Title

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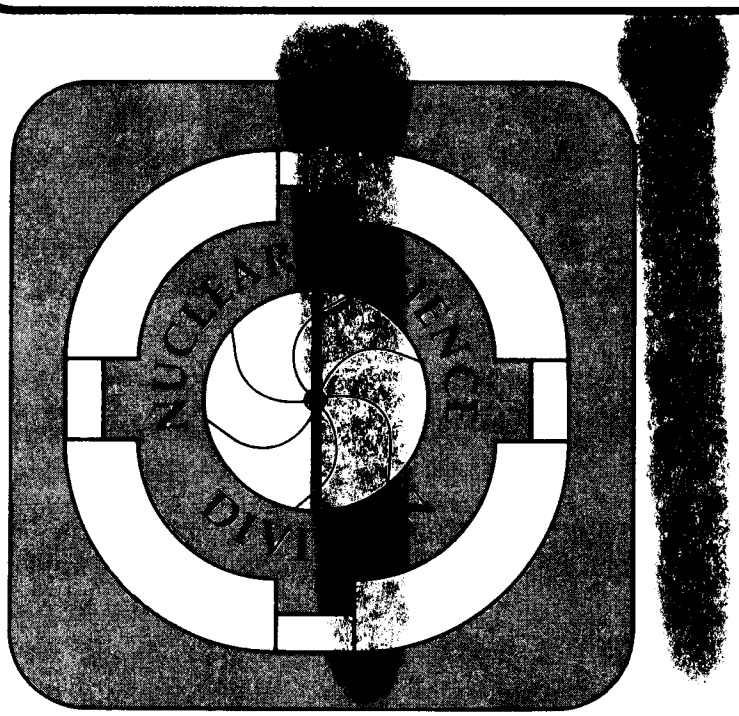

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An Analysis of Angular Momentum Projected Hartree-Fock-Bogoliubov Wave Functions in Terms of Interacting Bosons[+]

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Abstract:

Angular momentum- and number-projected Hartree-Fock-Bogoliubov (HFB) wave functions of transitional and deformed Rare Earth nuclei are analyzed in terms of Fermion pairs coupled to angular momenta L = 0(S), 2(D), 4(G), ... The Fermion space is truncated to contain only S-D or S-D-G pairs. The variation is carried out before and after angular momentum projection and also with different truncations. The influence of the truncation on physical quantities such as moments of inertia, quadrupole moments or pair transfer matrix elements is discussed.

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1. INTRODUCTION

The Interacting Boson Model (IBM) of Arima and Iachello[1]) has proved to be a very successful phenomenological description of collective properties in nuclear structure. One would like, of course, to understand this fact on a more microscopic basis. In particular one would like to make the connection between the Bosonic degrees of freedom used in the IBM as the building blocks of the nucleus and the conventional Fermionic degrees of freedom of protons and neutrons which are used for instance in the nuclear shell model. Usually this link is made by interpreting the Bosons in a first approximation as collective pairs of Fermions.

In fact many years ago it was shown that a system of interacting Fermions can be exactly represented by a system of interacting Bosons (for a review see ref. 2). In nuclear physics this idea was introduced by Belyaev and Zelevinskii[3]) and by Marumori, Yamamura and Tokunaga[4]). These authors used collective ph- (or two-quasi-particle-) pairs as the Fermionic counterpart of the Bosons. Much work has been done in this framework[5-8]) and considerable success has been achieved. There are, however, still a number of open problems as to the convergence of these "conventional" Boson expansions, the possible admixtures of single particle degrees of freedom and the occurrence of spurious modes. These problems show up in all Boson theories and can cause serious mistakes in practical applications if not properly treated.

The microscopic counterpart of the Bosons in the IBM are usually assumed to be pp-pairs of Fermions[9,10]). These pairs can be thought as the building blocks of a shell model calculation. Taking into account a sufficiently large number of different Fermion pairs one thus has in principle an exact

description of the many-body problem for the valence shell of transitional and deformed nuclei. Of course this concept can only be carried out in practice if the number of different types of Fermion pairs is restricted. In fact the ground state of spherical nuclei seems to be built to a very large extent by pairs coupled to angular momentum L = 0(S). Low lying excited states carry angular momentum L = 2(D). A number of calculations in spherical nuclei, where only very few broken pairs are present, has shown that one obtains a qualitative understanding of the microscopically fitted IBM-parameters already using only S- and D-pairs[11-13]). By taking into account the influence of higher pairs, such as G,I... and S',D'..., by a renormalization procedure one can even find a quantitative agreement[14,15]). In that sense there is a microscopic foundation of the IBM for spherical nuclei.

Of course the IBM model has its biggest success for the description of transitional and deformed nuclei. There the situation is much more complicated. The transition from spherical shapes to deformed shapes can be described as a kind of a phase-transition in a finite system. Such a phase-transition is connected with the freezing out of a soft mode. It is evident that this soft mode is a quadrupole vibration and therefore one expects the deformed ground state to contain a large number of D-pairs. A number of investigations have been carried out to understand quantitatively the structure of deformed HFB-states in terms of S,D,G... pairs[16-18]). It has been found that HFB wave functions of deformed nuclei lie, to a large extent, in the SD-space. Essential physical quantities, however, can only be understood on the basis of higher pairs. For a microscopic understanding of the properties of deformed nuclei one has to take into account at least the G-pair. These results are in agreement with detailed phenomenological

investigations of K. Heyde et al.[31,32]), which show that the fits to experimental data in ^{156}Gd can be considerably improved by including a g-Boson.

All these microscopic investigations used deformed HFB-states. IBM-model states, however, are states in the laboratory frame with good angular momentum. In fact one of the big advantages of pp-Bosons, as compared to the ph-Bosons based on quasi-particle pairs, is the fact that the former preserve the symmetries. The microscopic counterpart of the IBM-groundstate in spherical nuclei is a state with generalized seniority zero[19-21]), or a number projected BCS-state. Using symmetry conserving wave functions in the Fermion picture is certainly more complicated, but it has the advantage that one avoids the admixture of spurious states.

A consistent extension of these ideas to deformed nuclei requires, in addition to number projection, the restoration of rotational invariance using angular momentum projection. For the analysis of the microscopic background of the IBM-model in deformed nuclei we therefore used angular momentum and number projected deformed HFB wave functions in this paper. In fact it is well known that the groundstate and the members of the groundstate band for not too large angular momenta can be described to a fairly good approximation by such wave functions. These wave functions have only a very small overlap with the intrinsic HFB wave function[22-24]) and thus it is not at all clear from the outset if the conclusions obtained from the analysis of intrinsic unprojected wave functions remain valid.

The analysis was carried out in different stages. We start out in section 2 with a fixed HFB wave function, decompose it into SD-,SDG-,... parts and calculate overlaps of wave functions and matrix elements of physical

observables with these truncated wave functions. We are thus in a position to investigate which quantities can be reproduced already in the SD-space and which are sensitive to admixtures of higher pairs. This analysis is carried out first for a model containing nucleons in a single j-shell and later on extended to the case of a realistic wave function of Rare Earth nuclei.

In these investigations the structure of the collective Fermion pairs is completely determined by the intrinsic wave function. In section 3 we go a step further and use pairs optimized for the different truncations. We carry out a variation of the energy calculated after truncation and projection. Thus we are able to work with optimally adjusted pairs. We study how their structure changes in going from spherical shapes through transitional cases to deformed nuclei and discuss again to what extent this shape-change may be represented in such truncated spaces.

In section 4 we summarize the conclusions we can draw from this investigation regarding the validity of the IBM model in deformed and transitional nuclei.

2. CALCULATIONS WITH FIXED INTRINSIC WAVEFUNCTIONS

2.1 THE TRUNCATION OF ANGULAR MOMENTUM PROJECTED HFB-STATES

It is well known that the groundstate and the low lying members of the groundstate rotational band of deformed nuclei can be written to a good approximation as a number- and angular-momentum projected state:

$$|\Psi\rangle^{IN} = P^I P^N |\Phi\rangle \tag{1}$$

where P^I and P^N are projection operators onto good angular momentum and particle number. The intrinsic function $|\Phi\rangle$ is a generalized Slater determinant. According to the theorem of Thouless[25]) it can be represented in the form

$$|\Phi\rangle \propto \exp(x\Lambda^+)|0\rangle \tag{2}$$

where x is a normalization constant determined be the condition $\langle|0[\Lambda,\Lambda^+]|0\rangle = 1$ and the operator Λ^+, the so-called deformed Cooper-pair, is a collective superposition of Fermion-pairs.

$$\Lambda^+ = \sum_{\alpha<\beta} \Lambda_{\alpha\beta} a^+_\alpha a^+_\beta \tag{3}$$

The quantum numbers $\alpha = (a,m_\alpha) = (n_\alpha,l_\alpha,j_\alpha,m_\alpha)$ describe a spherical oscillator basis and the coefficients $\Lambda_{\alpha\beta}$ can be obtained from the usual representation of HFB wave functions in terms of the matrices $U_{\alpha k}, V_{\alpha k}$ of the Bogoliubov-transformation

$$\alpha_k^+ = \sum_\alpha U_{\alpha k} a_\alpha^+ + V_{\alpha k} a_\alpha \tag{4}$$

by matrix inversion (see ref. 24, p. 615):

$$\Lambda_{\alpha\beta} = \frac{1}{x}(V\ U^{-1})^*_{\alpha\beta} \tag{5}$$

Since we are dealing with deformed nuclei, the collective pair Λ^+ violates rotational symmetry. As in ref. 17,18 it can be decomposed into pairs of good angular momentum:

$$\Lambda^+ = \sum_L x_L Q_L^+ \tag{6}$$

with

$$Q_L^+ = \sum_{a\leq b} \alpha_L(a,b) A_{L0}^+(a,b) \tag{7}$$

$$A_{LM}^+(a,b) = \frac{1}{\sqrt{1+\delta_{ab}}} \sum_{m_a m_b} C^{j_a j_b L}_{m_a m_b M}\ a_\alpha^+ a_\beta^+ \tag{8}$$

$$x_L \alpha_L(a,b) = \frac{1}{\sqrt{1+\delta_{ab}}} \sum_{m_a m_b} C^{j_a j_b L}_{m_a m_b M}\ \Lambda_{\alpha\beta} \tag{9}$$

The pairs Q_0, Q_2, Q_4... are called in the following S,D,G,... . They are normalized in the sense

$$\langle 0|[Q_L, Q_L^+]|0\rangle = 1 \tag{10}$$

which defines the quantities x_L^2. They can be interpreted as the probability of finding a pair with angular momentum L in the Cooper pair A^+ and have been calculated by several authors[16-18]). It has been found that a large percentage (between 80% and 90%) of the Cooper pair is already given by the S and D pair. We investigate in the following different truncations, i.e., we use intrinsic states of the form

$$|\Phi\rangle_{02} \propto \exp\{x(x_0 S^+ + x_2 D^+)\}|0\rangle \tag{11}$$

$$|\Phi\rangle_{024} \propto \exp\{x(x_0 S^+ + x_2 D^+ + x_4 G^+)\}|0\rangle \tag{12}$$

From these wave functions we project onto good particle number and onto good angular momentum as indicated in eq. 1. We use the projection operators in the form introduced by Wigner[26]). Projected wave functions are in the following denoted by $|\Psi\rangle^{IN}$, $|\Psi\rangle^{IN}_{02}$ and $|\Psi\rangle^{IN}_{024}$ indicating the different truncations.

