Title

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STRUCTURE STUDIES OF LOW-LYING 0^+ STATES IN THE DEFORMED RARE-EARTH REGION

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Abstract

To better understand the structure of the low lying 0^+ states of even-even nuclides in the deformed rare-earth region, we have carried out calculations to generate the wavefunctions, energies and pair transfer rates from/to these states within a framework of exact diagonalization of the residual pairing and n-p forces. First we carried out exact diagonalization for the neutron and proton systems separately, using as a basis space the 126 vector space of four/five pairs within nine appropriate deformed Nilsson orbitals. For the pairing force we included both monopole an quadrupole terms. Next, we used the lowest eight eigenfunctions from both the neutron and the proton systems to generate a new basis space composed of the 64 possible neutron-proton product vectors. The n-p force was approximated by a quadrupole-quadrupole force term which was then diagonalized within the new basis space. The resulting wave functions were used to calculate the neutron pair transfer strength from and to the various low 0^+ states below 3 MeV in the even-even Gd, Dy and Er isotopes. Furthermore, for the case where the deformation parameters do not change appreciably between the pair of nuclides involved in the pair transfer reaction, reasonable global agreement was obtained for the measured (t,p) and (p,t) pair transfer reaction strengths both to the ground and excited states 0^+ states accessible in these isotopes. The observed enhancement of (t,p) pair transfer strength to excited states in some of these isotopes was reproduced by the calculation. The enhancement is due to subshell gap and large relative pair transfer amplitude for an orbital near the Fermi surface.

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1. Introduction

There have been theoretical calculations[1-8] of the 0^+ states of even-even spheroidal nuclei dating back many years. Why now make yet another approach? First, new-data have appeared, of special importance being 2-neutron transfer studies via (p,t) and (t,p) Reactions.[9-13] Second, the 0^+ excited states pose special difficulties for quasi-particle and RPA methods due to spurious states, particle number fluctuations and, for some number-projection methods, non-orthogonality problems. Third, new computing power is ever more available, making "brute force" shell-model matrix diagonalization methods more feasible. Fourth, in nuclei where 4 or more 0^+ states are known previous model calculations have enjoyed only limited success.[14-18] Fifth, we have long suspected that the energies and properties of the low-lying 0^+ excited states are very sensitive to the detailed order, spacing, and properties of single-particle levels nearest the Fermi surface. Thus, a more fundamental Hartree-Foch-Bogolyubov model may have greater difficulty than the more empirical Nilsson deformed-potential model, where the parameters have been fine-tuned in the past to reproduce correctly the orbitals near the Fermi surface.

2. Method

Our basis consists of all unbroken-pair combinations in 9 Nilsson orbitals centered in energy about the Fermi energy, taking 4 and then 5 pairs. This basis set for neutrons (or protons) separately is of size 126, the binomial coefficient $\binom{9}{4}$ or $\binom{9}{5}$. Thus, we first diagonalize two 126×126 matrices, separately for neutrons and protons. Matrix elements from both simple pairing and quadrupole pairing[19] are taken into account.

When we compared with experiment the calculated 0^+ energies and 2-neutron transfer results with no neutron-proton coupling, we found poor agreement. Therefore, we added neutron-proton coupling, of quadrupole-quadrupole form. The lowest eight 0^+ solutions from neutron and proton 126×126 matrix diagonalization were taken to form a 8×8=64 basis set. Then the np QQ force was diagonalized in a 64×64 matrix.

$$H = \sum_{i=n,p} \left({}_{i}H_{Nils} + {}_{i}H_{pair} + {}_{iQ}H_{pair}\right) + H_{QQnp}, \qquad (1)$$

where

$$H_{pair} = -G_{(x)} \sum_{\substack{j>0 \\ k>0}} a_{k}^{+} a_{\bar{k}}^{+} a_{\bar{j}} a_{j}$$

$$(x) = n \text{ or } p$$

$$H_{Q\ pair} = -G_{Q(x)} \sum_{\substack{j>0 \\ k>0}} \frac{5}{4} q_{k} q_{j} a_{k}^{+} a_{\bar{k}}^{+} a_{\bar{j}} a_{j} / \langle r_{j}^{2} \rangle \langle r_{k}^{2} \rangle$$

where q_j is the mass quadrupole moment of the jth Nilsson orbital

$$q_k = \langle k|2r_k^2\, P_2(\cos\,\theta_k)|k\rangle$$

$$H_{QQnp} = \chi_{np} \sum_{jn} q_j a_j^+ a_j \sum_{kp} q_k a_k^+ a_k$$

Of the many possible parameters to vary we have constrained the calculations to only a few. First, we have constrained the single-particle Nilsson calculation to the Nilsson parameters and equilibrium deformation parameters ε_2, ε_4 and ε_6 published by P. Möller and R. Nix.[20*] We have adjusted the monopole pairing-force strengths to reproduce generally the gap from ground to first-excited 0^+ states. For the rare earths we need $G_p \approx 0.23$ MeV and $G_N \approx 0.20$ MeV. These values are, as expected, somewhat larger than those generally used, since our 9-orbital basis is much smaller than the basis set usually used in pairing calculations.

The quadrupole pairing strength is a more uncertain parameter. Most pairing calculations have not included it, but the Surface Delta Interaction Model, which enjoyed considerable success, implies quadrupole (and higher multipole) pairing for equal coefficients [7,8,21,22] to the monopole pairing. We have made most of our calculations here for these two extremes plus half strength, between the limits, as would be appropriate for a finite-range pairing interaction.

To take into account the variation in the pair transfer amplitudes for individual Nilsson orbitals, we took the values calculated by Oothoudt and Hintz.[23] It must be noted here that these authors have carried out for ^{174}Yb an exact diagonalization of the monopole pairing force among the 30(56) lowest summed Nilsson single-particle energies. The agreement of their calculation with experiment was not satisfactory.

