation was obtained and the point of minimal energy was considered the equilibrium deformation of the configuration.

Marshalek, Person and Sheline[3] have extended the calculations to a wide region of nuclei, predicting some new regions of deformed nuclei.

In all these calculations the pairing correlations which were found to be very important, for example, for moments of inertia[4], have not been taken into account. The explicit Coulomb term has also been dropped. However, the single-particle energy levels used, were different for neutrons and protons and fitted to experimental odd nuclei data. The theoretical estimations by Belyaev[5] indicated that the pairing correlations might be important for equilibrium deformations, especially at the boundaries of the deformation regions.

Detailed calculations taking the pairing forces into account and including the explicit Coulomb term have been performed by Bès and Szymański[6] and Szymański[7] for even nuclei and by Hassan, Skladanowski and Szymański[8] for odd nuclei.

The Hamiltonian used by Bès and Szymański has the form

$$H = H_{qp} + H_{pair} = \sum_{\nu} \epsilon_{\nu} (c^{+}_{\nu+} c_{\nu+} + c^{+}_{\nu-} c_{\nu-}) - G \sum_{\nu,\omega} c^{+}_{\nu+} c^{+}_{\nu-} c_{\omega-} c_{\omega+} \qquad (1)$$

for neutrons and for protons separately.

Here ϵ_ν is the energy of a twofold degenerate single-particle Nilsson state $|\nu>$, c_ν^+ is the corresponding creation operator and G is the pairing force strength.

The minimization of the mean value of the Hamiltonian (1) in the BCS ground state[9] under the condition that the mean value of the number of particles in this state is given, leads to the expression for the energy

$$\mathcal{E} = \sum_\nu \epsilon_\nu 2v_\nu^2 - \Delta^2/G \quad , \tag{2}$$

where

$$2v_\nu^2 = 1 - (\epsilon_\nu - \lambda)/E_\nu \tag{2a}$$

with

$$E_\nu = \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2} \quad .$$

The chemical potential λ and the energy gap 2Δ are obtained from the equations

$$\begin{aligned} 2/G &= \sum_\nu 1/E_\nu \\ n &= \sum_\nu 2v_\nu^2 \end{aligned} \tag{3}$$

where n is the number of particles (neutrons or protons) in the nucleus.

After the inclusion of the Coulomb term $\mathcal{E}_C$, the expression for the energy of the nucleus is

$$\mathcal{E} = \mathcal{E}_n + \mathcal{E}_p + \mathcal{E}_C \quad , \tag{4}$$

where $\mathcal{E}_n$ and $\mathcal{E}_p$ are given by eq. (2) and correspond to neutrons and protons, respectively. The Coulomb term is assumed to be equal to the electrostatic energy of a charged ellipsoid. Its dependence on the deformation $\bar{\epsilon}$ of the ellipsoid is given, up the third order in $\bar{\epsilon}$, by[10]

$$\mathcal{E}_C(\bar{\epsilon}) = (1 - \frac{4}{45}\bar{\epsilon}^2 - \frac{92}{2835}\bar{\epsilon}^3)\mathcal{E}_C(0). \tag{5}$$

Here $\mathcal{E}_C(0)$ is the Coulomb energy of the sphere with a spherically symmetric charge distribution. The trapezoidal form of the radial charge density distribution has been accepted, taking the parameters from electron scattering data[11].

The deformation parameter $\bar{\epsilon}$ of the charge density of a nucleus is obtained from the quadrupole moment Q_0, calculated for a given deformation of the single-particle potential. The relation is

$$Q_0(\epsilon) = \bar{\epsilon}(1 + \tfrac{1}{2}\bar{\epsilon})\,\frac{4}{5} Z \int \rho(r') r'^2 \, d\vec{r}' \qquad (6)$$

with

$$Q_0(\epsilon) = \sum_{\nu\,(\text{protons})} q_{\nu\nu}(\epsilon) 2v_\nu^2(\epsilon) \,, \qquad (7)$$

where $\rho(r')$ is the charge density and $q_{\nu\nu}$ is the matrix element of the quadrupole moment operator in the single-particle state $|\nu>$. The integral over the sphere in eq. (6) has been calculated with the same trapezoidal charge distributions as taken in the calculation of the energy $\delta_C^{(0)}$ in eq. (5).

