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The effect of pair correlation on the moment of inertia and the collective gyromagnetic ratio of deformed nuclei

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THE EFFECT OF PAIR CORRELATION ON
THE MOMENT OF INERTIA AND
THE COLLECTIVE GYROMAGNETIC RATIO
OF DEFORMED NUCLEI

BY

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i kommission hos Ejnar Munksgaard

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Synopsis

The moment of inertia and the collective gyromagnetic ratio of even-even nuclei are calculated on the basis of wave functions that take a pairing interaction into account through the quasi-particle formalism. The results obtained theoretically are found to be in reasonable agreement with experiments. The strength of the characteristic pair-correlation matrix element to be employed is estimated on the basis of data on odd-even mass differences. The dependence of the calculational results on the central-field parameters, as e. g. the eccentricity and the single-particle energy scale, is discussed. Other possible effects with particular relevance to the odd-even mass difference and the experimentally occurring energy gap are also surveyed.

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Introduction

The regions of deformed nuclei are empirically characterized by the occurrence of rotational bands in the nuclear excitation spectra. The characteristic energy spacings within these bands exhibit the well-known $I(I+1)$ dependence. The occurrence of such collective rotational states is largely independent of the detailed character of the intrinsic motion.

If one writes the rotational energy in the form

$$E_{\text{rot}} = \frac{\hbar^2}{2\mathfrak{J}} I(I+1), \quad (1)$$

the magnitude of the moment of inertia \mathfrak{J} , entering in the proportionality constant, provides, however, more of a test of the detailed nuclear model. For even-even nuclei two more intrinsic constants determine most of the properties of the low-lying states. One is the intrinsic quadrupole moment which determines the $E2$ transition strengths for gamma decay and for Coulomb excitation. The other constant, g_R , the gyromagnetic ratio of the collective flow, enters, for instance, when one measures the magnetic moment of a higher member of the ground-state rotational band. While \mathfrak{J} measures the mass of the collective flow, g_R is associated with the magnetic properties of the flow.

For odd-A nuclei, magnetic moments and decay probabilities within a rotational band also depend on some of the details of the odd-particle orbital in addition to the said quantities connected with the even-even ground-state band.

The present work is based on the "cranking model"⁽¹⁾. This model corresponds to the approximation that the self-consistent field determining the single-particle orbitals is cranked around externally. The rotational energy of the system is then calculated as the extra energy necessary for the nucleons to follow a slow rotation. The cranking model applied on the basis of a completely-independent-particle description gives a value of the moment of inertia approximately equal to that of rigid motion, provided one chooses

the equilibrium value of the deformation of the nuclear field^(2,3). The empirical values amount, however, to only 20-50 % of the rigid moment of inertia.

BOHR and MOTTELSON⁽²⁾ gave general arguments to the effect that a residual short-range attractive interaction between the particles—the latter being assumed in the first approximation to move independently in a common field—would decrease the value of the moment of inertia. They also studied the effects explicitly in terms of a very simplified "two-particle model". The strength that such an additional interaction must have to reproduce the empirical situation was found to be of the order usually attributed to the short-range inter-particle force. It remained, however, to treat such an inter-particle force in the case of a large number of particles outside of closed shells.

Such an additional inter-particle force, the pair-correlation force, which allows a complete treatment even when many particles are involved, has recently been introduced into nuclear physics by BOHR, MOTTELSON and PINES^(4,3,5), by BELYAEV⁽⁶⁾, and by SOLOVIEV⁽⁷⁾ and other authors of the Bogolubov school. These authors employ and adapt to nuclear physics the elegant and powerful methods developed by BARDEEN and others⁽⁸⁾ to explain the phenomenon of superconductivity. Such a pairing interaction is first of all capable of explaining the empirically encountered energy gap in the spectra of even-even nuclei. For an example of the empirical occurrence of such a gap, take for instance the region of rare-earth nuclei $150 < A < 190$. The empirical average energy spacing of intrinsic excitations appears to be of the order of 150 keV (which seems to indicate a single-particle level density of about one level per 300 keV). In even-even nuclei in this region, however, there exist experimentally no excited states that are not of collective character below ~ 1000 keV. Such an energy gap cannot be explained by the mere assumption of an additional diagonal pairing energy, effective between the pair of particles filling the degenerate orbitals K and $-K$. This would indeed forbid the breaking of such a pair, but could not prevent low-lying two-particle excitations; the latter would occur with an average level density of one state per 300 keV or so, where about half the states would correspond to excited proton pairs and half to neutron pairs.

As pointed out, the pair-correlation interaction is capable of explaining this very conspicuous feature of even-even spectra. Expressed in terms of the single-particle states of the average nuclear potential, the pair-correlation interaction thus scatters pairs of particles from the originally filled lower-lying, doubly degenerate single-particle orbitals into the higher-lying levels which are left unoccupied according to the earlier description. The new

total intrinsic wave function that most effectively utilizes this additional type of interaction and represents the ground state is then a state with a diffuse Fermi surface. In this state there exists a particular correlation between all the scattering pairs of particles within the region of diffuseness of the Fermi surface. Any excited state which thus involves the formation of a state orthogonal to the ground state then necessarily spoils some of the correlation and is therefore associated with an excitation energy of at least about the width of the diffuseness of the Fermi surface.

The investigation reported in this paper appears to bear out the contention that the introduced pair-correlation interaction in the regions of deformed nuclei is capable of explaining quantitatively at the same time the occurrence and magnitude of the energy gap in the spectra of even-even nuclei, the even-odd-mass difference, and the magnitude of the moment of inertia associated with the collective rotation. A computation of the moment of inertia rather similar in scope to the one reported here has been carried through by GRIFFIN and RICH⁽⁹⁾. Also the investigations by MIRDAL⁽¹⁰⁾ and by HACKENBROICH⁽¹¹⁾ contain some numerical results largely in line with the results obtained in the publication cited above as well as with those of the present paper.

A preliminary report of the present calculations was presented at the Conference of the Swedish Physical Society in June, 1959⁽¹²⁾.

I. The Hamiltonian Describing the Intrinsic Motion of Deformed Nuclei with the Inclusion of the Pair Correlation

The application of the quasi-particle formalism in the nuclear case is described in detail in the paper by BELYAEV⁽⁵⁾. For the reader's convenience we shall, however, give a short account of the most important results.

Let the Hamiltonian of the (static) self-consistent nuclear field be denoted H_s . The corresponding single-particle eigenfunctions are first characterized by the eigenvalue K of the angular-momentum component along the nuclear axis. This component is a constant of the motion provided H_s exhibits cylindrical symmetry. Furthermore, under the condition that the system is invariant under time reversal there always exist two states degenerate in energy, each of which is the time reverse of the other. Under the additional requirement of cylinder symmetry these may be labelled by the components of angular momentum K and $-K$.

We define such a single-particle state as $|\nu\rangle$, where ν denotes both the K -value and the additional quantum numbers necessary for the complete specification of the state. It is sometimes convenient to consider such a state expanded in terms of eigenstates of the angular momentum j as follows:

$$|\nu\rangle = \sum_j c_j^{\nu} \chi_K^j. \quad (2)$$

We then define the conjugate $|\bar{\nu}\rangle$ state, which corresponds to the nucleonic orbit with a completely reversed direction of motion compared with $|\nu\rangle$, as*

$$|\bar{\nu}\rangle = \sum_j (-)^{l+j-K} c_j^{\nu} \chi_{-K}^j, \quad (3)$$

where the phases of χ_K^j and χ_{-K}^j are defined in accordance with the conventions of CONDON and SHORTLEY⁽¹³⁾. As already pointed out, this definition of the conjugate state makes it equal to the time-reversed state $T|\nu\rangle$, possibly apart from a conventional phase. In the following we shall employ the relation

$$T|\nu\rangle = |\bar{\nu}\rangle, \quad (4)$$

which then fixes the arbitrary phase of T . We denote the eigenvalues of H_s by ε_ν . Furthermore we assume that both ε_ν and $|\nu\rangle$ can be taken with sufficient accuracy from the calculations by MORTELSON and NILSSON^(15,16). The remaining, most important features of the inter-particle forces, which correspond to the very short range components of these forces, may now (cf. references 3, 5, 6) be simulated by the said pair-correlation interaction. In its simplified form this interaction may be written in second-quantization language

$$H^{\text{pair}} = -G \sum_{\nu\nu'} a_{\nu'}^{\dagger} a_{-\nu'}^{\dagger} a_{-\nu} a_{\nu}. \quad (5)$$

Eq. (5) represents the limiting assumption that the residual force acts only when two particles move in a $J = 0$ state. The said force displays the main features of the δ -force, although the latter has minor but non-negligible effects on pairs of particles in states of non-vanishing but small angular momentum.

In this notation a one-particle state is expressed as follows in terms of the creation operator a_{ν}^{\dagger} :

$$|\nu\rangle = a_{\nu}^{\dagger} |0\rangle. \quad (6)$$

* By redefinition of the spherical harmonics as $Y_{lm} = i^l Y_{lm}$, where Y_{lm} is the conventional spherical harmonic defined in accordance with the CONDON-SHORTLEY⁽¹³⁾ phase conventions, the parity sign in (3) or $(-)^j$ may be absorbed into $|\bar{\nu}\rangle$ (see EDMONDS⁽¹⁴⁾). This parity sign is furthermore unimportant in our calculations.

With the inclusion of H_s the total Hamiltonian takes the form

$$H = \sum_{\nu} \varepsilon_{\nu} (a_{\nu}^{\dagger} a_{\nu} + a_{-\nu}^{\dagger} a_{-\nu}) - G \sum_{\nu\nu'} a_{\nu'}^{\dagger} a_{-\nu'}^{\dagger} a_{-\nu} a_{\nu}. \quad (7)$$

The great advantage of the second-quantization formalism is that it automatically ensures compliance with the Pauli principle. This principle is built into the formalism by the usual anti-commutation relations which the a_{ν}, s are required to obey.

The obvious aim is now to find an eigenfunction of the Hamiltonian (7) that is in addition an eigenfunction of the number operator

$$N = \sum_{\nu} (a_{\nu}^{\dagger} a_{\nu} + a_{-\nu}^{\dagger} a_{-\nu}). \quad (8)$$

BARDEEN et al. find a convenient but approximate eigenfunction of (7) at the cost of weakening the latter condition* and replacing it by a condition for the average value of N :

$$\langle \Psi | N | \Psi \rangle = n. \quad (9)$$

In conformity with the fact that the number of particles is conserved only on the average, the solution corresponds physically to an ensemble of nuclei having slightly different numbers of nucleons. The procedure for treating this new simplified problem is then to introduce an auxiliary Hamiltonian H' :

$$H' = H - \lambda N, \quad (10)$$

where λ , treated as a Lagrangian multiplier, takes the role of the chemical potential. Thus λ represents the energy of the last added particle.

* A method for obtaining wave functions which fulfil this condition exactly has recently been discussed by B. BAYMAN⁽¹⁷⁾.

II. The Bardeen-Cooper-Schrieffer Trial Function and the Canonical Transformation of the Hamiltonian Considered to a Hamiltonian Describing Independent Quasi-Particles

BARDEEN et al. employ a trial wave function of the following type to minimize H' :

$$\Psi_0 = \prod_{\nu} (u_{\nu} + v_{\nu} a_{\nu}^{\dagger} a_{-\nu}^{\dagger}) |0\rangle. \quad (11)$$

In eq. (11), u_{ν} and v_{ν} are free parameters, subject only to the normalization condition, which can be fulfilled by the requirement

$$u_{\nu}^2 + v_{\nu}^2 = 1, \quad (12)$$

and to the auxiliary condition (9), which takes the form

$$n = 2 \sum_{\nu} v_{\nu}^2 \quad (13)$$

in terms of the parameters introduced.

The variational calculation leads to the equations^(3, 6)

$$(\epsilon_{\nu} - \lambda) 2 u_{\nu} v_{\nu} - G \sum_{\nu'} u_{\nu'} v_{\nu'} (u_{\nu}^2 - v_{\nu}^2) - 2 G v_{\nu}^2 u_{\nu} v_{\nu} = 0. \quad (14)$$

The last term in (14) is small compared with the second (except in a region near the Fermi surface) and is usually neglected or assumed to be included in the self-consistent field energies ϵ_{ν} .

If one chooses to neglect the third term, one obtains for u_{ν} and v_{ν} the simple expressions

$$u_{\nu}^2 = \frac{1}{2} \left(1 + \frac{\epsilon_{\nu} - \lambda}{E_{\nu}} \right), \quad (15 a)$$

$$v_{\nu}^2 = \frac{1}{2} \left(1 - \frac{\epsilon_{\nu} - \lambda}{E_{\nu}} \right), \quad (15 b)$$

and for the energy of the ground state the expression

$$\langle H' \rangle + \lambda \langle N' \rangle = \sum_{\nu} \epsilon_{\nu} 2 v_{\nu}^2 - \frac{\Delta^2}{G} - G \sum_{\nu} v_{\nu}^4, \quad (16)$$

* Concerning a method of accounting for this term by perturbation theory, see Appendix I.

where the third term is again of self-energy origin and is usually neglected as small compared with the second term (see the discussion below).

In eqs. (14) and (15) we have used the definitions

$$E_{\nu} = \sqrt{(\epsilon_{\nu} - \lambda)^2 + \Delta^2} \quad (17)$$

and

$$\Delta = G \sum_{\nu} u_{\nu} v_{\nu}. \quad (18)$$

Provided the ϵ_{ν} 's (the single-particle energies of the deformed field) are given and G is known, the auxiliary parameters λ and Δ can be determined from eqs. (18) and (13). The interpretation of v_{ν}^2 as the probability of the state ν being populated by a pair is borne out by eq. (13).

An equivalent way to obtain the ground-state energy given by eq. (16) and the corresponding wave function is provided by the BOGOLUBOV-V ALA-TIN⁽⁸⁾ transformation to quasi-particles (the creation operator of a quasi-particle is a linear combination of the corresponding particle operator and the operator creating a hole of opposite angular momentum)

$$\alpha_{\nu} = u_{\nu} a_{\nu} - v_{\nu} a_{-\nu}^{\dagger}, \quad (19 a)$$

$$\alpha_{-\nu} \equiv \beta_{\nu} = u_{\nu} a_{-\nu} + v_{\nu} a_{\nu}^{\dagger}. \quad (19 b)$$

In terms of α_{ν} and β_{ν} the transformed Hamiltonian H' is

$$H' = U' + H'_{11} + H'_{20} + H'_{\text{int}} \quad (20)$$

when written in its normal form, i. e. with α^{\dagger} , β^{\dagger} in front of β , α . In terms of the quasi-particle operators, U' is then a constant, H'_{11} is an operator that can destroy and recreate one quasi-particle at a time (and, furthermore, contains only the particular combinations $\alpha_{\nu}^{\dagger} \alpha_{\nu}$ and $\beta_{\nu}^{\dagger} \beta_{\nu}$), while H'_{20} can either destroy or create two quasi-particles. The operator H'_{int} contains products of four-quasi-particle operators and can be split up into the terms H'_{22} , H'_{31} and H'_{40} (the notation should be obvious from the above). It is discussed in more detail by BELYAEV⁽⁶⁾ and in Appendix I of the present paper.

The imposed condition that H'_{20} vanishes identically leads to eq. (14), whereby u_{ν} and v_{ν} are determined. As H'_{11} is a function only of the occupation number of the quasi-particles, we are then left with a system of non-interacting quasi-particles in the approximation that H'_{int} may be neglected. Indeed, as far as the ground state, i. e. the no-quasi-particle state, is concerned, only H'_{40} of the neglected H'_{int} term has non-vanishing matrix

elements connected with this state. The magnitude of this coupling is thus a measure of the lack of generality of the trial function (11). In this respect the quasi-particle formalism forms a complement to the variational procedure. The effect of H'_{40} on the ground-state wave function is fundamentally small of the order $\frac{G}{2\Delta}$. One may take the quantity:^{*}

$$\Omega_{\text{eff}} = \frac{2\Delta}{G} = \sum_p \frac{1}{\sqrt{(\epsilon_p - \lambda)^2 + 1}} \quad (21)$$

as a measure of the accuracy of the approximation. The definition may be less suitable in cases where the level density of single-particle states is very different above and below the Fermi surface. It is quite satisfactory for our purposes as the single-particle levels are rather evenly distributed in the cases treated here.

It should be noted at this point that the neglected term in (14) is also small of just this order $\frac{G}{2\Delta}$.

The ground state Ψ_0 of an even-even nucleus, given by (11), thus defines the quasi-particle vacuum; it will be denoted $|0\rangle\rangle$ in the following and is characterized by the condition

$$\alpha_p \Psi_0 \equiv \alpha_p |0\rangle\rangle = 0. \quad (22)$$

We now turn to the ground state of an odd-A nucleide. The odd particle here occupies, say, the orbital ϵ_p . This particle is entirely unaffected by the pairing force, which only scatters pairs of particles. The trial function of the ground state of such an odd-particle system is obviously

$$\Psi^{\text{odd}} = a_p^+ \prod_{p \neq p'} (u_p + v_p a_p^+ a_{-p}^+) |0\rangle. \quad (23)$$

Now u_p and v_p are still given by eqs. (15), but the sums over states in eqs. (13) and (18), which determine Δ and λ , now exclude the "blocked" p' state; furthermore, n in (13) has to be replaced by $(n-1)$.

The effect on λ is a trivial one; if p' lies near the Fermi surface (as it must for the ground state of an odd system), λ is not appreciably changed with respect to the "even" case of $n/2$ pairs. As Ω_{eff} terms in fact contribute to (18), the exclusion of one term appears again to imply an error of the order $\frac{1}{\Omega_{\text{eff}}}$, the

* The formula (21) gives values of Ω_{eff} about 5-10 for the actual calculations we have performed.

fundamental inaccuracy of the BCS-solution. If we neglect this blocking effect for the moment, we end up with the same u_p and v_p as in the "even" cases. Therefore we still have the same quasi-particle vacuum, and we may write Ψ^{odd} in a form identical with (23):^{*}

$$\Psi^{\text{odd}} = \alpha_p^+ |0\rangle\rangle. \quad (23')$$

The additional energy of this one-quasi-particle state compared with the vacuum state (the "even" case of $n/2$ pairs) is most easily obtained from

$$H'_{11} \equiv \sum_p \{ (\epsilon_p - \lambda) (u_p^2 - v_p^2) + \Delta^2 u_p v_p - G v_p^2 (u_p^2 - v_p^2) \} (\alpha_p^+ \alpha_p + \beta_p^+ \beta_p). \quad (24)$$

The last term in (24) is small, again of the order $\frac{G}{2\Delta}$, compared with the sum of the first two terms, and often much smaller because of the factor $(u_p^2 - v_p^2)$. The neglect of this term thus amounts to an approximation of the same order as that due to the neglect of H'_{40} etc. We then arrive at the simple relation

$$H'_{11} \simeq \sum_p E_p (\alpha_p^+ \alpha_p + \beta_p^+ \beta_p). \quad (24')$$

The odd-even mass difference, which we have here defined as the difference in mass between an odd-system and the "even" system^{**} having $n/2$ pairs and thus no orbital blocked, in this approximation simply equals E_p . This quantity is in turn very near to Δ for the ground state of the odd-n system, as $(\epsilon_p - \lambda)^2$ is very small compared with Δ^2 (usually of the order of a few per cent).