3. Results

In this section we present in graphical form some illustrative results of our calculations for a few cases in the rare earth region. In Fig. 1 we show the results of our calculations for ^{164}Dy. The Figure contains the calculated energies and the (t,p) population rates for the lowest eight 0^+ states (including g.s.) corresponding to 12 sets of (G0, G2,χ_{np}) parameters. At the left of the figure all experimentally known 0^+ states are shown together with the reported experimental (t,p) rates when available.[12] As can be seen from this figure, the calculations reproduce the doublet excited 0^+ states at 1.66 and 1.75 MeV and the observed strong enhanced (t,p) rates to these states, though the order

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[*] We are grateful to Dr. Peter Möller for making available his FORTRAN computer codes calculating Nilsson functions by diagonalization over a large number (10 or 11) oscillator shells. His codes retain energies, $\langle r^2\rangle$ and $\langle q\rangle$.

of the relative enhancement is reversed in the calculation. This can be easily taken care of by minor adjustment to the proton and neutron pairing strengths. It is to be noted from Fig. 1 that parameter sets I-3 and I-4 give the closest agreement with experiment, suggesting the need for inclusion of strong quadrupole pairing and moderate n-p coupling. Also to be noted from this figure is the persistent presence in the calculation of an excited 0^+ state with very high (t,p) enhancement at around 2.2 MeV.

In a similar fashion, we show in Figure 2 the results of our calculations for the energies and (t,p) rates for the lowest eight 0^+ states in ^{168}Er together with known data from experiments.[11] For this case the agreement between the calculations and experiment for the lowest three excited 0^+ states is less satisfactory, though again it will be easy to obtain improved agreement with minor fine tuning of the calculation parameters. To show the effect of increasing n-p force coupling on our results we present in Figure 3 the results for ^{168}Er extending the n-p coupling strength to about 7.8×10^{-3}MeV/fm^4 (corresponding to parameter value 0.02 in the figure) At such high values of the n-p coupling the pairing coherence of the ground state is destroyed.

We turn now to the (p,t) rate calculations and show in Figs. 4 and 5 the results of our calculations for ^{168}Er and ^{164}Er together with known experimental[11,24] data. It is satisfying to see that no significant (p,t) rate enhancement to low-lying excited 0^+ states is predicted by the calculation, in agreement with experimental results. For ^{164}Er a significant (p,t) rate enhancement is predicted for the third excited 0^+ state at about 1.6 MeV, with no data or limits reported from experiments. It would indeed be interesting to see if some of the key and compelling predictions of our calculations can be borne out by future experiments. As an example we show in Figure 6 the results of our calculations for the (t,p) ^{166}Er, predicting strong enhancement to two 0^+ states at about 1.7 and 2.4 MeV. Such an experiment(and others) is possible, though difficult because of the need for highly isotopically enriched targets.

4. Discussion

We have barely begun to explore this model of exact pairing solutions in a few-Nilsson-state basis for spheroidal nuclei, so any conclusions must be tentative.

The most optimistic hopes were that a set of strength parameters, slowly varying with mass number, could be found that would reproduce the energies and collective properties of all the low-lying 0^+ band heads. These hopes now seem unrealistic. However, for reasonable values of the input parameters the model does seem to reproduce the general features for numbers of states in a given energy range and for the regions of neutron-pair transfer strength. (Our codes calculate E0 and E2 matrix elements among the bands, but we have not yet begun to correlate these results with data. Clearly the truncated basis will require larger-than-usual effective charges for the E2 transitions. Effective charges for E0 are less certain, but will be taken initially as equal to the E2 effective charges. Our codes also return values of quadrupole-transfer matrix elements, with which we can begin to study the variation of pair transfer strength with particular zones on the nucleus from polar to equatorial, but we have not yet studied this in any detail.)

We thought at the outset that this successive matrix diagonalization computation would have difficulty reproducing close-lying doublets of 0^+ states, since there always should be some kind of mixing that would cause roots to be spaced out. (Of course, the case of zero n-p coupling will have cases of accidental near-degeneracy between pure proton excitations and pure neutron excitations.) Even with substantial n-p coupling we do see calculated close doublets, implying underlying cancellations or symmetries. There can be some "intruder" 0^+ states not included in our basis of no broken Nilsson pairs. For example, two gamma vibrational phonons can couple to 0^+, or the proton system with a broken pair can couple to some K and parity other than 0^+, with the neutron system coupling likewise and combining to overall 0^+.

It is satisfying but not surprising that our model shows pair transfer strength strongly enhanced among ground-to-ground transitions. Our model seems to reproduce more than just the qualitative enhancement, but the trends in the Gd (Fig. 7) and Dy compare well with experiment. Fig. 7 shows that at unphysically large values of the neutron-proton coupling the pairing scheme begins to break down with a loss of ground pair transfer enhancement.

Our model calculations also show that when the chemical potential is in regions of neutron subshells (wider spacing between orbitals), an appreciable fraction of the pair transfer strength may shift to higher states. This phenomenon has long been understood generally. Some 20 years ago at a Dubna Conference Aage Bohr[4] set forth an elegant formalism with the example of nuclei at a major closed shell. At the same conference a paper by Rasmussen[5] showed exact pairing solutions to show a similar property at the 114-neutron subshell in the Sn nuclei. Experimental studies have showed this splitting of pair transfer strength at the 152-neutron subshell in Pu and Cm,[9,10] and examples are found also in the rare-earth region. (See the review article[2] of Broglia, Hansen and Riedel).