The calculation by Bès and Szymański has showed a rather good consistency between the potential deformation and the density one i.e. $\epsilon = \bar{\epsilon}$. The calculated quadrupole moments are in good agreement with experiments in the middle of the deformation region and show some discrepancies at the boundaries of the region.

It has been suggested [7] that these discrepancies might be connected with the use of BCS wave functions which were not eigenfunctions of the particle number operator and that the use of projected wave functions might improve the results.

The effect of projecting the BCS wave functions on the space of the particle number operator eigenfunctions has been investigated by a number of authors [12-23]. In particular some of them have compared the BCS wave functions and the projected ones with the exact solutions of the Hamiltonian (1), for simple systems. The projected wave functions (PBCS in the nomenclature of ref. [23]) were obtained by projecting fixed-particle terms from the BCS functions. Pawlikowski and Rybarska [14] have studied the system of $n = 6$ particles located on the $\Omega = 5$ equidistant, twofold degenerate levels. The system imitated the situation in a deformed nucleus. It has been shown that the PBCS ground state energy was much closer to the exact energy than the BCS one. The improvement was the better, the stronger was the pairing force. For example, in the case of the weakest pairing forces considered in ref. [14]; $G = 0.5\,\Delta\epsilon$ ($\Delta\epsilon$ was the distance between the levels) the error of the PBCS ground state energy amounted to 17% of the error of the BCS energy. For $G = \Delta\epsilon$ it reduced to 1.8% of the BCS error.

Similar results have been obtained by Rho and Rasmussen [22] for the system of $\Omega = 6$ equidistant twofold degenerate levels with $n = 6$ particles. They have shown that with the pairing force strength G tending to its critical value, at which the nontrivial solution in the BCS approximation disappears, the PBCS and BCS ground state energy errors tend to the same limit, the PBCS error being always lower than the BCS one.

In all the calculations of the equilibrium deformation, quoted above [2,3,6-8] axial symmetry of the nuclei has been assumed. Thus, only the dependence of the energy on the ϵ deformation has been studied. The analysis by Das Gupta and Preston [24] of the γ - deformation dependence of the energy has revealed that the assumption of the axial symmetry was well founded, possible except for the nuclei in the neighbourhood of the Os isotopes, which appear to be quite soft with respect to the γ-deformation [25]. The same results have been obtained in the calculations based on the pairing-plus-quadrupole forces model [26].

The aim of the present investigation is to calculate the ground state equilibrium deformations and deformation energies, for the axially symmetric even nuclei, using the PBCS wave functions instead of the BCS ones.

2. Description of the Calculation

We choose the part of the BCS function corresponding to a definite number of particles as the ground state wave function. After the normalization it is of the form [17,23]

$$|\mathrm{PBCS}\rangle = \beta_1^+ \ldots \beta_\ell^+ N \sum_{\nu_1<\nu_2<\ldots<\nu_k} \gamma_{\nu_1} \ldots \gamma_{\nu_k} \beta_{\nu_1}^+ \ldots \beta_{\nu_k}^+ |\mathrm{vac}\rangle , \qquad (8)$$

where $\gamma_\nu = v_\nu / u_\nu$, $\beta_\nu^+ = c_{\nu+}^+ c_{\nu-}^+$ and the normalization factor

$$N = \Big(\sum_{\nu_1<\nu_2<\ldots<\nu_k} \gamma_{\nu_1}^2 \ldots \gamma_{\nu_k}^2 \Big)^{-1/2} .$$

The indices $i = 1 \ldots l$ enumerate the levels for which $v_i = 1$, while the indices $\nu_i > \ell$ correspond to the levels for which $0 < v_{\nu_i} < 1$ i.e. the levels between which the scattering of particles, due to the pairing forces, takes place. We have the equality $2(\ell + k) = n$, where n is the number of particles (neutrons or protons). The summation extends over all the combinations of k states (ordered with respect to the energy) chosen from the states for which $0 < v_{\nu_i} < 1$. The symbol $|\mathrm{vac}\rangle$ denotes the vacuum for the particles described by the creation operators $c_{\nu_i}^+$ or c_i^+ .