2.2 INVESTIGATIONS IN A SINGLE-j-SHELL

The conclusions about the validity of SD- and SDG-... truncation depend certainly on the dynamics of the system, i.e., on the underlying many-body Hamiltonian. Since there is no unique prescription which Hamiltonian one should use, these conclusions can be somewhat arbitrary. We therefore begin this section with an investigation, which is completely independent of the

dynamics. We use as intrinsic state a fixed wave function of the Nilsson-BCS type, truncate it, project it onto good angular momentum and particle number and discuss the effect of the truncation and projection on overlaps and matrix elements of physical operators. In the following sections we will also take into account the dynamics, by treating a realistic Hamiltonian.

As in ref. 17 we use a model wave function $|\Phi\rangle$ of the Nilsson-BCS type in a single $j = 41/2$ shell with fixed deformation $\beta = -0.3$, a fixed gap parameter $\Delta = 1$ MeV and particle number mean value $N = \langle\Phi|\hat{N}|\Phi\rangle$. In contrast to ref. 18 we shall not minimize with respect to some Hamiltonian. Since we only wish to study the influence of projection we shall always work with the same intrinsic wave function.

In Fig. 1a we show the probabilities x_L^2 as a function of the particle number N, starting from small particle numbers (where certainly a deformed intrinsic state is a bad approximation) up to N = 20, where the shell is nearly half filled. With increasing number we observe that the sum of the probabilities of the S- and D-pair $x_0^2 + x_2^2$ increases from 70% to 95%. The relative importance of the D-pair increases too, and it reaches its saturation value of ≈55% at N = 10. The probability for the G-pair has a maximum for N = 6 and decreases slowly thereafter, a fact which has been seen already in an early paper by A. Klein and C. Dasso[33]).

In Fig. 1b we show the overlap integrals of the various normalized functions. Only the overlap between the number and angular momentum projected Nilsson + BCS state and the SDG-approximation to it stays close to unity for all particle numbers. This indicates that the relative contribution of G-pairs increases for larger particle numbers, although the G-pair content in a single Cooper-pair x_4^2 decreases, a fact which can be understood only by

appealing to the Pauli principle. For large particle numbers we have a considerable cancellation of S- and D-pairs, such that the contribution of the G-pair (also small in a single Λ-pair) becomes important in the total wave function. The corresponding overlaps for unprojected and number only projected functions are smaller, but we find qualitatively the same features. In particular the SD-approximation becomes very poor in the intrinsic scheme for large particle numbers.

We have, however, to bear in mind the well known fact that a small overlap in a many-body wave function does not necessarily mean a bad description of the physical properties, because we are mainly interested in certain matrix elements of a few observables.

We therefore calculate projected and unprojected matrix elements for the quadrupole operator. Since we cannot compare spectroscopic quadrupole moments with intrinsic values, we show in Fig. 2 the intrinsic quadrupole moments $\langle Q \rangle$ and $\langle Q \rangle^N$ and in the angular momentum projected case an effective intrinsic quadrupole moment $\langle Q \rangle^{IN}$ defined through the rotor model:

$$\sqrt{B(E2,2 \to 0)} = \langle 2\ 0\ 2\ 0 | 0\ 0 \rangle\ \langle Q \rangle^{IN} \tag{13}$$

As one can see, the unprojected intrinsic matrix element $\langle Q \rangle$ provides for all particle numbers a very reasonable approximation to the projected value $\langle Q \rangle^{IN}$. This is of course a well known fact and a justification for introducing an intrinsic scheme with a deformed potential. In detail the projected matrix element is roughly 5% larger than the unprojected, indicating that angular momentum projection usually yields somewhat larger deformations in a self-consistent calculation.

For small particle numbers the SD-approximation seems to work properly (at least for the quadrupole operator), but for more than 10 particles we observe a strong reduction of the unprojected quadrupole moment $\langle Q\rangle_{02}$. This effect is due mainly to the fact that the SD-part of the unprojected wave function $|\Phi\rangle_{02}$ gives the wrong mean value of the particle number:

$$\langle\Phi|N|\Phi\rangle_{02} \neq \langle\Phi|N|\Phi\rangle \tag{14}$$

and this strong reduction disappears after projection onto the right particle number.

The additional projection onto good angular momentum only increased the matrix elements by a small amount, but gives no great change to this picture.

$$\frac{\langle Q\rangle_{02}^{IN}}{\langle Q\rangle^{IN}} \approx \frac{\langle Q\rangle_{02}^{N}}{\langle Q\rangle^{I}} \approx 0.88 \tag{15}$$

If the G-pair is included, one obtains nearly the full value for the quadrupole operator. This is not true for other quantities such as the pairing gap Δ, which is proportional to the pair transfer matrix element $\langle\Phi|S^{+}|\Phi\rangle$

Summarizing our investigations for a single j-shell we can say that restoration of the broken symmetries in a HFB calculation (particle number and angular momentum) is necessary for a discussion of the validity of the SD-approximation. It turns out that the main effect comes from the projection onto good particle number. The proper treatment of the rotational symmetry, however, has little influence on the effects connected with the truncation to SD- or SDG-space. In order to verify these results obtained for a single j-shell we investigate in the following section a realistic case with many non degenerate j-shells.

2.3 INVESTIGATIONS OF MULTI-j-SHELL CONFIGURATIONS

In contrast to the single j-shell case, where we have only analyzed the structure of a given wave function, we now refer explicitly to an effective two-body Hamiltonian. We use the configuration space and the residual interaction of Kumar and Baranger[27]), which has been widely used in the literature and has been very successful in microscopic descriptions of collective excitations in Rare Earth nuclei. The Hamiltonian is of the form

$$H = H_o - \frac{\chi}{2} Q^+ \cdot Q - G\, P^+ P \qquad (16)$$

The model takes into account only the residual interaction between the valence nucleons in the oscillator shells $N = 4,5$ for protons and $N = 5,6$ for neutrons. This is compatible with the ideas of the Interacting Boson Model, where the Bosons are assumed to be pairs of nucleons in the valence shell.

The configuration space in this calculation therefore includes the j-shells:

Protons: $1g_{9/2}$, $1g_{7/2}$, $2d_{5/2}$, $2d_{3/2}$, $3s_{1/2}$
$1h_{11/2}$, $1h_{9/2}$, $2f_{7/2}$, $2f_{5/2}$, $3p_{3/2}$, $3p_{1/2}$

Neutrons: $1i_{13/2}$, $1i_{11/2}$, $2g_{9/2}$, $2g_{7/2}$, $3d_{5/2}$, $3d_{3/2}$, $4s_{1/2}$
$1h_{11/2}$, $1h_{9/2}$, $2f_{7/2}$, $2f_{5/2}$, $3p_{3/2}$, $3p_{1/2}$

In the following we shall discuss results for the Dy-isotopes ^{156}Dy-^{164}Dy, a chain which leads from the transitional region in ^{156}Dy into the well deformed region in ^{164}Dy. We use the intrinsic HFB-functions of Kumar and Baranger, which are obtained by a variation of the unprojected

energy subject to the constraint of fixed average particle numbers for protons and neutrons. Truncation and projection is carried out after the variation. It should perhaps be emphasized that variation in a truncated space may yield totally different results, as we will see in the section 3.

As we have already seen in the j = 41/2 model, number projection is crucial. Thus we have for every case in the following included particle number projection (for protons and neutrons) and look for effects coming only from the additional angular momentum projection.

An essential difference to the single j-shell case is that we now have a spherical single particle field H_0. Figure 3 shows the expectation values of this operator and compares results obtained in the full Fermion space with the SD- and the SDG-truncation. On the l.h.s. we use angular momentum projection as well as number projection, on the r.h.s. we use only number projection. Going from the transitional region in ^{156}Dy to the well deformed region in ^{164}Dy we observe a large decrease of $\langle H_0 \rangle$, which is obviously connected with the increase in total binding with increasing particle number. At the beginning (A = 156-160) $\langle H_0 \rangle$ drops slowly, because in this region the deformation changes drastically and the increase in binding is partially compensated by the fact that we have to mix in deformed wave function components from higher lying j-shells (which are nearly empty in the less deformed region). Beyond A = 160 deformation is only increased a little and therefore $\langle H_0 \rangle$ drops more rapidly. These general features are found in all cases shown in Fig. 3. But there is a difference in the absolute values. In the SD-space we obtain roughly 8-10 MeV less binding than in the full space. Taking into account the G-pair closes this gap to less then 2 MeV. One could argue that this difference amounts to only 5% of the total value in the

SD-space and less then 2% in the SDG-space. However it is clear that those percentages contain little information, because an arbitrary shift in the energy scale would change them. Physically interesting properties depend only on the vicinity of the Fermi surface.

We also see in Fig. 3 that angular momentum projection has little influence on $\langle H_0 \rangle$. The curves on the r.h.s. obtained after number projection only, look very similar to those on the l.h.s.

In Fig. 4 we show intrinsic quadrupole moments. As in section 2.2 they are obtained from eq. 14 in the case of angular momentum projected wave functions. These quantities are connected with the deformation parameter (in simple HFB-theory we have $\hbar \omega_0 \beta = \chi \langle Q \rangle$). We observe an increase of the deformation on the way from ^{156}Dy to ^{164}Dy in all cases. Again there is no qualitative difference between the calculations with and without angular momentum projection; in detail angular momentum projection increases all expectation values a little. There is, however, a large difference between the SD-truncation and the full wave functions, which increases with deformation: In the well deformed region we find only 80% of the quadrupole deformation in the SD-space. Surprisingly the inclusion of the G-pair produces nearly the full value. We can say that the SD-approximation shows the same features as in the single j-shell: little influence of angular momentum projection and an increasing contribution coming from the G-pair with growing deformation. The relative influence of the G-pair increases although the coefficient x_4 remains rather small ($x_4^2 = 0.07\text{-}0.1$). This has to be understood again as an effect of the Pauli principle. In detail the SDG wave function reproduces the full value for the stronger deformed isotopes ($\beta > 0.3$) whereas for the somewhat weaker deformed isotopes ($0.25 < \beta < 0.3$) we find only 98-99%.

A difference to the above results, concerning the SD- or SDG-approximation, is found, if one looks at the pair transfer matrix elements:

$$\langle P^+ \rangle = \langle \Psi | (a^+ a^+)_0 | \Psi \rangle \tag{17}$$

This is related to the pairing gap parameter (in the mean field approach we have $\Delta = G\langle P^+ \rangle$). As one can see from Fig. 5 it is clearly not enough to take into account the SDG-pairs to reproduce the result obtained with the full wave function.

Another interesting quantity which is crucial for the description of rotational spectra is the moment of inertia.

$$\mathcal{J}(I) = (2I - 1)/\Delta E_{I\,I-2} \tag{18}$$

We obtain it from angular momentum projected energies E_I and assume that the intrinsic wave function is the same for all the I-values under consideration. Fig. 6 shows the moments of inertia obtained in this way for the two isotopes ^{158}Dy ($\beta = 0.289$) and ^{164}Dy ($\beta = 0.328$). In the first case the influence of SD-truncation is a reduction of more then 20%, which increases with angular momentum. In the second case we find only 20-30% of the moment of inertia in the SD-space. Again the inclusion of the G-pair gives nearly the full value. These results are similar to the results found for the quadrupole moments: The SDG-approximation works better in the stronger deformed cases and gives for not too large angular momenta nearly the full value of $\mathcal{J}$.

Going to the region of higher angular momenta is not meaningful because it is well known that this region is characterized by alignment processes, which cannot be described in the original version of the IBM model and which are not included in our wave functions.

Thus far our investigations have been restricted to fixed intrinsic wave functions determined before truncation and projection. In the following section we investigate the influence of truncation and projection on the variation.

