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ABSTRACT

The Bogoliubov method of general linear transformations is applied to a selfconsistent calculation of deformed shapes of Rare Earth Nuclei and light nuclei around Mg^{24}. Nucleon-nucleon forces of finite range and different spin-dependence and exchange character are used. The dependence of the deformation on the particle number and the different components of the nuclear interaction is investigated.

* Work done at the "Lawrence Radiation Laboratory" Berkeley, California (Nuclear Chem. Division).

I- INTRODUCTION

Nuclei in the mass regions $20 < A < 30$, $155 < A < 185$, and $A > 225$ (A = number of nucleons) exhibit quadrupole moments considerably larger than the single particle values and lowlying excited states which can be interpreted as rotational states of a symmetric top. The unified model of Bohr and Mottelson[1,2] provides a satisfactory description of such nuclei. In this model the nucleus is pictured as a system of independent nucleons moving in a deformed shell model potential. A collective rotation is superimposed on this single particle motion. In the case of strongly deformed nuclei, the single particle motion is approximately decoupled from the collective rotation ("adiabatic hypothesis"), and the nuclear wave function can be factorized into a rotational and an intrinsic part. Under this assumption, we may ask for the shape of the nucleus irrespectively of its rotational state.

The question of the nuclear equilibrium deformation has been discussed by many authors[3,4,5]. Most of these papers deal with the problem of finding the equilibrium shape of a single particle potential with a given number of nucleons[3,4]. Usually, this potential was assumed to be axially symmetric[3]; some authors made allowance for arbitrary ellipsoidal deformations[4]. An important step towards more quantitative investigations was to take residual interactions into account[5]: The nucleons were confined to a given average potential and the parameters of this potential were determined such that the system of interacting nucleons had a maximal binding energy. In these calculations, the long-range part of the nuclear interaction is supposed to be incorporated in the average potential whereas the attractive short-range part is represented by a residual interaction.

In the first detailed calculations of this type, Moszkowski[5] used a δ-force. Arima applied the Nilsson model to light nuclei above O^{16} also using

δ -forces as residual interactions[5]. Belyaev described the short-range part of the nucleon-nucleon potential by a constant pairing interaction applying the superconductivity formalism[5]. Using the same theoretical approach, Bés and Szymanski performed extensive calculations in the rare earth and actinide region[5].

The present work tries to improve the existing calculations in mainly two respects; 1) We use forces with finite range, spin-dependence and exchange character.

2) We determine the average single particle potential selfconsistently from the nuclear interactions. Thus we can find out how accurate it is to represent the average nuclear field by a Nilsson-potential. Furthermore, the results are expected to reveal the interrelation of the presence of pairing forces and the requirement of selfconsistency of the field and we hope to learn about the dependence of the nuclear deformation on the different components of the nuclear interaction.

We would like to mention that similar calculations were performed by Baranger, Nagata, Ikeda et al, Bando et al, and Kelson et al[6].

We use the variational formulation of the superconductivity method[7]. This formalism is described in chapter II. Chapter III contains numerical results for rare earth nuclei and also for Mg^{24} and neighbouring deformed nuclei. In chapter IV, we discuss the approximations involved and summarize the main results.

In the appendix, the connection between our special variational ansatz and the method of general linear transformations of Bogoliubov[8] is presented and an outline of the numerical procedure is given.

II- THEORY

The Hamiltonian for a system of identical fermions is :

$$H = \sum_{K_1 K_2} \mathcal{E}_{K_1 K_2} a^+_{K_1} a^+_{K_2} + \frac{1}{4} \sum_{K_1 \ldots K_4} \langle K_1 K_2 | V | K_3 K_4 \rangle a^+_{K_1} a^+_{K_2} a_{K_4} a_{K_3} \quad (2.1)$$

a^+_K and a_K are creation and annihilation operators for a fermion in a quantum state K. K represents all the quantum numbers which specify a single particle state in a given representation.

$\langle K_1 K_2 | V | K_3 K_4 \rangle$ are the matrix elements of the interaction between normalized, antisymmetrized products of single-particle wave functions. In case V is the complete nucleon-nucleon interaction, the quantities $\mathcal{E}_{K_1 K_2}$ are the matrix elements of the kinetic energy operator T

$$\mathcal{E}_{K_1 K_2} = \langle K_1 | T | K_2 \rangle \quad (2.2)$$

If, however, V is some residual interaction, $\mathcal{E}_{K_1 K_2}$ is the matrix element of a Hamiltonian H_o which contains already a part of the interaction in terms of an average potential.

$$\mathcal{E}_{K_1 K_2} = \langle K_1 | T + V | K_2 \rangle \quad (2.2')$$

We describe our system by the trial state of Bardeen, Cooper, and Schrieffer[7] ("BCS-state") :

$$\Psi = \prod_{\nu > 0} (u_\nu + v_\nu b^+_\nu b^+_{\bar{\nu}}) | 0 \rangle \quad (2.3)$$

$|0\rangle$ is the vacuum state . V_ν and u_ν are probability amplitudes for the pair of states $(\nu, -\nu)$ to be occupied and unoccupied, respectively. They can be chosen real and are, of course, subject to the normalisation conditions

$$u_\nu^2 + v_\nu^2 = 1 \tag{2.4}$$

The operators b_ν^+ and $b_{-\nu}^+$ are creation operators for particles in quantum states ν and $-\nu$ of a new representation. They are connected with the operators of the original representation by a unitary linear transformation :

$$b_\nu^+ = \sum_\kappa D_\nu^\kappa \, a_\kappa^+ \tag{2.5}$$

$$b_{-\nu}^+ = \sum_\kappa D_{-\nu}^\kappa \, a_\kappa^+ \tag{2.5'}$$

We choose the coefficients D_ν^κ to be real . Then the unitarity conditions are simply :

$$\sum_\kappa D_{\nu_1}^\kappa \, D_{\nu_2}^\kappa = \delta_{\nu_1 \nu_2} \tag{2.6}$$

$$\sum_\nu D_\nu^{\kappa_1} \, D_\nu^{\kappa_2} = \delta_{\kappa_1 \kappa_2} \tag{2.6'}$$

In full generality, the conjugate state $-\nu$ is defined by the requirement that the density matrix and the pairing tensor be canonical in the ν -representation[9]. In the actual calculations we shall assume rotational symmetry with respect to the symmetry axis of the nucleus. In this case it can be shown that with a suitable phase convention[9,18] the state $-\nu$ is obtained by time-reversal and thus we have

$$D_{-\nu}^\kappa = D_\nu^\kappa \tag{2.7}$$

Since Ψ is not an eigenstate of the number operator $\underline{N}$

$$\underline{N} = \sum_{\kappa} a_{\kappa}^{+} a_{\kappa} \tag{2.8}$$

we have to assure that the average particle number is equal to the number of particles A :

$$\langle \Psi | \underline{N} | \Psi \rangle = A \tag{2.9}$$

We now consider the variational principle $\delta \mathcal{L} = 0$ (2.10)

with $$\mathcal{L} = \langle \Psi | H - \lambda \underline{N} | \Psi \rangle - \sum_{\nu_1 \nu_2 \kappa} K_{\nu_1 \nu_2} D_{\nu_1}^{\kappa} D_{\nu_2}^{\kappa} \tag{2.10'}$$

The Lagrange multiplier λ and $K_{\nu_1 \nu_2}$ are to be chosen such that the subsidiary condition (2.9) and the orthogonality relations (2.6) are fulfilled. (Iti is easily seen that it is sufficient to satisfy only one group of orthogonality conditions.) Furthermore, the variations of the quantities u_ν and v_ν are restricted by the normalisation conditions (2.4).

The Euler-Lagrange equations of this problem are :

$$\frac{\delta \mathcal{L}}{\delta v_\nu} = \frac{\partial \mathcal{L}}{\partial v_\nu} - \frac{v_\nu}{u_\nu} \frac{\partial \mathcal{L}}{\partial u_\nu} = 0 \tag{2.11}$$

$$\frac{\delta \mathcal{L}}{\delta D_\nu^{\kappa}} = \frac{\partial \mathcal{L}}{\partial D_\nu^{\kappa}} = 0 \tag{2.12}$$

It turns out to be advantageous to eliminate the Lagrange multipliers $K_{\nu_1 \nu_2}$ by using the conditions (2.6), but to retain the "chemical potential" λ explicitly in the equations. λ is, of course, a function of all the other parameters.