The occupation factors v_ν^2 ($u_\nu^2 = 1 - v_\nu^2$) obtained from the formulae (2a) and (3) correspond to the minimization of the energy in the BCS state.

One could obtain a better wave function minimizing the energy already in the projected state. The wave function obtained in such a manner (FBCS in the nomenclature of ref.[23]) has been studied by Mang et al. in their calculations for heavy elements[23]. They have shown that for the system of $Z = 96$ protons and the system $N = 152$ neutrons the error of the PBCS ground state energy (calculated with respect to FBCS energy) amounts to 13% and 25% of the BCS error, respectively. The numbers $Z = 96$ and $N = 152$ are just the cases of the maximal BCS error, in connection with a decrease in the density of the Nilsson levels (and consequently with the lowest pairing effect) for these numbers of particles at the deformation $\eta = 5$ used. For larger level densities ($Z = 88, 90$; $N = 132, 134, 136$) the PBCS error reduces to about 8% of the BCS one.

The results of Mang et al. correspond to the picture obtained in the calculations for simple systems[14,22], where the PBCS ground state energy is much better than the BCS one.

Moreover, the difference between the PBCS and FBCS energies appears to be quite small.

For the energy in the state (8) we obtain

$$\mathcal{E} = \sum_{i=1}^{i=\ell} 2\varepsilon_i + N^2 \Big\{ \sum_{\nu_1<\nu_2<\ldots<\nu_k} 2(\varepsilon_{\nu_1} + \ldots + \varepsilon_{\nu_k}) \gamma_{\nu_1}^2 \ldots \gamma_{\nu_k}^2 - \tag{9}$$

$$- G \sum_{\sigma_1,\sigma_2} \gamma_{\sigma_1} \gamma_{\sigma_2} \sum_{\nu_1<\nu_2<\ldots<\nu_k \neq \sigma_1,\sigma_2} \gamma_{\nu_1}^2 \ldots \gamma_{\nu_k}^2 \Big\}$$

and for the quadrupole moment

$$Q = \sum_{i=1}^{i=\ell} 2q_{ii} + N^2 \sum_{\nu_1<\nu_2<\ldots<\nu_k} 2(q_{\nu_1\nu_1} + \ldots + q_{\nu_k\nu_k}) \gamma_{\nu_1}^2 \ldots \gamma_{\nu_k}^2 . \tag{10}$$

To obtain the pure effect of using the PBCS wave functions instead of the BCS ones, we perform all the calculations in full analogy with those of Bès and Szymański[6]. We use only the formula (9) instead of (2) for the expressions $\mathcal{E}_n$ and $\mathcal{E}_p$ in eq. (4), and the formula (10) (with the summation extended over protons) instead of (7) for the quadrupole moment. All the values of the parameters are taken the same as in the variant (III + VI) of ref.[6] which gave there the best agreement with experiment.

3. Results and Discussion

As an example the dependence of the energy on the deformation is presented in Fig.1 for Gd^{158}. The independent particle curve (IP) has been obtained by summing up the energies of the twofold degenerate Nilsson levels from the lowest one to the Fermi level, just as in refs.[2,3]. No Coulomb term has been included. The comparison of the PBCS and BCS curves shows that the dependence of the PBCS energy on the deformation does not differ much from that of the BCS energy, although the PBCS energy itself is lowered significantly with respect to the BCS energy (just this lowering of the ground state energy was the significant improvement obtained by taking the PBCS wave function insted of the BCS one in the calculations for simple systems[14,22]).

Comparing the IP curve with the PBCS and BCS ones, one can see that the inclusion of pairing forces decreases the equilibrium deformation slightly (from 0.31 to 0.29) and that the inclusion of pairing forces together with the Coulomb term increases it (from 0.31 to 0.34 for BCS).