3. VARIATION AFTER PROJECTION AND TRUNCATION

3.1 SELF-CONSISTENT CALCULATION OF DEFORMATION AND GAP PARAMETERS

It is well known that a projection after variation violates the basic idea of the variational principle. Besides the fact that in the case of translational motion it does not reproduce the exact total mass of the nucleus, which is perhaps only an esthetic shortcoming, this method completely fails in the description of high spin states, where alignment processes (which depend on the angular momentum) produce drastic changes in the intrinsic wave function. Nevertheless unprojected HFB-theory is very successful in the description of groundstate properties of deformed nuclei. This means that one has to investigate for each case separately whether a projection before the variation (required by the variational principle) can be replaced by projection after variation, which is considerably simpler. In certain cases projection can be neglected completely.

In our case we not only project onto good angular momentum and particle number, but in addition truncate the intrinsic wavefunction. According to the variational principle we should do this before the variation. In order to avoid too large a numerical effort, in the following calculation, we restrict the variation to a few crucial parameters. In particular we take only the deformation parameter β and the gap parameters Δ_p and Δ_n for protons and neutrons into account. This restriction of the variation is physically meaningful because quadrupole deformation and pairing properties are the crucial properties which determine the low lying collective states and our Hamiltonian in eq. 16 contains only quadrupole and pairing terms. In fact the variation of the intrinsic untruncated HFB-functions is completely determined by these three parameters.

In detail we calculate as a first step for each set of parameters $\beta, \Delta_p, \Delta_n$ the corresponding Nilsson + BCS wave function $|\Phi(\beta,\Delta_p,\Delta_n)>$ by diagonalizing the HFB-matrix

$$\begin{pmatrix} H_o - \beta Q - \lambda & \Delta \\ -\Delta & -H_o + \beta Q + \lambda \end{pmatrix} \tag{19}$$

The chemical potential λ is determined by the constraint on the particle number.

In a second step we evaluate the energy after truncation and projection

$$E(\beta,\Delta_p,\Delta_n) = \frac{<\Phi(\beta,\Delta_p,\Delta_n)|HP^I P^N|\Phi(\beta,\Delta_p,\Delta_n)>}{<\Phi(\beta,\Delta_p,\Delta_n)|\ P^I P^N|\Phi(\beta,\Delta_p,\Delta_n)>} \tag{20}$$

For the third step we determine the minimum of this energy surface with respect to the parameters $\beta, \Delta_p, \Delta_n$. The actual calculation was carried out for the chain of Sm isotopes ^{148}Sm, ^{150}Sm, ^{152}Sm, ^{154}Sm, in order to study the effects of projection and truncation in the region of the phase transition from spherical to deformed. Again the configuration space and the residual interaction of Kumar and Baranger were used. In order to avoid a too large computational effort an independent variation of the parameters Δ_p and Δ_n has been carried out only for a few test cases. It turned out that the approximation $\Delta_n = \Delta_p + (\Delta_n - \Delta_p)_{\text{Baranger Kumar}}$ gives rather good results. We therefore used in all other calculations only β and Δ_p as independent parameters. For each isotope we took the difference $\Delta_p - \Delta_n$ from Baranger and Kumar (ref. 27).

From Figs. 7 and 8 we may recognize how sensitive the variation is to a truncation of the wave function. Fig. 7 shows the dependence of the total

energy on the deformation parameter β for ^{152}Sm. The other two parameters Δ_p and Δ_n were kept fixed at their values at the minimum. Although the SD-part of the Cooper-pair A^+ has $x_0^2 + x_2^2$ is ≈90%, the result obtained from a variation in the SD-space is totally different from the results in the full space. The origin of this surprising effect can be studied in Fig. 8, where the total energy in the vicinity of the minimum is split up into the different contributions coming from the single particle Hamiltonian, the quadrupole correlations and the pairing force. Due to the fact that the minimum is rather flat, its position is strongly shifted even by very small contributions and one has to take into account the L = 6 pair to reproduce the correct position of the minimum. It is also seen that the main effect comes from the interplay between $\langle H_o \rangle$, a quantity which is steeply increasing with deformation, and $-\frac{x}{2}\langle Q^+Q \rangle$, which drops dramatically. The contribution of the pairing-interaction shows much smaller variations, because we keep the gap parameters fixed in Fig. 8.

In Figs. 9 and 10 we show the equilibrium values for the parameters β, Δ_p and Δ_n, i.e., the minima of the different energy surfaces. We see the well known fact that angular momentum projection, which takes into account fluctuations in the orientation of the deformed nucleus, smears out the sharp phase transition observed in pure mean field theory. Between A = 148 and A = 150 we have, for the unprojected case, a sharp onset in the deformation. In the angular momentum projected case, we find a smooth transition; even the spherical nucleus ^{148}Sm shows small deformation. Similar results have been found earlier[28]). Apart from this effect, there is no qualitative difference between the angular momentum projected and unprojected results.

With varying neutron number, the parameters show the same behavior to those derived from the unprojected theory of Kumar and Baranger. The deformation increases to $\beta = 0.3$ in going from ^{148}Sm to ^{154}Sm and as a result the proton gap Δ_p decreases because of the decreasing level density. The neutron gap Δ_n stays roughly constant, because as one adds additional neutrons to the semi-magic configuration ^{146}Sm (having 82 neutrons), two effects (increasing pairing by the addition of particles to a closed shell and decreasing pairing caused by the growing deformation) tend to cancel each other.

In Fig. 9 we compare the full HFB-values with results obtained in the framework of SD-truncation; in Fig. 10 we do the same for SDG-truncation. The reduction of the quadrupole matrix element found after truncation to SD in the static calculation (Fig. 4) is responsible for the reduction of the deformation after variation. Here, however, because of the non-linearity of the variation, the effect is much larger. We find a reduction of roughly 50% in ^{154}Sm. The smaller deformations in the SD-space obviously lead to larger gap parameters.

Including the G-pair (in Fig. 10) improves the situation, but, as mentioned previously, because the variation procedure is quite sensitive to the truncation one cannot fully reproduce the results obtained with full HFB wave functions using the SDG-framework.

3.2 CHANGES IN THE STRUCTURE OF THE WAVEFUNCTION

In the next figures some light is shed on the structure of the wave functions for the Sm isotope chain. We remember that $|\Phi\rangle$ is completely characterized to be the structure of the Fermion pair A^+. Indeed the number projected wave function

$$P^N|\Phi\rangle \propto (\Lambda^+)^{N/2}|0\rangle \tag{21}$$

is a condensate of Λ-pairs. This pair is decomposed in normalized pairs with definite angular momentum.

$$\Lambda^+ = \sum_L x_L Q_L^+ \tag{22}$$

In a single j-shell there is for each L-value only one Fermion pair and Λ^+ is uniquely determined by the x_L coefficients. In the general case of many non-degenerate j-shells one needs in addition the structure coefficients $\alpha_L(a,b)$ of eq. 9, which characterize the collective pairs S,D,G,... . In the philosophy of the IBM model they determine the microscopic structure of the Bosons used in the theory.

Since we have calculated the wave functions in the chain of Sm nuclei self-consistently, we are now able to study the changes in the structure of these wave functions, i.e., the change in the x_L-parameters and the change of the structure of the Fermion pairs, as we go through the phase transition from spherical to deformed.

In Fig. 11 we show the dependence of these structure coefficients on the neutron number, i.e., on the deformation. It is remarkable how little they change when we go through the phase transition. The changes for the neutron pairs are somewhat larger than those for the proton pairs. This probably has to do with the larger neutron number and reflects the fact that we are dealing with Fermions, which feel the Pauli principle. Similar results have been found by the authors of refs. 29 and 30 without angular momentum projection.

Since the structure of the Fermion pairs changes so little, the main effect of the phase-transition has to be understood by changes of the x_L-coefficients. In fact we see in Fig. 12 that they change dramatically as we go from ^{148}Sm to ^{154}Sm. The amplitude of the S-pair, which is close to one in ^{148}Sm (the "spherical case"), decreases, whereas the amplitudes of the D- and G-pairs increase. In terms of these Fermion-pairs, deformation is therefore produced by an increasing admixture of mainly D- and a few G-pairs having a rather constant structure. Theories, which describe the phase transition from spherical to deformed in terms of the variables x_L but with A-independent Fermion pairs Q_L seem to be justified by these results[34]).

In Fig. 13 we finally show the same x_L-coefficients for the well deformed region of the Dy-nuclei discussed in section 2.3. Here the situation is very different. Going form ^{158}Dy to ^{164}Dy we have only minor changes in the deformation. Correspondingly the x_L-coefficients stay rather constant.

Of course the full many-body wave function contains components with many different numbers of S-, D-, and G-pairs. Because of the Pauli principle these different components in the Fermion space are not orthogonal. Therefore the average number of S-, D- or G-pairs is not a well defined quantity. Only to get a very rough estimate we neglect for a moment the Pauli principle and investigate a wave function in the Boson-space, with the same structure as the number projected HFB-function of eq. 21. and restrict ourselves to sdg configurations only

$$|sdg) = \frac{1}{\sqrt{\frac{N}{2}!(x_o^2 + x_2^2 + x_4^2)}} (x_o s^+ + x_2 d^+ + x_4 g^+)^{N/2} |0) \qquad (23)$$

This Boson wave function is than decomposed into orthogonal components with different numbers of s-, d- and g-Bosons:

$$|sdg) = \sum_{\nu_2\nu_4} c_{\nu_4\nu_4} (s^+)^{N/2-\nu_2-\nu_4} (d^+)^{\nu_2} (g^+)^{\nu_4} |0) \qquad (24)$$

The coefficients $c_{\nu_2\nu_4}$ are straightforward expressions in the amplitudes x_L. The quantities

$$c_{\nu_2}^2 = \sum_{\nu_4} |c_{\nu_2\nu_4}|^2 \qquad \text{and} \qquad c_{\nu_4}^2 = \sum_{\nu_2} |c_{\nu_2\nu_4}|^2 \qquad (25)$$

measure the probability of finding ν_2 d-Bosons or of finding ν_4 g-Bosons in the wave function $|sdg)$. In Fig. 14 we show these quantities for the nucleus ^{154}Sm. Following these arguments we would estimate that we need up to 5 proton d-Bosons and up to 6 or 7 neutron d-Bosons and at the same time up to one or two g-Bosons in order to describe the deformed nucleus ^{1154}Sm within a Boson model. From this we may conclude that a two-broken-pair approximation, which takes into account not more then two D-pairs, cannot be used to describe deformed nuclei. A calculation, however, which includes many d-bosons and only one or two g-bosons might eventually be reasonable.

4. SUMMARY AND CONCLUSIONS

Angular momentum and number projected HFB wave functions have been used in order to study the possibility of truncations of the underlying Cooper-pair so as to contain only components coupled to angular momentum $L = 0,2,4,\ldots$. In the first place we carried out this truncation after variation on a fixed intrinsic wave function and found that the SD-truncation is a very poor approximation to the full HFB wave function. Although the Cooper-pair comprises more than 80% S- and D-pairs, important physical observables cannot be reproduced in this approximation. We obtain only 25% of the moment of inertia in the well deformed region. The inclusion of the G-pair, which amounts to only a few percent of the Cooper-pair, gives, however, surprisingly good results for the quadrupole moments and the moments of inertia in the well deformed region.

In the second part we studied the influence of projection and truncation on the variation. We found that the phase transition from spherical to deformed cannot be represented in the SD-space, and even the inclusion of the G-pair does not give the full deformation.