By a straightforward calculation we then obtain the following equations.

$$H_{\nu\nu} u_\nu v_\nu + \frac{1}{2} \Delta_{\nu,-\nu} \left(u_\nu^2 - v_\nu^2 \right) = 0 \tag{2.13}$$

$$H_{\nu_1\nu_2}\left(V_{\nu_1}^2 - V_{\nu_2}^2\right) + \Delta_{\nu_1-\nu_2}\left(u_{\nu_1}V_{\nu_1} - u_{\nu_2}V_{\nu_2}\right) = 0 \qquad (2.14)$$

The matrix $H_{\nu_1\nu_2}$ is given by

$$H_{\nu_1\nu_2} = \mathcal{E}_{\nu_1\nu_2} + \Gamma_{\nu_1\nu_2} - \lambda\delta_{\nu_1\nu_2} \qquad (2.15)$$

and the quantities $\mathcal{E}_{\nu_1\nu_2}$, $\Gamma_{\nu_1\nu_2}$ and $\Delta_{\nu_1-\nu_2}$ are defined as follows :[xx]

$$\mathcal{E}_{\nu_1\nu_2} = \sum_{K_1K_2} \mathcal{D}_{\nu_1}^{K_1}\mathcal{D}_{\nu_2}^{K_2}\,\mathcal{E}_{K_1K_2} \qquad (2.16)$$

$$\Gamma_{\nu_1\nu_2} = \sum_{\nu>0} \langle\nu_1\nu\,|\,V\,|\,\nu_2\nu\rangle V_\nu^2 \qquad (2.17)$$

$$\Delta_{\nu_1-\nu_2} = \sum_{\nu} \langle\nu_1-\nu_2\,|\,V\,|\,\nu-\nu\rangle u_\nu V_\nu \qquad (2.18)$$

The matrix-elements $\langle\nu_1\nu_2|V|\nu_3\nu_4\rangle$ are related to the matrix-elements in the K-representation by a formula analogous to equ. (2.16) :

$$\langle\nu_1\nu_2\,|\,V\,|\,\nu_3\nu_4\rangle = \sum_{K_1\cdots K_4} \mathcal{D}_{\nu_1}^{K_1}\mathcal{D}_{\nu_2}^{K_2}\mathcal{D}_{\nu_3}^{K_3}\mathcal{D}_{\nu_4}^{K_4}\langle K_1K_2\,|\,V\,|\,K_3K_4\rangle \qquad (2.19)$$

The quantity $\Gamma_{\nu_1\nu_2}$ is obviously a generalized Hartree-Fock potential, whereas $\Delta_{\nu_1-\nu_2}$ is the so-called "pairing potential". It vanishes in the absence of pairing correlations.

Equations (2.13) are the well-known BCS-equations. They define the probability amplitudes and for a given selfconsistent field, i.e. for a given set of coefficients.

[xx] From now on, all sums over states ν are to be taken only over the states $\nu > 0$ if not mentioned otherwise.

Equations (2. 14) are called Hartree-Bogoliubov equations ("HB"- equations). In the case of a sharp Fermi-surface, they degenerate into the usual Hartree-Fock equations. The solution of the coupled set of BCS - and HB-equations (2. 13) and (2. 14) is of course, a much more difficult task than the solution of the BCS-equations alone. We have obtained numerical solutions by a simple interaction method (see appendix). A rapid convergence is achieved, if one starts the iteration with a reasonably good approximation of the selfconsistent field.

A suitably chosen Nilsson potential provides such an approximation. In order to apply to a realistic nuclear case the treatment must still be generalized : We describe the nuclear system by the product of a BCS-configuration for neutrons and BCS-configuration for protons disregarding the possibility of pairing between neutrons and protons :

$$\Psi = \prod_{\nu_1>0} \left(u_{\nu_1}^{(n)} + v_{\nu_1}^{(n)} b_{\nu_1}^{(n)\dagger} b_{\bar{\nu}_1}^{(n)\dagger} \right) \prod_{\nu_2>0} \left(u_{\nu_2}^{(p)} + v_{\nu_2}^{(p)} b_{\nu_2}^{(p)\dagger} b_{\bar{\nu}_2}^{(p)\dagger} \right) |0\rangle \quad (2.19)$$

The superscripts (n) and (p) refer to neutrons and protons , respectively. The meaning of the quantities in (2. 19) is obvious from what has been said. The variational equations corresponding to such a trial are derived in a completely analogous way and contain additional contributions to the Hartree-Fock potential due to the interaction between neutrons and protons .

III RESULTS

III 1) General remarks

In the actual calculations, we have assumed that the intrinsic nuclear wave function is invariant with respect to rotations around a symmetry axis which is chosen as the z-axis. This means that the magnetic quantum number m is conserved and the sum in (2. 5) is not to be extended over magnetic substates. With the special phase convention made[9, 18] this also leads to the relation

$$\mathcal{D}^{\kappa}_{-\nu} = \mathcal{D}^{\kappa}_{\nu} \tag{3.1}$$

As initial set of single-particle states $a^{+}_{\kappa}|o\rangle$ we use eigenfunctions of an isotropic harmonic oscillator in j -representation. Under these assumptions, the expansion (2. 5) can be written as follows :

$$b^{+}_{km} = \sum_{n l j} \mathcal{D}^{n l j}_{k}(m)\, a^{+}_{n j l m} \tag{3.2}$$

where j is the total angular momentum, l the orbital angular momentum, and n the radial quantum number. k labels the different states of equal m (and equal parity).

Because of the restricted storing capacity of the computer, it was not possible to include all those single-particle states $a^{+}_{njlm}|o\rangle$ which are expected to contribute noticeable amplitudes $\mathcal{D}^{njl}_{k}(m)$ to the final single-particle state.

In the case of light nuclei we included all single-particle states of principal quantum number $N = 0, 1, 2, 3$ $(N = 2n + l)$ for neutrons and protons, i. e. for a deformed nucleus like Mg^{24} we took into account the polarization of the O^{16} core.

In the case of rare earth nuclei we took into account all single particle states of principal quantum number $N = 5$ and the $i_{\frac{13}{2}}$ level for neutrons,

all states of $N = 4$ and the $h_{\frac{11}{2}}$ level for protons. The core formed of all nucleons in energetically lower states was assumed to be spherically symmetric.

This assumption is, of course, not realistic and, as a result, our quadrupole moments for rare earth nuclei are too small by a factor of two and more. Nevertheless, qualitative features like the gradual appearance and disappearance of deformation as a major shell is filled are obtained satisfactorily. Furthermore, other quantities of physical interest like the moments of inertia and the lowest quasi-particle energies depend less critically on this assumption.

Another critical question is the choice of the nucleon-nucleon potential: The formalism as it stands can be used for any nucleon-nucleon potential V which leads to finite matrix-elements in a single-particle representation. If no assumption is made of an inert core and an average field due to it, one could in principle use realistic nuclear forces fitted to the scattering data. Since our wave function does not allow for those two-particle correlations which are produced by the repulsive components of the nuclear forces at small distances, such an effort would be of questionnable value without improving at the same time the theory. We were less ambitious and chose nucleon-nucleon potentials of Gaussian shape and reasonable strength and varied range, exchange character and spin-dependence in order to see how these different properties of the nucleon-nucleon potential affect the formation of deformed shapes and the position of the lowest quasi-particle excitations. Some of our forces would probably satisfy the low-energy data not too badly, but surely these forces are not saturating and, as a consequence, the total binding energies we obtain are not meaningful quantities.

It turns out (see sect. III, 3) that the physical quantities we are interested in, i e; above all the equilibrium deformations, are quite insensitive to the presence of a short-range repulsion (see sect. III, 3). Furthermore, since we include only a few states of different radial quantum number n in expansion (3. 2) (2 in the case of light nuclei , 1 in the case of rare earth nuclei) , and since we choose the frequency ω of the basis oscillator wave functions such as to correspond to an approximately correct nuclear radius ($\hbar\omega = \frac{41\,Mev}{A^{1/3}}$) the non-saturating character of the forces does not lead to a collapse of the nucleus .

Thus keeping the average density artificially at correct values , we do not perform a fully selfconsistent calculation. We do , however , determine the parameters of the wave function from the Hartree-Bogoliubov and BCS-equations, (2. 13) and (2. 14) , without imposing subsidiary conditions such as the ones used by Nilsson[3] and Bés and Szymanski[5].

It is in this sense that we speak of "self-consistency" in this paper .

For light as well as for rare earth nuclei, we perform two types of calculations :

a) selfconsistent calculations , i. e. the solution of the full set of equ. (2. 13) and (2. 14)

b) calculations in which we describe the angular dependence of the deformation by the spherical harmonic Y_{20} ('Nilsson"-calculation) .

In detail we proceed as follows : We introduce a single-particle Hamiltonian H_0 in the original k-representation

$$\langle K_1 | \mathcal{H}_0 | K_2 \rangle = \mathcal{E}_{K_1 K_2} + \langle K_1 | V^{spher} + \eta r^2 Y_{20}(\Theta) | K_2 \rangle$$

In the case of light nuclei, $\mathcal{E}_{K_1 K_2}$ is the matrix-element of the kinetic energy operator , eventually plus a phenomenological spin-orbit term, in the case of Rare Earth nuclei , $\mathcal{E}_{K_1 K_2}$ contains in addition the average field produ-

ced by the core.