The dependence on the deformation of the ground state energy change due only to the pairing forces ($\Delta\mathcal{E}_{NC}$) and to the pairing forces together with the Coulomb term ($\Delta\mathcal{E}_{C}$) is presented in fig. 2. It is seen that the tendencies to change the deformation in the opposite directions by pairing forces on one hand and the Coulomb term on the other, approximately compensate each other in a rather wide region of deformation (from $\epsilon \approx 0.15$ to $\epsilon \approx 0.30$ for Gd^{158}). However, at the equilibrium deformation obtained in the independent particle case, the tendency of increasing the deformation by Coulomb term already predominates over the tendency of lowering the deformation by pairing forces.

This situation is rather typical for the whole region of deformed nuclei excluding only the region of the lowest equilibrium deformations, where the pairing forces seem to be dominant (see e.g. the Pt isotopes in table 1).

For the most strongly deformed nuclei the influence of the Coulomb term seems to be dominant, so that the equilibrium deformations of these nuclei obtained in the IP case are more close to the deformations obtained in the case with no Coulomb term (NC) than to the deformations obtained with the Coulomb term (C).

Table 1 gives the equilibrium deformations calculated with the PBCS wave functions both in the (C) and (NC) case. The equilibrium deformations calculated in the BCS case by Bès and Szymański[6] [their variant (III + VI)] and in the IP case - by Marshalek, Person and Sheline[3] (their single-particle level

scheme is quite close to variant (III+VI) of ref.[6]) are also given for comparison. Since the PBCS and BCS energy curves are rather flat (cf. fig. 1) and defined only in the six points (η = 0,2,4,5,6,7) the minimum points (ϵ_{eq}) are not very exact, so that the purpose of table 1 is only to illustrate the general tendencies.

The ϵ_{eq} values in the independent particle case are especially rough as read from the diagram of ref.[3].

The quadrupole moments are given in fig. 3. The experimental points are deduced from the Coulomb excitation data quoted in the table of Lindskog et al. in ref.[27]. If more than one experimental point is available the point with the lowest experimental error was chosen. For Os^{188} fig. 3 gives two experimental points measured with almost the same acçuracy. For Os^{190}, the lower experimental point given in fig. 3 was measured with larger error than the upper one, but in two independent experiments. The theoretical PBCS results with the Coulomb term (C) are always larger than the corresponding BCS. Thus the discrepancy with the experiment in the beginning of the deformation region increases. Moreover, the PBCS calculation predicts a large deformation already for the Ce^{142} nucleus.

A better agreement with the experiment in the beginning of the deformation region and also for the most strongly deformed nuclei (i.e. for the nuclei, for which the inclusion or not of the Coulomb term has the largest effect on the equilibrium deformation) is obtained in the NC case. As the Coulomb effect is to some extent taken already into account in the single-particle levels, fitted to experiment, it is possible that the addition of the electrostatic Coulomb term to the energy overestimates the real Coulomb repulsion. However, it is not very probable that the part of Coulomb effect, included through the single-particle levels has the correct dependence on deformation.

Fig. 4 illustrates the dependence of the quadrupole moment calculated with the PBCS wave function [eq. (10)] for Z = 64 on the deformation η of the potential. The BCS values of Q [eq. (7)] are found to be quite close to the PBCS ones, so that the corresponding curve would not be distinguishable from the curve plotted in fig. 4.

Fig. 5 gives the deformation energy defined as the difference in the energy of a nucleus at the zero and the equilibrium deformations i.e. $\mathcal{E}_{def} = \mathcal{E}(0) - \mathcal{E}(\eta_{eq})$. Two of the five curves are calculated with the PBCS wave functions, including the Coulomb term (C) and not (NC). The next curve calculated in the indepen-

dent particle case (IP) is read from the diagram of the paper by Marschalek, Person and Sheline [3]. The last two curves are deduced from the recent extensive semi-empirical analysis by Myers and Swiatecki [28] (see also refs. [29,30]). The mass of a nucleus and its dependence on deformation have been obtained in Myers and Swiatecki analysis from the four parameter liquid drop formula, supplemented by the three parameter shell correction. The shell correction was assumed to come from the bunching of the energy levels and the effect of bunching was assumed to disappear with increasing deformation of the nucleus. Such a shell correction has allowed to reduce significantly the systematic discrepancy between the liquid drop masses and the experimental ones for almost the whole region of the stable nuclei (excluding only the light nuclei, for which the Wigner term appears to be important).