The investigations of this paper differ from earlier investigations by the fact that full angular momentum and number projection is used. It turns out that number projection is crucial, because the truncation procedure can cause major changes in the average particle number. The influence of angular momentum projection is very small in the well deformed region. In the transitional regions of small deformations angular momentum projection has more influence; the essential qualitative results, however, are not changed.

Summarizing we can conclude that the concept of SD-truncation does not work in transitional and deformed nuclei. In particular it seems to fail even

more for well deformed nuclei than for weakly deformed nuclei. On the other hand SDG-truncation seems to reproduce many of the full results surprisingly well. For a microscopic understanding of the success of the phenomenological IBM models it is therefore not enough to neglect the effects of the G-pair. It is still an open problem, which will require further investigation, to establish if all the effects of the G-pair and the corresponding g-Boson can be taken care of by a suitable renormalization of the force-parameters, or if the g-Boson has to be treated dynamically.

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REFERENCES:

[1] A. Arima and F. Iachello; Lett. 35 (1975) 1069

[2] P. Garbaczewski; Phys. Rep. 36C (1978) 65

[3] S. T. Belyaev and V. G. Zelevinskii; Nucl. Phys. 39 (1962) 582

[4] T. Marumori, M. Yamamura, and A. Tokunaga; Progr. Theor. Phys. 31 (1964) 1009

[5] S. C. Pang, A. Klein, and R. M. Dreizler; Ann. Phys. (New York) 49 (1968) 477

[6] E. R. Marshalek; Nucl. Phys. A224 (1974) 221,245

[7] S. G. Lie and G. Holzwarth; Phys. Rev. C12 (1975) 1035

[8] T. Kishimoto and T. Tamura; Nucl. Phys. A270 (1976) 317

[9] T. Otsuka, A. Arima, F. Iachello, and I. Talmi; Phys. Lett. 76B (1978) 139

[10] Y. K. Gambhir, P. Ring, and P. Schuck; Nucl. Phys. A384 (1982) 37

[11] Y. K. Gambhir, P. Ring, and P. Schuck; Phys. Rev. C25 (1982) 2858

[12] S. Pittel, D. Duval, and B. R. Barrett; Phys. Rev. C25 (1982) 2834

[13] O. Scholten and S. Pittel; Phys. Lett. 120B (1983) 9

[14] T. Otsuka; Phys. Rev. Lett. 46 (1981) 710

[15] A. v. Egmond and K. Allaart; Nucl. Phys. A425 (1984) 274

[16] J. Dudelsky, G. G. Dussel, and H. M. Sofia; Phys. Lett. 100B (1981) 367

[17] T. Otsuka, A. Arima, and N. Yoshinaga; Phys. Rev. Lett. 48 (1982) 387

[18] D. R. Bes, R. A. Broglia, E. Maglione, and A. Vitturi; Phys. Rev. Lett. 48 (1982) 1001

[19] I. Talmi; Nucl. Phys. A172 (1971) 1

[20] Y. K. Gambhir, A. Rimini, and T. Weber; Phys. Rev. 188 (1969) 1573

[21] B. Lorazo; Ann. Phys. (New York) 92 (1975) 95

[22] F. Gruemmer, K. W. Schmidt, and A. Faessler; Nucl. Phys. A306(1978) 134

[23] S. Islam, H. J. Mang, and P. Ring; Nucl. Phys. A326 (1979) 161

[24] P. Ring and P. Schuck; The Nuclear Manybody Problem (Springer Verlag, New York 1980)

[25] D. J. Thouless; Nulc. Phys. 21 (1960) 225

[26] E. P. Wigner; Gruppentheorie und Ihre Anwendungen in der Quantenmechanik der Atomspektren, Vieweg Verlag, Braunschweig 1931

[27] K. Kumar and M. Baranger; Nucl. Phys. 110 (1968) 529

[28] R. Beck; Z. Phys. 243 (1971) 409

[29] F. Catara, A. Insolia, E. Maglione, and A. Vitturi;

[30] O. Scholten; Phys. Rev. C28 (1983) 1783

[31] K. Heyde, P. van Isacker, M.Waroquier, and G. Weues; Nucl. Phys. A380 (1982) 383

[32] P. van Isacker, K. Heyde, M.Waroquier, and G. Weues; Phys. Lett. 104B (1981) 5

[33] A. Klein and C. Dasso; Phys. Rev. C9 (1974) 414

[34] T.D. Cohen; Preprint University of Pennsylvania, Philadelphia 1984

FIGURE CAPTIONS:

Fig. 1 Properties of the j = 41/2 model with respect to truncation: a) The probabilities x_L of finding pairs Q_L coupled to angular momentum L in the Cooper-pair of eq. 3 as a function of the number N of Fermions. The sum of the probabilities for L = 0 and 2 and for L = 0, 2 and 4 are also given. b) Overlap integrals between various projected (full) and unprojected (dashed) wave functions as a function of N. The indices 0,2,4 give L-values taken into account. Functions without lower index are calculated in the full Fermion space. The upper indices I,N indicate angular momentum projection (I = 0) and number projection. All overlaps are obtained from normalized wave functions.

Fig. 2 Quadrupole moments as defined in eq. 13 as a function of the particle number N at angular momentum zero. Values obtained in the full Fermion space are compared with those in the SD-space. Details of the notation are given in Fig. 1. On the l.h.s. We compare full projected values with completely unprojected values. On the r.h.s. we compare values with and without angular momentum projection.

Fig. 3 The expectation value of the spherical single particle part of the Hamiltonian $\langle H_0 \rangle$ in eq. 16 as a function of the neutron number in the Dy isotope chain. Various truncations are compared: a) with particle number (N) and angular momentum projection (I = 0), b) only with number projection. The different curves correspond to full HFB-wave functions and to truncations to the SD-space (02) and to the SDG-space (024).

Fig. 4 Mass quadrupole moments as defined in eq. 13. The units are fm^2 and details of the notation are given in Fig. 3. We also show to what extend the truncated quantities exhaust the values obtained in the full Fermion space.

Fig. 5 Pair transfer matrix elements as defined in eq. 17. Details of the notation are given in Figs. 3 and 4.

Fig. 6 Moments of inertia defined in eq. 18 for the nuclei ^{164}Dy and ^{158}Dy as a function of the angular momentum. Full HFB-results are compared with SD-truncation (02) and SDG-truncation (024).

Fig. 7 The angular momentum and number projected energy surface for the nucleus ^{152}Sm. The full line corresponds to a calculation in the full Fermion space; the dashed curve is obtained after a truncation to the SD-space.

Fig. 8 Different contributions to the projected energy in ^{152}Sm: the pairing part $-G\langle P^+P\rangle$ (scale on the r.h.s.), the quadrupole part $-\frac{x}{2}\langle Q^+Q\rangle$ (scale on the r.h.s.), the single particle part $\langle H_o\rangle$ (scale on the l.h.s.) and the total energy. Full lines are calculated in the full Fermion space without truncation; dashed lines are obtained in the SGD-space and dotted lines are found in the SDGI-space.

Fig. 9 Equilibrium values of the deformation and gap parameters in the chain of Sm isotopes as a function of the neutron number. The full lines correspond to calculation in the full space, dashed lines are obtained after truncation to the SD-space (02). Angular momentum and number projection (IN) is compared with number projection alone (N). Since we are dealing with the ground state we always project onto angular momentum I = 0.

Fig. 10 Equilibrium values of the deformation parameters in the chain of Sm isotopes as a function of the neutron number. Calculations in the full space (full lines) are compared with those after SDG truncation (dashed lines). For details see Fig. 9.

Fig. 11 The structure coefficients $\alpha_L(a,b)$ for proton- and neutron-pairs with different angular momenta in the chain of Sm-nuclei as a function of the mass-number A. Not all the coefficients are given in detail. Many of them are close to zero; others lie in the shadowed areas. The underlying wave functions are obtained by a variation after angular momentum and number projection without truncation. The numbers $1^+,2^+,\ldots$ characterize the single particle levels a,b. For the protons we used $1^+ = g_{9/2}$, $2^+ = g_{7/2}$, $3^+ = d_{5/2}$, $4^+ = d_{3/2}$, $5^+ = s_{1/2}$, $1^- = h_{11/2}$, $2^- = h_{9/2}$, $3^- = f_{7/2}$, $4^- = f_{5/2}$, $5^- = p_{3/2}$, $6^- = p_{1/2}$ and for the neutrons we use $1^+ = i_{13/2}$, $2^+ = i_{11/2}$, $3^+ = g_{9/2}$, $4^+ = g_{5/2}$, $5^+ = d_{5/2}$, $6^+ = d_{3/2}$, $7^+ = 5_{1/2}$ $1^- = h_{11/2}$, $2^- = h_{9/2}$, $3^- = f_{7/2}$, $4^- = f_{5/2}$, $5^- = p_{3/2}$, $6^- = p_{11/2}$.

Fig. 12 The coefficients x_L of eq. 6, which characterize the admixture of S-,D-,G-,... pairs in the Cooper-pair A^+ for the Sm-isotopes as a function of the mass-number. Full lines correspond to neutrons and dashed lines correspond to protons.

Fig. 13 The coefficients x_L of eq. 6 for the Dy-chain discussed in section 2.3. For details see Fig. 12.

Fig. 14 The probabilities $c^2_{\nu_2}$ and $c^2_{\nu_4}$ for finding ν_2 d-Bosons or ν_4 g-Bosons in the deformed Boson state of eq. 25. Full lines correspond to neutrons and dashed lines correspond to protons. The x_L-coefficients for the deformed nucleus ^{154}Sm are used for the calculation of these quantities.