Our model provides a conceptual picture for better understanding the role of the various interactions. Quadrupole pairing along with monopole pairing makes a step toward a more realistic pairing interaction in that it brings about an enhanced pairing between orbitals with Nilsson wave functions in the same angular zones of the nucleus.[19] That is, orbitals corresponding to probability densities largest in the ends of spheroidal nuclei ("downgoing orbitals") interact most strongly among one another. They interact less strongly with "flat orbitals" and least strongly with "up-going orbitals," with their probability densities near the equator. If there were nuclei with deformations and Fermi energies in a region of the Nilsson level diagram having only strongly up-going and strongly downgoing orbitals, the inclusion of quadrupole pairing may nearly decouple the two level systems, which would each develop their own characteristic pairing correlations. We would not argue that anything we have calculated yet "proves" the need for inclusion of quadrupole pairing. Rather, we are convinced by arguments elsewhere that it should be included. (Note added post- workshop: Arima's talk at this workshop set forth one of the clearest arguments for quadrupole pairing. He pointed out that the near constancy of the energies of the first excited states (2^+) of the even tin nuclei required quadrupole pairing in the shell model.) For our calculations we favor the intermediate value of quadrupole pairing, that is, half the strength corresponding to the surface delta interaction, such as, a finite-range attractive interaction might give.

We were forced to include neutron-proton coupling and the attendant great complication of the computation because the existence of a set of pure proton excitation states with no neutron-transfer strength seemed to violate experimental data and general intuition. While it may not be a bad approximation for nuclear ground states to assume a factorizable wave function of neutron and proton parts, it is not realistic to expect that close-lying excited proton and excited neutron states will not mix through n-p residual interactions. We initially began our mixing code to include both monopole-monopole and quadrupole-quadrupole n-p interactions. However, to limit the number of parameters we implemented just the quadrupole-quadrupole residual interaction. As to the appropriate strength, we felt we had fewer guidelines. A good deal of the n-p interaction in a spherical shell model is accounted for in the deformed field of the Nilsson potential, and it is only in the quadrupole fluctuations that neutrons and protons need to be coupled by a residual interaction. Accordingly, we varied the n-p QQ interaction strength over a wide range, from zero to values that caused a drastic spreading of excited states and a breakup of ground transition pairing enhancement. For general best agreement of energies and pair transfer we favor a value of n-p QQ strength of about 1.17×10^{-3}MeV/fm^4 (corresponding to a parameter value of 0.003 in the figures).

Viewed as a mathematical system of coupled matrices we see regions in parameter space where the excited state energy patterns show earmarks of chaotic systems. That is, small changes in input parameters cause large changes in eigenvalue patterns. Such near-chaotic situations make the hope of near-exact agreement between nuclear models and experiment on the higher 0^+ excited states comparable to the hope that near-term weather forecasting can be made exact if only we get bigger computers, better input data, and better models. In the early days of nuclear collective models we thought we had schemes for understanding excited 0^+ states. In the spherical case we knew that 2-phonon, and 3-phonon quadrupole vibrational states should have 0^+ members. In the spheroidal case we had the n-phonon beta vibrational family and the 2-gamma-phonon state, and so on. The independent-particle early shell model had a difficulty of too many low-lying 0^+ states arising from the rearrangement of pairs near the Fermi energy. Pairing theory with its superfluidity gap helped that problem, and RPA dispersion theory calculations gave us predictions of 0^+ excited states above the gap, many more states than the collective models showed. The IBM-2 models in more recent times have added more realism to the collective picture, (cf. review of Arima and Iachello[1]) but to get the first few ^{156}Gd excited 0^+ states correctly required introduction of s' and d' bosons.

We believe that only microscopic calculations can be expected to address study of the lowest dozen excited states of a given spin and parity. The collective models essentially are calculating strength functions, which may settle on one or a group of states, and the most refined collective models should take into account the influence of the properties of the nucleon orbitals nearest the Fermi surface.

Acknowledgments

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Figure Legends

Fig. 1. For $^{164}_{66}$Dy are shown experimental and calculated 0^+ level energies and (t,p) reaction strengths in percent of ground-to-ground strength. There are four clusters of calculations for increasing n-p coupling strengths ($\chi'_{np} = 2.56\ \chi_{np}$ = 0.0, 0.002, 0.003, and 0.004, labeled 1, 2, 3 and 4 respectively). Within each cluster there are three pairing parameter sets, I, II, and III. In all cases G_{0P} = 0.23 MeV and G_{0N} = 0.20 MeV. Cases I, II, and III correspond to quadrupole pairing (G_Q) equal, half, and zero the monopole pairing G_0, respectively.

Fig. 2. Same as Fig. 1 except for $^{168}_{68}$Er.

Fig. 3. Same as Fig. 2 except for higher n-p coupling strengths of (χ'_{n-p} = 0.005, 0.0075, 0.01 and 0.02, cases 5, 6, 7 and 8, respectively).

Fig. 4. Same as Fig. 2, except for (p,t) reaction strengths instead of (t,p). Also neutron pairing strength was increased slightly to be equal to proton pairing.

Fig. 5. Same as Fig. 1, except for ^{164}Er and (p,t) relative strengths.

Fig. 6. Same as Fig. 4, except for ^{166}Er and the (t,p) reaction. Note that we predict substantial strength to two levels in the region of 1.7-2.5 MeV. No (t,p) data exist.

Fig. 7. For Gd isotopes we show experimental and calculated relative ground state (t,p) reaction strengths for various coupling strengths. The pairing strengths (MeV) are noted within parentheses (G_0,G_Q).