The curve denoted in fig.5 as "semi-emp MS" was obtained from the calculated curve ("calc MS") by taking the experimental mass of a nucleus instead of the mass calculated in the equilibrium point.

The comparison of the PBCS results with the semi-empirical ones shows much better agreement for the NC variant.

Table 2 shows the rather good consistency of the potential and the density deformations i.e. $\epsilon \approx \bar{\epsilon}$, similarly as was the case for BCS functions [6].

The results of this paper show that the projecting itself of the wave functions improves the values of the quadrupole moments only in the second half of the rare earth region i.e. for Yb and heavier isotopes.

The comparison of the experimental quadrupole moments and the semi-empirical deformation energies with the results of the two variants of the calculation: C and NC shows much better agreement for the variant with no Coulomb term, especially at the beginning of the investigated region.

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Table 1

Equilibrium deformations ϵ_{eq}. The second and the third columns give the values for the PBCS cases with the Coulomb term included and not, respectively. The results of variant (III+ VI) of ref. [6] are quoted in the fourth column and those of ref. [3] in the fifth

Nucleus	PBCS		BCS	IP
	C	NC	C	NC
Ce^{142}	0.32	0		0.14
Nd^{144}	0.34	0		0.22
Nd^{146}	a)	0		0.22
Nd^{148}	a)	0.29		0.27
Sm^{146}	0.30	0	0	0.22
Sm^{148}	a)	0.23	0.30	0.29
Sm^{150}	a)	0.26	0.33	0.30
Sm^{152}	a)	0.29	0.34	0.31
Sm^{154}	a)	0.32		0.32
Gd^{152}	a)	0.26	0.31	0.30
Gd^{154}	0.35	0.29	0.33	0.30
Gd^{156}		0.30		0.31
Gd^{158}	0.35	0.29	0.34	0.31
Gd^{160}	0.34	0.29	0.34	0.30
Dy^{160}	0.33	0.29	0.31	0.30
Dy^{162}	0.32	0.28	0.31	0.30
Dy^{164}	0.31	0.27	0.30	0.29
Er^{164}	0.31	0.27	0.30	0.30
Er^{166}	0.30	0.26	0.29	0.28
Er^{168}	0.29	0.26	0.28	0.27
Er^{170}	0.28	0.25	0.27	0.26
Yb^{170}	0.28	0.25	0.27	0.26
Yb^{172}	0.28	0.25	0.26	0.26
Yb^{174}	0.27	0.24	0.25	0.25
Yb^{176}	0.25	0.22	0.24	0.25

Nucleus	PBCS		BCS	IP
	C	NC	C	NC
Hf^{176}	0.24	0.21	0.24	0.25
Hf^{178}	0.23	0.20	0.22	0.22
Hf^{180}	0.22	0.19	0.21	0.22
W^{180}	0.22	0.19	0.21	0.21
W^{182}	0.20	0.18	0.20	0.20
W^{184}	0.18	0.17	0.18	0.17
W^{186}	0.17	0.16	0.17	0.16
Os^{186}	0.17	0.15	0.17	0.17
Os^{188}	0.16	0.14	0.14	0.14
Os^{190}	0.15	0.13	0.11	0.14
Pt^{190}	0.11	0.10		0.12
Pt^{192}	0.10	0.09		0.11

a) The energy curve decreases with deformation in the whole region investigated $0 \leq \epsilon \leq 0.35$, so that the equilibrium deformation is probably greater than 0.35.

Table 2

Quadrupole moments (in units of 10^{-24} cm^2) calculated with the help of eq. (10) and the values of the density deformation parameter $\bar{\epsilon}$, obtained from the quadrupole moments by eq. (6), for the deformations of the potential: ϵ = 0.10, 0.20 and 0.30. The integral in eq.(6) has been calculated with the trapezoidal charge distribution.