V^{spher} is the spherically symmetric part of the average potential. We define it by the Hartree-Fock potential $\Gamma^{spher}_{\kappa_1\kappa_2}$ (see defin. (2. 17))

$$\langle \kappa_1 | V^{spher} | \kappa_2 \rangle = \Gamma^{spher}_{\kappa_1\kappa_2} \qquad (3.4)$$

$\Gamma^{spher}_{\kappa_1\kappa_2}$ is obtained from the solution of the BCS-equations for a spherically symmetric configuration defined by

$$D^{\kappa}_{\nu} = \delta_{\nu\kappa} \qquad (3.5)$$

Following Nilsson[3] we describe the non-spherical part of the average potential by a spherical harmonic Y_{20} and a quadratic dependence on the radial coordinate r (see (3. 3)).

The transformation coefficients D^{κ}_{ν} are then obtained as the unitary transformation which diagonalizes the matrix $\langle \kappa_1 | \mathcal{H}_0 | \kappa_2 \rangle$. In this diagonalization matrix-elements of H_0 between single-particle states of different principal quantum number N are put equal to zero. This is the approximation used in chapter II of Nilsson's paper[3].

Then the BCS-equations (2. 13) are solved in the representation defined by the D^{κ}_{ν} and the total energy E is calculated.

The D^{κ}_{ν} and E are still functions of the deformation parameter η.

The absolute minimum of $E(\eta)$ defines the equilibrium deformation η_{min} (see for instance fig. 1)

The set of D^{κ}_{ν} and Γ_{ν} which belong to $\eta = \eta_{min}$ are expected to be an approximate solution of the full set of BCS- and HB-equations (2. 13) and (2. 14) and provide a good initial set for an iterative solution of these equations.

III- 2) Results for rare earth nuclei

Fig. 1 shows the gradual appearance and disappearance of deformations as a function of the number of neutrons and protons outside the closed configuration of the core. The nuclear interaction used in these "Nilsson" -calculations was a superposition of a δ- and a quadrupole force :

$$V(\vec{r}_1' - \vec{r}_2') = c\,\delta(\vec{r}_1' - \vec{r}_2') + f(|\vec{r}_1' - \vec{r}_2'|)\,Y_{20}(\cos\vartheta_{12}) \quad (3.6)$$

The matrix-elements of f(r) were all put equal. The parameters c and f and the single-particle matrix -elements $\varepsilon_{\kappa_1\kappa_2}$ were adjusted such as to reproduce correctly the odd-even mass-differences throughout the shell and the one-hole excitations of Pb^{207}

This procedure resulted in values for the parameters c and f which were very close to the ones used by Kisslinger and Sorensen[5].

Analogous calculations were performed with a Rosenfeld-and a Serber force of Gaussian radial dependence.

This investigation lead to the following results :

1)The dependence of the energy E on deformation and the number of extra-core nucleons which is exhibited in fig. 1 is rather unaffected by spin-dependence and exchange character of the nuclear interaction, it is, however, a sensitive function of the range of the interaction.

It is seen that a δ -function as the limiting case of a short-range force does not lead to any deformation. Fig. 1 shows that.

2) In accordance with experimental results the quadrupole moments of rare earth nuclei are all positive. But only if the single-particle parameters $\varepsilon_{\kappa_1\kappa_2}$ are chosen in close correspondence to a Wood-Saxon potential or generally a potential with steep walls, then the cigar-shaped configurations

are energetically favoured. If we choose $\mathcal{E}_{K_1K_2}$ as the matrix elements of a harmonic oscillator, the groundstate deformations turn out to be negative in the second half of the major shell for all force mixtures we investigated. This result confirms the statement by Lemmer and Weisskopf[3] that the preponderance of positive deformations is due to the steepness of the walls of the average potentials.

Fig. 2 shows a comparison of experimental and theoretical values of the intrinsic quadrupole moment

$$Q_0 = \langle \Psi | \underline{Q}_0 | \Psi \rangle$$

$$\underline{Q}_0 = \sum_{\substack{n l j m \\ n' l' j' m'}} \langle n j l m | r^2 Y_{20} | n' j' l' m' \rangle \, a^+_{n j l m} \, a_{n' j' l' m'}$$

as a function of particle number. The theoretical values are obtained from a selfconsistent calculation with the Rosenfeld force of table I. The single-particle energies $\mathcal{E}_{K_1K_2}$ were adjusted in the same way as before and are given in table 2. The sudden rise of quadrupole moments in the group of Sm isotopes and the gradual decrease towards shell closure is correctly reproduced, the absolute values, however, are too small by a factor of 2 to 3 for the reasons we mentioned in section III, 1.

Again, this result was qualitatively the same for a Serber force and for the $\vec{\sigma}\vec{\tau}$ quadrupole force.

Because of the r^2-dependence of the quadrupole operator, the quadrupole moment depends more sensitively than other physical quantities (see fig. 4) on small admixtures of single-particle wave functions of higher radial quantum numbers. Furthermore, the polarization of the core which we neglected is believed to enhance the quadrupole moments by about a factor of 2 for medium heavy and heavy nuclei.

Fig. 3 shows in greater detail the result of a "Nilsson" calculation for Sm^{152} . The parameters were again those of table 1 and 2 . According to the "Nilsson" calculation the groundstate deformation is negative , whereas the selfconsistent calculation leads to a positive quadrupole moment for the groundstate . An analogous result was obtained for Mg^{24} (see section III, 3). Furthermore, this result shows that admixtures of higher multipoles (l = 4, 6. .) to the selfconsistent field lead to an energy gain of about 0. 5 Mev.

Fig. 4 shows a comparison of experimental and theoretical values of the moments of inertia . The calculated moments of inertia are obtained from the Inglis-formula :

$$\mathcal{J} = \hbar \sum_{\lambda\lambda'} \frac{|\langle \psi_{\lambda\lambda'} | I_x | \psi \rangle|^2}{E_\lambda + E_{\lambda'}} \qquad (3.9)$$

I_x is the x-component of the angular momentum operator , for the definition of the two-quasi-particle state $\psi_{\lambda\lambda'}$ and the quasi-particle energies E_λ , see appendix I.

In making a comparison of our results with those of other authors as Nilsson and Prior[9] for instance one should keep in mind that after having selected a nuclear interaction and single particle energies ε_{jj}, we have no more parameters to adjust .

Table 3 contains a comparison of the quasi-particle energies $\tilde{E}_{\nu\nu}$ and E_λ before and after the diagonalisation of H (see appendix I)

$$E_\lambda = \langle \omega | \xi_\lambda \, H \, \xi_\lambda^+ | \omega \rangle - \langle \omega | H | \omega \rangle \qquad (3.10)$$

$$\tilde{E}_{\nu\nu} = \langle \tilde{\omega} | \xi_\nu \, H \, \xi_\nu^+ | \tilde{\omega} \rangle - \langle \tilde{\omega} | H | \tilde{\omega} \rangle \qquad (3.11)$$

$$= \sqrt{(\varepsilon_{\nu\nu} + \Gamma_{\nu\nu} - \lambda)^2 + \Delta_{\nu-\nu}^2} \qquad (3.12)$$

The differences are negligibly small. They are more considerable for the wave functions, but still the dominant component was larger than 0.9 in all the cases considered.

III-3) Results for deformed light nuclei

Fig. 6 shows again the gradual appearance and disappearance of strong deformations as a function of particle number. The calculations were performed with a Serber-force (see table 4). Within the frame work of the effective range theory this potential is equivalent to the one used by Mang and Wild [11] in their study of H^3 and He^4. It reproduces the low-energy data approximately.

The frequency ω of the basic oscillator was adjusted to the experimental RMS-radius of Mg^{24}, which lead to $\hbar\omega = 14.2$ Mev.

Since this potential does not contain any tensor and spin-orbit components, a phenomenological spin-orbit splitting was incorporated in the single-particle matrix-elements $\mathcal{E}_{K_1 K_2}$ i.e.

$$\mathcal{E}_{K_1 K_2} = \langle K_1 | T | K_2 \rangle + C_{LS} \langle K_1 | \vec{l}\vec{s} | K_2 \rangle \quad (3.13)$$

Contrary to the case of rare earth nuclei, negative ground state deformations do occur for light nuclei with $A > 24$. We obtained negative quadrupole moments for S^{32} and Si^{28}. For the case of Mg^{24} and Mg^{26}, the energies of the oblate and prolate configurations were very close to each other. In the selfconsistent calculation, the prolate configuration turned out to correspond to the absolute minimum, whereas this was not so in the "Nilsson" calculation (see fig. 6)

The fact that a selfconsistent calculation lowers the energy of the prolate configuration more than the one of the oblate configuration may be attributed to the polarization of the O^{16} core which is not taken into account in our "Nilsson"-calculation but which is included in the selfconsistent solution. According to Das Gupta and Preston[12] it can be inferred from a simple single-particle model that the polarization of the core favours prolate shapes. Recently, Glover[13] found strong indications that the quadrupole moment of Mg^{27} is negative. If this is true, one would also expect a negative intrinsic quadrupole moment for the groundstate band of Si^{28}

Fig. 7 presents a comparison between experimental and theoretical values of quadrupole moments. The calculated values are too small by about 10% to 20%. This may be due to our neglecting admixtures of higher single-particle states ($N > 3$) in (3. 2) or to the insufficiency of the forces we used.