FIG. 1 - (p,t)^{164}Dy

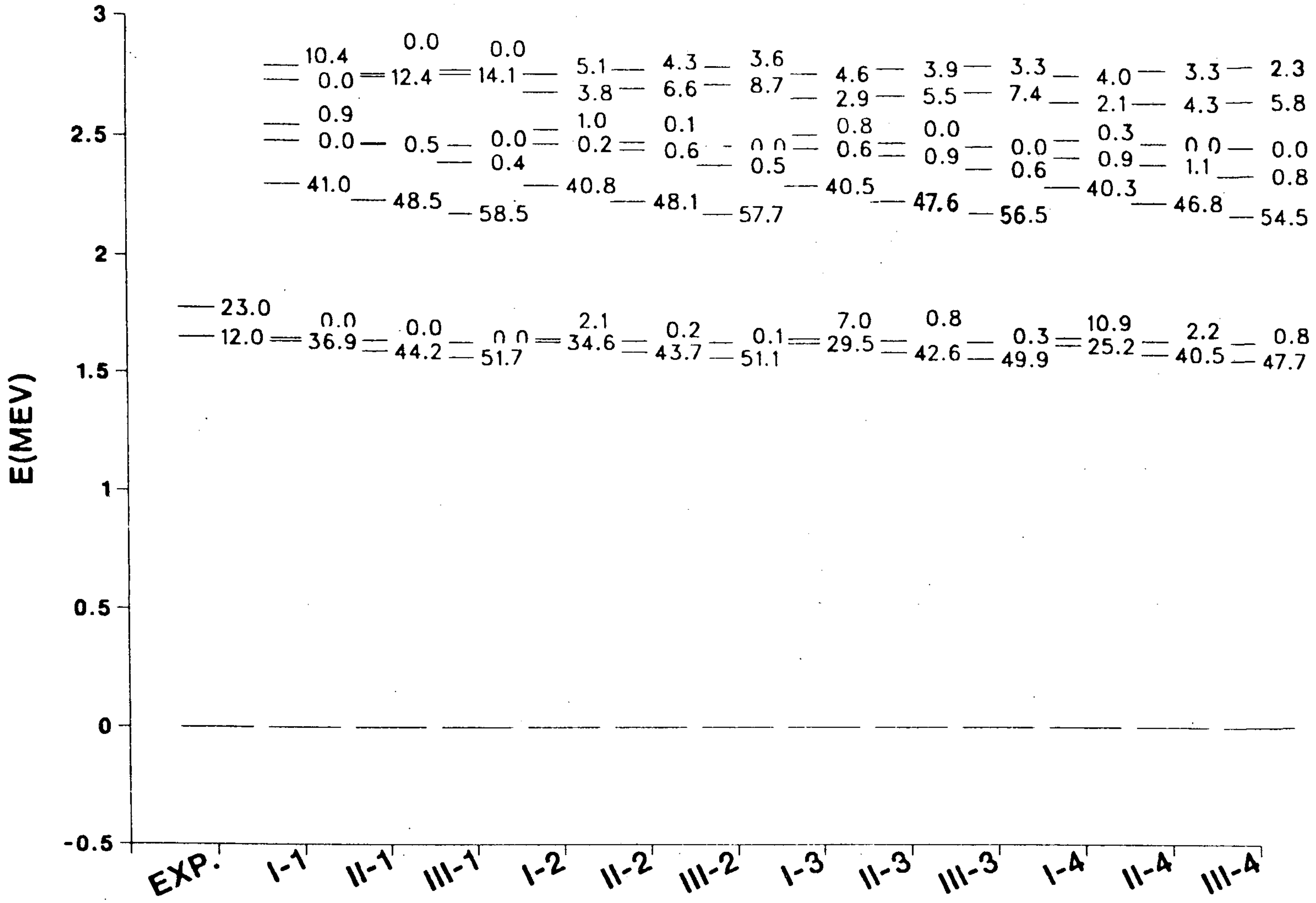


Fig. 1

FIG 2. - $(t,p)^{168}Er$

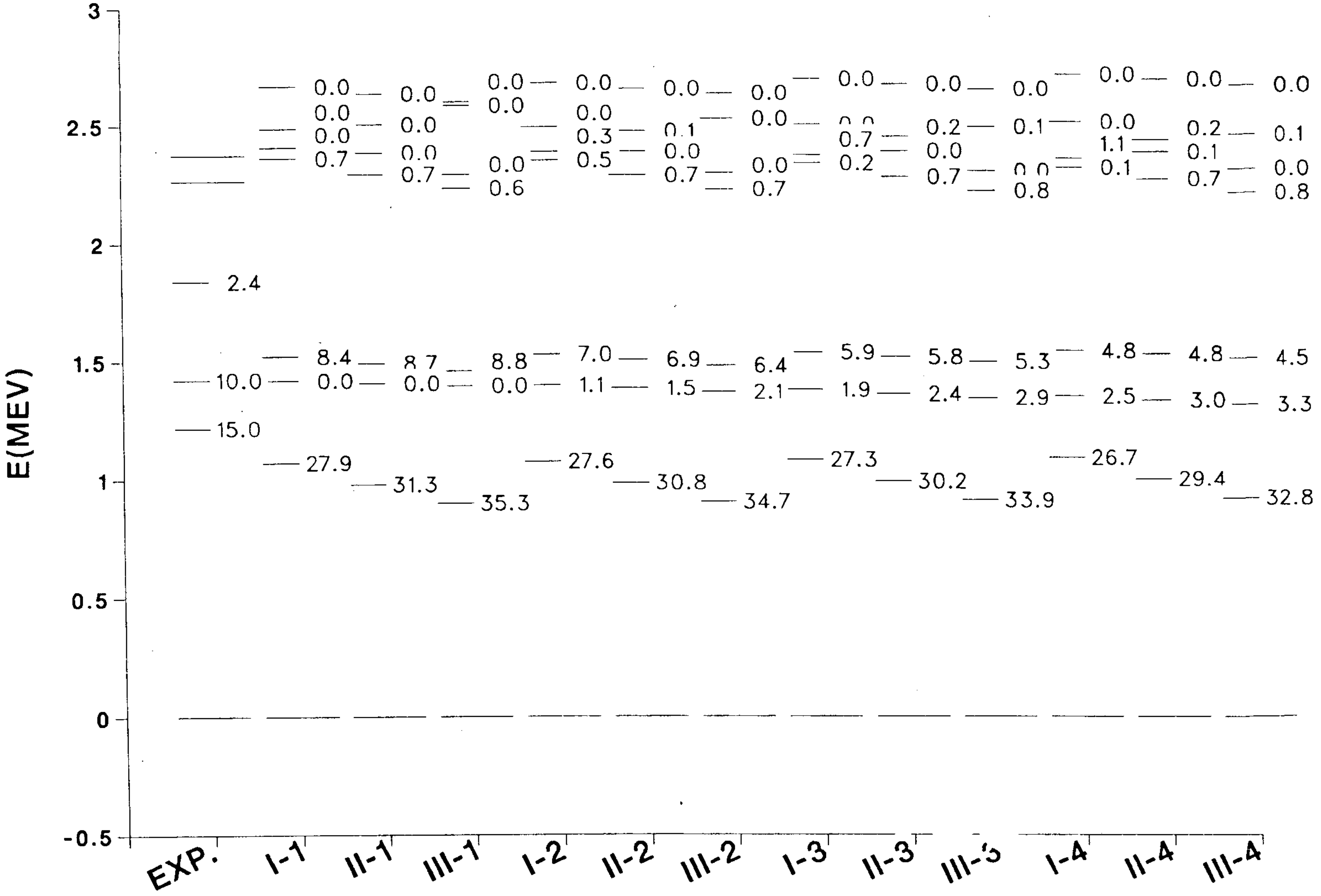


Fig. 2

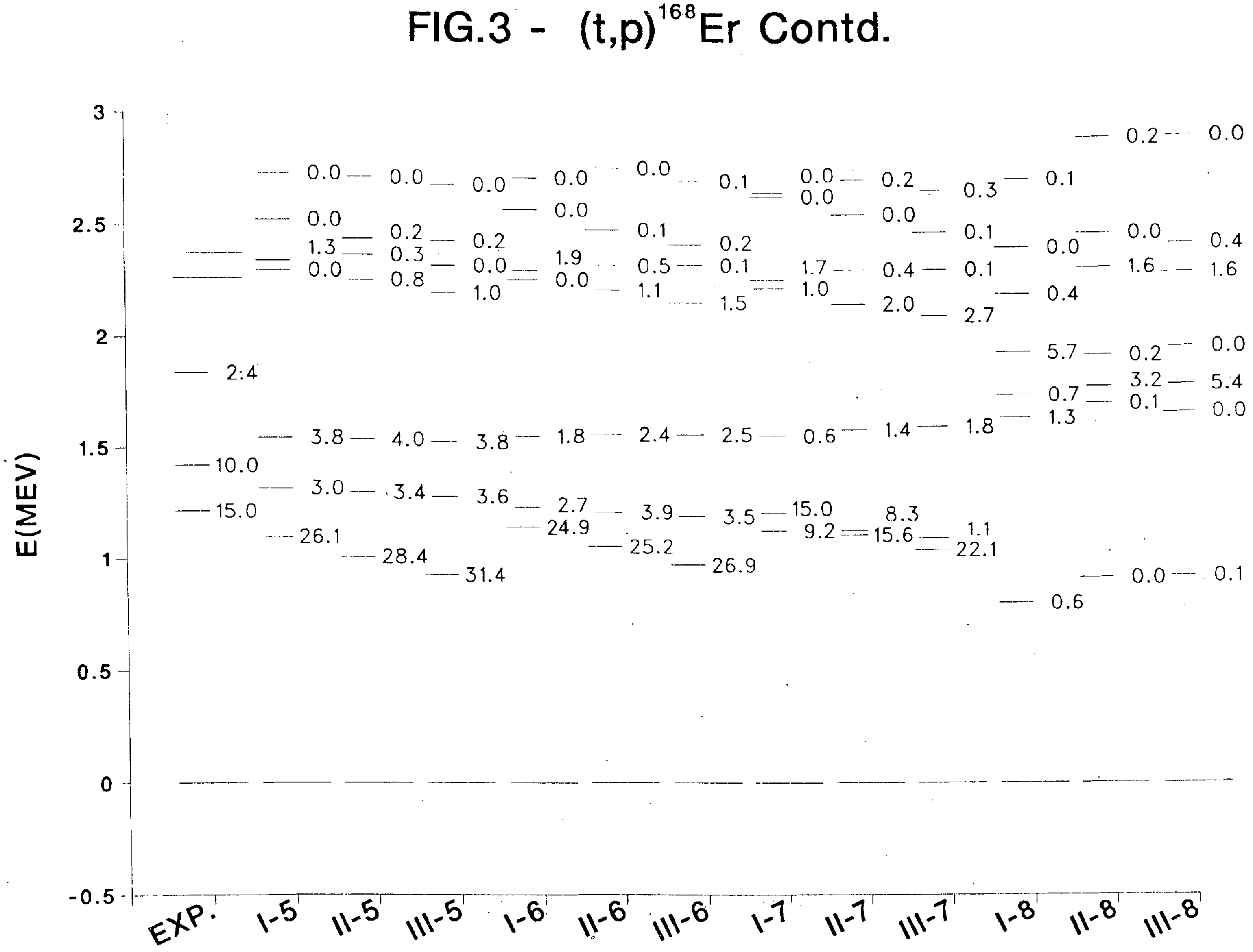


FIG.3 - $(t,p)^{168}$Er Contd.
E(MEV)
3
2.5
2
1.5
1
0.5
0
-0.5
EXP.
I-5
II-5
III-5
I-6
II-6
III-6
I-7
II-7
III-7
I-8
II-8
III-8
2.4
10.0
15.0
0.0
0.0
1.3
0.0
3.8
3.0
26.1
0.0
0.2
0.3
0.8
4.0
3.4
28.4
0.0
0.2
0.0
1.0
3.8
3.6
31.4
0.0
0.0
1.9
0.0
1.8
2.7
24.9
0.0
0.1
0.5
1.1
2.4
3.9
25.2
0.1
0.2
0.1
1.5
2.5
3.5
26.9
0.0
0.0
1.7
1.0
0.6
15.0
9.2
0.2
0.0
0.4
2.0
1.4
8.3
15.6
0.3
0.1
0.1
2.7
1.8
1.1
22.1
0.1
0.0
0.4
5.7
0.7
1.3
0.6
0.2
0.0
1.6
0.2
3.2
0.1
0.0
0.0
0.4
1.6
0.0
5.4
0.0
0.1