Z	ϵ = 0.10		ϵ = 0.20		ϵ = 0.30	
	Q_0	$\bar{\epsilon}$	Q_0	$\bar{\epsilon}$	Q_0	$\bar{\epsilon}$
58	1.99	0.11	4.28	0.22	6.64	0.33
60	2.16	0.11	4.63	0.23	6.99	0.33
62	2.32	0.12	4.94	0.23	7.21	0.33
64	2.47	0.12	5.22	0.23	7.42	0.32
66	2.60	0.12	5.46	0.23	7.62	0.31
68	2.70	0.12	5.62	0.23	7.83	0.31
70	2.78	0.11	5.69	0.22	8.03	0.30
72	2.82	0.11	5.64	0.21	8.12	0.29
74	2.82	0.11	5.52	0.20	7.66	0.27
76	2.76	0.10	5.38	0.19	7.86	0.26
78	2.55	0.09	5.08	0.17	8.14	0.26

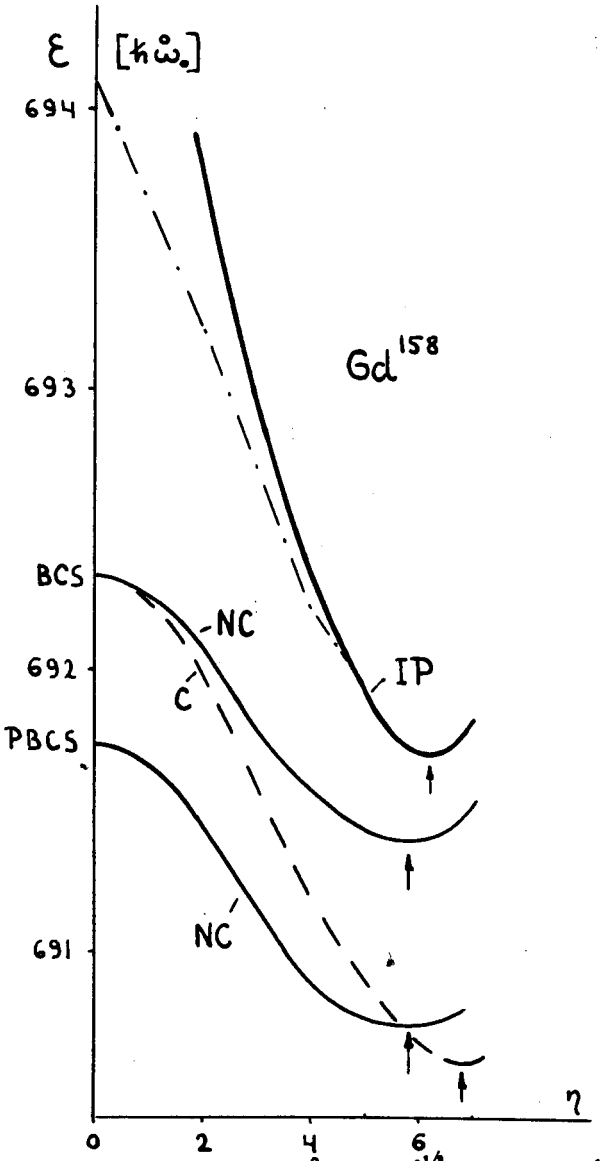

Fig. 1. The ground state energy (in $\hbar\omega_0 = 41A^{-1/3}$ MeV) for Gd^{158}, calculated using three types of wave functions: independent particle (IP) BCS and PBCS. The IP solid line corresponds to the configuration giving the absolute minimum. The IP dotted-dashed line connects the ground state energy points for $\eta = 0,2,4,5$. The solid lines of the BCS and PBCS cases correspond to the energy with no coulomb term (NC). The dashed line of the BCS case corresponds to the energy with the decrease [i.e. $\delta_0(\eta) - \delta_0(0)$] of the Coulomb term included (C). The arrows indicate the minimum points.