The spectrum of excited states of an odd-A nucleus is given in this approximation by the quasi-particle energies E_p . As the single-particle level density is of the order of one state per 300 keV on the average, compared with an average Δ of between 500 and 1000 keV, this would lead to a level density in odd-A nuclei of the order of one state per 50-100 keV for excitation energies smaller than Δ , which is contrary to experience⁽¹⁶⁾. It appears that of the approximations made, involving terms of the order of $\frac{G}{2\Delta}$, the neglect of the blocking effects described on page 10 may be the most serious^{***}.

* i.e. a system described by eq. (11) treated formally as if n were an even number.

** A comparison with the results of an exact diagonalization performed for a particular case of six levels and three pairs (corresponding to a 20×20 matrix) clearly bears out this contention.

*** This effect has also been studied recently by SOLOVIEV⁽¹⁶⁾.

One may estimate the change in Δ between the even and the odd case due to the blocking of one level by the odd particle as*

$$\Delta^{\text{odd}} \simeq \Delta^e - \frac{1}{(\Delta^e)^2} \left(\sum_{\nu \neq \nu'} \frac{1}{E_\nu^3} \right)^{-1}. \quad (25)$$

In obtaining this formula we have neglected terms of the type $\sum_{\nu} (\epsilon_\nu - \lambda) E_\nu^{-n}$ as being small compared with $\Delta \sum_{\nu} E_\nu^{-n}$. As is obvious from (25), the difference $(\Delta^e - \Delta^{\text{odd}})$ depends somewhat on the cut-off of the sum over ν in $\sum_{\nu} \frac{1}{E_\nu^3}$. The change in Δ , leading to a change in u_ν and v_ν also for $\nu \neq \nu'$, also affects the odd-even mass difference. If one makes the same approximations as in deriving (25), one obtains for the odd-even mass difference P the expression

$$P \simeq \Delta^e + \frac{1}{(\Delta^e)^2} \left(\sum_{\nu \neq \nu'} \frac{1}{E_\nu^3} \right)^{-1} G + \frac{2}{4} \Delta^e \left(\sum_{\nu \neq \nu'} \frac{E_\nu^4}{E_\nu^3} \right)^{-1} \left(\sum_{\nu \neq \nu'} \frac{(\epsilon_\nu - \lambda)^2}{E_\nu^3} \right)^{-1}. \quad (26)$$

In deriving (26) we have included the "self-energy" terms from (16). They give as a result the third term in (26). While the neglect of these terms leads to the relation $P > \Delta^e$ to first order in $\delta\Delta$, the inclusion of these and of terms of higher order results in a P smaller than Δ^e by a magnitude of the order of 10^{-10} in the present cases (see table II). The results of table II correspond to an exact inclusion of the blocking effect, but are generally in line with eq. (26).**

Of interest to us here are finally the lowest excited states in an even-even nucleus, which correspond to the excitations of two quasi-particles. Take as an example a state reached from the ground state by the j_x operator considered in section III. Such a state is e. g.

$$\Psi_{\nu'-\nu''} \equiv \alpha_{\nu'}^{\dagger} \beta_{\nu''}^{\dagger} | 0 \rangle \rangle \equiv \alpha_{\nu'}^{\dagger} \alpha_{-\nu''}^{\dagger} \prod_{\nu \neq \nu', \nu''} (u_\nu + v_\nu a_{\nu}^{\dagger} \alpha_{-\nu}^{\dagger}) | 0 \rangle. \quad (27)$$

* On account of the rapid convergence of the sum in eq. (25) the choice of the cut-off energies $\lambda \pm D$ is not very critical provided $D \gg \Delta$. Assuming a constant level density ϱ and furthermore $\Delta \gg \frac{1}{\varrho}$, one obtains the estimate $\Delta^{\text{odd}} \simeq \Delta^e - \frac{1}{2\varrho}$. The actual calculations, in which the "blocking" effects have been included exactly, indicate a difference in Δ between systems with even and odd numbers of particles of the order of 20% , as exhibited in table II. These results are roughly in agreement with eq. (25) and the estimate above.

** The arbitrariness in the choice of the cut-off energy enters (26) through the relation between G and Δ , which depends more critically on the cut-off energy than does eq. (25).

In the approximation implied by this equation (where, for $\nu \neq \nu', \nu'', u_\nu$ and v_ν are the same as in the no-quasi-particle ground state) the excitation energy is given simply by application of H_{II}^+ as

$$\mathcal{E}^{(\nu', -\nu'')} - \mathcal{E}^{(0)} = \bar{E}_{\nu'} + E_{\nu''} \geq 2\Delta. \quad (28)$$

As the reduction in the effective Δ , i. e. in the diffuseness of the Fermi surface, is considerable in this two-quasi-particle state, owing to the blocking of two levels, one might be tempted to correct for this error in line with what is done above for the one-quasi-particle state, and write as an alternative to eq. (27)*

$$\Psi_{\nu'-\nu''} \equiv \alpha_{\nu'}^{\dagger} \alpha_{-\nu''}^{\dagger} \prod_{\nu \neq \nu', \nu''} (u_\nu^{(\nu', \nu'')} + v_\nu^{(\nu', \nu'')} \alpha_{\nu}^{\dagger} \alpha_{-\nu}^{\dagger}) | 0 \rangle, \quad (27')$$

where $u_\nu^{(\nu', \nu'')}$ and $v_\nu^{(\nu', \nu'')}$ are thus calculated from (14) with two single-particle levels blocked. The excitation energy of this state (27') must be calculated via the total energies (16) obtained from variational calculations applied to the excited state, respectively to the ground state. It is obvious that a quasi-particle description has no advantage if one wants to include the effects of blocking, as we should then be forced to assume a vacuum for the excited state different from that of the ground state.

III. General Formula for the Moment of Inertia and the Collective Gyromagnetic Ratio in Terms of the Quasi-Particle Formalism

A derivation of the formula for the moment of inertia based on the cranking approximation has already been given in the quasi-particle formalism by BELVAEV⁽⁶⁾. The exposition of ref. 6 appears not explicitly to include the case of the single-particle angular-momentum component being equal to $1/2$. Although the explicit inclusion of this case only amounts to a minor modification, we shall repeat the general lines of the derivation.

We first express j_x , the operator associated with the rotation of the field of an individual particle, in terms of creation and annihilation operators α^{\dagger} and α . By the indices ν, ν' we denote combinations of states for which K_ν

* It is easily verified that this state is orthogonal to the ground state.

and K_{ν} do not both equal $1/2$. The indices μ, μ' are then reserved for combinations of orbitals that both have $K = 1/2$.

$$\begin{aligned}
 j_x^{\text{op}} = & \sum_{\nu\nu'} \left\{ \langle \nu | j_x | \nu' \rangle a_{\nu}^+ a_{\nu'} \right. \\
 & + \langle -\nu | j_x | -\nu' \rangle a_{-\nu}^+ a_{-\nu'} \left. + \sum_{\mu\mu'} \left\{ \langle \mu | j_x | -\mu' \rangle a_{\mu}^+ a_{-\mu'} \right. \right. \\
 & \left. \left. + \langle -\mu | j_x | \mu' \rangle a_{-\mu}^+ a_{\mu'} \right\} \right\} \quad (29)
 \end{aligned}$$

Employing the phase convention implied by eq. (4), one can readily prove the relations

$$\langle \nu | j_x | \nu' \rangle = -\langle -\nu' | j_x | -\nu \rangle \quad (30)$$

and

$$\langle \mu | j_x | -\mu' \rangle = \langle -\mu | j_x | \mu' \rangle. \quad (31)$$

To prove (30) one may for instance use the fact that the time reflection operator T is a product of a unitary operator and the complex conjugation operator, to obtain

$$\langle \nu | j_x | \nu' \rangle = \langle T\nu | Tj_x T^{-1} | T\nu' \rangle^* \quad (32)$$

To arrive at (30) one has then only to employ the facts a) that j_x is a Hermitian operator, b) that it changes sign under time reversal. To derive eq. (31) one must in addition use the fact that the matrix elements of j_x are real in the representation employed here.

The next step is to transform eq. (29) by the canonical transformations (19 a, b), using (30) and (31). We may then write

$$j_x^{\text{op}} = (j_x)_{11} + (j_x)_{20}, \quad (33)$$

where $(j_x)_{11}$ thus first destroys and then creates a quasi-particle. It can therefore have no matrix elements with the ground state of an even-even nucleus, which is just the quasi-particle vacuum. On the other hand, $(j_x)_{20}$ creates a two-quasi-particle state from the quasi-particle vacuum $|0\rangle\rangle$:

$$\begin{aligned}
 j_x^{\text{op}} |0\rangle\rangle = & \sum_{\nu\nu'} \langle \nu | j_x | \nu' \rangle (u_{\nu} v_{\nu'} - v_{\nu} u_{\nu'}) \alpha_{\nu}^+ \beta_{\nu'}^+ |0\rangle\rangle \\
 & + \sum_{\mu\mu'} \langle \mu | j_x | -\mu' \rangle (u_{\mu} v_{\mu'} - v_{\mu} u_{\mu'}) \frac{1}{2} (\alpha_{\mu}^+ \alpha_{\mu'}^+ + \beta_{\mu}^+ \beta_{\mu'}^+) |0\rangle\rangle. \quad (34)
 \end{aligned}$$

Now the two-quasi-particle states $\alpha_{\nu}^+ \beta_{\nu'}^+ |0\rangle\rangle$ and $\alpha_{\nu}^+ \beta_{\nu'}^+ |0\rangle\rangle$ both correspond to an excitation energy $E_{\nu\nu'} + E_{\nu'}$, measured with respect to the energy of the quasi-particle vacuum. These two states differ in their sign of the

angular-momentum component. Similarly, $\alpha_{\mu}^+ \alpha_{\mu'}^+ |0\rangle\rangle$ and $\beta_{\mu}^+ \beta_{\mu'}^+ |0\rangle\rangle$ both have the energy $E_{\mu} + E_{\mu'}$, but have $K = 1$ and -1 respectively. Thus the contributions from these transitions do not interfere. Although in eq. (34) the ν - and μ -sums do not at first glance appear quite symmetrical with respect to one another, their contributions to the moment of inertia are quite analogous. We finally obtain the following formula for the moment of inertia:

$$\begin{aligned}
 \mathfrak{J} = 2\hbar^2 \left\{ \sum_{\nu\nu'} \frac{|\langle \nu | j_x | \nu' \rangle|^2}{E_{\nu} + E_{\nu'}} (u_{\nu} v_{\nu'} - v_{\nu} u_{\nu'})^2 \right. \\
 \left. + \sum_{\mu\mu'} \frac{|\langle \mu | j_x | -\mu' \rangle|^2}{E_{\mu} + E_{\mu'}} (u_{\mu} v_{\mu'} - v_{\mu} u_{\mu'})^2 \right\} \quad (K_{\mu} = K_{\mu'} = 1/2). \quad (35)
 \end{aligned}$$

Indeed the second term can be formally included in the first, provided one remembers to take also the matrix elements between $K = 1/2$ and $K' = -1/2$ into account. Really there is no asymmetry between the ν and μ terms, as to every $\langle \nu | j_x | \nu' \rangle$ transition there corresponds a $\langle -\nu | j_x | -\nu' \rangle$ transition, of which only the first is counted formally in (35); further, to every $\langle \mu | j_x | -\mu' \rangle$ transition counted in (35) there corresponds a $\langle -\mu | j_x | \mu' \rangle$ transition which is not written out explicitly in (35).

The collective rotation takes place perpendicularly to the nuclear symmetry axis and is associated with the collective angular momentum \vec{R} . In an odd-A nucleus \vec{R} couples with the angular-momentum component K of the odd particle to form the total angular momentum \vec{I} , the nuclear spin. On the other hand, in the ground state of an even-even nucleus we have simply $\vec{R} = \vec{I}$. The collective flow of protons and neutrons building up the \vec{R} also gives rise to an instantaneous magnetic moment associated with the operator

$$\vec{\mu}_{\text{coll}} = \sum_{\nu} \vec{\mu}_{\nu} = \sum_{\nu} (g_{\nu}^i \vec{s}_{\nu} + g_{\nu}^i \vec{l}_{\nu}), \quad (36)$$

where the sum runs over the paired nucleons. One may express this magnetic moment in terms of a collective gyromagnetic ratio g_R defined by the relation

$$\vec{\mu}_{\text{coll}} \equiv g_R \vec{R}. \quad (37)$$

(The definition is of course limited to matrix elements of the operator $\vec{\mu}_{\text{coll}}$ that are diagonal with respect to the intrinsic nuclear wave function.)

In the cranking approximation the gyromagnetic ratio g_R takes the form⁽²⁾

$$g_R = \frac{\hbar^2}{\mathfrak{S}} \sum_{\beta} \frac{\langle \Phi_{\alpha} | \mu_x | \Phi_{\beta} \rangle \langle \Phi_{\beta} | J_x | \Phi_{\alpha} \rangle}{\varepsilon_{\beta} - \varepsilon_{\alpha}} + \text{c. c.}, \quad (38)$$

where $J_x = \sum_{\beta} j_x^{\beta}$ is the angular-momentum operator associated with the rotation. As μ_x transforms under time reflection in the same way as J_x , the inclusion of the pair-correlation interaction is completely analogous to the procedure employed on pp. 13-15. We just give the final expression

$$g_R = \frac{\mathfrak{S}^p}{\mathfrak{S}} + (g_s^p - 1) \frac{W_n^p}{\mathfrak{S}} + g_s^m \frac{W_n^m}{\mathfrak{S}}, \quad (39)$$

where

$$\frac{1}{2} \frac{W}{\hbar^2} = \left. \begin{aligned} & \sum_{\nu\nu'} \frac{\langle \nu' | j_x | \nu \rangle \langle \nu | s_x | \nu' \rangle}{E_{\nu} + E_{\nu'}} \langle u_{\nu} u_{\nu'} - v_{\nu} v_{\nu'} \rangle^2 \\ & + \sum_{\mu\mu'} \frac{\langle \mu | s_x | -\mu' \rangle \langle -\mu' | j_x | \mu \rangle}{E_{\mu} + E_{\mu'}} \langle u_{\mu} v_{\mu'} - v_{\mu} u_{\mu'} \rangle^2 \end{aligned} \right\} \quad (40)$$

Thus, apart from the spin contributions (given by the last two terms of (39)) to the magnetic moment of the collective flow, g_R is just the relative fraction contributed by the protons to the moment of inertia or, in other words, the effective charge of the collective flow. Of the last two terms of (39), W_p is the sum over all proton states and W_n the sum over all neutron states of the expression (40). The contribution from the terms containing W is small and is largely cancelled, as $(g_s^p - 1)$ is very nearly of the same magnitude as g_s^m and of opposite sign.

It has already been pointed out that the quasi-particle description used here involves the neglect of terms of the order $\frac{G}{2\Delta}$ at various stages. The errors connected with the neglect of H'_{40} for the ground state and with the neglect of H'_{40} , H'_{31} and H'_{22} in calculating the excited two-quasi-particle states enter in a fundamental way, and they are also the errors that it is most difficult to correct for. On the other hand, the errors associated with the blocking effects may, in many respects, be the most severe. We have therefore attempted a programme taking this blocking fully into account through the use of (27') instead of (27) as the form of the two-quasi-particle state. Including the said corrections, one obtains the following expression for the even-even moment of inertia:

$$\mathfrak{S} = 2 \hbar^2 \sum_{\nu, \nu'} \frac{|\langle \nu' | J_x | \nu \rangle|^2}{\varepsilon^{(\nu, \nu')} - \varepsilon^{(0)}} \frac{(v_{\nu}^{(0)} u_{\nu'}^{(0)} - u_{\nu}^{(0)} v_{\nu'}^{(0)})^2}{\varepsilon^{(\nu, \nu')} - \varepsilon^{(0)}} + (\text{terms involving } \mu' \text{ and } \mu''). \quad (35')$$

In this formula the superscript 0 refers to the ground state, while the superscripts ν' and ν'' refer to the states in which the single-particle orbitals ν' and ν'' are blocked.

The modification of eq. (40) is completely analogous to that of (35).

IV. Numerical Calculations of the Moment of Inertia and the Collective Gyromagnetic Ratio

a. Energy scale of the single-particle energies ε_p and determination of the deformation δ

The relative order of the single-particle energies is probably rather well represented by the calculations of ref. 15. A minor readjustment of the energy differences within a shell, as may be suggested by the analysis of experimental nuclear spectra by MORTELSON and NILSSON⁽¹⁶⁾, does not very significantly affect either \mathfrak{S} or g_R of an even-even nucleus. Even though the level order is fairly well established, the total energy scale $\hbar\omega_0$ is determined from a condition on the extension of the nuclear matter which is somewhat arbitrarily formulated⁽¹⁵⁾ as $5/3 \langle r^2 \rangle = R_0^2$, where, furthermore, the nuclear radius R_0 has been set equal to $1.2 \times A^{1/3}$ fermis. This then corresponds to choosing $\hbar\omega_0 = 41 \times A^{-1/3}$ MeV. As the uncertainty of R_0 must be regarded as being, say, of the order of 10%, the inaccuracy of $\hbar\omega_0$ is probably larger than 20%. Now the scale $\hbar\omega_0$ enters first of all in the energy denominator, so from this effect alone there appears at first glance to be an uncertainty in \mathfrak{S} of, say, 20%. However, the ratio $\frac{\Delta}{\hbar\omega_0}$, which determines the u and v values, obviously decreases when $\hbar\omega_0$ is increased, and vice versa. This effect largely cancels the first effect. Indeed, as seen from figs. 22 and 23, a 10% decrease of $\hbar\omega_0$ results in a net change of \mathfrak{S} by only $\pm 2\%$ or less in the range of parameters used in these calculations.

Furthermore, the single-particle energy parameters ε_p are also connected with the eccentricity parameter δ . Indeed, for the use of the energy diagram

of ref. 15 it is necessary to know δ . To obtain values of δ we have employed the empirical values of the quadrupole moments as determined from Coulomb-excitation data. We have made use of the measurements and compilations* of Q_0 recently made by ELBEK et al.⁽¹⁹⁾ in the mass region $150 < A < 190$ (often denoted region I in the following) and by BELL et al.⁽²⁰⁾ in the region $A > 220$ (region II). The experimental values of the quadrupole moments in region I exhibit an estimated accuracy of the order of 3% compared with one another⁽¹⁹⁾. The absolute uncertainty may be greater, however. In particular the values of ELBEK et al. appear systematically to be a few per cent lower on the average than those of most other authors, as pointed out in ref. 19.

Assuming a homogeneous charge distribution, one obtains the well-known relation between the intrinsic quadrupole moment and δ

$$Q_0 = \frac{4}{5} \delta Z R_2^2 \left(1 + \frac{1}{2} \delta + \dots \right). \quad (41)$$

The main uncertainty connected with the use of this formula probably lies in the specification of the parameter R_2 . We have, in using formula (41), put R_2 equal to the average nuclear radius R_0 , which, as pointed out, is related to the energy scale $\hbar\omega_0$. Also the analysis by RAVENHALL⁽²¹⁾ of electron scattering data indicates a proton charge distribution such that the charge radius R_2 defined as $[5/3 \langle r^2 \rangle]^{1/2}$ equals about $1.2 \times A^{1/3}$ fermis.