Fig. 3

FIG.4 - (p,t)^{168}Er

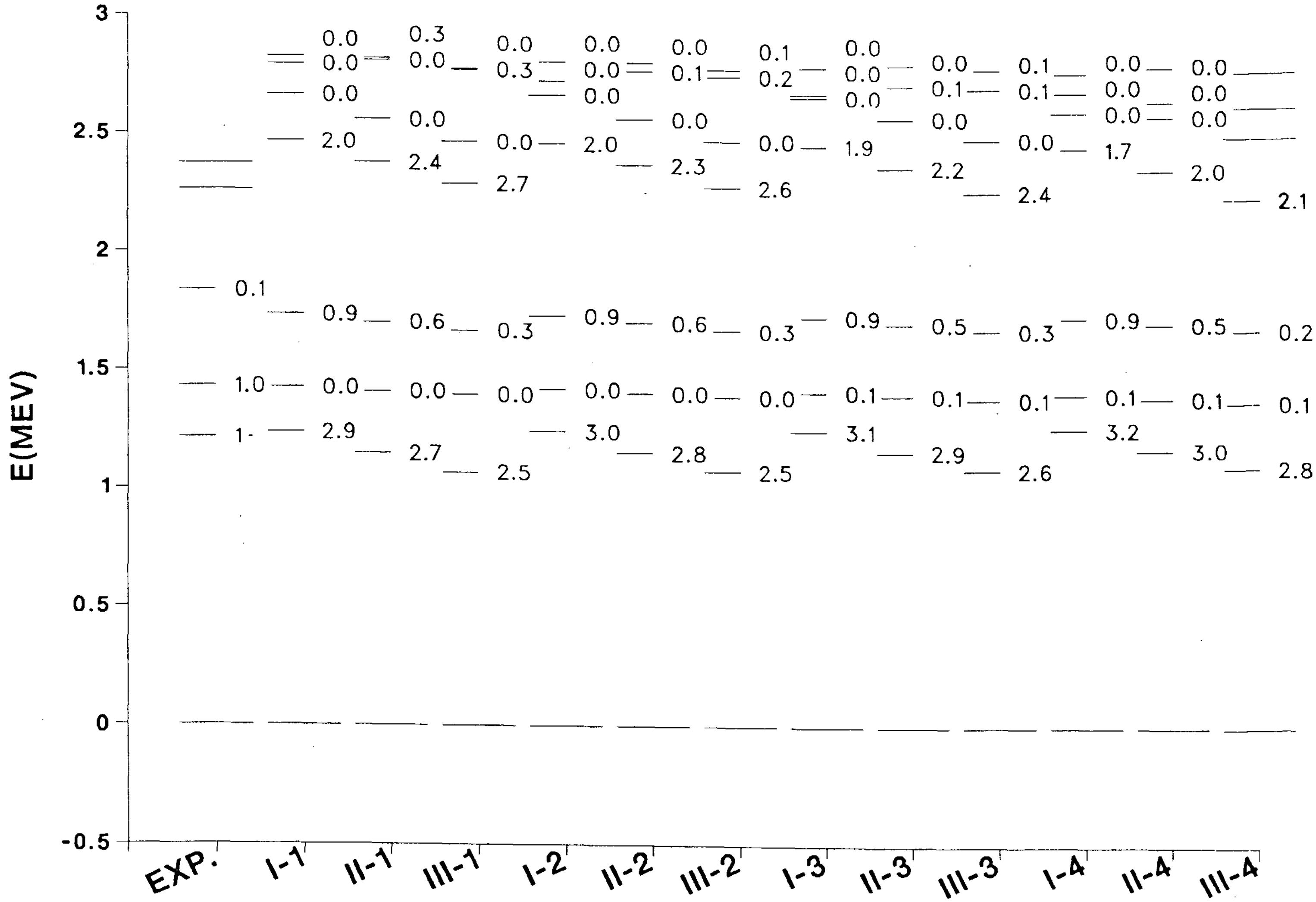


Fig. 4

FIG.5 - (p,t)^{164}Er

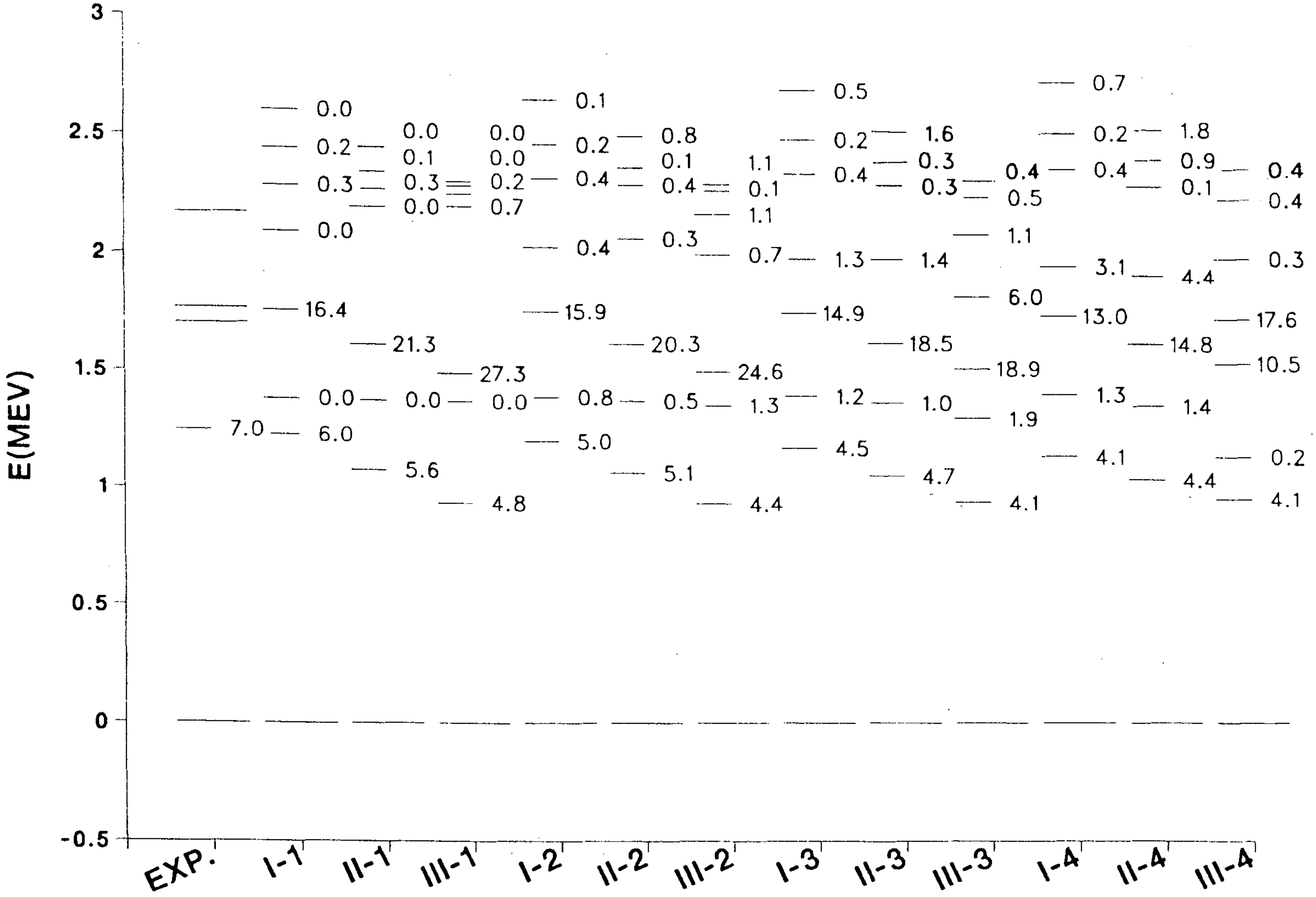


Fig. 5

FIG.6 - (t,p)^{166}Er