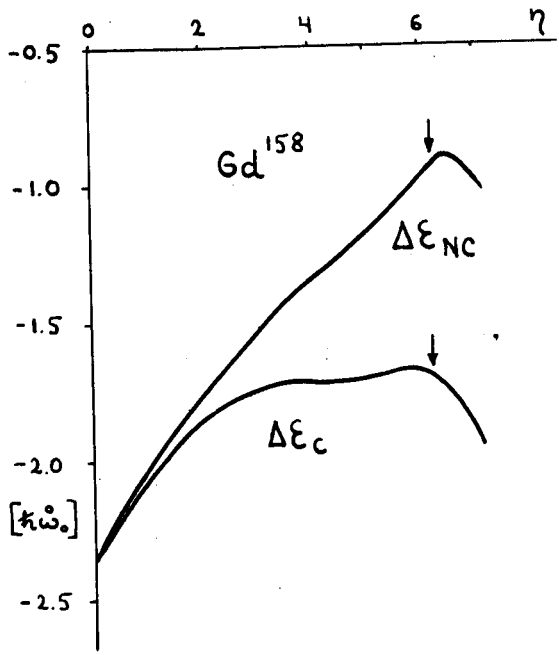

Fig. 2. The dependence of the energy differences (in $\hbar\omega_0$) on the deformation: $\Delta\mathcal{E}_{NC}(\eta) = \mathcal{E}^{PBCS}_{NC}(\eta) - \mathcal{E}^{IP}(\eta)$ and $\Delta\mathcal{E}_C(\eta) = [\mathcal{E}^{PBCS}_C(\eta) - \mathcal{E}_0(0)] - \mathcal{E}^{IP}(\eta)$. The arrows indicate the equilibrium deformation point in the independent particle case.

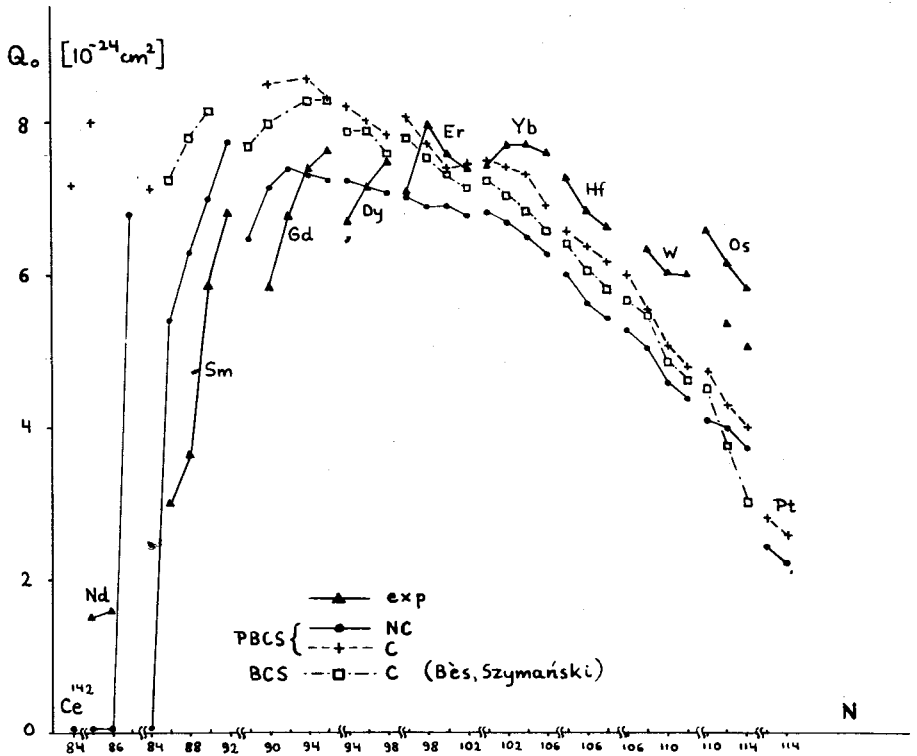

Fig. 3. Equilibrium quadrupole moments versus neutron number N.