It turns out that δ is a most critical parameter in the calculation of the moments of inertia. The very large uncertainty in its determination is thus due mostly to the inaccurate knowledge of R_2 , furthermore to the experimental inaccuracies in the Q_0 determination, and finally to the approximate assumptions underlying formula (41). Indeed, as the nucleonic wave functions are known in the pairing approximation, they may be used to calculate an expectation value of the quadrupole operator. For the quasi-particle vacuum, one obtains the simple relation⁽⁶⁾

$$Q_0 = \sum_{\nu} q_{\nu\nu}^0 2b_{\nu}^2, \quad (42)$$

where

$$q_{\nu\nu}^0 = \sqrt{\frac{16\pi}{5}} \langle \nu | r^2 Y_{20} | \nu \rangle. \quad (43)$$

As the population numbers of the single-particle states as well as $q_{\nu\nu}^0$ are functions of δ , eq. (42) provides a relation between Q_0 and δ in which,

* We are grateful to the authors cited for access to their values in advance of publication.

however, $\hbar\omega_0$ (and thereby R_0) enters as a parameter. Formula (42) should be considered somewhat of an improvement on (41). However, the preliminary calculations by SZYMANSKI and BÉŠ⁽²²⁾, until now limited to region I, indicate that the approximation (41) is accurate to within a few per cent in the entire region. This corresponds to a matter distribution displaying approximately the same eccentricity as the potential shape.

SZYMANSKI and BÉŠ go further to seek the equilibrium deformations δ_{eq} . Using the relation (42), they then compare the magnitude and trend of the calculated Q_0 corresponding to δ_{eq} with the empirical Q_0 -values. The preliminary results indicate deviations from the experimental values of the order of 20%.

As pointed out, the use of formula (42) instead of (41) does not remove the uncertainty in the specification of the nuclear charge radius. The δ obtained from equilibrium calculations appears rather sensitive to details of the model, and therefore uncertain.

b. The gap parameters Δ_n and Δ_p

The moment of inertia is very sensitive to the choice of Δ_n and Δ_p , the energy-gap parameters of neutrons and protons. Thus a 10% increase in the magnitude of Δ_n and Δ_p results in an average decrease in \mathfrak{J} of the order of magnitude of 10% (cf. figs. 20 and 21).

Now, Δ_n and Δ_p are determined from the average pair-correlation matrix elements G_n and G_p and the single-particle level density. The exact relation is given by eq. (18). A separate and independent treatment of neutrons and protons, which we have implied here, appears to be adequate in the two regions of deformed nuclei to which the calculations have been confined, as neutrons and protons fill different shells. The assumption that the pairing matrix element can always be set equal to a constant, G , is of course also approximate. Indeed, as the single-particle states on the average become less and less similar as they get more distant from one another in energy, it appears that the overlap of two such wave functions should on the average decrease with increasing energy difference. The contribution from the states far below and above the Fermi surface to the sum in (18) is thus effectively limited. This we may approximately simulate by including in the sums only a certain number of states nearest above and nearest below the Fermi surface. The effect of the arbitrariness in the choice of a cut-off point is less severe as outside of a certain region the inclusion of some extra terms beyond

the cut-offs in many respects corresponds only to a renormalization of G (cf. refs. 5 and 6)*.

In our calculations we have included all states of the $N = 3, 4, 5$ shells (N is the total number of oscillator quanta) for protons in region I (56 levels). Furthermore, we have taken into account all states of the $N = 4, 5, 6$ shells for protons in region II and neutrons in region I (64 levels), and finally all states of the shells $N = 5, 6, 7$ (85 levels) for the neutrons in region II. Compared with an earlier calculation in which only altogether 20 levels near the Fermi surface were taken into account, the inclusion of this great number of levels implied an increase in \mathfrak{S} by an amount of the order of 10% for nuclei at the beginning and the end of region I, provided Δ_n and Δ_p were kept the same in the two calculations. In the middle of region I the effect was even smaller. On the other hand, to obtain the same Δ -value in the two cases we had to use G -values 30-50% larger in the calculation in which the fewer levels were taken into account.

KISSLINGER and SORENSON⁽²³⁾ have analysed systematically sequences of isotopes and isotones of single-closed-shell nuclei, such as the Pb and Sn isotopes, in terms of the known shell-model states with the inclusion of the pair-correlation interaction and a long-range P^2 -force. They conclude that the strength of the pair correlation that best fits the data corresponds to $G = \frac{\text{const}}{A}$ with $G \times A = 17.28$ MeV when they take single-particle levels of one shell into account. They do not explicitly point out any systematic difference between the $G \times A$ values for neutrons and protons. Similar calculations by BRO-JØRGENSEN and HAATUFT^(23a) in progress, treating nuclei that exhibit low-lying vibrational states, also indicate that the values of $G \times A$ that best reproduce the experimental material lie between 20 and 25 MeV. SZYMANSKI and BÉSI⁽²²⁾, taking always the 24 levels nearest to the Fermi surface into account, give $G_p \times A \simeq 32$, $G_n \times A \simeq 25.5$. Previously MORTELSON⁽³⁾ had suggested a value of $G \times A \simeq 25$ -30 MeV, based on an analysis of nucleon-nucleon scattering data.

In the present calculations we have first attempted to obtain a direct estimate of the energy-gap parameters Δ_n and Δ_p , based on empirical evidence other than the rotational-band spacing. We have then studied how well one value of $G_n \times A$ and one value of $G_p \times A$ can reproduce the empirical Δ_n and Δ_p values in both regions. The result of this analysis (cf. figs. 7-14) is discussed below.

* On examination of the effects of "blocking" it appears that the choice of the cut-off limits is much more critical e. g. in the determination of the odd-even mass difference (see section II).

TABLE I. Parameters Defining the Single-Particle Level Spectrum Employed in the Calculations.

Region	Treated shells	κ	μ	Energies to be found in reference:	Additional shifts in units of $\hbar\omega_0$ (in line with reference MN)		
					Case A	Case B	Case C
I	Protons $62 \leq Z \leq 74$	0.05	0.45	N	—	—	The same as case A. (plus some very small shifts of a few individual levels)
		0.05	0.55	N	—	—	
		0.05	0.55	*	{ h 11/2: -0.075 others: +0.1 }	{ -0.075 }	
II	Neutrons $90 \leq N \leq 112$	0.05	0.45	N	—	—	
		0.05	0.45	N	—	—	
		0.05	0.45	N	{ i 13/2: unchgd. others: +0.15 }	{ — }	
I	Protons $Z \geq 88$	0.05	0.55	N	-0.38	-0.15	(plus some very small shifts of a few individual levels)
		0.05	0.70	MN	{ h 11/2: -0.2 i 13/2: -0.35 others: unchgd. }	{ -0.05 -0.35 }	
		0.05	0.45	N	{ — }	{ — }	
II	Neutrons $N \geq 138$	0.05	0.45	N	-0.38	0.15	
		0.05	0.45	N	{ i 13/2: -0.23 j 15/2: -0.06 others: unchgd. }	{ -0.075 -0.06 }	
		0.05	0.40	MN	{ — }	{ — }	

N: S. G. NILSSON [1955], ref. 15

MN: B. MORTELSON and S. G. NILSSON [1958], ref. 16

*: S. G. NILSSON, unpublished calculations.

Regions I and II refer to the so-called rare-earth region ($150 < A < 190$) and the actinide region ($A > 220$) of elements respectively. The parameters κ and μ of columns four and five are defined in ref. 15. Note that we have employed only one κ -value ($\kappa = 0.05$). A few ad hoc changes have been made in the level scheme obtained on the basis of the parameters listed. These are indicated in columns seven, eight and nine for the cases A, B and C, which are discussed in the text. Case C should correspond to the level scheme that is in best agreement with the empirical data on level spectra of odd-A nuclei (cf. ref. 16).

When searching for empirical information from which estimates of Δ_n and Δ_p may be obtained, one first thinks of the empirical energy gap in the excitation spectra of even-even nuclei and of the odd-even mass differences. As pointed out on p. 13, the quasi-particle description gives an energy gap $\geq 2\Delta$, where Δ is the smaller of Δ_p and Δ_n . Indeed, the gap should be very nearly equal to 2Δ , as pointed out in section 2. In region I the lowest excited states clearly identified as two-quasi-particle states occur in Hf¹⁷⁸ and Hf¹⁸⁰ at about 1150 keV, in Er¹⁶⁸ at about 1100 keV, in Dy¹⁶² at about

1450 keV, and in Gd¹⁵⁶ at about 1500 keV. One would, however, be inclined to regard the empirical identification of such lowest-lying states merely as setting a lower limit on 2Δ . The neglected additional interactions, as for instance the fluctuating part of the long-range P^2 -force which is not already included in the spheroidal field, would split apart the two-quasi-particle states lying very densely just above the energy gap. Furthermore, the inclusion of the H'_{22} term of H'_{int} would tend to pull some of these states down below 2Δ . An estimate of the magnitude of the depression due to this term is rather difficult as a large part of its effect is spurious (see Appendix I) and related to the fluctuations in the number of particles introduced by the BCS wave function. A somewhat better measure of the energy gap is probably provided by spectra in which a great number of higher-lying two-quasi-particle states are identified, as is the case in W¹⁸². Here the level density becomes very high at ≈ 1400 keV, which seems to indicate a gap of such magnitude for this nucleus*. Finally there are also the effects associated with the effective reduction of Δ in the two-quasi-particle case due to 'blocking', as discussed in section 2.

Thus a more detailed experimental study of even-even spectra above one MeV would be very informative. In particular one should be able to see whether the lowest-lying two-quasi-particle excitations correspond to broken neutron rather than broken proton pairs, as the evidence from mass differences suggests**.

Probably the best available information on the gap parameters can be obtained from the study of even-odd mass differences. The mass measurements by JOHNSON and BHANOT⁽²⁵⁾ are the main source of empirical knowledge in region I, while the extensive compilation, based on many empirical sources including beta and alpha systematics, by FOREMAN and SEABORG⁽²⁶⁾ covers region II. We have also exploited systematics of beta-decay energies in region I, where more extensive binding-energy data are available for neutrons only.

The total binding energies of, for instance, a series of isotopes having an even value of Z , exhibit a smooth variation with N for all even-even nucleides and a parallel smooth variation with N for the odd ones. According to the present theory, the displacement should correspond to the quasi-particle energy of the last nucleon.

Consider first the neutrons. We have defined the empirical odd-even mass difference P_n by the formula***

* We are grateful to Professor B. R. MOTTELSON for an enlightening discussion of this point.
** Indeed a recent analysis by C. GALLAGHER⁽²⁴⁾ of beta-decays populating higher-lying states of even-A nuclei in region I appears to lend support to this supposition.

*** This quantity would more correctly be labelled $P_n(Z, N-1/2)$.

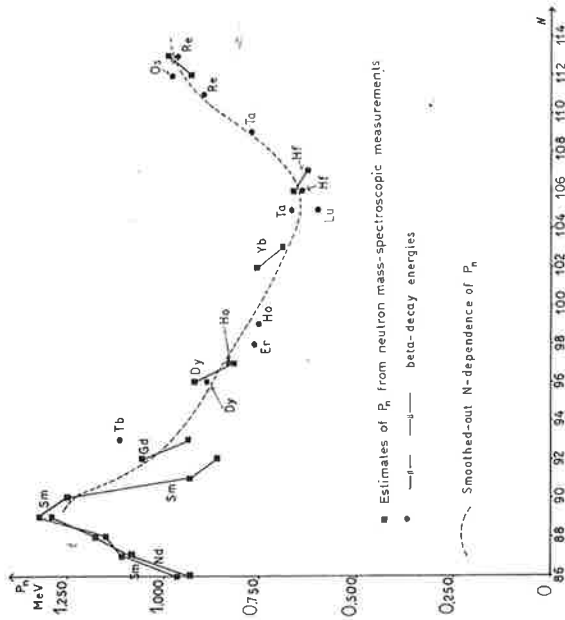


Fig. 1. The odd-even mass difference parameter P_n for neutrons in region I ($150 < A < 188$). The squares refer to mass-spectroscopic measurements by JOHNSON and BHANOT⁽²⁵⁾, while the circles refer to beta-decay energy data. The dashed curve represents averaged values used in the moment -of- inertia calculation.

Added in proof: Recently published more complete mass-spectroscopic measurements by BHANOT, JOHNSON and NIER⁽²⁶⁾ give 100-200 keV lower P_n -values in the region $N = 108-112$; see furthermore fig. 28.

$$P_n(Z, N) = \frac{1}{4} \left\{ -E(Z, N+1) + 3E(Z, N) - 3E(Z, N-1) + E(Z, N-2) \right\} \quad (44)$$

$$= \frac{1}{4} \left\{ -S_n(Z, N+1) + 2S_n(Z, N) - S_n(Z, N-1) \right\},$$

where the neutron separation energy $S_n(Z, N)$ is related to the total binding energies $E(Z, N)$ by the formula

$$S_n(Z, N) = E(Z, N) - E(Z, N-1). \quad (45)$$

Analogous relations hold for the proton binding energy. Eq. (44) thus corrects for a second-order N -dependence of the mass valley. In fig. 2 of the present paper the values of P_n have been extracted from FOREMAN and SEABORG's binding energies by means of eq. (44). This figure may be compared with fig. 3 of ref. 27, where the same data have been exploited, but the following relation has been used:

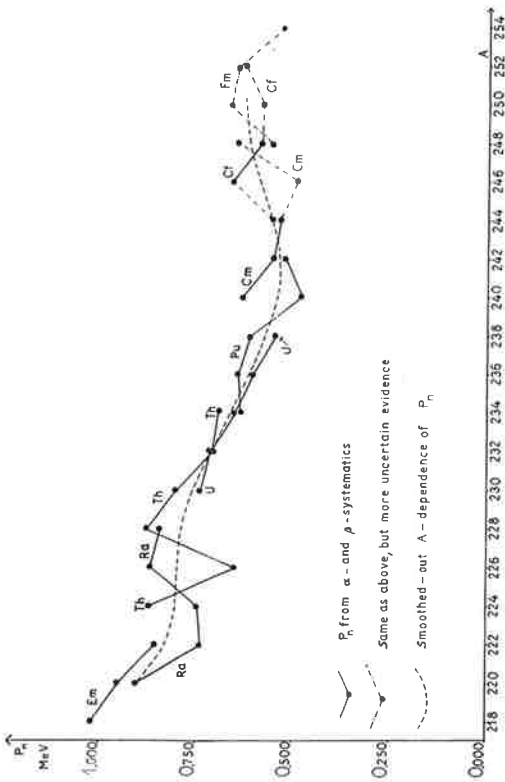


Fig. 2. The odd-even mass difference parameter P_n for nuclei in region II ($A > 224$). The circles correspond to data collected by FOREMAN and SEABORG⁽²⁶⁾. The dashed curve represents the smoothed-out values of P_n on which the calculations were based.

$$P_n(Z, N) = \frac{1}{2} \{ S_n(Z, N) - S_n(Z, N-1) \}, \quad (44')$$

which allows only for a first-order N -dependence of the masses. The use of (44) appears to give smaller fluctuations. In region I, where the data are meagre, the difference between (44) and (44') also appears significant. The values of P_n derived from (44) turn out usually 50-100 keV higher than those obtained by the use of eq. (44').

In region I, as already pointed out, the beta-decay energy systematics are a valuable complementary source of information. From a comparison of sequences of odd isobars connected by beta decay or electron capture one obtains an estimate of $(P_p - P_n)$, as an odd- Z isobar corresponds to a proton quasi-particle state and an odd- N nucleide to a neutron quasi-particle state. In addition to using beta-decay energies from isobars it turns out to be advantageous to study also elements having $(N - Z) = \text{constant}$ (isodiaspheres⁽²⁸⁾) or $(3N - Z) = \text{constant}$. Indeed, one could employ any systematic cut through the mass valley other than those mentioned. For isobars, usually only a few energy differences are known. In particular, electron capture energies are very uncertain; furthermore the elements soon get very short-lived as one moves away from the stability minimum. Contrary to iso-

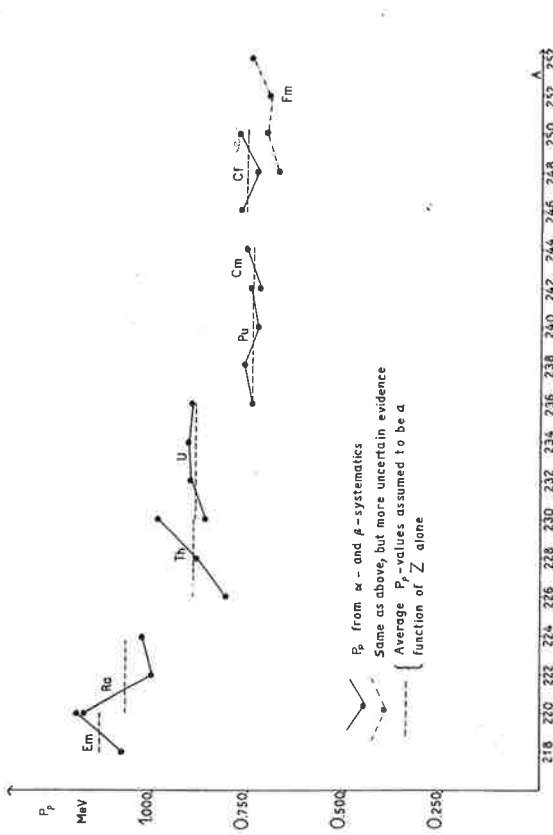


Fig. 3. The odd-even mass difference parameter P_p for nuclei in region II. For further explanation see fig. 2.

bars, which correspond to lines of elements almost perpendicular to the direction of the mass valley, isodiaspheres, as well as elements corresponding to $(3N - Z) = \text{constant}$, represent cuts exhibiting a small inclination to the direction of the valley. Such lines thus contain many more studied nucleides. On the other hand, for instance isodiaspheres also correspond to an averaging over a larger region of elements.