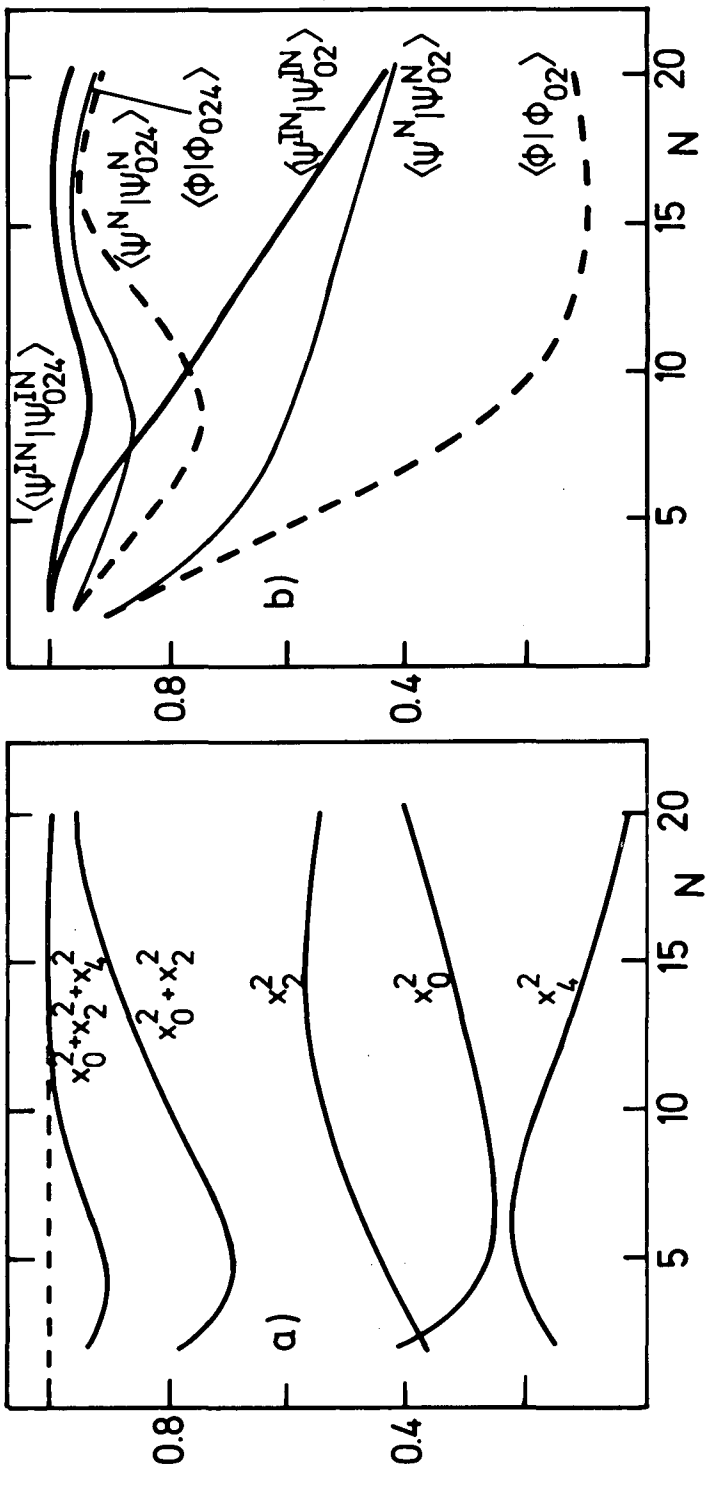

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Fig. 1

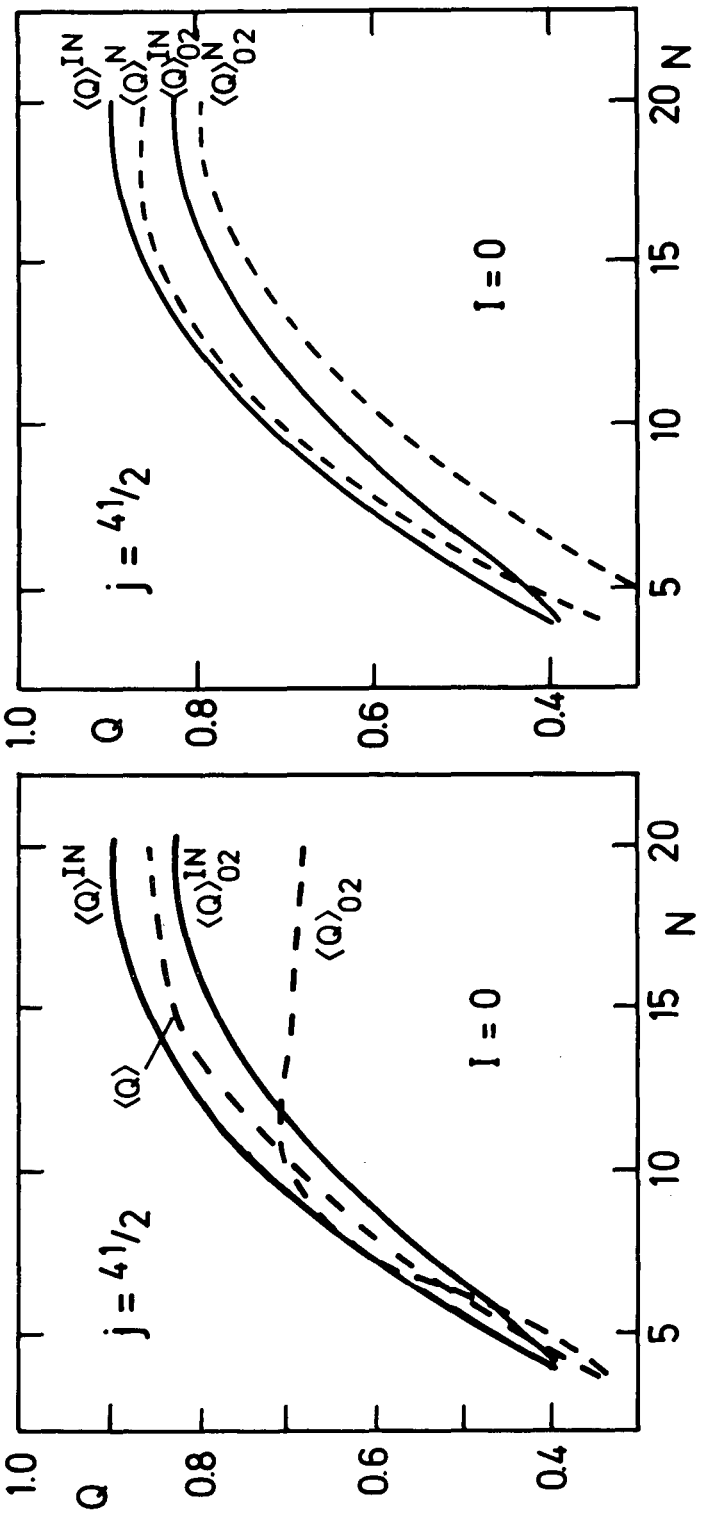

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Fig. 2

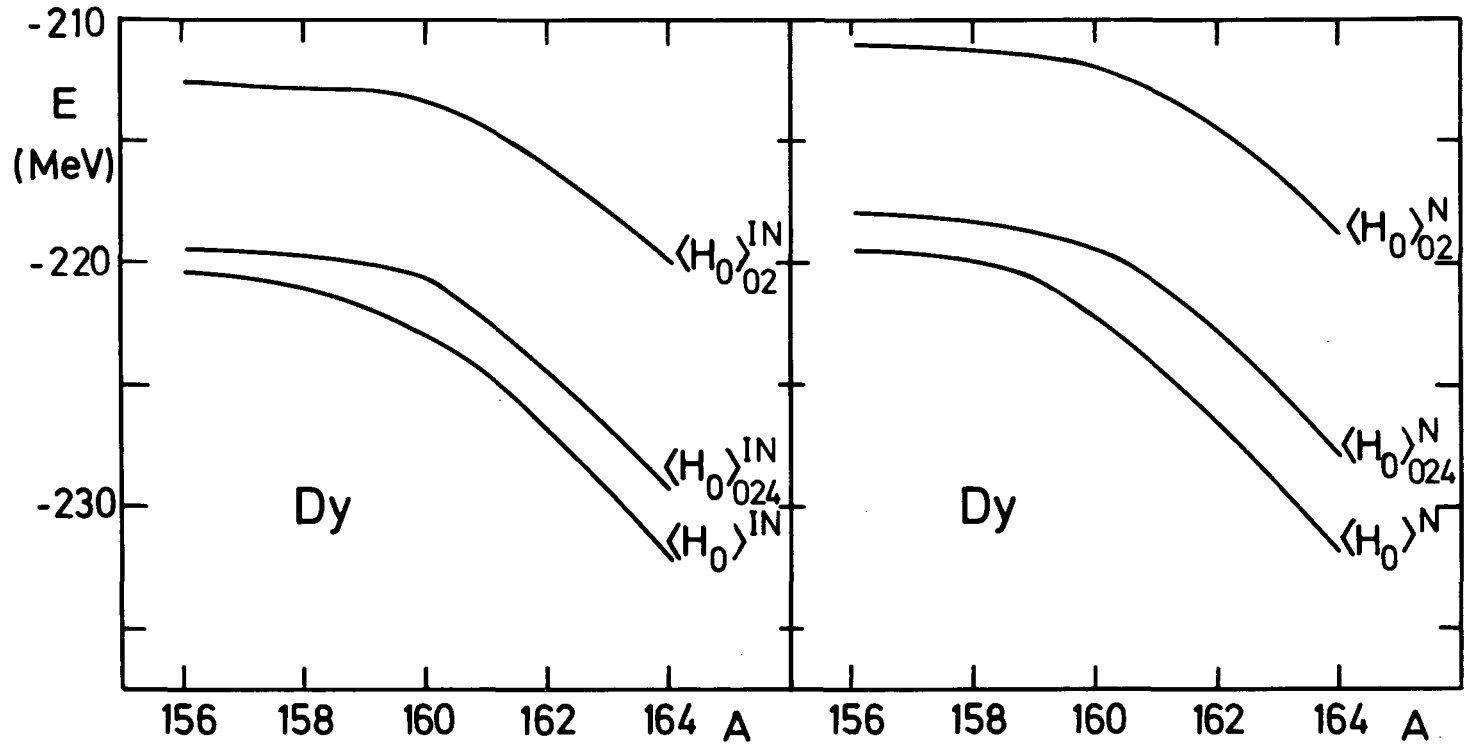

Fig. 3

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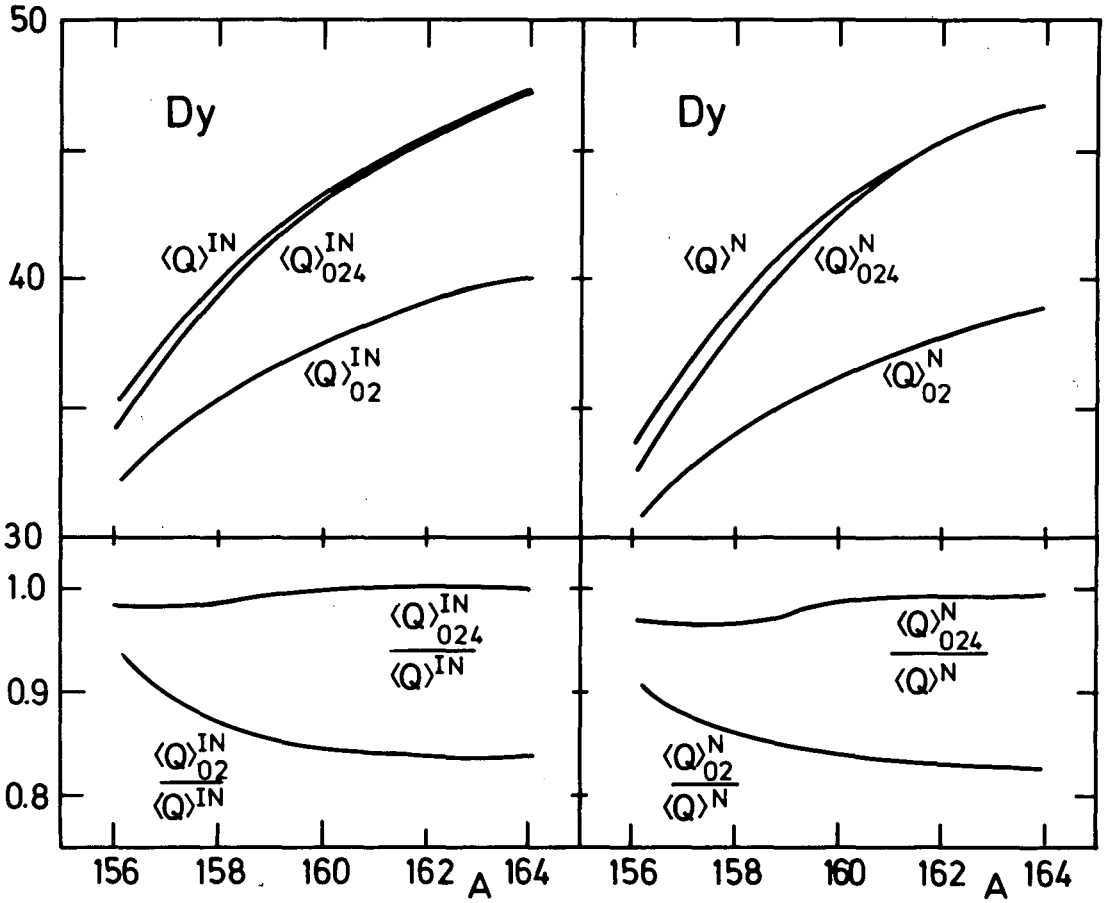