The polarized core of the lowest 16 nucleons contributed about 20% to 35% of the total quadrupole moment. No strong dependence of this contribution on the number of extra-core nucleons was observed. We did not, however, check systematically whether a stronger dependence on the forces exists.

In order to study the influence of the tensor-force on the formation of deformed shapes we performed calculations with one of the force mixtures given by Pease and Feshbach[14]. These forces reproduce the low-energy data and give fairly correct values for the binding energy of the triton. They contain a relatively strong tensor component. In this calculation we did not include a phenomenological spin-orbit term in $\mathcal{E}_{\kappa_1\kappa_2}$ ($C_{LS} = 0$).

There was no strong dependence of the equilibrium deformation on the strength of the tensor component. Furthermore, the spin-orbit splitting produced by the tensor contribution was too small by a factor of 4 to 5. Concerning the reliability of these two last-mentioned results one should keep in mind that the BCS-state (2. 3) emphasizes configurations which depend sensitively on the triplet - and singlet - components of the central potential, but

much less on the tensor force. It is, therefore, possible that the contribution of the tensor force will be larger, if other configurations not included in (2. 3) are taken into account.

In table 5 the squares of the amplitudes D_ν^κ resulting from a "Nilsson"-calculation are compared with the ones resulting from a selfconsistent calculation. Since we have neglected the coupling between states of different principal quantum number in the "Nilsson" calculation, the differences are likely to be smaller in reality. The rather considerable deviation found for single particle components near the Fermi surface are sure to persist. This is what one would expect from the Hartree-Bogoliubov equation. The diffuseness of the Fermi surface i. e. the occupation amplitudes V_ν depend sensitively on the level density at the Fermi surface. Even slight differences of the level spacing as they are produced by the selfconsistent and the "Nilsson" calculation, can lead to quite different occupation amplitudes V_ν. This can be seen from the BCS-equations (2. 13). Different V_ν will in turn lead to different coefficients D_ν^κ through the HB-equations (2. 14). The single particle wave functions of the lower-lying states, however, are quite successfully represented by Nilsson wave functions.

In this context we would like to mention that the coupling of the HB-equations (2. 14) to the BCS-equations (2. 13) is mainly produced by the Hartree-Fock potentials $\Gamma_{\nu_1\nu_2}$ which depend quite sensitively on the occupation probabilities V_ν^2. The second term in (2. 14), $\Delta_{\nu_1-\nu_2}\,(U_{\nu_1} V_{\nu_1} - U_{\nu_2} V_{\nu_2})$, is usually considerably smaller than the first and can be completely neglected in a 1st approximation.

The selfconsistent results for light nuclei were indeed obtained with this approximation.

Finally we would like to point out that pairing configurations apparently play a less important role for light nuclei than for medium-heavy and heavy nuclei. So we did not obtain any diffuseness of the Fermi-surface ("trivial" solution of the BCS-equations), if we used the Rosenfeld force of table I for light

nuclei , and a rather small diffuseness for the Serber force (table 4). The reason is that the ratio of the average pairing matrix element to the average level distance is smaller for light nuclei than for heavy ones .

In order to check how strongly our results are falsified by the fact that the nucleon-nucleon potentials are not saturating , we performed some test calculations with an additional repulsive soft-core potential[16] . The effect of the repulsive core on the quadrupole moment was completely negligible (less than L 5%) , it was, of course, larger on other quantities of interest, like the decoupling factors[16] .

IV. Discussion

The main results of this investigation may be summarized as follows :

1) The appearance of strongly deformed nuclei between shell closures depends sensitively on the range and very little on the spin-dependence and the exchange character of the nucleon-nucleon forces .

2) The Nilsson-representation for the deformed field is a fairly good approximation of the selfconsistent single-particle states provided the single particle Hamiltonian is defined according to eq. 3.3. Deviations are found for those components which correspond to single-particle energies close to the Fermi surface .

3) Pair configurations play a less important role for light nuclei than for medium-heavy and heavy nuclei.

4) The reciprocal dependence of the diffuseness of the Fermi surface and the selfconsistent field , which is reflected in the coupling between the two sets of equations (2.13) and (2.14) , cannot be overlooked when a selfconsistent description is attempted . It is mainly contained in the dependence of the Hartree-Fock matrix $\Gamma_{\lambda,\lambda'}$ on the occupation probabilities .

No great care has been given to the choice of nucleon-nucleon potentials and especially in the case of light nuclei interesting additional work could be done along these lines . We still wish to discuss the main approximations underlying our treatment : Besides the technically necessary restriction on the configurations admitted in (2.5) , the theory involves a number of approximation which we want to mention shortly .

1) The particle number is not conserved and , instead , only the average numbers of neutrons and protons are kept fixed . This approximation is expected to be good as long as the number Ω of partially occupied single-particle orbitals is large compared to one [17] . A more detailed investigation shows that Ω = 3-4 is already sufficient for the justification of this method[18] . If the diffuseness of the Fermi surface is very small such as for rotational states of high angular momentum and generally for light nuclei , the non-conservation of particle number can introduce serious errors .

2) If the selfconsistent field is not spherically symmetric , the BCS-wave function (2.3) is not an eigenstate of angular momentum . Only the projection K of the angul ar momentum on the symmetry axis remains a good quantum number as long as the summation in eq. (2. 5) is not extended over magnetic substates .

Thus , the wave function (2. 3) as it stands can only be interpreted as the wave function of intrinsic motion , χ_K^{intr} , in the adiabatic rotational model .

$$\Psi = \chi_K^{intr} \tag{4.1}$$

In this model , the wave function Ψ_{IM} of rotational states of angular momentum I and magnetic quantum number M is given by the well-known formula

$$\Psi_{IM} = \mathcal{D}^{I}_{KM}(\Theta)\,\chi_K^{intr} \tag{4.2}$$

$D^{I}_{KM}(\vartheta)$ are the eigenfunctions of the symmetric top which depend on the Euler angles ϑ.

The "adiabatic approximation" is known to hold only in the case of strongly deformed nuclei. In the transition region of small deviations from spherical symmetry our results have at most a qualitative meaning and more elaborate variational methods ought to be applied [19].

3) The wave function (2.3) contains also an undesirable centre-of-mass motion which, supposedly, falsified values of the total energy E by terms of the order $1/A$ (A = mass number). We expect, however, that the differences of energies of the spherically symmetric and deformed configurations depend less sensitively on the spurious centre-of-mass motion. Only these energy differences are meaningful quantities in our theory.

4) In spite of the rather large number of parameters, the BCS-state comprises only a small subgroup of all possible configurations.

A very apparent deficiency is that the state (2.19) does not allow for pairing between neutrons and protons. In the case of heavy and medium-heavy nuclei the Fermi surface for neutrons and protons occurs at very different single-particle levels and thus pairing between neutrons and protons will be less important than pairing between identical particles.
This argument does not hold for light nuclei and a generalization of the method including α-clusters would be of great interest. There is a general argumer according to which pairing between identical particles should be predominant: The most important contributions to pairing are due to singlet states of relative angular momentum O. In the case of identical particles, only singlet states may occur for S-states of relative motion while for nonidentical

particles the triplet-configuration competes with the singlet configuration and thereby reduces its statistical weight . In a recent investigation[20] Camiz, Covello and Jean conclude that indeed a product of two BCS wave functions is a good approximation . By not summing over states of different magnetic quantum number in (3.2) we do not allow for non-axially symmetric deformations . The formalism as it stands could be immediately used to study the importance of " γ -deformations " . One is , however , faced with the technical difficulty that considerably more matrix-elements of the nuclear interaction will enter into the calculation .

5) A more general problem which includes the questions raised in the last paragraphs is the importance of that part H_4 of the Hamiltonian (see appendix I) which is neglected in the Bogoliubov theory . H_4 is usually treated by special perturbation methods like the quasi-boson approximation .

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We highly appreciated helpful and encouraging discussions with Prof. J. Rasmussen . We are grateful to Dr. N. Glendenning and M. Redlich for many discussions and for providing us programs for the computation of nuclear matrix-elements . We are also grateful to Dr. V. Gillet for stimulating discussions .

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Appendix

A . I) Connection of the variational method with the theory of linear transformations of Bogoliubov .

The variational principle formulated in chapter II does not show whether the theory can serve as a basis of a more complete treatment . This becomes apparent in the method of linear transformations[21] which can be shown to be equivalent to the variational principle[22 , 23] .

We shall briefly restate this equivalence because certain results we obtained are beyond the scope of the variational principle of chapter II .
Bogoliubov introduces the most general unitarity transformation of the creation and annihilation operators of the initial basis .

$$\xi_\lambda^+ = \sum_\kappa \left(A_\lambda^\kappa a_\kappa^+ + B_\lambda^\kappa a_\kappa \right) \qquad (A.1)$$

and chooses the transformation coefficients A_λ^κ and B_λ^κ such as to bring the Hamiltonian into the following form :

$$H - \lambda N = U + H_{11} + H_{\phi} \qquad (A.2)$$

In (A.2) U is a c-number and up to a term $N.\lambda$ equal to the total energy E of the system . H_{11} is diagonal

$$H_{11} = \sum_\lambda E_\lambda \xi_\lambda^+ \xi_\lambda \qquad (A.3)$$

and H_4 is the sum of all terms of four ξ -operators in normal order. In this procedure, the coefficients of the unitary transformation (A.I) are defined by the requirement that H_2, the sum of all terms with two creation or two annihilation operators of "quasi-particles", vanish

$$H_2 = 0 \tag{A.4}$$

and H_{11} be diagonal (A.3).