A collection of such available data on $(P_p - P_n)$, mostly taken from Nuclear Data Sheets⁽²⁹⁾ and ref. 16, is given in fig. 4. The diagram shows clearly that P_p is rather consistently much greater than P_n in region I. This is also the case in region II, where the evidence is more complete (cf. figs. 2 and 3). The difference is of the order of 100 keV in region I and about 150-200 keV in region II. Fig. 4 also indicates a trend in the value of $(P_p - P_n)$ from 0-50 keV around $A = 155$ up to 150-200 keV around $A = 175$, and then a decline towards zero again beyond $A = 180$. However, it must be borne in mind that the uncertainty of these energy differences is probably more than 50 keV. If the mass valley were exactly parabolic in shape, the beta energies would lie on straight lines. There is, however, a systematic curvature, especially conspicuous for isodiaspheres, which we have in some

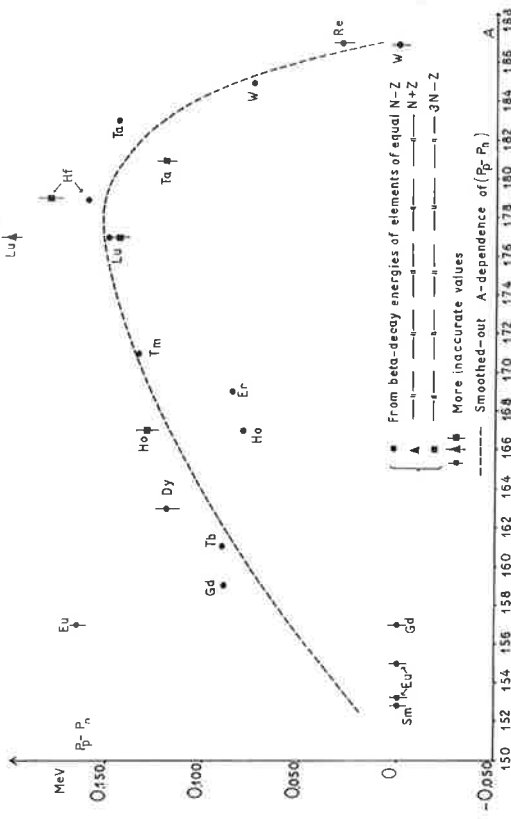


Fig. 4. The difference $P_p - P_n$ for nuclei in region I from beta-decay energy systematics. The circles correspond to cuts through the mass valley characterized by $(N-Z)$ being constant (isodispheres), the triangles to series of isobars, and the squares to series of elements with $(3N-Z)$ equal to a constant. Uncertainties associated with the points are of the order of 50-100 keV.

measure taken into account graphically by drawing smooth curves through the points. This deviation corresponds to a higher-order $(N-Z)$ -dependence of the mass-valley*.

Furthermore, a study of beta decay energies of even- A nucleides gives a measure of $(P_p + P_n)$. However, a study of the available wealth of mass data in region II indicates clearly that there is an additional coupling energy^(27, 28) between the odd neutron and the odd proton that makes the mass difference between the odd-odd and even-even nuclei smaller than $P_p + P_n$. We define such an empirical coupling energy R_{np} as

* The somewhat astonishing conclusion that empirically P_p is greater than P_n is suggested already by the fact that of the stable odd- A elements the odd- N nucleides are more numerous than the odd- Z ones in the mass regions of interest here. For instance, among the elements $A = 153, 155, \dots, 185$ there are 10 odd- N nucleides and seven odd- Z ones. If we assume the distribution of masses to lie on the parabolic surfaces

$$M(I) = M_0 + \frac{1}{2}b(I - I_0)^2 + \left\{ \begin{matrix} P_n \\ P_p - P_n \end{matrix} \right\},$$

where $I = N - Z$, the probability of the odd- N nucleide being stable is apparently

$$\frac{1}{2} \left(1 + \frac{P_p - P_n}{2b} \right).$$

For the elements mentioned above one then obtains the estimate $(P_p - P_n) \approx 100$ keV as an average for the whole region.

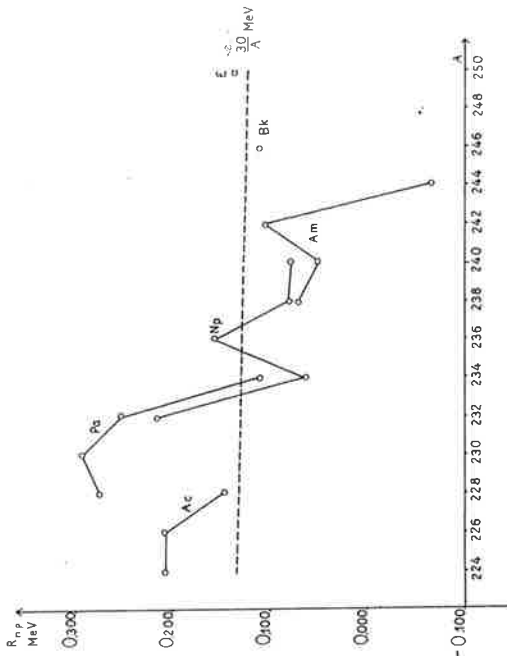


Fig. 5. Coupling energies R_{np} between the odd proton and the odd neutron in odd-odd nuclei. The experimental binding energies of series of nucleides, as given in ref. 26, are exploited by means of eq. (46) of the present article for a determination of R_{np} . The uncertainty in the obtained values of R_{np} is at least of the order of 50 keV. The squares in fig. 5 correspond to particularly uncertain points.

$$R_{np}(Z, N) = \frac{1}{8} \left\{ \begin{aligned} &[-S_n(Z+1, N) + 2S_n(Z, N) - S_n(Z-1, N)] \\ &+ [-S_p(Z, N+1) + 2S_p(Z, N) - S_p(Z, N-1)] \end{aligned} \right\} \quad (46)$$

where (Z, N) refers to the odd-odd nucleus. Values of R_{np} are collected in fig. 5. As expected, there are great fluctuations (to some extent probably indicating a difference between the overlaps of the neutron and proton orbitals in the different cases). However, R_{np} appears to be greater than zero in almost all the cases. On the inclusion of the data from other regions of elements, as collected e. g. in ref. 28, one might conclude that, on an average,

$$R_{np} \approx \frac{20-30}{A} \text{ MeV.} \quad (47)$$

This correction has been employed in region I in obtaining the values of $P_p + P_n$ from beta-decay systematics. The corrected energies have then been used together with the smoothed-out $(P_p - P_n)$ -values of fig. 4 in obtaining the P_n -values exhibited in fig. 1.

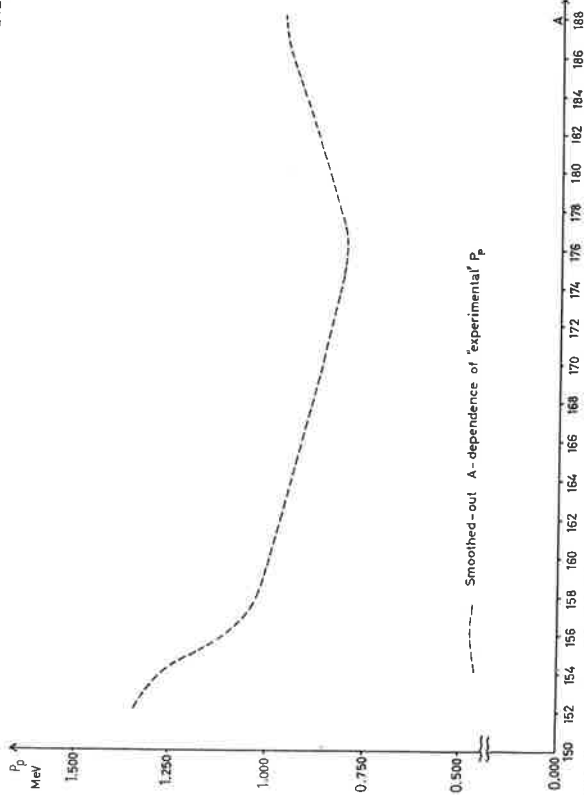


Fig. 6. Average empirical values of the proton odd-even mass difference parameter P_p in region I used in the calculations. This dashed curve is obtained by addition of the smoothed-out ($P_p - P_n$) function of fig. 4 to the averaged P_n -values of fig. 1.

Note added in proof: The recent mass-spectroscopic measurements by BHANOT, JOHANSON and NIJER⁽²⁰⁾ allow more accurate P_p -values as displayed in fig. 29. The deviation from fig. 6 is notable only for $A > 180$.

The main problem now concerns the relation between P and Δ . It has already been discussed in some detail in section 2, where it is pointed out that, if one assumes the same quasi-particle vacuum for the odd and the even case, this leads to $P = \Delta$. The results of a calculation that allows for the fact that the odd particle blocks the scattering of the pairs by its presence and thereby changes the occupation numbers also of the other single-particle levels, are exhibited in table II. This calculation gives the result that P is smaller than Δ by a magnitude of the order of 10% on the average, both for neutrons and protons. The relation between P and Δ is unfortunately very uncertain as, first, the correction is somewhat dependent on the cut-off, secondly, an important contribution comes from the "self-energy" term displayed in eq. (26), thirdly, still other effects of the order $\frac{G}{2\Delta}$ are neglected, some of which are discussed in Appendix I. In the calculations presented in this article we have simply started from the assumption $\Delta_n = P_n^{\text{exp}}$ and $\Delta_p = P_p^{\text{exp}}$ (or rather some smoothed-out experimental values of P_n^{exp} and P_p^{exp}).

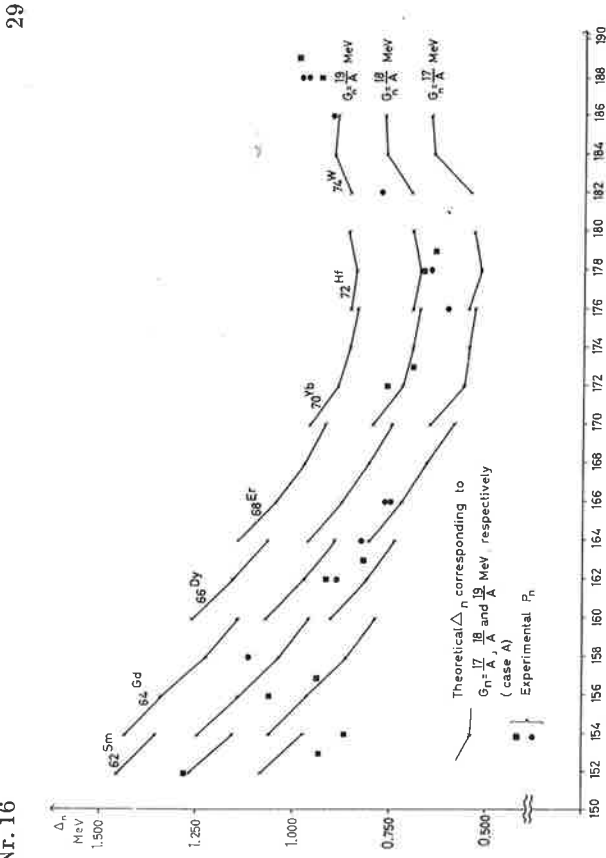


Fig. 7. The relation between values of Δ_n and G_n in region I obtained in the calculations. For details of the single-particle spectrum employed, denoted as "case A", see table I. The points exhibited for comparison refer to the P_n -values of fig. 1.

In figs. 7-10 and 11-14 we have compared the values of Δ_n and Δ_p obtained in the detailed calculations corresponding to constant values of G_n and G_p with the empirically given values of P_n and P_p . It is found that values of $G_n \times A \simeq 18$ MeV and $G_p \times A \simeq 25-26$ MeV both in region I and II and for a given set of ϵ_p 's, denoted case A, reproduce rather well the "empirical" trends. For an alternative set of ϵ_p 's, denoted case B, we find instead that $G_p \times A \simeq 16-17$ MeV and $G_n \times A \simeq 23$ MeV give the best fit. It seems plausible that case A represents rather well the situation in region I, while region II is presumably better described by a set of ϵ_p 's intermediate between case A and case B and probably closest to case B (cf. case C of table I). Still the similarity of the G -values used in the two regions appears encouraging*.

* One might also point out in connection with figs. 7-14 that the illustrated relation between G and Δ appears to be described rather well by the expression $\Delta \sim e^{-\frac{G}{\rho}} \frac{1}{\rho}$, where ρ is the single-particle level density. The conditions for this relation to hold are that the level density is roughly constant, that there is approximately the same number of levels above and below the Fermi surface, that $\rho G \ll 1$, and furthermore that $\Delta \gg d$, which is implied by the replacement of sums by integrals in obtaining the expression above (d is the magnitude of the cut-off energy above and below the Fermi surface).

Nr. 16
 TABLE II. The Odd-Even Mass Difference Parameter P when the Effect of Blocking due to the Odd Particle is Included, Referring to Odd- N Nuclei in Region I (TABLE IIa) and Region II (TABLE IIc) and to Odd- Z Nuclei in Region I (TABLE IIb) and Region II (TABLE IId).

Nuclide	$G_n \times A$ (MeV)	Δ_n^e (keV)	Δ_n^{odd} (keV)	$\frac{\Delta_n^e - \Delta_n^{\text{odd}}}{\Delta_n^e}$ (%)	$P_n^{\text{theor.}}$ (keV)	$\frac{\Delta_n^e - P_n^{\text{theor.}}}{\Delta_n^e}$ (%)	P_n^{exp} (keV)
$^{91}\text{Gd}^{155}$ ₆₄	17	1047	895	15	977	7	
	18	1215	1068	12	1122	8	1145
	19	1396	1247	11	1294	7	
$^{88}\text{Gd}^{157}$ ₆₄	17	958	796	17	868	9	
	18	1122	960	14	1028	8	990
	19	1303	1134	13	1232	5	
$^{95}\text{Dy}^{161}$ ₆₆	17	895	744	17	874	2	
	18	1050	887	16	1046	0	904
	19	1231	1049	15	1276	-4	
$^{87}\text{Dy}^{163}$ ₆₆	17	809	643	21	837	-3	
	18	965	802	17	986	-3	846
	19	1141	969	15	1150	-1	
$^{89}\text{Er}^{167}$ ₆₈	17	711	516	27	618	13	
	18	859	677	21	730	15	787
	19	1030	846	18	903	12	
$^{101}\text{Yb}^{171}$ ₇₀	18	783	557	29	733	6	
	19	946	732	23	881	7	732
	20	1121	914	18	1048	7	
$^{103}\text{Yb}^{173}$ ₇₀	18	699	397	43	531	24	
	19	869	604	30	736	15	684
	20	1049	811	23	926	12	
$^{105}\text{Hf}^{177}$ ₇₂	18	677	374	45	503	26	
	19	845	581	31	704	17	659
	20	1022	786	23	892	13	
$^{107}\text{Hf}^{179}$ ₇₂	18	677	375	45	488	28	
	19	846	585	31	701	17	690
	20	1021	790	23	893	13	
$^{109}\text{W}^{183}$ ₇₄	18	733	529	28	700	5	
	19	883	692	22	849	4	788
	20	1040	858	18	997	4	
$^{109}\text{W}^{183}$ ₇₄ (1.1 δ)	18	686	452	34	613	11	
	19	839	623	26	785	6	788
	20	997	796	20	945	5	

TABLE IIa

TABLE IIb

Nuclide	$G_p \times A$ (MeV)	Δ_p^e (keV)	Δ_p^{odd} (keV)	$\frac{\Delta_p^e - \Delta_p^{\text{odd}}}{\Delta_p^e}$ (%)	$P_p^{\text{theor.}}$ (keV)	$\frac{\Delta_p^e - P_p^{\text{theor.}}}{\Delta_p^e}$ (%)	P_p^{exp} (keV)
$^{63}\text{Eu}^{153}$	24	1270	1041	18	1149	10	
	25	1421	1185	17	1320	7	1309
	26	1586	1337	16	1532	3	
$^{65}\text{Tb}^{159}$	24	1098	854	22	982	11	
	25	1244	991	20	1157	7	1013
	26	1409	1133	20	1399	1	
$^{67}\text{Ho}^{165}$	24	985	713	28	834	15	
	25	1127	856	24	1001	11	925
	26	1285	1000	22	1226	5	
$^{69}\text{Tm}^{169}$	24	917	613	33	742	19	
	25	1060	771	27	918	13	883
	26	1220	922	24	1151	6	
$^{71}\text{Lu}^{175}$	24	883	644	27	821	7	
	25	1025	770	25	1015	1	809
	26	1208	895	26	1369	-13	
$^{73}\text{Ta}^{181}$	24	839	632	25	830	1	
	25	951	733	23	945	1	869
	26	1078	844	22	1100	-2	
$^{75}\text{Re}^{185}$	25	822	496	40	715	13	
	26	948	661	30	860	9	937
	27	1090	815	25	1040	5	
$^{75}\text{Re}^{187}$	25	803	476	41	718	11	
	26	923	638	31	854	7	961
	27	1057	790	25	1012	4	

Column one identifies the nuclide; column two lists the chosen G -values; columns three, four and five give the corresponding Δ -values for the even and the odd case, and the relative difference in per cent. Column six shows the calculated P -value, which is compared with the experimental P -value of the even case in column seven. The last column gives the averaged here the so-called "even" case corresponds to a nuclide having $n/2$ pairs and no single-particle state blocked.)

The result that G_p comes out considerably larger than G_n is in agreement with the fact that near the Fermi surface the velocity of the protons is smaller than that of the neutrons owing to the Coulomb repulsion. Now the S -wave, phase shift, with which the pair-correlation force is directly associated, falls off rapidly with increasing relative energy because of the increasing importance of the repulsive core. This in turn follows from the fact that particles of higher velocity may penetrate closer to each other*.

* The authors are indebted to Professor B. R. MOTTISON for valuable comments on this point.

TABLE IIc

Nuclide	$G_p \times A$ (MeV)	Δ_p^e (keV)	$\frac{\Delta_p^e - \Delta_p^{\text{odd}}}{\Delta_p^e}$ (%)	$\frac{\Delta_p^e - \Delta_p^{\text{theor.}}}{\Delta_p^e}$ (%)	$P_p^{\text{theor.}}$ (keV)	$\frac{\Delta_p^e - P_p^{\text{theor.}}}{\Delta_p^e}$ (%)	P_p^{exp} (keV)
$^{139}_{90}\text{Th}^{229}$	16	639	16	2	627	2	777
	17	781	15	4	746	4	
	18	935	13	3	909	3	
$^{141}_{90}\text{Th}^{231}$	16	587	30	14	504	14	737
	17	732	20	12	642	12	
	18	890	15	11	791	11	
$^{144}_{92}\text{U}^{233}$	16	573	30	14	491	14	687
	17	714	20	12	625	12	
	18	869	15	11	777	11	
$^{148}_{92}\text{U}^{235}$	16	532	34	18	438	18	639
	17	669	22	15	568	15	
	18	825	17	12	723	12	
$^{145}_{94}\text{Pu}^{239}$	16	488	36	19	397	19	561
	17	615	25	16	514	16	
	18	767	19	11	680	11	
$^{147}_{94}\text{Pu}^{241}$	17	576	28	18	473	18	543
	18	725	21	14	626	14	
	19	927	21	-5	976	-5	
$^{149}_{96}\text{Cm}^{245}$	17	529	34	17	440	17	574
	18	665	24	16	558	16	
	19	839	20	7	777	7	

TABLE II d

Nuclide	$G_p \times A$ (MeV)	Δ_p^e (keV)	$\frac{\Delta_p^e - \Delta_p^{\text{odd}}}{\Delta_p^e}$ (%)	$\frac{\Delta_p^e - P_p^{\text{theor.}}}{\Delta_p^e}$ (%)	$P_p^{\text{theor.}}$ (keV)	$\frac{\Delta_p^e - P_p^{\text{theor.}}}{\Delta_p^e}$ (%)	P_p^{exp} (keV)
$^{91}\text{Pa}^{231}$	22	846	16	8	782	8	896
	23	949	14	7	887	7	
	24	1059	13	5	1008	5	
$^{93}\text{Np}^{237}$	22	742	593	9	676	9	821
	23	841	690	7	779	7	
	24	949	792	5	904	5	
$^{95}\text{Am}^{241}$	22	615	400	6	579	6	745
	23	718	526	3	693	3	
	24	832	648	1	827	1	
$^{95}\text{Am}^{243}$	22	601	383	6	563	6	745
	23	702	508	4	676	4	
	24	813	630	1	802	1	

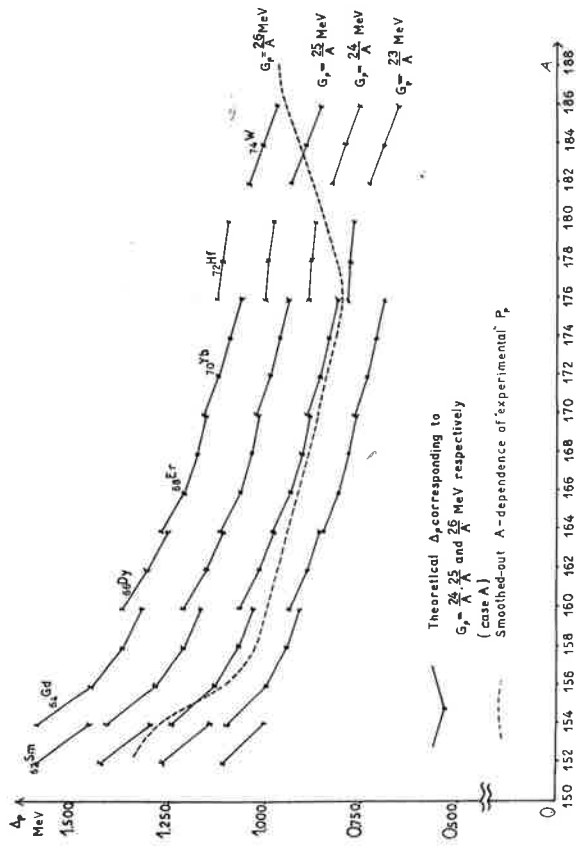


Fig. 8. The relation between Δ_p and G_p in region I (case A). The "empirical" dashed curve refers to the averaged P_p curve of fig. 6.