Fig. 4

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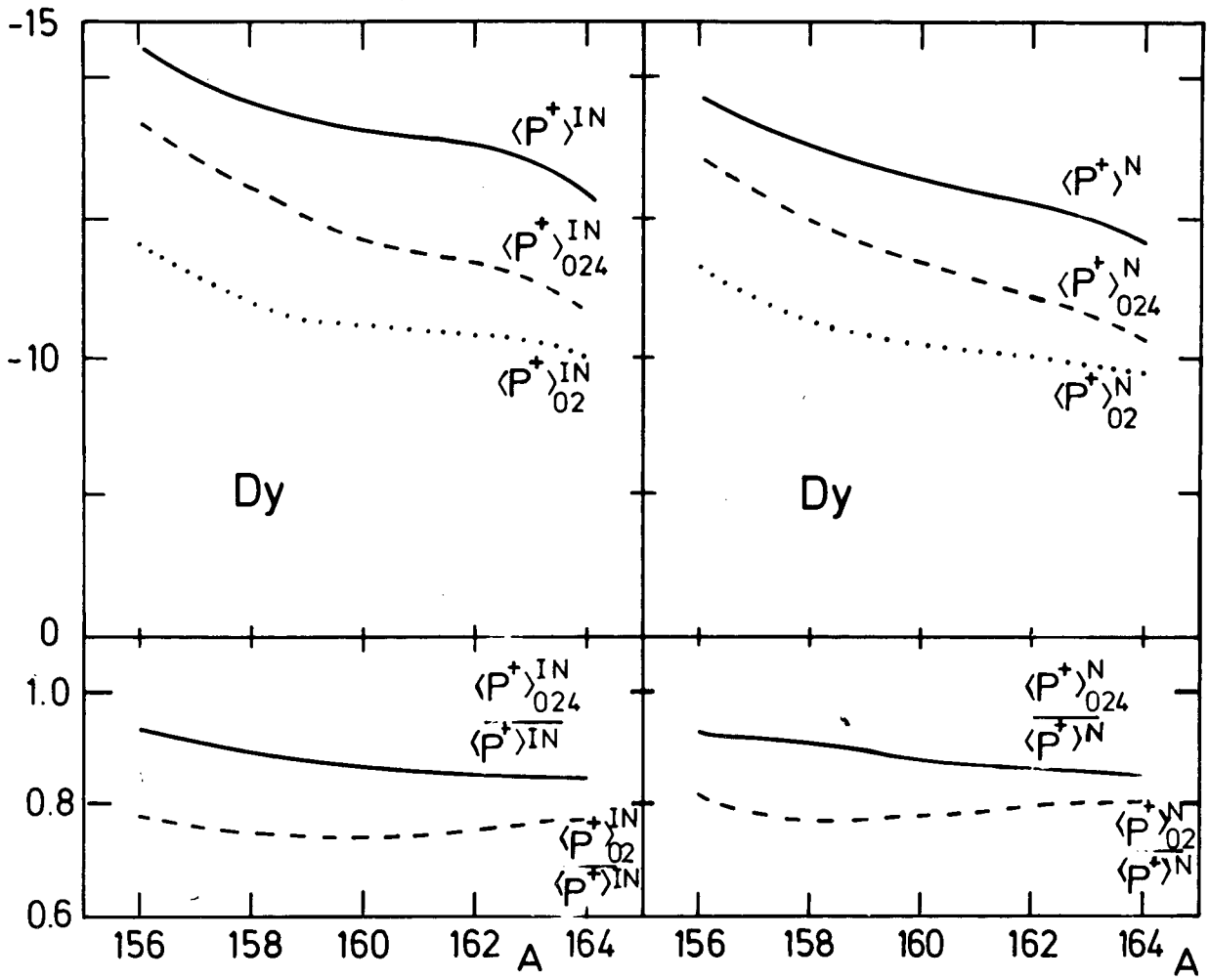

Fig. 5

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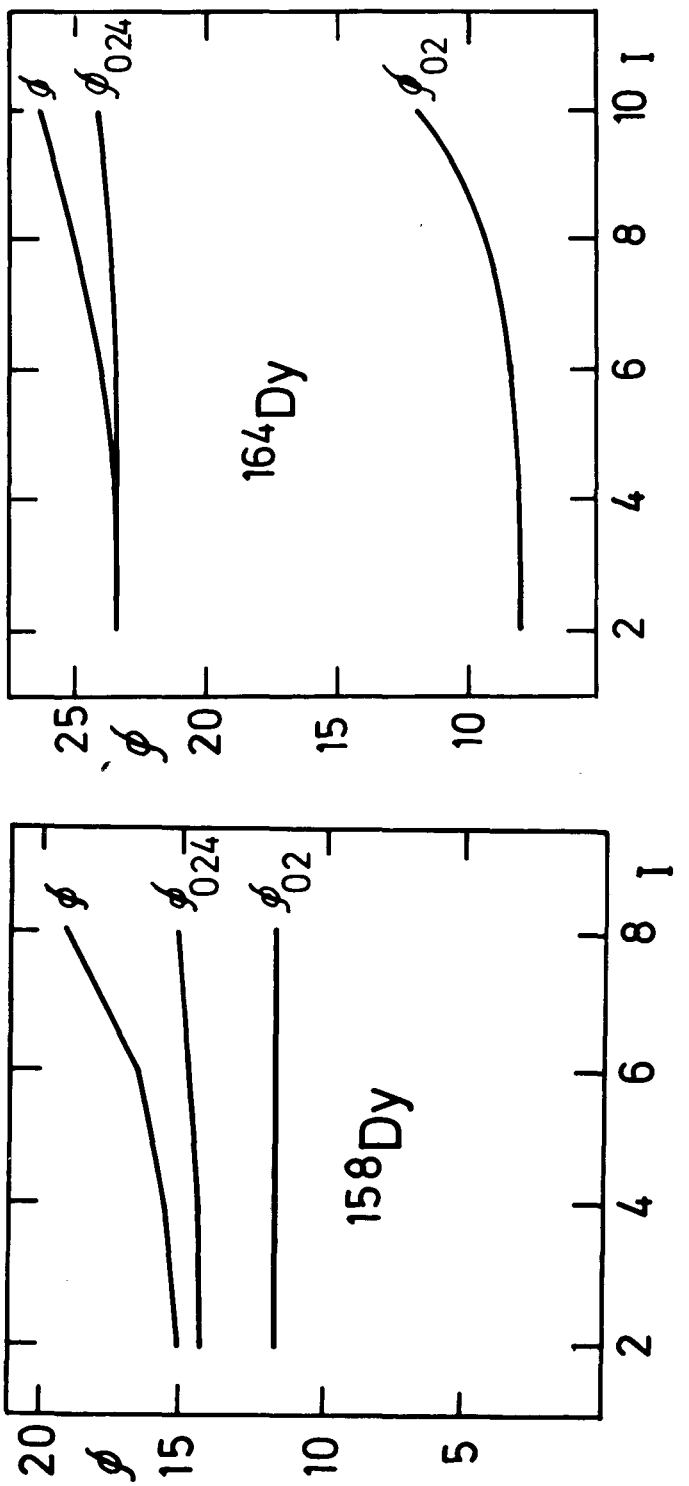