For any Bogoliubov transformation (A.I) there is a "quasi-vacuum" $|\omega\rangle$ defined by

$$\xi_\lambda |\omega\rangle = 0 \tag{A.5}$$

The relationship between this method and the variational principle of chapter II can be most easily established by using a theorem proved by Bloch and Messiah and by Zumino [10].

Any general Bogoliubov transformation $\mathcal{B}$ can be written as a product of 3 linear unitary tranformations

$$\mathcal{B} = U_2 P U_1 \tag{A.6}$$

of the form

$$U_1 : \quad b_\nu^+ = \sum_\kappa D_\nu^\kappa a_\kappa^+ \tag{A.7}$$

$$P : \quad \xi_\nu^+ = u_\nu b_\nu - v_\nu b_{-\nu}^+ \tag{A.8}$$

$$U_2 : \quad \alpha_\lambda^+ = \sum_\nu C_\lambda^\nu \xi_\nu^+ \tag{A.9}$$

where the coefficients u_ν, v_ν have to satisfy the normalization conditions (2.4) and the coefficients D^κ_ν, C^ν_k the usual unitarity conditions. For a given Bogoliubov transformation $\mathcal{L}$ the ψ-representation is defined by the requirement that the density matrix ρ and the pairing tensor t be canonical:

$$\rho_{\nu_1\nu_2} := \langle\omega | b^+_{\nu_1} b_{\nu_2} | \omega\rangle = \delta_{\nu_1\nu_2}\rho_{\nu_1\nu_1} \qquad (A.10)$$

$$t_{\nu_1-\nu_2} := \langle\omega | b_{\nu_1} b_{-\nu_2} | \omega\rangle = \delta_{\nu_1\nu_2} t_{\nu_1-\nu_1} \qquad (A.11)$$

We can now easily prove the following statement: we can always choose the two transformations P. U_1 such that H_2 vanishes

$$H_2 = 0$$

and this condition is equivalent to the variational principle of chapter II. Writing the Hamiltonian H in terms of the operators $\xi^+_{\nu_1}$ ξ_ν one obtains the following explicit form for H_2:

$$H_2 = \sum_{\nu_1\nu_2}\Big\{H_{\nu_1\nu_2}(u_{\nu_1}v_{\nu_2} + v_{\nu_1}u_{\nu_2}) + \qquad (A.12)$$

$$+ \Delta_{\nu_1-\nu_2}(u_{\nu_1}u_{\nu_2} - v_{\nu_1}v_{\nu_2})\Big\}\cdot\left[\xi^+_{\nu_1}\xi^+_{-\nu_2} + \xi_{-\nu_1}\xi_{\nu_2}\right]$$

where $H_{\nu_1\nu_2}$ and $\Delta_{\nu_1-\nu_2}$ are defined by (2.15) and (2.19) resp. The condition of vanishing H_2 leads to the set of equations

$$H_{\nu_1\nu_2}(u_{\nu_1}v_{\nu_2} + v_{\nu_1}u_{\nu_2}) + \Delta_{\nu_1-\nu_2}(u_{\nu_1}u_{\nu_2} - v_{\nu_1}v_{\nu_2}) = 0 \qquad (A.13)$$

For $\nu_1 = \nu_2$ this is the set of BCS-equations (2.13).

For $\nu_1 \neq \nu_2$ the equations (A.13) are equivalent to the HB-equations (2.14).

In order to see the equivalence , we multiply (A. 13) by $(u_{\nu_1} v_{\nu_1} - u_{\nu_2} v_{\nu_2})$. Writing $\mathcal{E}$ for the left side of eq. (2. 14) , we obtain :

$$\mathcal{E} \cdot (u_{\nu_1} u_{\nu_2} - v_{\nu_1} v_{\nu_2}) = 0$$

i. e.

$$\mathcal{E} = 0$$

With the help of (A. 13) , H_{11} can be shown to have the following form :

$$H_{11} = \sum_{\nu_1 \nu_2} \frac{H_{\nu_1 \nu_2}}{(u_{\nu_1} u_{\nu_2} - v_{\nu_1} v_{\nu_2})} \left(\xi^+_{\nu_1} \xi_{\nu_2} + \xi^+_{-\nu_1} \xi_{-\nu_2} \right) \tag{A. 14}$$

$$= \sum_{\nu_1 \nu_2} E_{\nu_1 \nu_2} \left(\xi^+_{\nu_1} \xi_{\nu_2} + \xi^+_{-\nu_1} \xi_{-\nu_2} \right)$$

i. e. , in general H_{11} is not diagonal as a result of the variational method . It can , however , be diagonalized by a simple unitary transformation of the form (A. 9) .

In many practical cases , H_{11} will be almost diagonal already in the form (A. 14) (see, sect. III 2) . The energies $E_{\nu\nu}$ or , more accurately , the energies E_λ (A. 3) are to be interpreted as "quasi-particle excitations " of neighbouring odd nuclei .

$E_{\nu\nu}$ can be written in the well-known form :

$$E_{\nu\nu} = \sqrt{(\varepsilon_{\nu\nu} + \Gamma_{\nu\nu} - \lambda)^2 + \Delta^2_{\nu,-\nu}} \tag{A. 15}$$

The elementary excitations of an even nucleus are given by two-quasi-particle states

$$\Psi_{\lambda_1 \lambda_2} = \xi^+_{\lambda_1} \xi^+_{\lambda_2} |\omega\rangle \tag{A. 16}$$

A . II) Remarks on the numerical method

Solutions of the eqs. (2-13), (2-14) were obtained by a straight-forward procedure : in a first step an initial set of coefficients $D^j_k(m)$ is calculated from a deformed single particle potential $V_{s.p.}$

$$V_{s.p.} = V^{spher} + \eta r^2 Y_{20}$$

With this set we then solve the coupled BCS-eqs. (2-13) for neutrons and protons . Using the amplitudes v_{km} and u_{km} thus obtained , we solve the non-linear Hartree-Bogoliubov-Eqs. (2-14) for the coefficients $D^j_k(m)$ by iteration . Each step in this iteration involves the solution of the eqs. (2-14) for given potentials $\Gamma_{k_1 k_2}$ and $\Delta_{k_1 - k_2}$. Such a solution cannot be achieved by diagonalizing a hermitian matrix unless the pairing potential $\Delta_{k_1 - k_2}$ is neglected . It was , however , not difficult to develop a method of solution very similar to the Jacobi Method for diagonalizing a symmetric matrix . With the new values of the coefficients $D^j_k(m)$ the BCS-equations are now solved again and the whole procedure is repeated until the occupation probabilities v^2_{km} change by less than 5×10^{-4} in subsequent iterations .

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Table 1 : Parameters of Rosenfeld force

Table 2 : Single-particle energies

Table 3 : Quasi-particle energies (Sm^{152})

Table 4 : Parameters of Serber force

Table 5 : Comparison of selfconsistent results with results of a Nilsson calculation

Fig. 1 : Binding energy as a function of deformation (η) for various nuclei in the rare earth region (δ + quadrupole force)

Fig. 2 : Calculated and experimental quadrupole moments for rare earth nuclei (Rosenfeld force mixture, selfconsistent calculation)

Fig. 3 : Binding energy as a function of deformation for Sm^{152} (Rosenfeld force). The lines below the minima indicate the result of the selfconsistent calculation.

Fig. 4 : Calculated (o) and experimental (x) values for the moment of inertia $\Im$ of rare earth nuclei (Rosenfeld force mixture, self-consistent calculation, experimental values are taken from ref. 9).

Fig. 5 : Binding energy as a function of deformation δ for deformed light nuclei (Serber force) (Parameter δ defined as by S. G. Nilsson[3])

Fig. 6 : Calculated (o) and experimental (x) values for the intrinsic quadrupole moments of deformed light nuclei.
(Serber force, selfconsistent calculation).
A basic oscillator of $\hbar\omega$= 13,5 MeV was chosen for S^{32} and of $\hbar\omega$ = 14,62 MeV for the other nuclei.