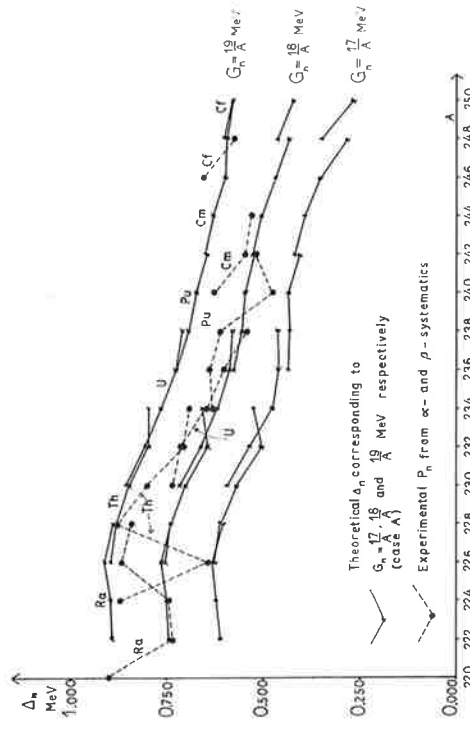


Fig. 9. The relation between Δ_n and G_n in region II (case A). The exhibited points refer to the P_n -values of fig. 2.

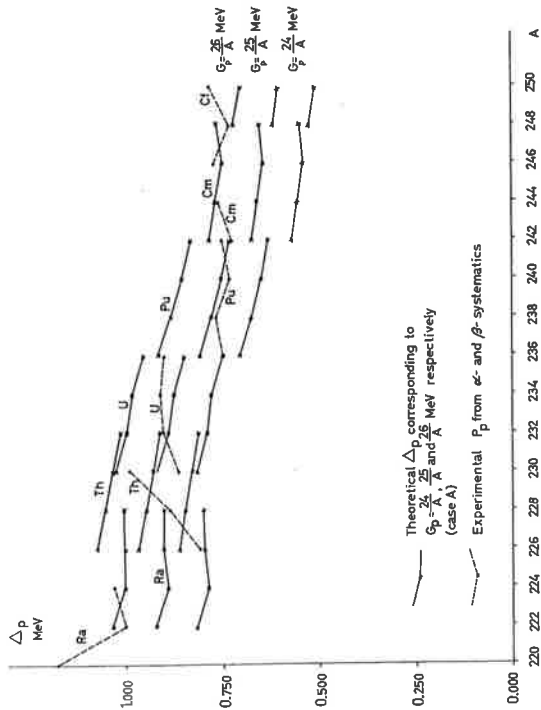


Fig. 10. The relation between Δ_p and G_p in region II (case A). The exhibited points refer to the P_p -values of fig. 3.

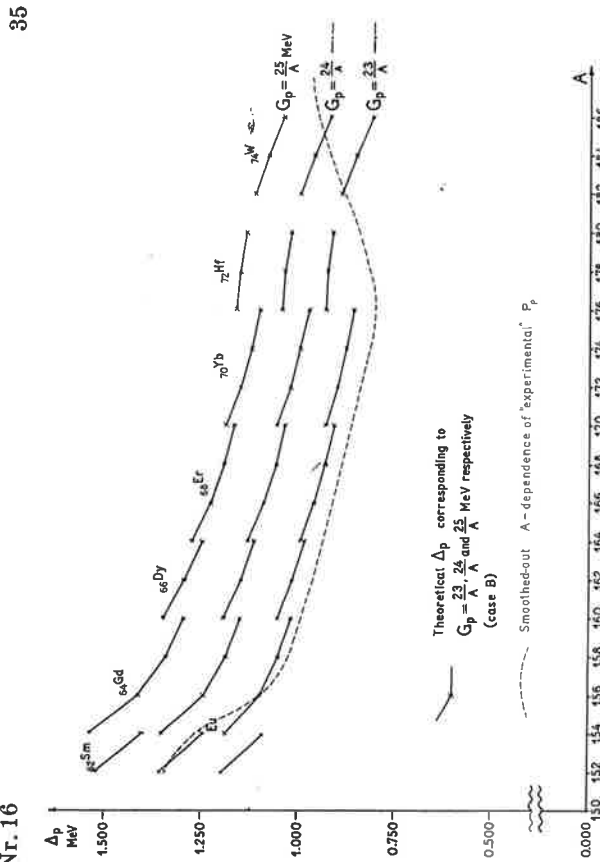


Fig. 12. The relation between Δ_p and G_p in region I (case B). The "empirical" dashed curve corresponds to the P_p -values of fig. 6.

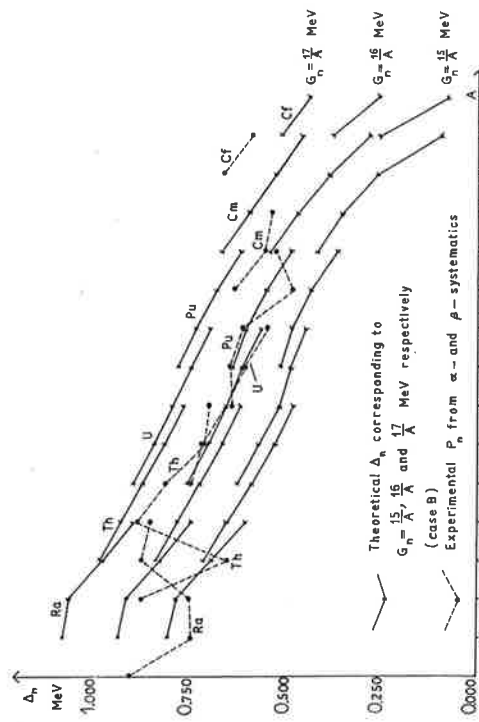


Fig. 13. The relation between Δ_n and G_n in region II (case B). The exhibited points refer to the P_n -values given in fig. 2.

to interpolate \mathfrak{S} and W for specific values of δ and Δ , by means of all the points computed, and also to find the relation between Δ and G for the given eccentricities, as exhibited in figs. 7-14.

In a later programme designed also for the treatment of moments of inertia of odd- A nuclei (see Appendix III), where the correct position of the chemical potential with reference to the level populated by the odd particle is very critical, we employed a different procedure. According to this latter programme the interpolation between ϵ_p 's, stored in the memory for a few deformations, to the correct deformation is performed first.

VI. Results of the Calculations

a. Moments of inertia of even-even nuclei

The values of the calculated moments of inertia of even-even nuclei, corresponding to the sets of single-particle states ϵ_p as given in table I (cases A and B), as well as to the eccentricities exhibited in figs. 15 and 16, and to the Δ -values equal to the P -values of figs. 1, 2, 3, and 6, are displayed in fig. 17 (region I) and in fig. 18 (region II). All the empirical and some of the calculated values are listed in table III, where the appropriate references of the former are also given. A correction to the empirical values for the rotation-vibration interaction is not employed for the plotted values of figs. 17-25. Information on this point is incomplete, but the effect is of some importance at the beginning of regions I and II, and its inclusion amounts to a depression in \mathfrak{S} of a few per cent, as can be studied in table III, thus very slightly improving the agreement with the theoretical calculations.

In region I the quantity $\frac{2}{\hbar^2} \mathfrak{S}$ in case A lies consistently $\sim 10 \text{ MeV}^{-1}$ below the experimental values. The calculations corresponding to case B (which case implies that the ad hoc raise of the shells above $Z = 82$ and $N = 126$, assumed according to case A, is very largely diminished) give values of \mathfrak{S} above those of case A, particularly at the end of the region. Nevertheless, the overall variation over the nucleides is probably less favourable than in case A. Furthermore, in case B the single-particle states of the above-lying shells are allowed to come down further than is tolerable on the basis of the detailed knowledge⁽¹⁶⁾ about the odd- A nuclear excitation spectra at the end of region I. Thus case A appears more realistic*.

* The interest in including case B lies, however, apart from its giving an estimate of the effects of the inaccuracies of the single-particle level scheme, in the fact that fewer ad hoc changes in the single-particle spectra are made in that case. Such changes are dangerous as they lead to violations of the sum rules otherwise fulfilled by any consistent model.

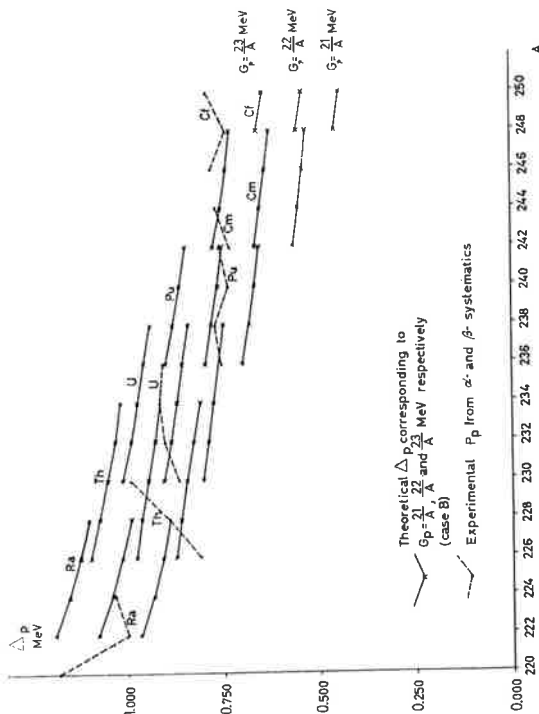


Fig. 14. The relation between Δ_p and G_p in region II (case B). The exhibited points refer to the P_p -values given in fig. 3.

V. Details of the Numerical Calculations

The numerical calculations were performed on the SMIL electronic digital computer of the University of Lund. In the first programme used* the ϵ_p 's were stored in the computer for three different eccentricities, $\delta = 0.20, 0.25$ and 0.30 , in region I and for $\delta = 0.20$ and 0.25 in region II. Furthermore the computer was provided with a set of four different Δ_n and Δ_p values, covering the whole region of variation of these parameters. For each value of δ and Δ the computer was instructed to find the correct λ fulfilling the condition (13) for the sequence of given Z and N values of the elements of regions I and II. About 1000 different matrix elements of s_x and j_x were also stored, connecting all single-particle states up to and including the $N = 7$ shell in terms of the wave functions of ref. 15 and computed for three, respectively two, different values of the eccentricity. When the u 's and v 's had been determined for each λ, Δ and δ , SMIL went on to compute $\mathfrak{S}_n, W_n, \mathfrak{S}_p, W_p, G_n, G_p$, the total energy, the fluctuation in the number of particles, etc. All this information was printed. A subroutine was then used

* The programme was constructed by Dr. C. E. FRÖBERG, Director of the Institute of Numerical Analysis of the University of Lund.

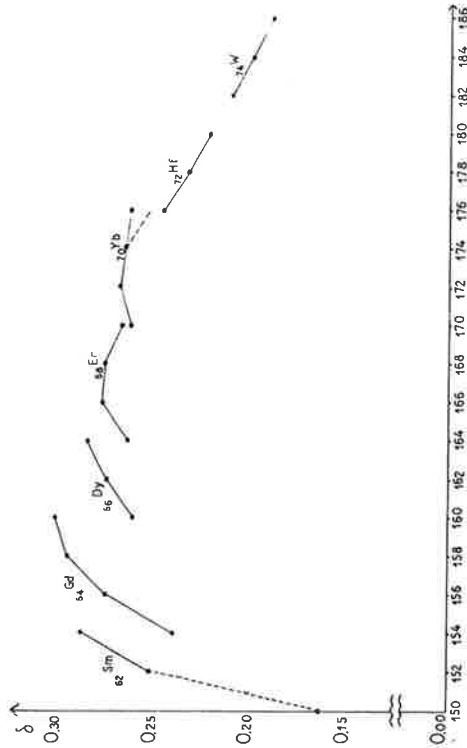


Fig. 15. Values of the eccentricity parameter δ in region I used in the calculations. The values of δ are obtained by means of eq. (41) from the quadrupole moments given by ELBEK et. al. (19), assuming $R_2 = 1.2 \times A^{1/3}$ f. Note that the dashed line ending at Yb-175 represents a slight ad hoc correction of the Yb-175 point. Such a correction is in line with the level diagram of ref. 15.

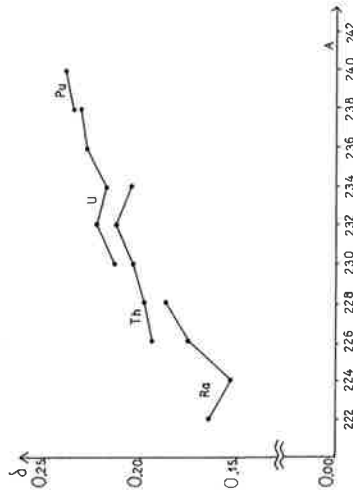


Fig. 16. Values of the eccentricity parameter δ in region II used in the calculations. For references to the experimental data see BELL et al. (20) and SROMINGER, HOLLANDER and SEABORG (49). The detailed fine structure of the A-dependence of δ appears less regular than in fig. 15, and some of the variations may be due to experimental uncertainties.

In region II both the calculations, corresponding to case A and case B, give results very much below the empirical energy moments, particularly at the beginning of the region, even when the vibration-rotation correction for the empirical values is applied.

Unfortunately, however, both δ , Δ_n and Δ_p are known too inaccurately

TABLE III. Experimental and Theoretical Values of the Moment of Inertia and the Collective Gyromagnetic Ratio in Region I (TABLE IIIa) and Region II (TABLE IIIb).

The nucleides are identified from columns one and two. Column three shows the experimental values of the moment of inertia based on the excitation energy of the first rotational states as found, e.g., in refs. 44 and 46. Column four gives the inertia values that include the correction for the rotation-vibration interaction. These values have been taken from ref. 45. Columns five, six and seven show the values of the parameters δ , Δ_n and Δ_p assumed in the calculations. The values of δ given in parentheses are extrapolated. Of the quantities listed in the last columns, the theoretical quantities \tilde{S} and W are defined from eqs. (A11-10) and (40). The indices n and p refer to neutrons and protons respectively. Columns 10 and 13 (respectively 14) give the final theoretical values of the moment of inertia and the collective gyromagnetic ratio. In table III a, columns 8-13 refer to "case A", only column 14 to "case B". For experimental values of g_R see refs. 33 and 40.

TABLE IIIa

Nucleide	A	$\frac{2}{h^2} \tilde{S}_{exp}$ (MeV) ⁻¹	$\frac{2}{h^2} S_{corr}$ (MeV) ⁻¹	δ	$\frac{\Delta_n}{\pi \hbar \omega_0}$	$\frac{\Delta_p}{\pi \hbar \omega_0}$	Case A						g_R	
							$\frac{2}{h^2} \tilde{S}_{exp}$	$\frac{2}{h^2} \tilde{S}_{exp}$	$\frac{2}{h^2} \tilde{S}_{exp}$	$\frac{2}{h^2} \tilde{S}_{exp}$	$\frac{2}{h^2} \tilde{S}_{exp}$	$\frac{2}{h^2} \tilde{S}_{exp}$	$\frac{2}{h^2} \tilde{S}_{exp}$	Case A
Sm	152	49.2	47.3	0.254	3.254	3.502	22.98	13.20	38.9	0.619	0.327	0.341	0.344	
	154	73.2		0.289	2.720	3.329	33.67	16.41	53.9	0.951	0.436	0.295	0.299	
Gd	154	48.8(a)	46.8	0.242	3.269	3.329	21.28	13.19	36.9	0.567	0.361	0.367	0.378	
	156	67.4	66.7	0.277	2.731	2.886	32.45	17.83	53.9	0.949	0.553	0.333	0.339	
	158	75.5	75.0	0.297	2.479	2.705	38.38	20.10	62.9	1.160	0.654	0.319	0.326	
	160	79.7		0.303	2.320	2.651	41.42	20.82	67.0	1.273	0.687	0.307	0.311	
Dy	160	69.0(a)	68.5	0.263	2.489	2.651	34.18	17.98	55.5	1.064	0.584	0.318	0.325	
	162	74.4	74.0	0.277	2.330	2.574	38.54	19.09	61.6	1.208	0.634	0.311	0.310	
	164	81.8		0.287	2.176	2.501	41.09	19.99	65.4	1.183	0.677	0.304	0.309	
Er	164	66.7		0.266	2.339	2.501	37.26	18.93	59.9	1.168	0.601	0.306	0.324	
	166	74.5	74.1	0.279	2.185	2.448	40.59	19.92	64.7	1.181	0.640	0.303	0.313	
	168	75.2	75.0	0.278	2.046	2.403	41.85	20.30	66.4	1.079	0.658	0.309	0.315	
Yb	170	75.6		0.269	1.905	2.358	44.25	20.38	68.7	1.118	0.665	0.296	0.298	
	170	71.2	70.9	0.265	2.053	2.358	41.07	20.48	65.4	1.066	0.627	0.313	0.329	
Yb	172	76.2	76.0	0.270	1.913	2.289	44.35	21.59	70.1	1.119	0.661	0.308	0.322	
	174	78.5		0.268	1.806	2.224	45.15	22.10	71.4	1.236	0.687	0.305	0.303	
Hf	176	73.1		0.265	1.788	2.190	41.41	21.62	67.1	1.163	0.700	0.324	0.305	
	176	67.9	67.5	0.248(b)	1.812	2.190	43.88	16.95	64.3	1.228	0.578	0.245	0.301	
W	178	64.4	64.1	0.235(b)	1.795	2.250	39.74	15.34	58.2	1.149	0.553	0.245	0.285	
	180	64.3	64.1	0.224(b)	1.997	2.338	32.14	14.30	50.1	0.876	0.517	0.280	0.292	
	182	60.0	59.6	0.213(b)	2.004	2.455	33.67	11.65	46.8	0.850	0.412	0.281	0.254	
W	184	54.1	53.6	0.202(b)	2.358	2.558	25.12	10.81	38.1	0.610	0.375	0.284	0.285	
	186	49.0		0.194(b)	2.659	2.651	18.41	10.23	30.6	0.434	0.340	0.352	0.334	

(a) J. O. RASMUSSEN and K. S. TORH, Phys. Rev. 116, 150 (1959).
 (b) from B. ELBEK, unpublished.