Fig. 6

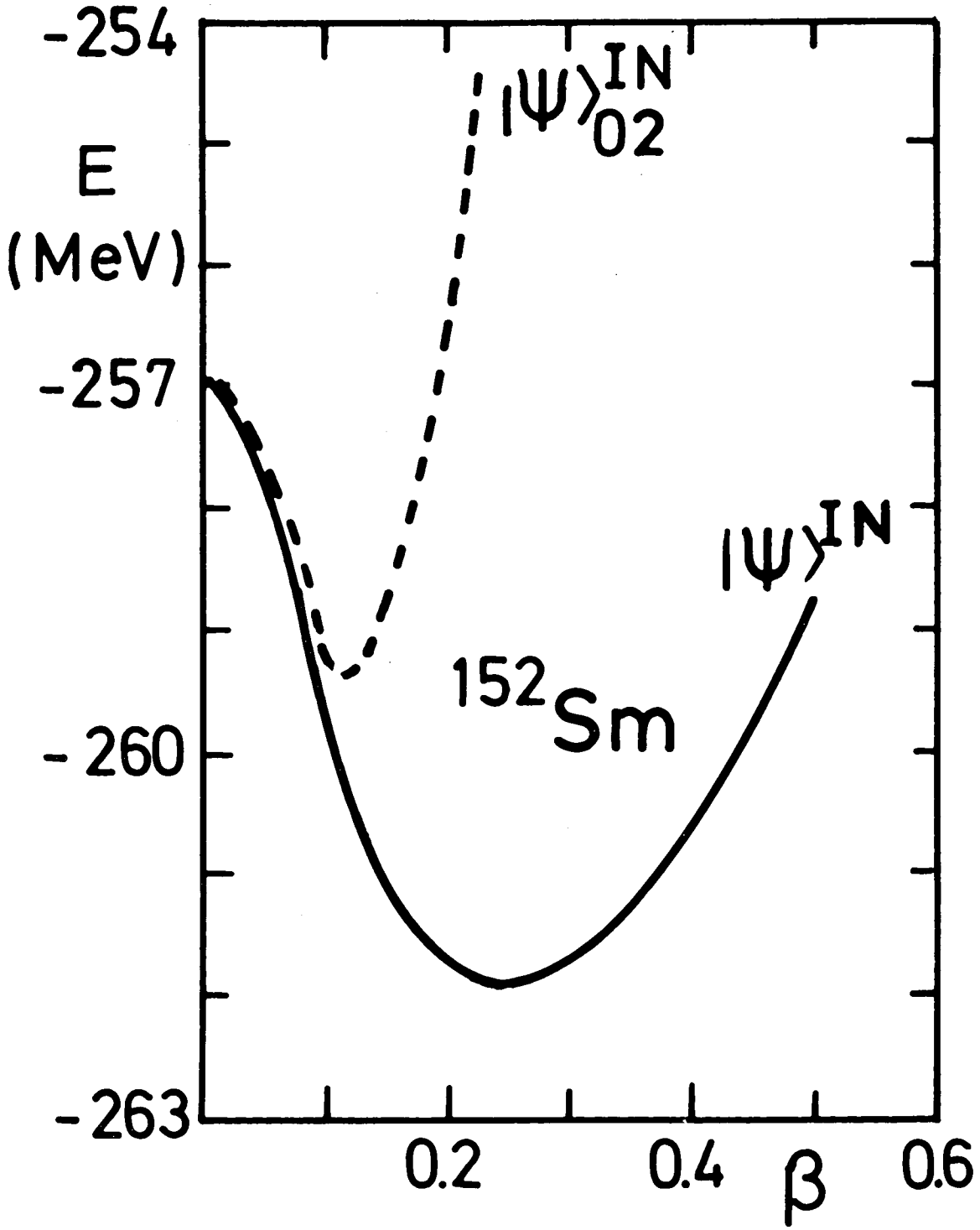

Fig. 7

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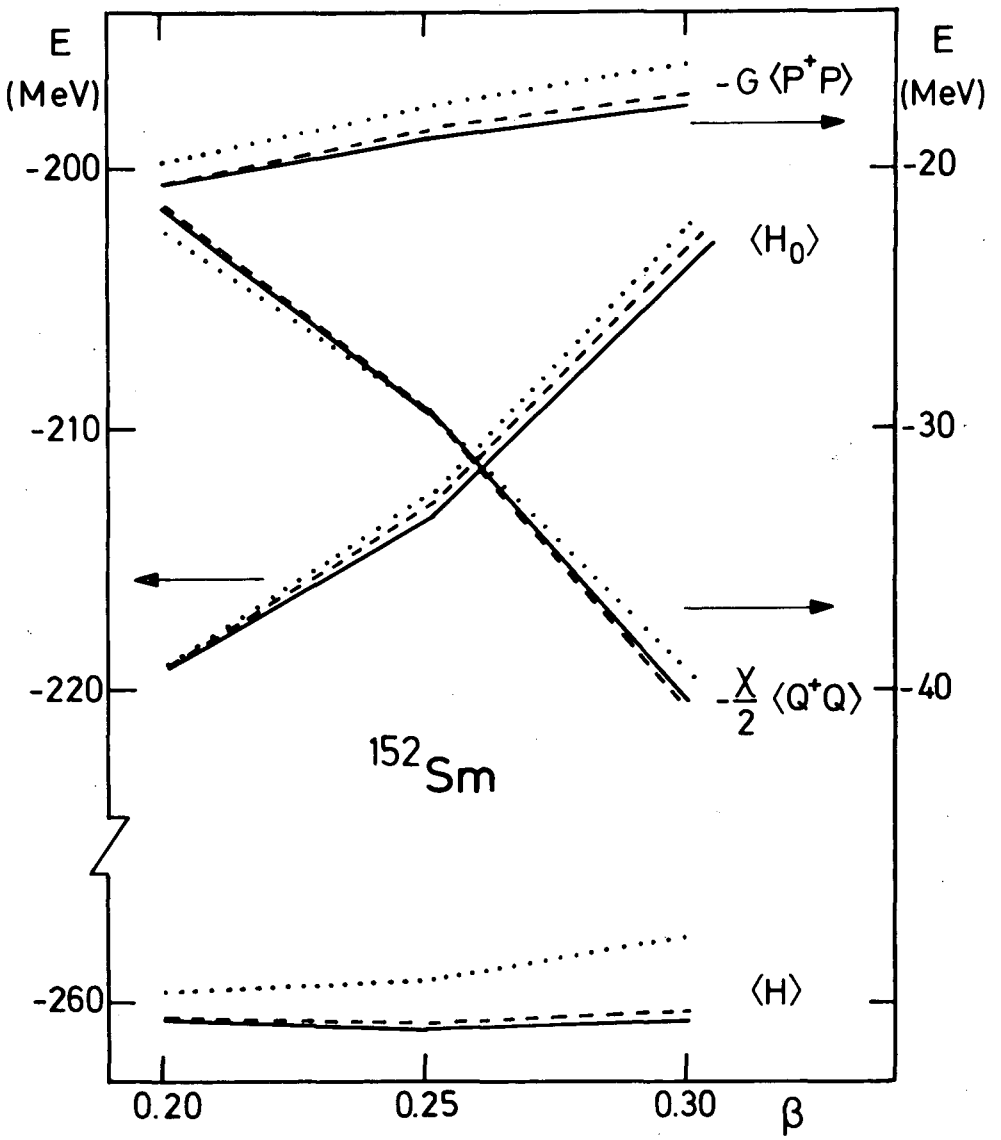

Fig. 8

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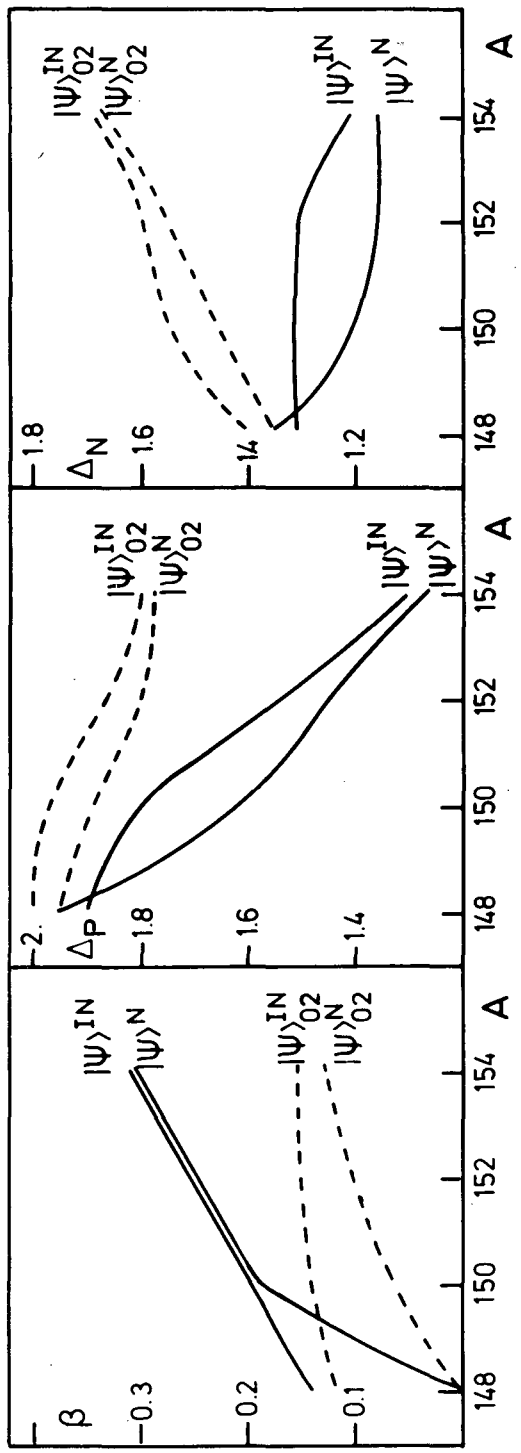

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Fig. 9

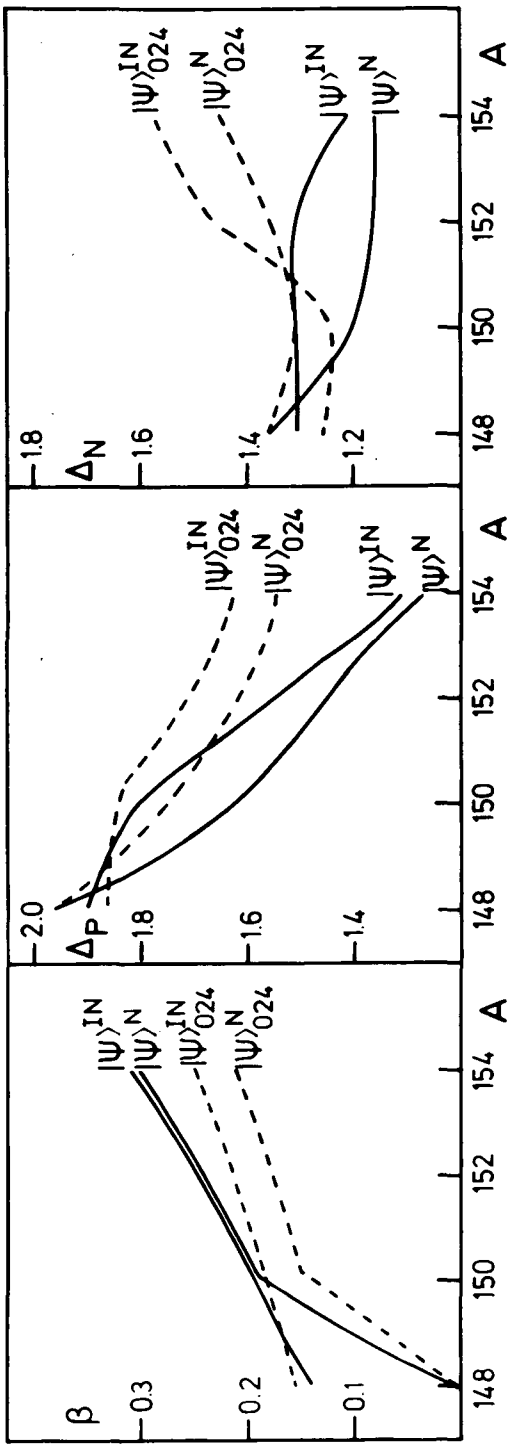

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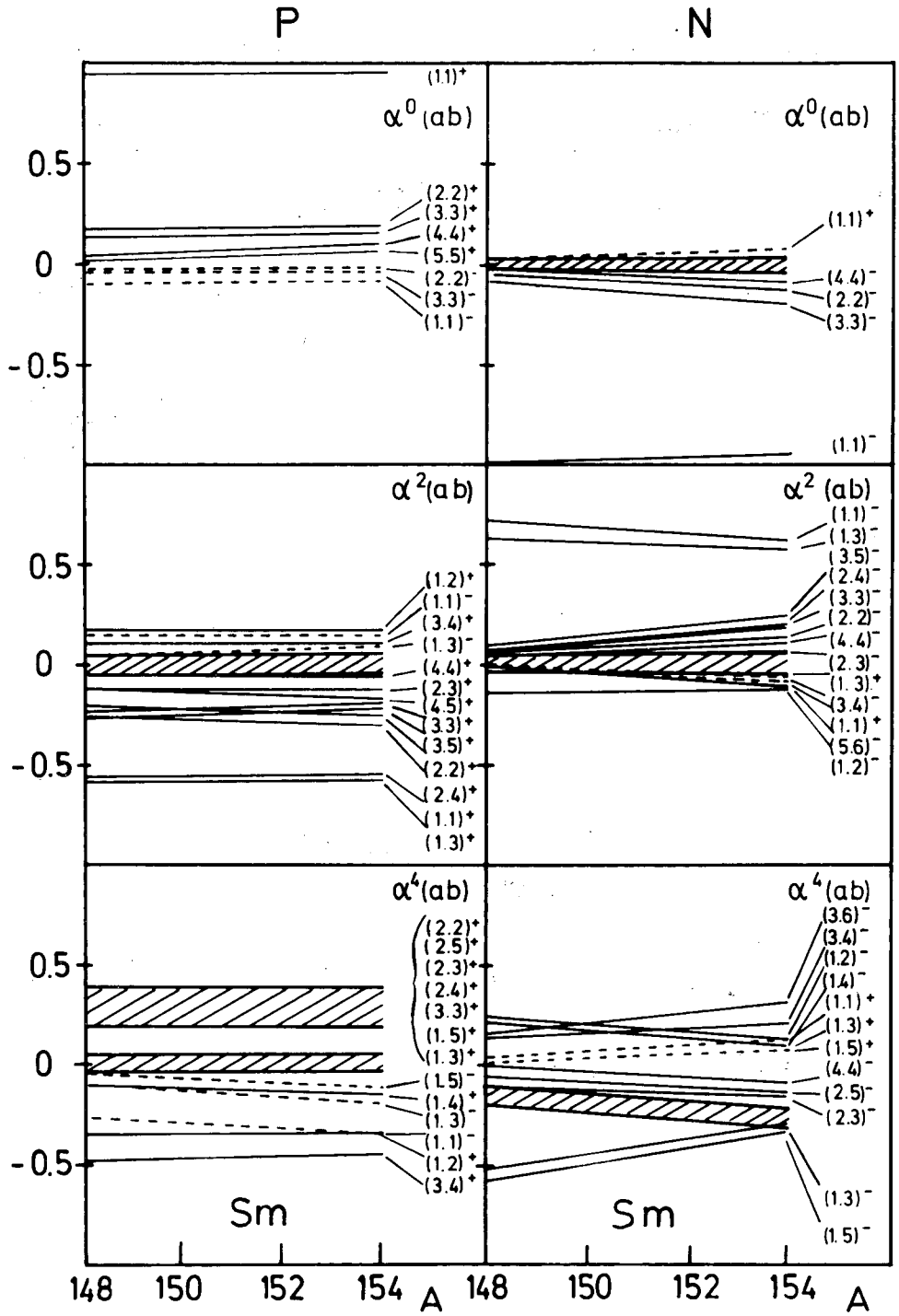
Fig. 10