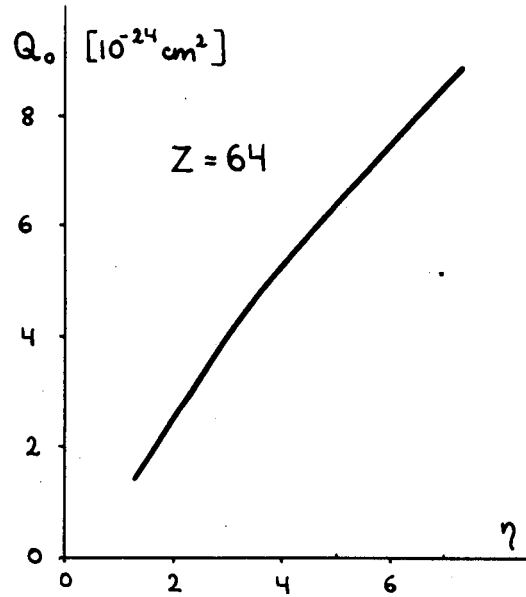

Fig. 4. Example of the dependence of the quadrupole moment on the deformation, for $Z = 64$.

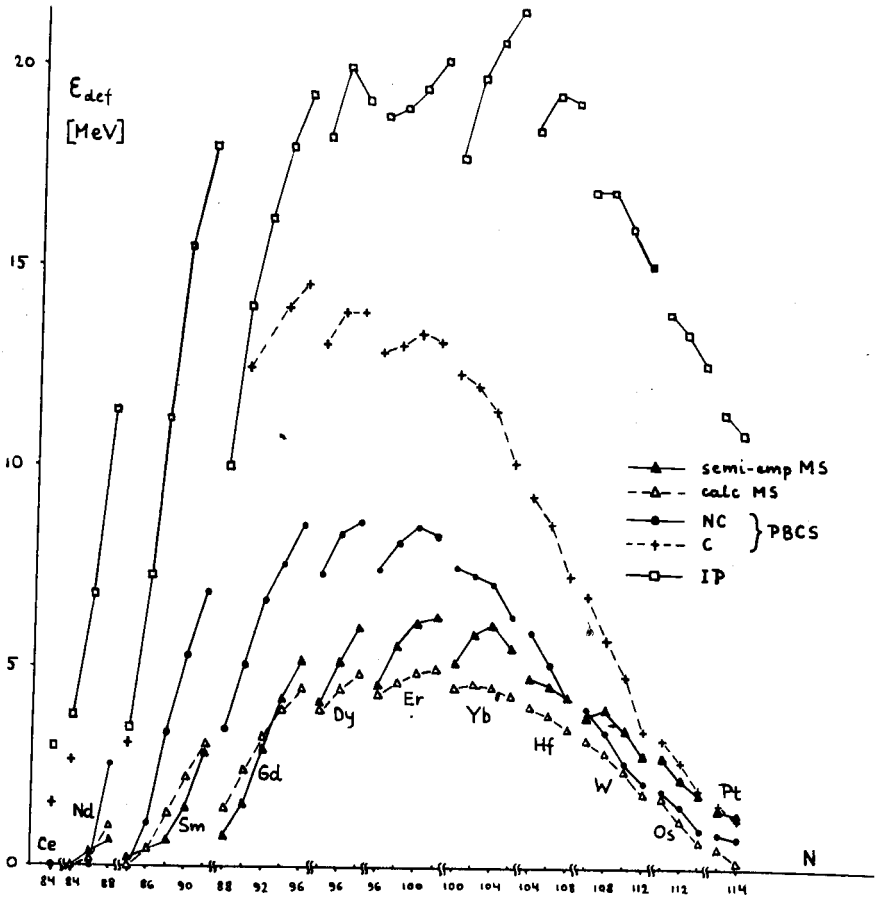

Fig. 5. Deformation energy in MeV versus neutron number N. Open and closed triangles correspond to the deformation energy deduced from the Myers and Swiatecki semi-empirical analysis.