TABLE IIIb

Nuclide	$\frac{2}{\hbar^2} S_{\text{exp}}$ (MeV) ⁻¹		$\frac{2}{\hbar^2} S_{\text{corr}}$ (MeV) ⁻¹	δ	$\frac{\Delta_p}{\pi \hbar \omega_0}$	Case B						
	88.5	102				$\frac{2}{\hbar^2} S_p$	$\frac{2}{\hbar^2} S_n$	$\frac{2}{\hbar^2} S$	$\frac{2}{\hbar^2} W_p$	$\frac{2}{\hbar^2} W_n$	$\frac{2}{\hbar^2} W$	g_R
Ra	226	228	86.2	0.176	2.377	3.179	35.14	9.14	46.5	0.841	0.041	0.14
Th	226	228	81.1	0.188	2.354	3.188	41.84	11.55	56.1	1.033	0.141	0.16
	226	228	103.6	0.195	2.377	2.665	40.24	18.98	62.2	0.990	0.389	0.29
	228	230	113.2	0.199	2.354	2.673	43.55	19.82	66.5	1.097	0.428	0.28
	232	234	120.5	0.205	2.281	2.681	48.82	21.11	73.3	1.217	0.487	0.27
	234	236	125	0.214	2.134	2.689	55.96	23.05	82.9	1.321	0.576	0.26
	234	238	116.1	0.206	1.990	2.696	58.33	21.27	83.2	1.337	0.495	0.23
U	230	232	127.1	0.215	2.281	2.673	51.25	24.58	79.7	1.341	0.666	0.30
	232	234	137.9	0.224	2.134	2.680	59.08	26.15	89.6	1.510	0.728	0.28
	236	238	132.5	0.219	1.990	2.687	62.32	25.23	91.8	1.499	0.691	0.26
	238	242	133.9	0.229	1.860	2.695	68.44	26.99	100.2	1.545	0.759	0.26
	238	242	134.8	0.232	1.741	2.703	73.76	27.48	106.2	1.662	0.778	0.25
Pu	236	238	134.4	(0.230)	1.860	2.252	70.04	35.25	110.3	1.703	1.072	0.32
	238	240	136.1	0.236	1.741	2.258	74.92	36.25	116.5	1.707	1.103	0.32
	240	242	139.9	0.240	1.652	2.264	79.50	36.85	122.0	1.777	1.124	0.30
	242	244	134.8	(0.242)	1.642	2.271	78.83	37.14	121.8	1.723	1.132	0.31
Cm	242	244	142.5	(0.243)	1.642	2.259	80.80	36.88	123.6	1.793	1.003	0.30
	244	246	139.9	(0.243)	1.698	2.265	76.82	36.87	119.6	1.655	1.001	0.31
	246	248	138.3	(0.243)	1.804	2.271	71.02	36.85	113.7	1.349	0.999	0.34
	248	248	138.3	(0.225)	1.891	2.277	69.94	36.48	112.2	1.221	0.990	0.34
Cf	248	250	142.2(a)	(0.240)	1.891	2.332	68.03	34.30	108.0	1.277	0.894	0.33
	250			(0.225)	1.922	2.339	69.09	34.28	109.1	1.200	0.893	0.33

(a) Van den Bosch, Diamond, Sjöblom, and Fields, Phys. Rev. 115, 115 (1959).

to admit any further definite conclusions. An increase of δ by about 20% corresponding to the use of an $R_2 = 1.08 \times A^{1/3}$ fermis in eq. (41) raises the curves by amounts that can be studied in fig. 19. A decrease in Δ_n and Δ_p by 10-20% is certainly admissible within the inaccuracy of the experimental data, particularly in view of the uncertain relation between P and Δ^s . The effect of choosing 20% smaller Δ -values may be studied in figs. 20 and 21.

* The recent very detailed and inclusive study of relative nucleic masses by EVERLING, KÖNIG, MATTAUCH, and WAPSTRA⁽²¹⁾, based on all relevant information available, indicates that a few per cent smaller P_n values should be chosen at the end of region I.

Added in proof: The recent more complete mass-spectroscopic data published by BHANOT, JOHNSON and NIER⁽²⁰⁾ lowers the values of Δ_n and Δ_p to be used for ${}_{84}\text{W}$ by up to 10-20% as exhibited in fig. 28. The adoption of these new Δ -values would considerably improve the agreement with theory for the W-isotopes.

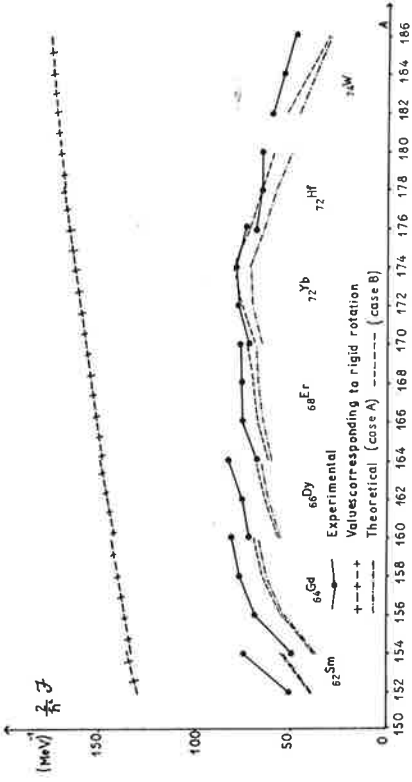


Fig. 17. Moments of inertia of even-even nuclei in region I. The figure exhibits by the crossed line the rigid moment of inertia corresponding to $R_0 = 1.2 \times A^{1/3} f$. The empirical values given as filled circles do not include any correction for the rotation-vibration interaction. The dashed and dot-and-dash lines refer to calculations corresponding to the choice of $\Delta_p = P_p$ and $\Delta_n = P_n$ with an assumed single-particle level spectrum ϵ_p , as given according to the alternative cases A and B of table I.

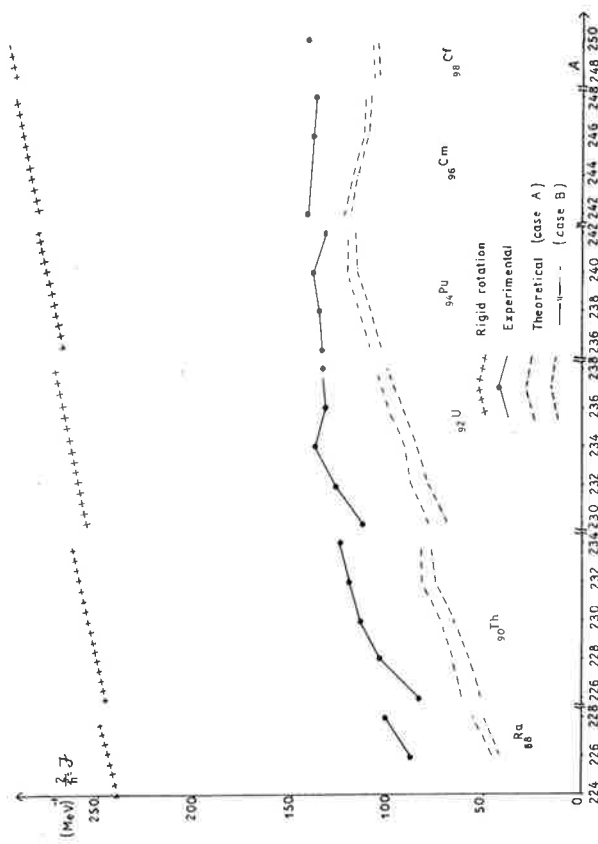


Fig. 18. Moments of inertia of even-even nuclei in region II. For explanation see fig. 17.

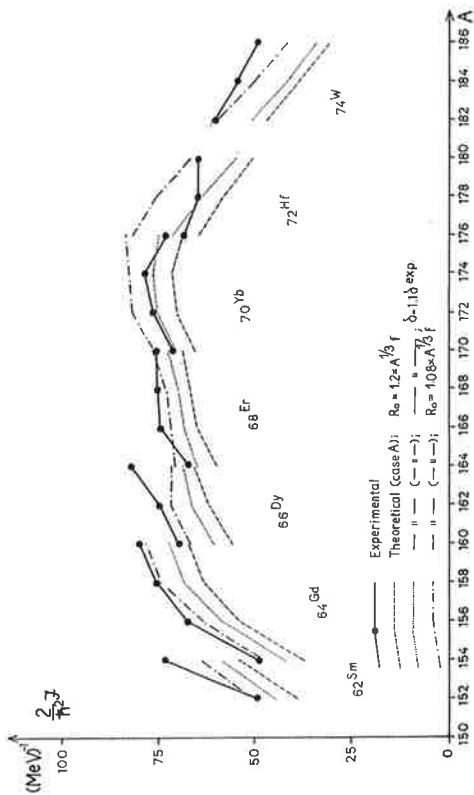


Fig. 19. The dependence of the calculated moment of inertia for nuclei in region I on the eccentricity parameter δ . Note that the dot-and-dash line corresponds to δ as obtained from the experimental Q_0 -values of eq. (41) with the charge radius R_0 chosen equal to $1.08 \times A^{1/3} f$.

It may also be of interest to note the great dependence on the type of wave functions employed in calculating the matrix elements of j_x and s_x . Thus the use of "asymptotic" (15) matrix elements, i. e. the employment of nucleonic wave functions corresponding to the limit of very large eccentricities, gives values considerably above the experimental points in region I and of the same order of magnitude as the experimental values in region II. As can be seen from fig. 25, the variation with (N, Z) is much less favourable than in the calculations where the more accurate nucleonic wave functions have been employed.

It may be argued that the use of the more detailed and realistic wave functions is consistent with the fact that we employ the level scheme of ref. 16 and the empirical estimate of the eccentricity parameter δ .

The greater magnitude of \mathfrak{J} when the asymptotic wave functions are employed corresponds to the fact that while a very large fraction of the whole j_x coupling strength lies between nearby states in the representation of the detailed wave functions, some of this strength and the strength connecting very far-away states is collected in states 2-3 MeV distant in the asymptotic case. When $\Delta \rightarrow 0$, the results are not very different in the two cases. In the case treated here the factor containing u and v cuts down the contribution from the very close-lying states most drastically (by a factor of

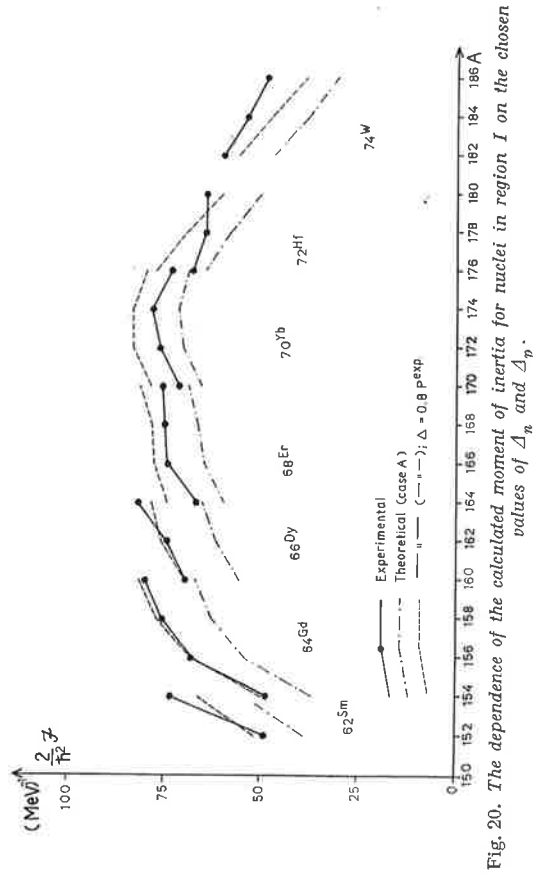


Fig. 20. The dependence of the calculated moment of inertia for nuclei in region I on the chosen values of Δ_n and Δ_p .

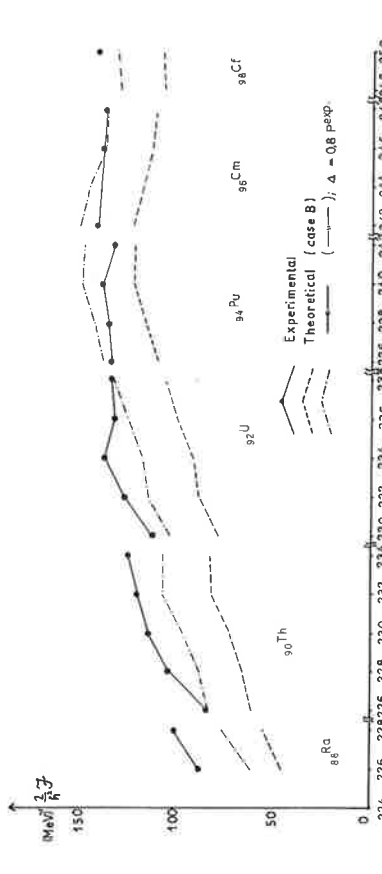


Fig. 21. The dependence of the calculated moment of inertia for nuclei in region II on the chosen values of Δ_n and Δ_p .

five or so). This cancellation therefore affects the asymptotic case less than the other.

In summary, we can only conclude first that, compared with the independent-particle value, the agreement in the magnitude of \mathfrak{J} is rather good; in particular the "fine structure" of the A-dependence of \mathfrak{J} is well reproduced.

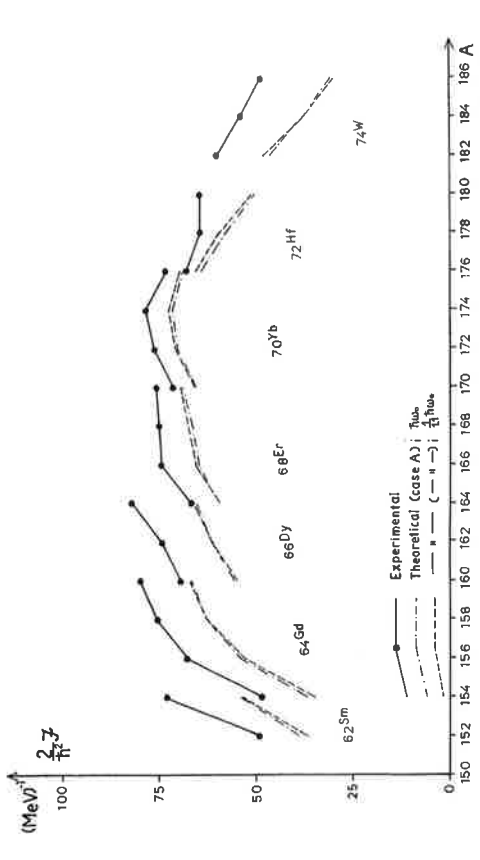


Fig. 22. The dependence of the calculated moment of inertia for nuclei in region I on the choice of the energy scale parameter $\hbar\omega_0$.

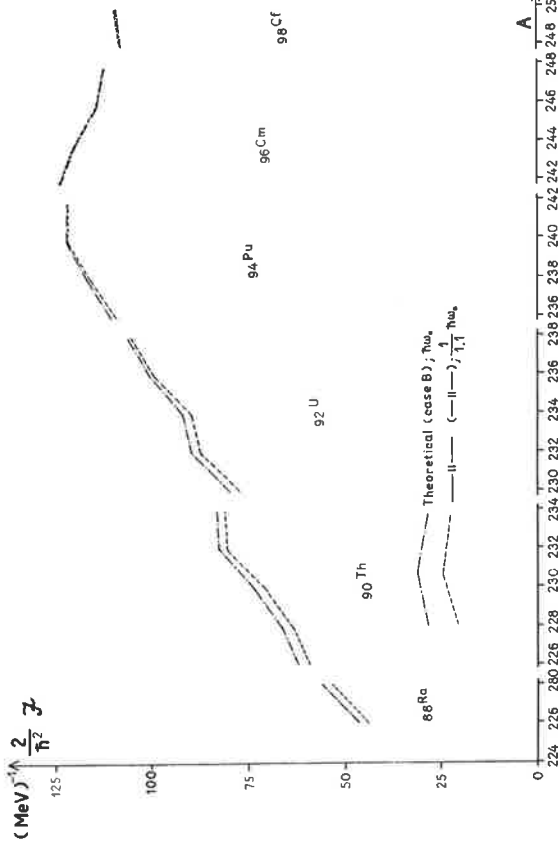


Fig. 23. The dependence of the calculated moment of inertia for nuclei in region II on the choice of the energy scale parameter $\hbar\omega_0$.

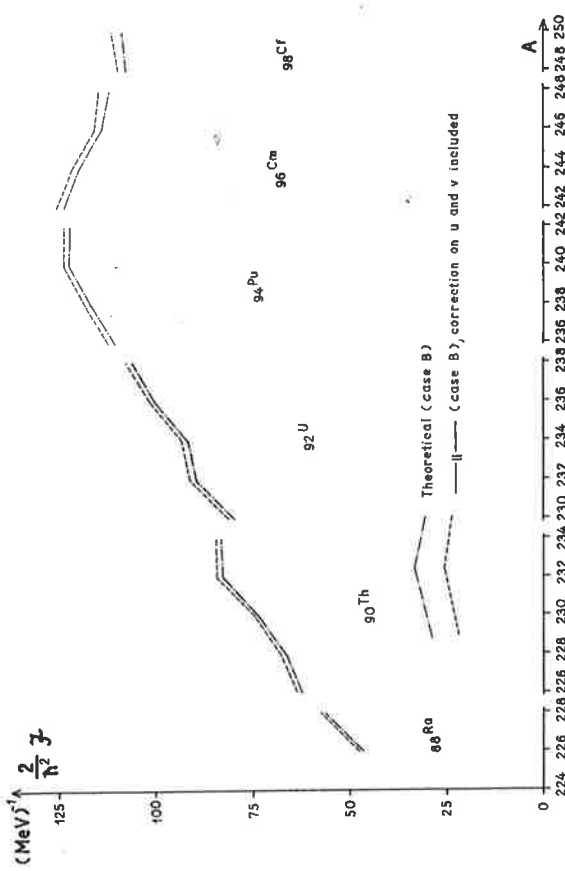


Fig. 24. Correction of the moment of inertia due to the inclusion of the otherwise neglected H_{20} terms in the calculation of u and v (cf. (A L-6) etc.).