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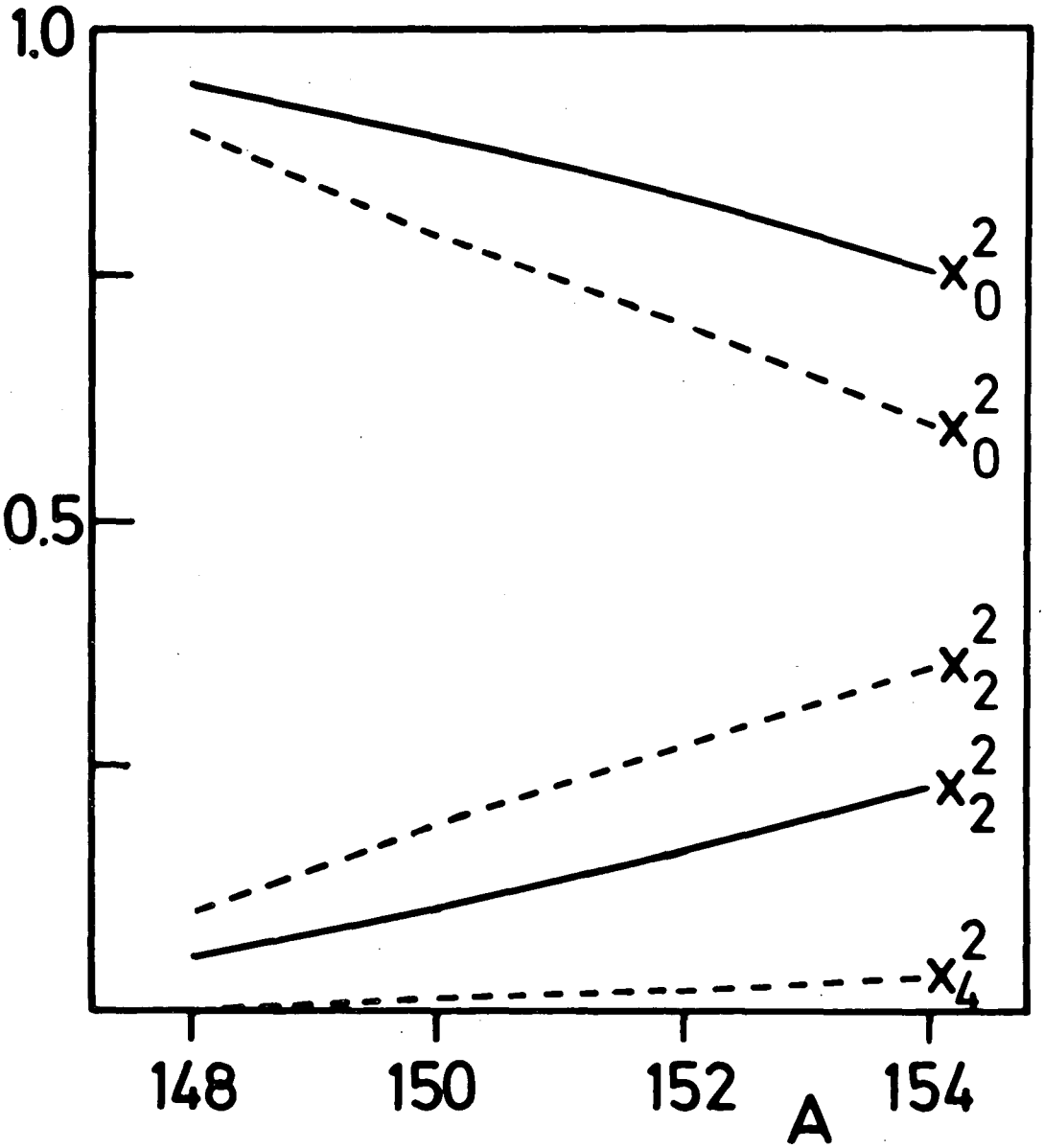

Fig. 12

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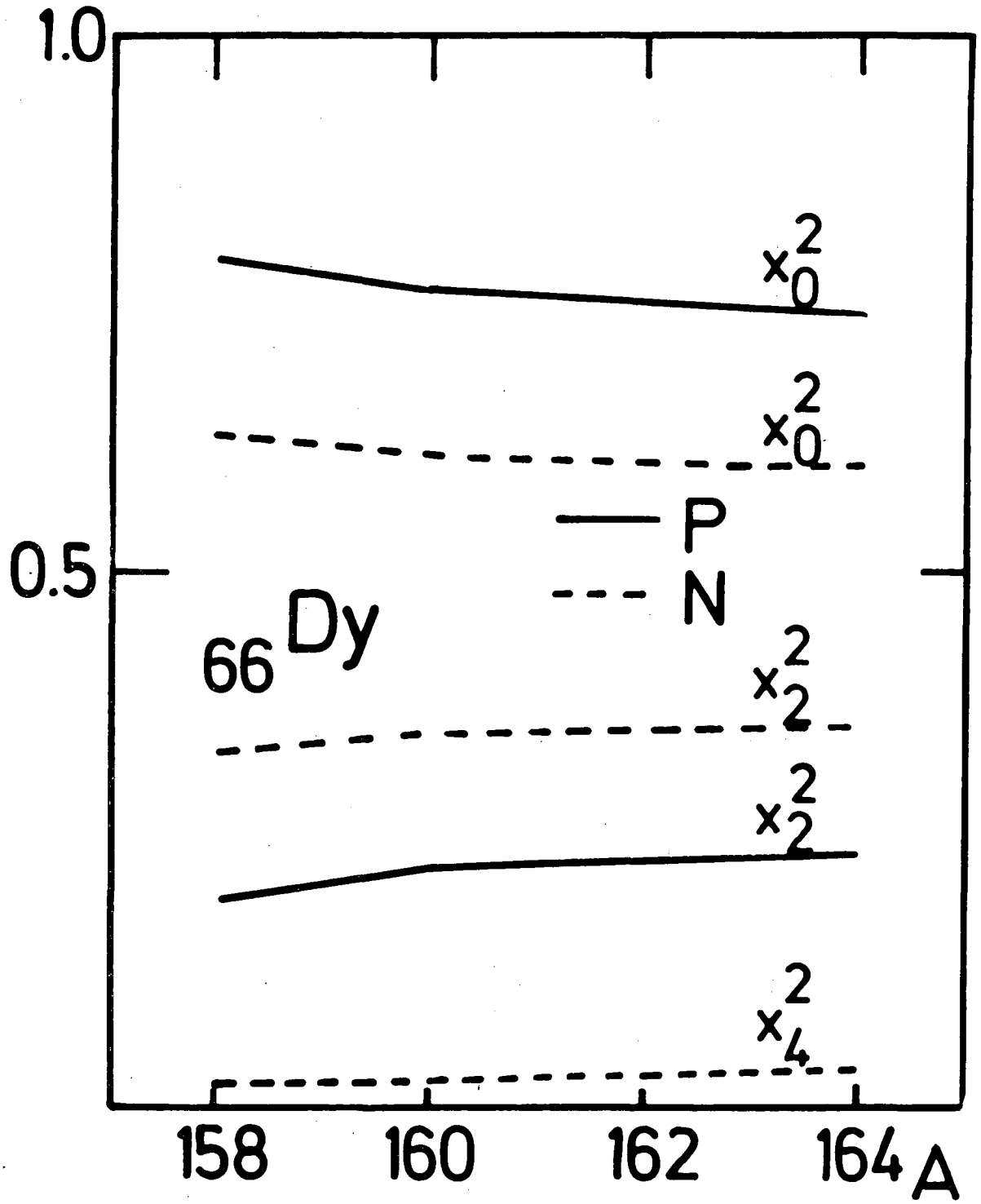

Fig. 13

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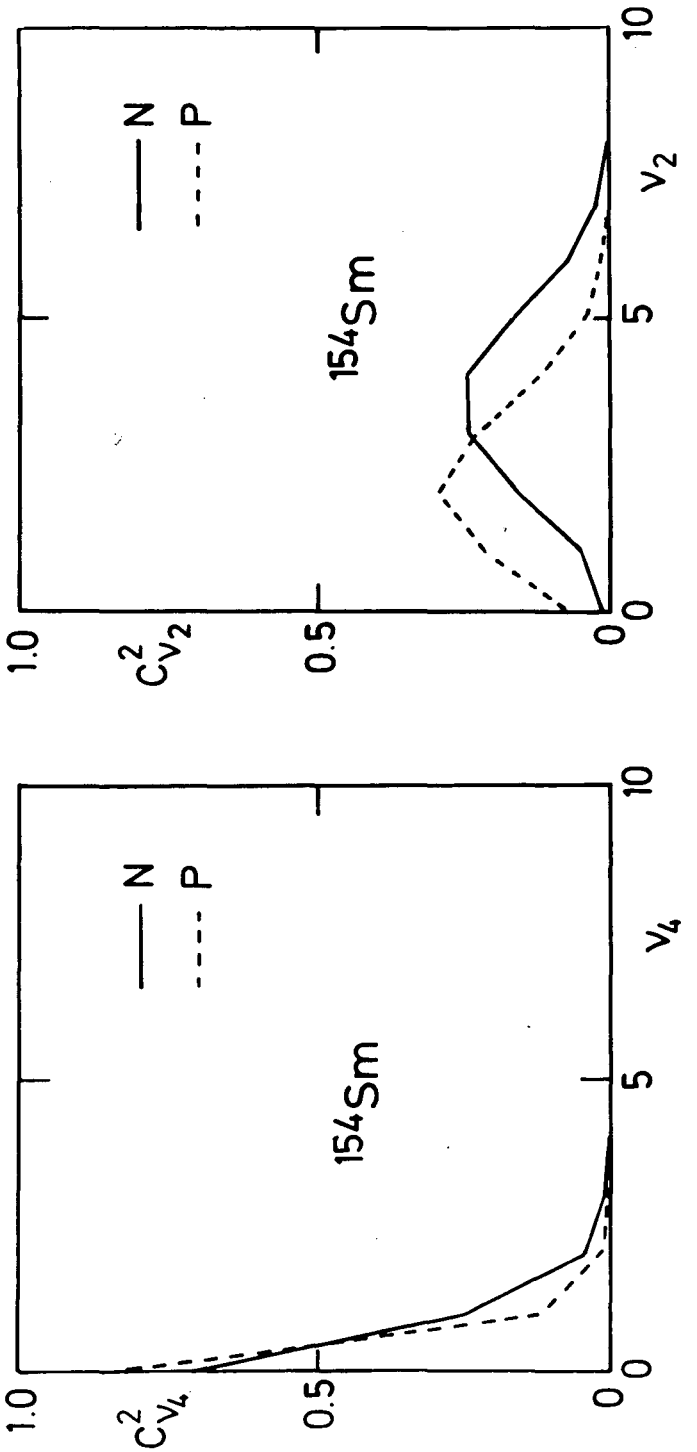

XBL 852-1328

Fig. 14

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