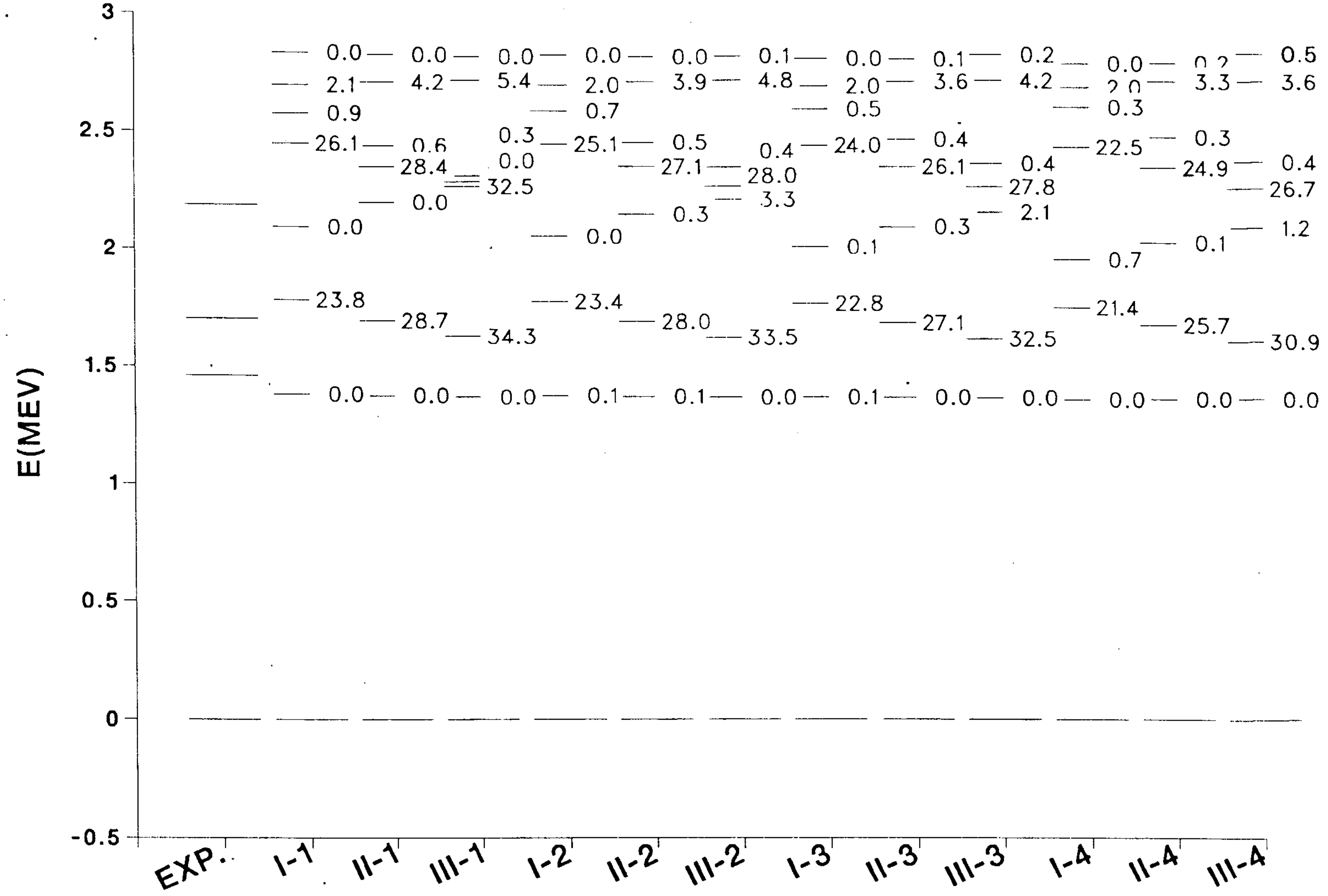
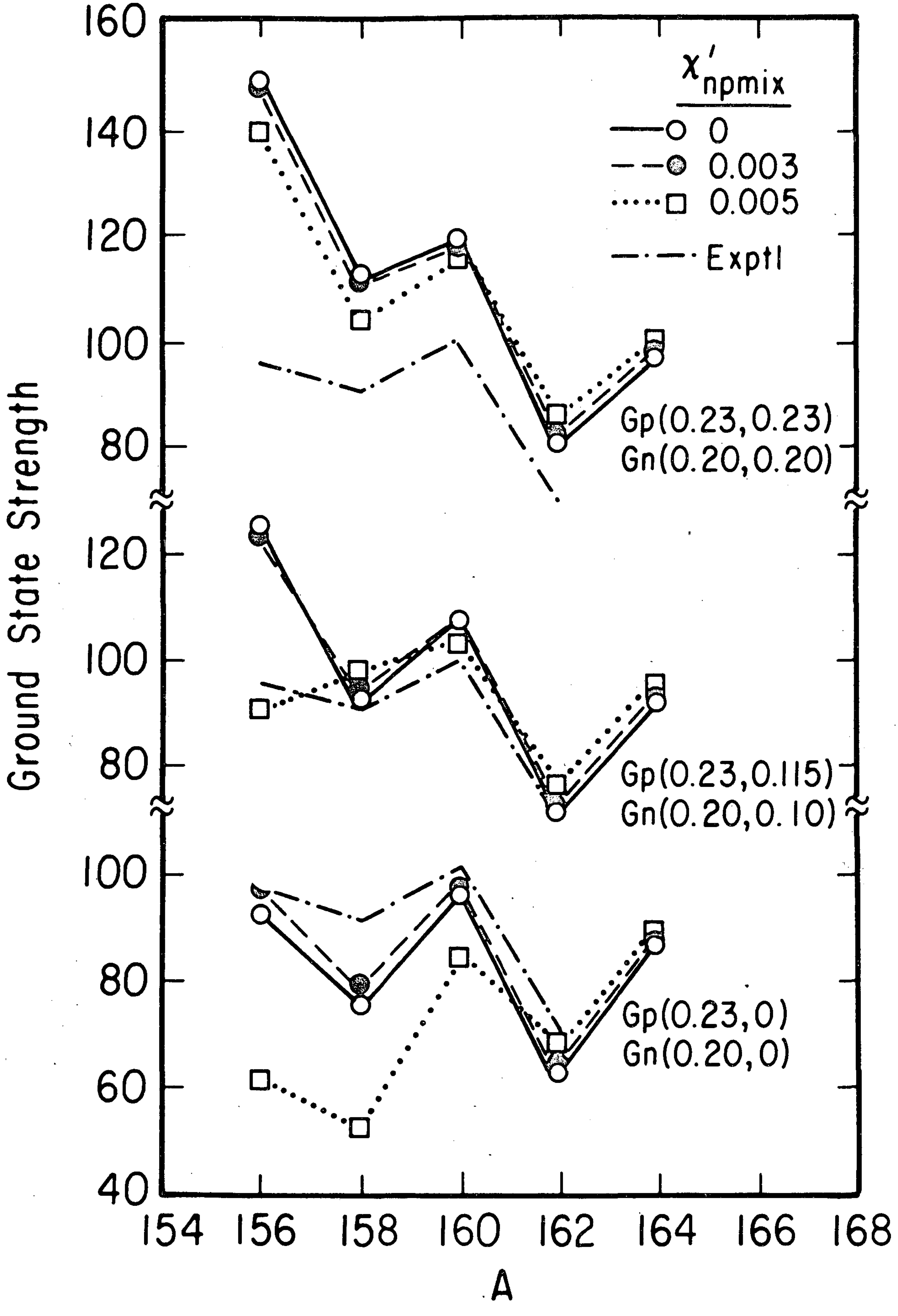


Fig. 6



160
140
120
100
80
120
100
80
100
80
60
40
154
156
158
160
162
164
166
168
A
Ground State Strength
χ'_{npmix}
0
0.003
0.005
Exptl
Gp(0.23,0.23)
Gn(0.20,0.20)
Gp(0.23,0.115)
Gn(0.20,0.10)
Gp(0.23,0)
Gn(0.20,0)

Fig. 7

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