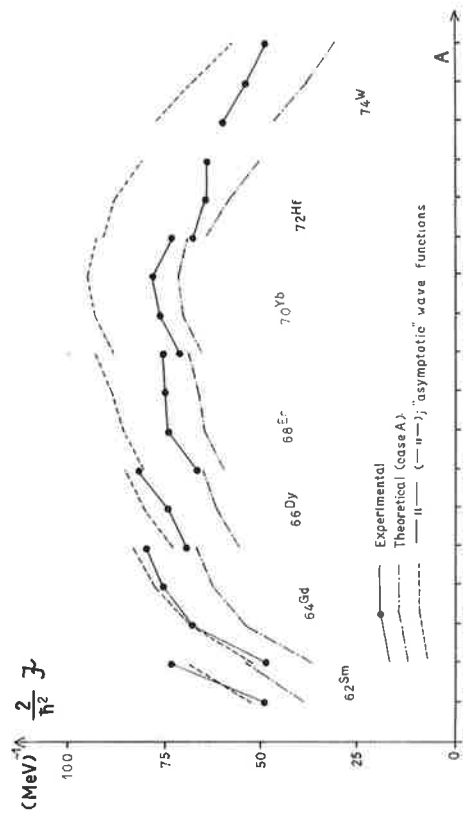


Fig. 25. The theoretical values of the moment of inertia when the asymptotic wave functions are used, compared with the case in which the more detailed wave functions of ref. 15 are employed.

The fine-structure variation appears largely a function of δ^* , which latter in the calculation is taken in turn from the accurate quadrupole determinations of refs. 19 and 20. The systematic deviation between the results of the present calculations and the empirical values may very well lie within the inaccuracies of the parameters δ and Δ and may also depend critically on the insufficient accuracy of the nucleonic wave functions**.

There are, however, also other effects which might be responsible for the deviation. They are connected with the limitations in the form of the interaction Hamiltonian assumed and with the approximate character of the BCS solution** corresponding to the given Hamiltonian.

As pointed out in connection with eq. (5), the assumed type of nucleonic interaction, given by that equation, admits scattering of pairs solely in $K = 0$ states. In particular, the scattering in the $K = 1$ state, that is the intermediate two-quasi-particle state in the cranking formula, is neglected. The inclusion of such an interaction would probably tend to depress somewhat the lowest-lying $K = 1$ states. By that effect alone the energy denominators of eq. (35) would be somewhat cut down and \mathfrak{J} correspondingly increased.

The inclusion of such effects is of interest also for the following reason: In the limit of an infinite nucleus, $A \rightarrow \infty$, the level density of single-particle states increases proportionally to A . As G , owing to the decreasing overlap, tends to zero as $\frac{1}{A}$, thus Δ in this limit goes towards a constant⁽⁶⁾. Finally, all the contributing states ϵ_i are swallowed up by the energy gap, and the term containing u and v makes \mathfrak{J} vanish identically in this limit. This consideration of the limiting behaviour of the solution appears to bear out the contention that some terms are missing in the Belyaev expression which would contribute the irrotational moment in the limit considered⁽¹⁰⁾. It remains to be shown, however, whether the terms present e. g. in the δ -force, but neglected in the pairing interaction, can bring about the expected behaviour in the limit of $A \rightarrow \infty$ ***.

* This is also concluded from an analysis of experimental data in ref. 19.

** The effect of the usually neglected terms in (14) and (24), largely taken care of by eqs. (A1-6)-(A1-8), was included in one calculation. It was found to increase \mathfrak{J} by only a few per cent, however (cf. fig. 24). Note added in proof: Calculations employing the expression (35') for the moment of inertia so far performed for neutrons of Sm^{152} , Gd^{156} , Dy^{160} , and W^{182} render a moment of inertia 6, 3, 2, and 16 per cent, respectively, lower than calculations on the basis of eq. (35), under the assumption of the same value of G_p . According to table II a calculation that take blocking into account in addition require slightly larger G -values to fit the odd-even mass difference. The preliminary results thus indicate that, all in all, the inclusion of the complicated "blocking effects" leads to values of the moment of inertia of the order of 10%, lower. The disparity with empirical findings is therefore increased.

*** The present calculations by PRANGE⁽³²⁾ appear to support such a supposition.

b. The collective gyromagnetic ratio g_R

The calculated value of g_R for even-even nuclei is exhibited in figs. 26 and 27. As g_R is approximately equal to $\frac{\mathfrak{J}_p}{\mathfrak{J}_n + \mathfrak{J}_p}$, it is less sensitive to e. g. an increase in δ , which affects \mathfrak{J}_p and \mathfrak{J}_n in very much the same way. That the value of g_R comes out smaller than the ratio $\frac{Z}{Z+N}$ is largely due to the fact that we have employed a value of Δ_p considerably larger than Δ_n . Furthermore, "fine structure" effects in figs. 26 and 27 are due in particular to the fact that it is mainly the nucleons outside of closed shells (z, n) that contribute to \mathfrak{J}_p and \mathfrak{J}_n , whence the relevant ratio of comparison should be $\frac{z}{z+n}$ rather than $\frac{Z}{Z+N}$. The former ratio exhibits a much faster variation

within a sequence of isotopes at the beginning and the end of shells. At the end of the shells the holes play the parts of the particles at the beginning of the shells, and so the trend of g_R within a series of isotopes is reversed. Fig. 26 also exhibits a comparison with experimental values of g_R for even-even nuclei, taken from a recent compilation by BODENSTEDT⁽³³⁾ *. The experimental errors are very large, as indicated in the figure. The values to the left correspond to measurements by GOLDRING and SHARENBERG⁽³⁴⁾, involving an angular-distribution measurement of the $E2$ gamma radiation emitted in the decay of the first rotational state. This state has been reached by Coulomb excitation and, during its very short lifetime, it is under the influence of a strong external magnetic field. Owing to paramagnetic effects connected with the unfilled atomic $4f$ shell the strength of this field is very much increased at the nucleus, which enhances the angular effects studied. However, as the atomic configurations are not known with sufficient accuracy, the interpretation of the angular-distribution measurements in terms of g_R becomes very uncertain. Indeed, on the basis of new atomic wave functions calculated by KANAMORI⁽³⁵⁾ and SÜSSMANN⁽³⁶⁾, BODENSTEDT et al.⁽³³⁾ have adjusted the values of g_R originally given⁽³⁴⁾. The experimental points on the right side in fig. 26 are based on very similar experiments⁽³⁷⁾, involving, however, a population of the rotational state by beta decay instead of by Coulomb excitation.

In view of the uncertainties of the experimental values, the agreement with the present calculations cannot be considered unsatisfactory.

* We are very much indebted to Dr. BODENSTEDT for his kind permission to quote his values of g_R in advance of publication.

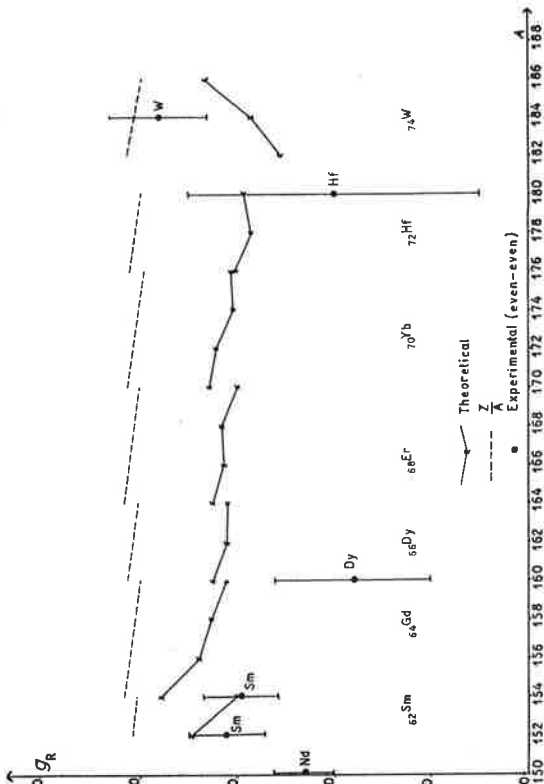


Fig. 26. Collective gyromagnetic ratios of even-even nuclei in region I. The theoretical values corresponding to the single-particle level scheme of "case B", $\Delta_n = P_n$, $\Delta_p = P_p$, and $R_0 = R_2 = 1.2 \times 10^{-13} f$, are represented by the solid line. The measured g_R -values, with experimental errors as listed by BODENREDT⁽³³⁾, are exhibited for comparison. (The calculated values of g_R corresponding to "case A", which can be found in table III b, show rather slight deviations from those of "case B".) Note added in proof: A recent measurement by BODENREDT et al. on Er-66 renders, with employment of the new $\langle r^{-3} \rangle$ values for 4 f electrons calculated by JUDN and LINDGREN (UCRL-9188, unpublished), a very accurate value of $g_R = 0.32 \pm 0.02$. This is in excellent agreement with the theoretical results. (Private communication from D. SHIRLEY.) Furthermore, a recent measurement by Stiening and Deutsch (Phys. Rev. Letters 6, 421 (1961)) gives $g_R = 0.36 \pm 0.06$ for Gd¹⁵⁴.

Turning now to odd-A nuclei, many data are available from magnetic-moment measurements and $M1$ branching ratios within the ground-state rotational bands. From such information g_R and g_K may be determined. In the limit in which the Coriolis coupling (and furthermore the difference in Δ between the odd and the even nucleide) may be neglected, this g_R is simply the same as that of the adjacent even-even nucleus. The effect of the Coriolis force, coupling the near-lying one-quasi-particle states, can now be accounted for in first approximation by a renormalization of g_K and g_R with respect to their adiabatic values⁽³⁸⁾. An analysis of the experimental material in terms of the simple unperturbed formulae therefore yields the renormalized values $g'_R = g_R + \delta g_R$ and $g'_K = g_K + \delta g_K$, where

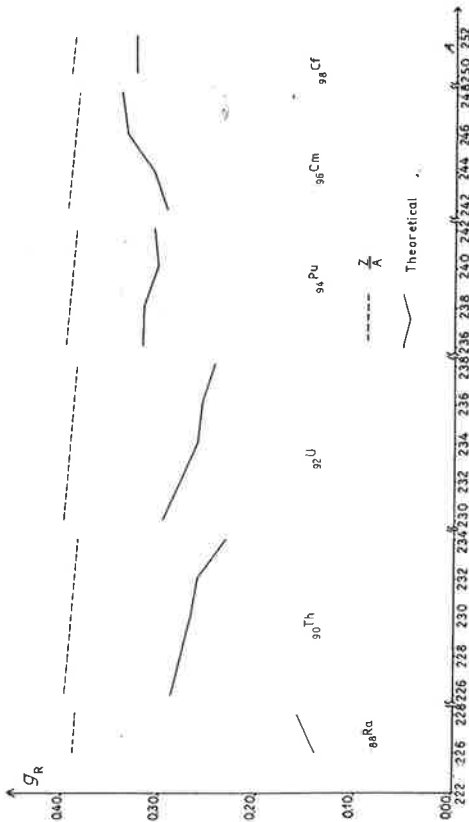


Fig. 27. Collective gyromagnetic ratios of even-even nuclei in region II. The theoretical values represented by the solid line correspond to the single-particle level scheme of "case B", and $\Delta_n = P_n$, $\Delta_p = P_p$. The dashed line represents the ratio Z/A corresponding to "homogeneous flow".

$$\delta g_R(\nu) = \frac{\delta \mathcal{J}^{(1)}(\nu)}{\mathcal{J}} (g_l - g_R) + \frac{\delta W^{(1)}(\nu)}{\mathcal{J}} (g_s - g_l). \quad (48)$$

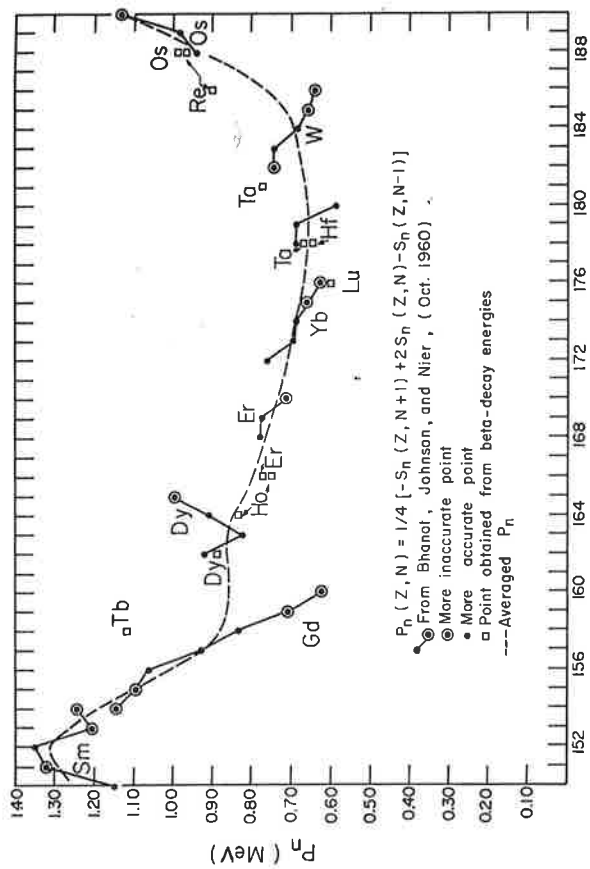
In eq. (48) $\delta \mathcal{J}^{(1)}$ is the contribution of the odd particle to the moment of inertia connecting the one-quasi-particle state ν with other states of the same kind. If the quasi-particle formulation is sufficiently accurate to estimate this difference, $\delta \mathcal{J}^{(1)}(\nu)$ should be very nearly equal to the odd-even difference in moments of inertia⁽³⁹⁾. Some of this difference, however, might be due to the effects of blocking. Blocking effects contributing to δg_R may also be included in eq. (48) through $\delta \mathcal{J}^{(1)}$. Similarly, $\delta W^{(1)}(\nu)$ is the contribution to the expression W of the odd particle occupying the orbital ν . Now $\delta \mathcal{J}^{(1)}$ is always a positive quantity. This is normally the case also with $\delta W^{(1)}$. As the first term always dominates, in all cases of practical interest δg_R is positive for protons ($g_l = 1$, $g_s = 5.56$) and negative for neutrons ($g_l = 0$, $g_s = -3.83$). Indeed, in their analysis of the empirical values of g_R and g_K for odd-A nuclei BERNSTEIN and DE BOER⁽⁴⁰⁾ find values of g_R for odd-N nuclei on the average 0.1 magneton lower than those for the odd-Z nuclei. This is qualitatively in agreement with (48). One might now attempt to apply (48) as a correction to the values found by the straightforward analysis, in order to obtain the unperturbed values g_R^0 . If one inserts

in this formula for $\delta_{\mathcal{N}}^{(1)}$ the empirical odd-even differences in the moment of inertia and estimates the somewhat smaller second term by its "asymptotic" expression⁽¹⁵⁾, one usually finds too large corrections δg_R . Now, the spin matrix elements empirically turn out to be systematically much smaller (about 50%) than those calculated from the single-particle wave functions. This is evidenced e. g. by the plots of magnetic moments (theoretical and experimental) exhibited in ref. 16. This reduction may be explained in terms of the spin polarization effect⁽⁴¹⁾ whereby e. g. in the case of an odd proton the spin polarization part of the two-nucleon interaction tends to align the spins of the neutrons parallel to, and the spins of the other protons antiparallel to, the direction of the odd-proton spin. This polarization then effectively diminishes the magnetic dipole strength. Even with a 50% reduction of the latter term the correction factor δg_R still appears somewhat too large. In view of the uncertainty of the correction δg_R , clearly one cannot point to a definite disagreement with the theoretical g_R -values. One might tentatively say, however, that the experimental g_R -values are on the whole 10-20% smaller than the calculated ones⁽⁴²⁾.

Acknowledgements

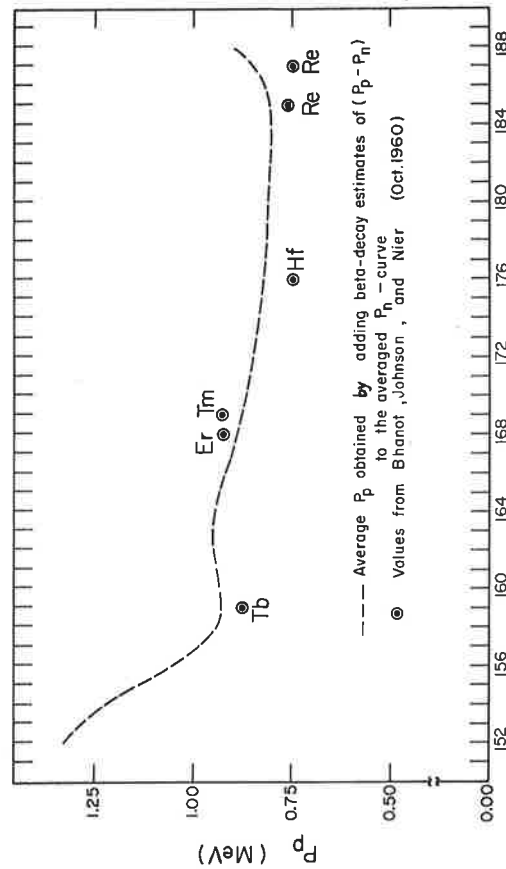
In this work we have profited greatly by valuable suggestions and generous advice from Professors A. BOHR and B. MOTTELSON, and by discussions with other members of the Copenhagen group. We are deeply indebted to Professor C. E. FRÖBERG and Mr. J. BOHRMAN of the Institute of Numerical Analysis in Lund for working out the large computational programme for SMIL. It is a pleasure for us to acknowledge the excellent working conditions of the Institute of Theoretical Physics in Lund and of NORDITA - Nordisk Institut for Teoretisk Atomfysik - in Copenhagen. We are also grateful to NORDITA and the Swedish Council for Atomic Research for financial support.

NORDITA, Copenhagen, and
The Institute of Theoretical Physics,
The University of Lund, Sweden



A

Fig. 28 (added in proof). Represents a revision of fig. 1 by the inclusion of recently published (Oct. 1960) mass-spectroscopic data, ref. 30.



A

Fig. 29 (added in proof). Empirical values of $(P_{\beta} - P_n)$ are added to the averaged P_n -function of fig. 28 in obtaining the dashed curve of this figure. The latter curve may then be compared with the six points of the figure which are based directly on masses of isotones as listed in ref. 30.

Appendix I

On the Quasi-Particle Approximation

The calculations reported in the main text rest on various approximations leading up to the simple quasi-particle formulation employed. We will start the discussion from the Hamiltonian (7) as given, including its diagonal parts. The trial wave function (11) and, analogously, the canonical transformation (19) introduce a non-conservation in the number of particles, leading to wave functions describing an ensemble of nuclei rather than a specific nucleide. Some problems, in particular the occurrence of spurious states, are associated with the resulting fluctuations in the number of particles. We will defer till later a few remarks on the relevance of these fluctuations to our present problems. First we will discuss the various approximations of relative magnitude $\frac{G}{2\lambda}$ that have to do with the neglect of H'_{int} etc.