TABLE 1

V_T^+ (MeV)	V_s^+	V_T^-	V_s^-	r_o(fe)
- 51. 9	- 31. 2	+ 17. 6	+ 92. 5	1. 732

TABLE 2

	$1h\frac{11}{2}$	$3p\frac{3}{2}$	$2f\frac{7}{2}$	$3p\frac{1}{2}$	$1i\frac{13}{2}$	$2f\frac{5}{2}$	$1h\frac{9}{2}$
$\varepsilon_{KK}^{(h)}$	- 5. 71	-1. 547	- 1. 400	-0. 58	0. 043	0. 7656	1. 70
	$1g\frac{9}{2}$	$2d\frac{5}{2}$	$1h\frac{11}{2}$	$1g\frac{7}{2}$	$3s\frac{1}{2}$	$2d\frac{3}{2}$	
$\varepsilon_{KK}^{(p)}$	-6. 24	-2. 73	-1. 03	- 0. 46	- 0. 43	-0. 317	

TABLE 3

$K = \frac{1}{2}$		$K = \frac{3}{2}$		$K = \frac{5}{2}$		$K = \frac{7}{2}$		$K = \frac{9}{2}$	
$\tilde{E}_{\gamma\gamma}$	E_γ	$\tilde{E}_{\gamma\gamma}$	E_γ	$\tilde{E}_{\gamma\gamma}$	E_γ	$\tilde{E}_{\gamma\gamma}$	E_γ	$\tilde{E}_{\gamma\gamma}$	E_γ
7. 40	7. 44	6. 78	6. 78	5. 56	5. 56	4. 50	4. 51	3. 96	3. 96
3. 75	3. 75	3. 46	3. 46	1. 47	1. 47	1. 41	1. 41	1. 79	1. 78
2. 82	2. 81	1. 41	1. 41	0. 931	0. 925	1. 145	1. 147		
2. 15	2. 14	0. 952	0. 951	0. 660	0. 660				
1. 58	1. 55	0. 903	0. 891						
1. 21	1. 21								

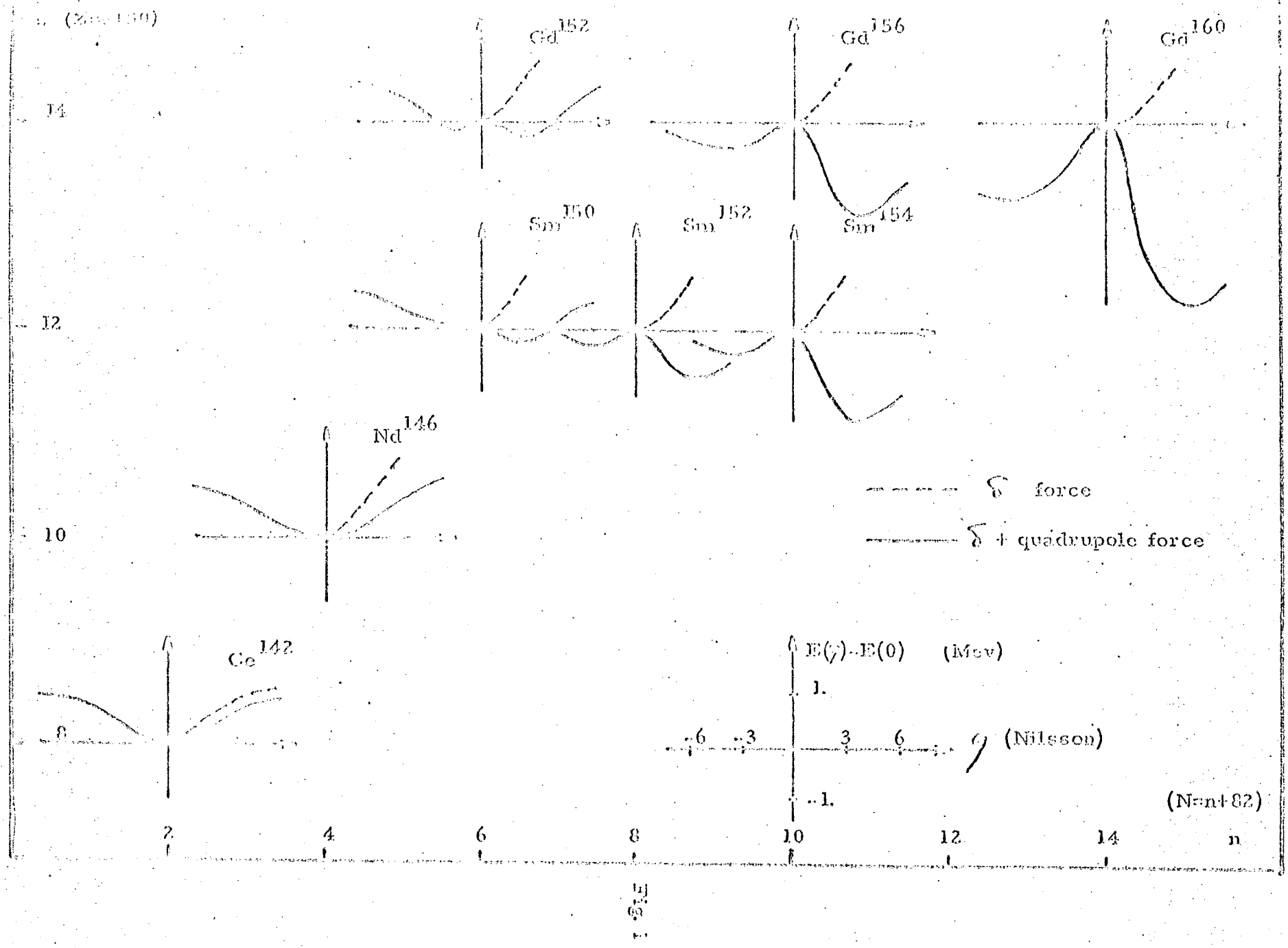
TABLE 4

	V_T^+ (MeV)	V_s^+	V_T^o	V_s^o	r_o (f_0)
Serberforce	- 48. 6	-33. 5	0	0	1. 7

			$K = 1p\frac{1}{2}$	$2p\frac{1}{2}$	$1p\frac{3}{2}$	$2p\frac{3}{2}$	$1f\frac{5}{2}$	$1f\frac{7}{2}$
$K = \frac{1^-}{2}$	$D_1 k^2$	s. c.	13. 6	0. 9	77. 2	7. 8	0. 1	0. 4
		N. P.	8	0	92	0	0	0
	$D_2 k^2$	s. c.	76. 5	8. 4	12. 2	2. 3	0. 5	0. 1
		N. P.	92	0	8	0	0	0
	$D_3 k^2$	s. c.	0. 8	11. 4	0. 8	16. 5	11. 5	59
		N. P.	0	25	0	5. 6	2	67
	$D_4 k^2$	s. c.	1. 5	17. 5	7. 2	56	6. 2	11. 6
		N. P.	0	8. 5	0	71	1	19. 5
	$D_5 k^2$	s. c.	0. 9	21. 8	0	3	54	20. 3
		N. P.	0	10. 6	0	0	89	0. 1
	$D_6 k^2$	s. c.	6. 7	40	2. 7	14. 2	27. 8	8. 6
		N. P.	0	55. 7	0	23	7. 9	13. 4

			$K = 1s\frac{1}{2}$	$2s\frac{1}{2}$	$1d\frac{3}{2}$	$1d\frac{5}{2}$
$K = \frac{1^+}{2}$	$D_1 k^2$	s. c.	93	6. 7	0. 1	0. 2
		N. P.	100	0	0	0
	$D_2 k^2$	s. c.	5	44	41	10
		N. P.	0	63	3	34
	$D_3 k^2$	s. c.	1	16	52	31
		N. P.	0	4	96	0
	$D_4 k^2$	s. c.	1	33	7	59
		N. P.	0	33	1	66

TABLE 5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12
10
8
Gd152
Gd156
Gd160
Sm150
Sm152
Sm154
Nd146
Ce142
δ force
δ + quadrupole force
E(γ)-E(0) (Mev)
1.
-1.
-6
-3
3
6
γ (Nilsson)
(N=n+82)
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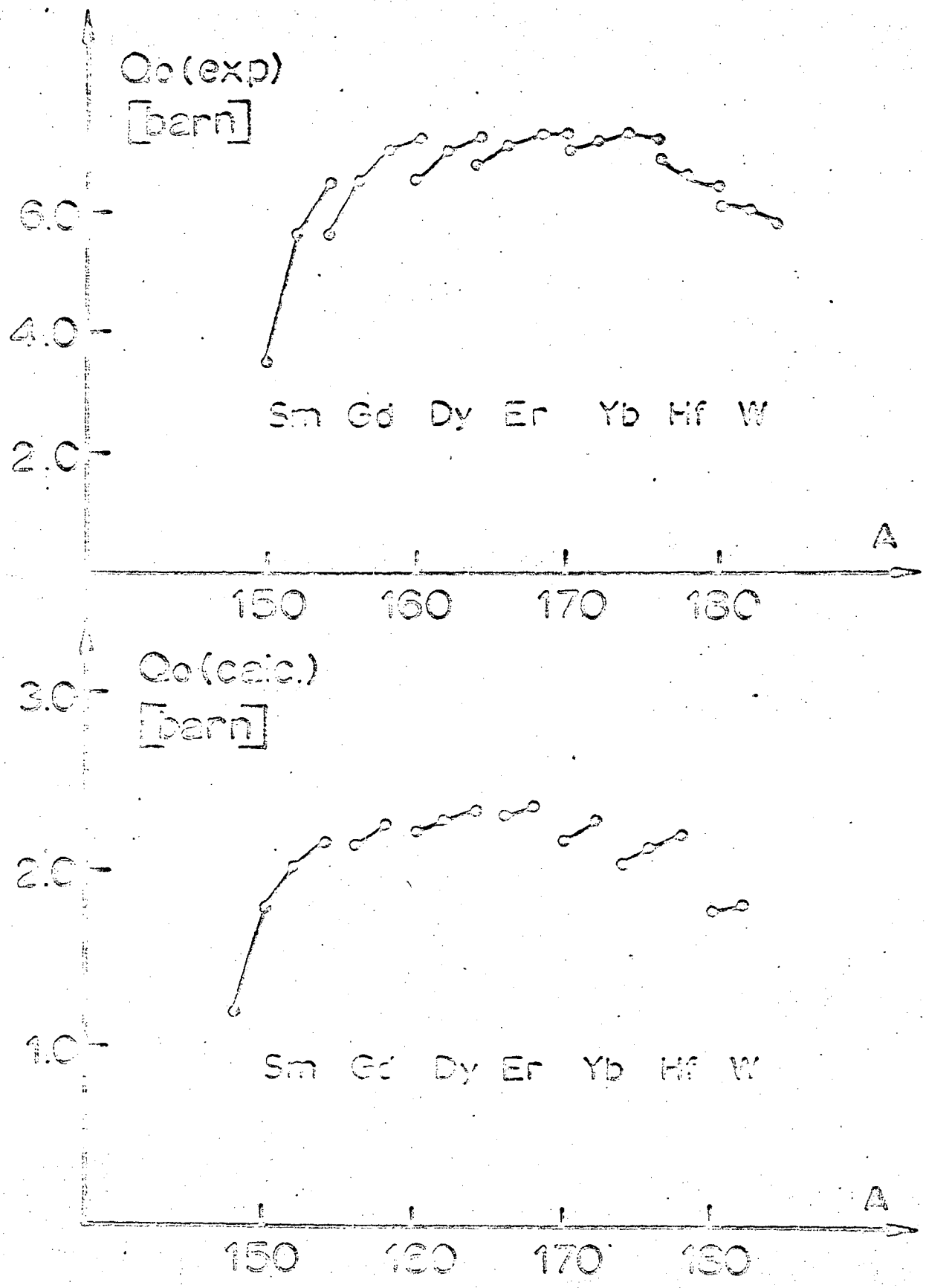
4
6
8
10
12
14
n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A
150 160 170 180

Figure 2

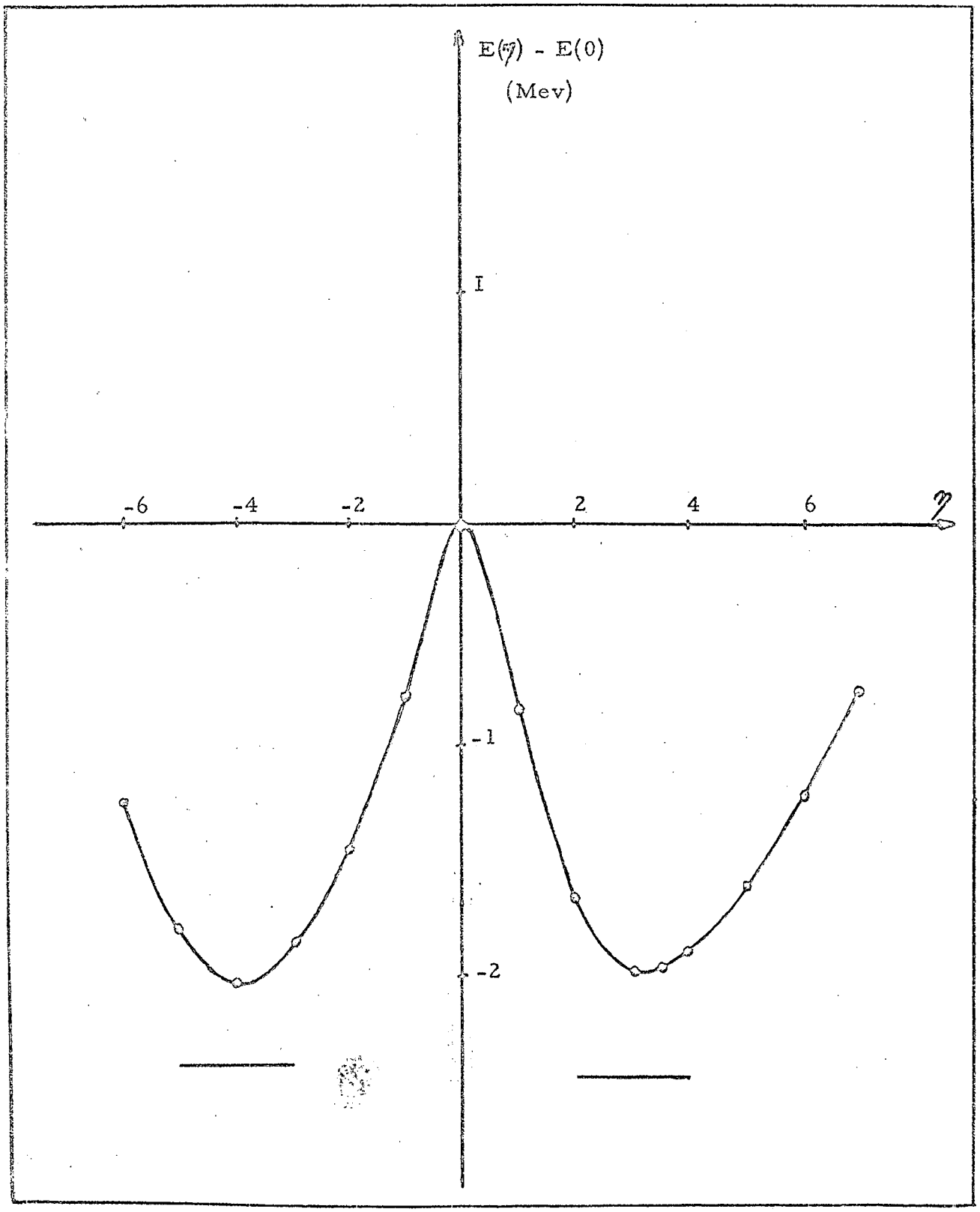
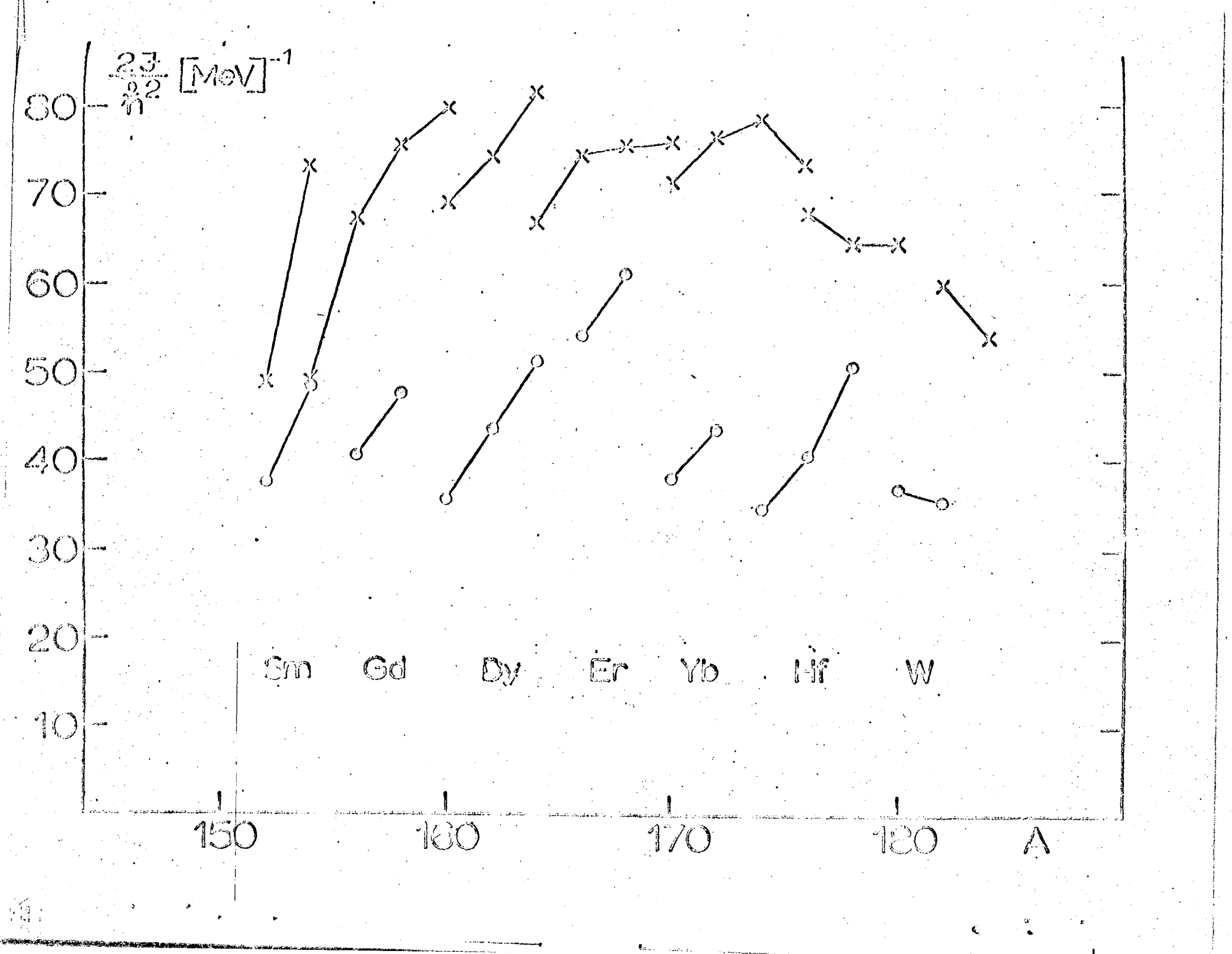