The Hamiltonian (7) after the canonical transformation (19a, b) takes the form (20). Of interest here are the explicit expressions of the H'_{int} terms H'_{22} , H'_{31} and H'_{40} . These have all been listed by BELYAEV⁽⁶⁾, but we give them here for the sake of completeness and in a form that is particularly simple as we have limited ourselves to the case of a constant matrix element G .

We first consider the problem of odd-even mass differences. The ground state of the odd system is affected by H'_{31} in contrast to the even ground state. This interaction is of the form

$$H'_{31} = G \sum_{\nu} (u_{\nu}^2 - v_{\nu}^2) \alpha_{\nu}^{\dagger} \beta_{\nu}^{\dagger} \sum_{\nu'} u_{\nu'} v_{\nu'} (\alpha_{\nu'}^{\dagger} \alpha_{\nu'} + \beta_{\nu'}^{\dagger} \beta_{\nu'}) + \text{c. c.} \quad (\text{A I-1})$$

The effect of H'_{31} on a one-quasi-particle state is therefore

$$H'_{31} \alpha_{\nu}^{\dagger} |0\rangle = +G \sum_{\nu'} (u_{\nu'}^2 - v_{\nu'}^2) u_{\nu'} v_{\nu'} \alpha_{\nu'}^{\dagger} \beta_{\nu'}^{\dagger} \alpha_{\nu}^{\dagger} |0\rangle. \quad (\text{A I-2})$$

The depression $-\delta E^{(1)}$ of the ground state ν' due to H'_{31} is given in lowest-order perturbation theory by

$$\delta E^{(1)}(H'_{31}) \simeq G^2 \frac{1}{8} \sum_{\nu} \frac{1}{E_{\nu}} \left(1 - \frac{\Delta^2}{E_{\nu}^2}\right). \quad (\text{A I-3})$$

Using (18), one easily obtains an upper limit to $\delta E^{(1)}$:

$$\delta E^{(1)}(H'_{31}) \leq \frac{G}{4}. \quad (\text{A I-4})$$

This perturbation estimate is actually rather accurate as the close-lying lower levels have small matrix elements because of the factor $(u_{\nu}^2 - v_{\nu}^2)$. We have computed (A I-3) numerically for some nuclei scattered over region I and have there obtained results between 50 and 80 % of the upper limit in (A I-4).

Furthermore, the H'_{40} -term is of the form

$$H'_{40} = G \sum_{\nu\nu'} u_{\nu}^2 v_{\nu'}^2 \alpha_{\nu}^{\dagger} \beta_{\nu'}^{\dagger} \alpha_{\nu'}^{\dagger} \beta_{\nu}^{\dagger} + \text{c. c.} \quad (\text{A I-5})$$

This couples the quasi-particle vacuum with four-quasi-particle states and the one-quasi-particle state with five-quasi-particle states. In both cases H'_{40} thus creates four new quasi-particles. Therefore, the first-order contribution is the same in the two cases within this formalism, except that in the second case the state ν' , with which one quasi-particle is associated, is excluded in the sum. An estimate of the difference in depression due to H'_{40} indicates that this energy difference is less than or of the order of $\frac{G}{4}$, i. e. a few tens of keV.

Furthermore, there is the effect of the neglect of the last term in eqs. (14), leading to the expressions (15) for u_{ν} and v_{ν} , which approximation is also of the order $\frac{G}{2\lambda}$.

It is of course possible to take the neglected term in eqs. (14) into account in an approximate way by treating it as a perturbation. The modified form of the population parameter v_{ν}^2 is then

$$v_{\nu}^2 = \frac{1}{2} \left(1 - \frac{(\overline{\epsilon_{\nu} - \lambda})}{E_{\nu}}\right), \quad (\text{A I-6})$$

where

$$(\overline{\epsilon_{\nu} - \lambda}) = (\epsilon_{\nu} - \lambda_0) \left(1 + \frac{G}{2E_{\nu}^2}\right) \quad (\text{A I-7})$$

and

$$E_{\nu} = \sqrt{(\overline{\epsilon_{\nu} - \lambda})^2 + \Delta^2}. \quad (\text{A I-8})$$

The quantities of the unperturbed case, given by eqs. (15a, b), (17) and (18), are denoted by an index zero in the relations above. Obviously, v_{ν}^2 is not at all affected at $\epsilon_{\nu} = \lambda_0$, and the correction also tends to zero for $|\epsilon_{\nu} - \lambda_0|$ very large, while the largest correction occurs for $|\epsilon_{\nu} - \lambda_0| \sim G$. On the assumption that the unperturbed solutions u_{ν} and v_{ν} fulfil (13) exactly, the perturbed

u_ν and v_ν given by (AI-6) correspond to a small error in the number of particles:

$$\delta n \simeq -\frac{G}{2} \Delta^2 \sum_\nu \frac{\varepsilon_\nu - \lambda_0}{E_\nu^4}, \quad (\text{AI-9})$$

which error may easily be compensated for ad hoc.

Furthermore, in terms of this same approximation, the expression for H'_{11} is simply

$$H'_{11} \simeq \sum_\nu \bar{E}_\nu (\alpha_\nu^+ \alpha_\nu + \beta_\nu^+ \beta_\nu). \quad (\text{AI-10})$$

Thus (AI-10) is formally identical with (24') although the last terms of (14) and of (24) have been included to obtain (AI-10). The energy gap is still associated with the same Δ . This Δ , however, now corresponds to a somewhat different value of G according to eq. (18), as u_ν and v_ν are slightly changed. It may also be pointed out that the modification of v_ν^2 brought about by this perturbation method is largely equivalent to a small renormalization of G . The effect on the moment of inertia of the inclusion of the perturbation terms discussed may be studied in fig. 24.

As far as the odd-even mass differences are concerned, the total result of the effects discussed should normally not exceed an order of magnitude of 50 keV. There remain effects due to fluctuations in the number of particles (see below), and the effects of the change of the quasi-particle vacuum due to the blocking by the odd particle, discussed in the main text.

It may be appropriate in this connection to make a few comments on the two-quasi-particle states and the empirical energy gap in even-even nuclei. The H'_{11} -term gives an excess energy of the lowest two-quasi-particle states compared with that of the ground state:

$$\delta E^{(2)}(H'_{11}) = 2E_\nu, \quad (\text{AI-11})$$

which is just twice the uncorrected value of the odd-even mass difference. Most important among the neglected H'_{int} -terms is here probably H'_{22} , which we write out explicitly below:

$$H'_{22} = -G \sum_\nu \left\{ (u_\nu^2 u_\nu^2 + v_\nu^2 v_\nu^2) \alpha_\nu^+ \beta_\nu^+ \beta_\nu \alpha_\nu + u_\nu v_\nu u_\nu v_\nu (\alpha_\nu^+ \alpha_\nu + \beta_\nu^+ \beta_\nu) \beta_\nu \alpha_\nu + 2 \alpha_\nu^+ \beta_\nu^+ \beta_\nu \alpha_\nu \right\}. \quad (\text{AI-12})$$

It gives rise to matrix elements of the following type (we here denote the two-quasi-particle state* $\alpha_\nu^+ \beta_\nu^+ |0\rangle\rangle$ by $|\nu - \nu\rangle\rangle$):

* We here limit ourselves to two-quasi-particle states in which the two-quasi-particles refer to the same orbital ν .

$$\langle\langle -\nu\nu | H'_{22} | \nu - \nu \rangle\rangle = -G \quad (\text{AI-13})$$

$$\langle\langle -\nu'\nu' | H'_{22} | \nu - \nu \rangle\rangle = -G(u_\nu^2 u_\nu^2 + v_\nu^2 v_\nu^2) \quad (\nu' \neq \nu). \quad (\text{AI-14})$$

There is thus first a negative diagonal element which is of the order of 5-10⁰/0 of the energy gap in our case. Even more important, however, appears the effect of the non-diagonal matrix elements (AI-14) connecting the rather dense-lying two-quasi-particle states with one another. The factor $(u_\nu^2 u_\nu^2 + v_\nu^2 v_\nu^2)$ can also be written as $\frac{1}{2} \left(1 + \frac{(\varepsilon_\nu - \lambda)}{E_\nu E_{\nu'}} \right)$. It has a value close

to 1/2 when ε_ν and $\varepsilon_{\nu'}$ refer to single-particle levels near the Fermi surface, as one would expect to be the case with the lowest-lying two-quasi-particle states. Thus the factor containing u and v causes no considerable reduction in the matrix elements. Furthermore, there are a number of states that are rather close-lying. The effect of the H'_{22} terms therefore at first sight appears disastrous to the whole concept of the energy gap; in fact it is very largely spurious, however. To elucidate this point it is useful to refer to the "degenerate model", where all the single-particle states ε_ν are degenerate in energy⁽⁶⁾. In this case all u : s and v : s are equal. Therefore, all off-diagonal matrix elements of H'_{22} are equal, and their value lies between $\frac{G}{2}$ and G ; let us call them $G\kappa$, where κ depends on the shell-filling parameter $\frac{n}{Q}$:

$$\kappa = 1 - \frac{n}{Q} \left(1 - \frac{1}{2} \frac{n}{Q} \right). \quad (\text{AI-15})$$

If we diagonalize the H'_{22} -matrix with respect to the two-quasi-particle states, we find that the state $\Psi'_s = \sum_\nu \alpha_\nu^+ \beta_\nu^+ |0\rangle\rangle$ exhausts the strength of the matrix apart from what is associated with the difference between the terms (AI-13) and (AI-14). The contribution to the energy in the state Ψ'_s is $[-G - (Q-1)\kappa G]$. The depression due to the H'_{22} interaction should thus amount to something of the order of half or more of the energy gap*. This state Ψ'_s is, however, just the lowest spurion occurring in the degenerate model, as is demonstrated by BOHR and MOTTELSON in ref. 5. Its occurrence as a BCS state is connected with the extra degree of freedom introduced through the ensemble of states having slightly different numbers of particles. In the non-degenerate case, to the extent to which there is an energy gap at all, there must be a certain number Q' of states ε_ν lying within a distance Δ above and below λ .

* Indeed the exact inclusion of couplings in higher orders brings this state all the way down to the ground state⁽⁵⁾ (communication from B. MOTTELSON).

The $K = 0$ quasi-particle states associated with these levels now all fall densely above the energy gap. In between them, all matrix elements given by eq. (AI-14) are roughly constant. With respect to these states we have a matrix representation of H'_{22} of the same type as that with respect to the \mathcal{Q} two-quasi-particle states in the degenerate case. The state that absorbs most of the strength of the coupling of H'_{22} between the near-lying two-quasi-particle states is largely spurious in analogy with the degenerate case.

There also remain to be discussed effects that have to do with the number of particles of the BCS wave function. The first effect, which is related to the variation in the average number of particles in the quasi-particle approximation, is of very small magnitude, and we include it only for the sake of completeness. The relative difference in the number of particles between a two-quasi-particle state $|\nu-\nu\rangle\rangle$ and the ground state is

$$\langle\langle \nu-\nu | N | -\nu\nu \rangle\rangle - \langle\langle 0 | N | 0 \rangle\rangle = 2(u_\nu^2 - v_\nu^2) = 2 \frac{\epsilon_\nu - \lambda}{E_\nu}. \quad (\text{AI-16})$$

Similarly, comparing the ground state of an odd-A nucleus with the even-even nucleide corresponding to the vacuum state, one obtains for the difference in the average number of particles

$$\langle\langle \nu | N | \nu \rangle\rangle - \langle\langle 0 | N | 0 \rangle\rangle = u_\nu^2 - v_\nu^2. \quad (\text{AI-17})$$

Provided ϵ_ν lies near the Fermi surface, as is the case for the ground odd-A state and the lowest excited even-even state, the deviation δn is rather small*. Now the solutions of $H' = H - \lambda N$ are stationary with respect to variations in the number of particles. That is to say, the quasi-particle solution corrects for the error in the number of particles δn by subtraction of an energy $\delta n \times \lambda_0$, where λ_0 refers to the quasi-particle vacuum. However, a small increase in the number of particles raises λ by $\frac{d\lambda}{dn} \times \delta n$. A good estimate of the error due to this effect should be

$$\delta E^{(1)}(\delta n) = \pm \frac{1}{2} \frac{d\lambda}{dn} (\delta n)^2, \quad (\text{AI-18})$$

where the plus sign corresponds to $\epsilon_\nu < \lambda$ and the minus sign to $\epsilon_\nu > \lambda$. In the cases treated in the present investigation the error from this source is

* It is thus apparent that in comparing odd-even mass differences of e. g. isotopes one should compare the odd-A nucleide with the average of the two adjacent even-even nucleides; this average is the appropriate quasi-particle vacuum in the odd-A case.

odd-even mass differences should be of the order of ± 5 keV. This effect obviously concerns also the energies of the two-quasi-particle states. The effect on the lower-lying excitations, according to eqs. (AI-16) and (AI-17), is twice that in the odd-A case, i. e. of the order of 10 keV. The higher-lying two-quasi-particle states are shifted by amounts of the order of a few hundred keV owing to this effect.

Furthermore there is an effect that is due to the fluctuations in the number of particles of the Bardeen wave functions. We introduce a mean square deviation defined by

$$\sigma_N^2 = \langle N^2 \rangle - \langle N \rangle^2. \quad (\text{AI-19})$$

For the ground state we have

$$\langle\langle 0 | N^2 | 0 \rangle\rangle - \langle\langle 0 | N | 0 \rangle\rangle^2 = \sum_p 4 u_p^2 v_p^2. \quad (\text{AI-20})$$

In the calculations performed for the regions of deformed nuclei a typical value of σ_N is 3. The fluctuations are somewhat smaller for a one-quasi-particle state, where

$$\langle\langle \nu | N^2 | \nu \rangle\rangle - \langle\langle \nu | N | \nu \rangle\rangle^2 = \sum_{p \neq \nu} 4 u_p^2 v_p^2, \quad (\text{AI-21})$$

which for the odd-A ground state is smaller by about one than the expression (AI-20). In the actual cases this leads to a σ_N -value about 5 % smaller. The actual wave function thus corresponds to an ensemble of nucleides with slightly different numbers of particles. Thus, for instance, the BCS wave function corresponding to U²³⁶ contains a very large fraction of U²³⁴ and U²³⁸ and also of Th²³⁴ and Pu²³⁸*. Now on the average the variation in the total energy of nucleides, as one moves between the shells, is expected to be somewhat concave upwards (at least if Δ_n and Δ_p are kept constant over the Bardeen ensemble). This effect in the Bardeen approximation would therefore cause a greater reduction of the binding energy of the state that displays the larger mean square deviation in the number of particles. An estimate of the influence this will have on the odd-even mass differences requires, however, a somewhat more detailed study of the parameters of the self-consistent field as functions of N and Z .

* One would think that this effect would iron out in the theoretical results the rather detailed dependence on Z and N exhibited by the experimental moment of inertia. That this is not the case is due to the fact that the mixed-in components correspond to fictitious nuclei having all parameters except λ in common with the $(Z_0 N_0)$ -nucleus in question, such as Δ_n , Δ_p and in particular the eccentricity parameter δ . As the dependence of \mathcal{J} on λ alone is weak, the fluctuations are therefore unimportant in this respect.

Appendix II

Single-Particle Matrix Elements of j_x

As pointed out in Appendix A of ref. 15, the interactions between the (spherical) harmonic oscillator shells N and $N+2$ due to the quadrupole deformation of the potential can easily be taken into account if one first transforms to the slightly distorted coordinates $\xi \sim x/\omega_x$ etc. as defined in eq. (A.5) of the reference cited. The wave function given in the tables of that reference should then be considered as expressed in these distorted coordinates, in terms of which we have

$$l_x = a l_x^t - b l_x^t, \quad (\text{AII-1})$$

$$l_x^t = -i \left(\eta \frac{\partial}{\partial \zeta} - \zeta \frac{\partial}{\partial \eta} \right) \quad (\text{AII-2})$$

$$f_x^t = -i \left(\eta \frac{\partial}{\partial \zeta} + \zeta \frac{\partial}{\partial \eta} \right). \quad (\text{AII-3})$$

where

and*

A similar relation holds for the y -component, while

$$l_z = l_z^t.$$

The exact expressions for a and b are given in (A13) of ref. 15. The expansions up to the lowest order in δ are

$$a = 1 + \frac{1}{8} \delta^2 + \dots \quad (\text{AII-4})$$

$$b = \frac{1}{2} \delta + \dots \quad (\text{AII-5})$$

The operator l_x^t now connects states only within the N -shell of these new coordinates, while f_x^t connects the shells N and $N+2$. This is most easily seen if we express l_x^t and f_x^t in terms of the operators I_z , R and S defined in ref. 43. Thus

$$l_x^t = \sqrt{2} [S I_z^* - R^* I_z] \quad (\text{AII-6})$$

$$f_x^t = \sqrt{2} [S^* I_z - R I_z^*] \quad (\text{AII-7})$$

* Such an operator f_x is encountered e. g. in the theory of elasticity.

$$f_+ = \sqrt{2} [R^* I_z^* - S I_z] \quad (\text{AII-8})$$

$$f_- = \sqrt{2} [R I_z - S^* I_z^*]. \quad (\text{AII-9})$$

We have defined f_+ as $f_x - i f_y$ and f_- as $f_x + i f_y$; f_+ is then associated with an increase in λ by one unit. The operator I_z^* gives rise to an increase in n_z by one unit, R^* and S^* both raise n_\perp by one unit, but R^* also raises λ by one unit while S^* lowers λ by one unit. From these relations it is obvious that \uparrow^t connects states with the same N while \uparrow^t has elements only between states with N values different by two. The matrix elements in the asymptotic representation are also trivially obtained from these relations.

In evaluating the contribution from \uparrow^t to the moment of inertia it proved essential, however, to employ the exact wave functions of ref. 15, as is discussed in the main text.

On the basis of eq. (AII-1) one may write the expression for the moment of inertia in the form

$$\mathfrak{S} = \mathfrak{S}^0 \left(1 + \frac{1}{4} \delta^2 \right) + \mathfrak{S}_f, \quad (\text{AII-10})$$

where \mathfrak{S}^0 is the moment of inertia obtained when the coupling of the quadrupole part of the nuclear potential between the shells N and $N+2$ is neglected. The term \mathfrak{S}_f represents solely the contribution of the term \uparrow^t in (AII-1). It only amounts to about 5% of the whole moment of inertia. As the states connected by \uparrow^t lie two shells apart, the pairing effects are negligible. The detailed level order within the shells is also unimportant for an estimate of this small correction term. In the case of a pure-harmonic oscillator model one finds

$$\mathfrak{S}_f = \frac{1}{4} \delta^2 \mathfrak{S}_{\text{rig}} = \frac{1}{4} \mathfrak{S}_{\text{irrot}}. \quad (\text{AII-11})$$

In addition, the effect of the coupling between the shells is manifested in the correction term $\frac{1}{4} \delta^2 \mathfrak{S}^0$. This term is associated with the extra nodes in the wave functions of one shell that are due to this coupling; it is smaller than \mathfrak{S}_f by a factor $\frac{\mathfrak{S}}{\mathfrak{S}_{\text{rig}}}$.

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