Fig. 3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60
50
40
30
20
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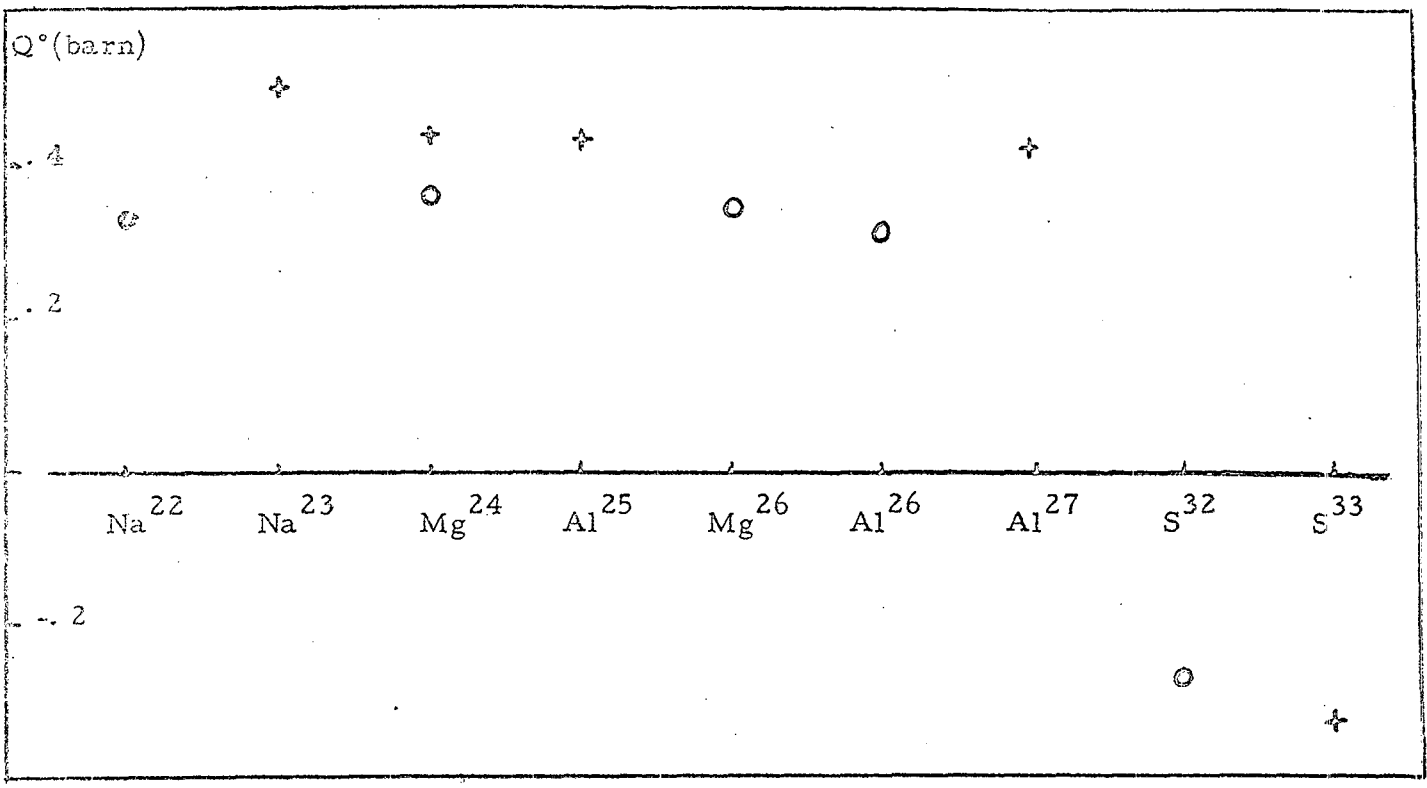
Sm
Gd
Dy
Er
Yb
Hf
W
150
160
170
180
A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-.2
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Na23
Mg24
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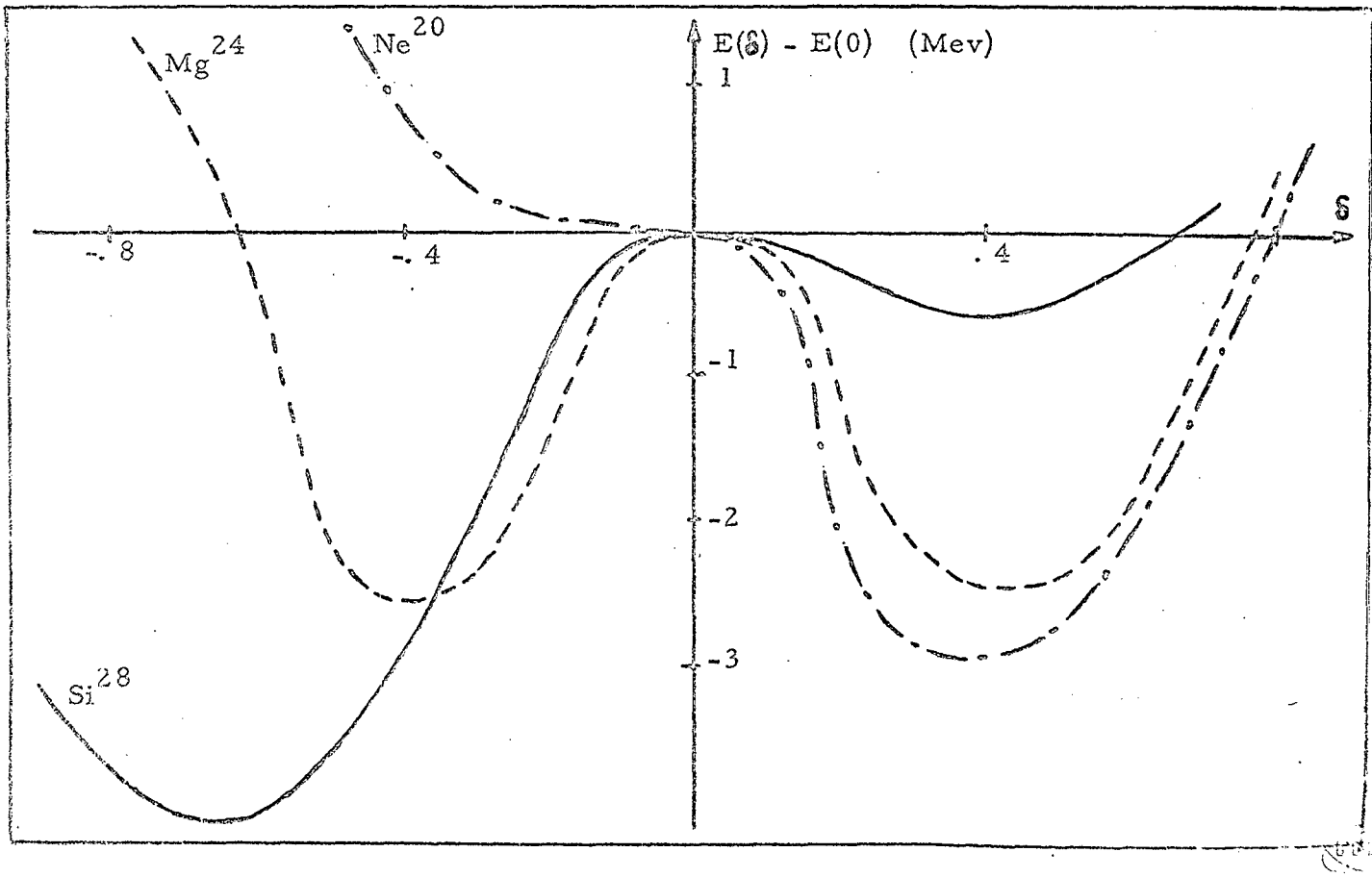
Mg26
Al26
Al27
S32
S33

Fig. 6

Fig. 5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E(δ) - E(0) (Mev)
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δ
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-.4
.4
-1
-2
-3
Si28