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ICAR-CODE for COMBINATORIAL CALCULATION OF LEVEL DENSITIES

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Abstract: ICAR-code for combinatorial calculations of level densities from ENEA Bologna, Italy, was implemeted for use on personal computer. It is available on diskettes from the NEA Data Bank, Saclay, and the IAEA Nuclear Data Section.

Implemented on PC by
V. Goulo

May 1988

ICAR-CODE for COMBINATORIAL CALCULATION OF LEVEL DENSITIES

Introduction

Code ICAR [1] was presented by M. Herman at the International Centre of Theoretical Physics (Trieste, Italy) Workshop on Applied Nuclear Theory and Nuclear Model Calculations for Nuclear Technology Applications, 15 February - 18 March 1988, with exercises on IBM compatible personal computers Olivetti M-24 and M-380. The code is short enough to be installed in 640K computer using DOS 3.2 and professional FORTRAN compiler 1.0.

1. Description of the program

Code ICAR makes combinatorial calculations of state and level densities with fixed exciton numbers. Shell model orbitals are used for generation of possible configurations. Pairing interactions are taken into account in the frame of Bardin-Cooper-Shriffer theory.

2. Changes in the text of program made while implementing

a. Operator DATA in the subroutine EXCESS was converted into BLOCK DATA module. COMMON block was used for data transmission into EXCESS subroutine.

b. Operators FORMAT were corrected.

3. Compiling and linking of the code text were done in accordance with PROFORT compiler manual [2], using compiler's library of standard procedures.

4. Example of batch file to run the code

```
SET FORT2 = ICAR1.OUT
SET FORT3 = ICAR1.INP
ICAR1 /R 90000 > ICAR5.LST < ICAR5.INP
```

where ICAR1.INP is table of data used in calculations
ICAR5.INP is input data file
ICAR1 is execution module of code
ICAR1.OUT is output file which is to be used for the further conversion with code CONV
ICAR5.LST is listing of the program

are presented on a diskette together with source file of the code.

5. Examples of input, output and data files used in exercises are described in the proceedings of the Workshop and are available together with the source file of the code.

   Running time of exercises: 12-20 minutes for 10 Mhz computer.

References

1. M. HERMAN, G. REFFO, Chain of Codes for the Combinatorial Calculation of Level Density, RT/TB/87/5, ENEA, Italy.

2. Installation and use of personal compiler professional FORTRAN, 1986.

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WORKSHOP ON

APPLIED NUCLEAR THEORY AND NUCLEAR MODEL CALCULATIONS
FOR NUCLEAR TECHNOLOGY APPLICATIONS

(15 February - 18 March 1988)

Combinatorial approach to few quasiparticle state densities

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COMBINATORIAL APPROACH TO FEW QUASIPARTICLE STATE DENSITIES

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ABSTRACT

The method for combinatorial calculation of state and level densities with fixed exciton numbers is presented. Shell-model orbitals are used as a basis from which all possible configurations are generated . The pairing interaction is taken into account by applying the BCS theory to each configuration. The role of the pairing interaction is discussed. The spin and parity distributions are obtained and analyzed. Effects of the restriction limiting configurations to only bound orbitals are also considered.

INTRODUCTION

The main deficiency of the formulae commonly used to estimate exciton level densities comes from the assumption of equidistant spacings for the single particle levels (s.p.l.) which is supplemented with the statistical approximations. Because only few-exciton configurations contribute significantly to preequilibrium emission and the population of low energy configurations is relevant as well, statistical approaches do not seem to be adequate for preequilibrium calculations. This has motivated calculations which provide the possibility of direct counting of the levels with a fixed number of excitons, so that at least some of the usual assumptions (equidistant single particle levels, saddle point approximation, no residual interactions) can be avoided. Combinatorial calculations seem to be well suited to this end. In this lecture we outline the theoretical model and summarize most important results. We refer to Refs.1,2, and 3 for more extensive discussion.

THE MODEL

We assume the finite set of basis vectors (single particle states) derived from the shell-model with appropriately deformed nuclear potential. The set consists of the time conjugated pairs of basis vectors. In each pair, both vectors have the same quantum numbers but differ in a sign of a spin projection. We further assume, that each nuclear state of a noncollective nature can be described by a simple sum of N and Z basis vectors, where N and Z stands for the number of neutrons or protons respectively. This assumption is equivalent to neglecting all residual interactions between the nucleons. The only exception is made for the pairing interaction which is included in terms of the BCS model with blocking according to Wahlborn /4/. For each state the set of two coupled BCS equations is solved in the subspace of the basis vectors. This subspace is formed after rejection of all those pairs of the time conjugated basis vectors for which one of the vectors, and only one, is involved in the formation of a nuclear state. In the following, we refer to these rejected pairs as configurations, which can be represented by the vectors with the components enumerating removed pairs of the basis vectors. The concept of the configuration greatly simplifies treatment of the excited states. First, it reduces the specification of a state to a few numbers specifying the corresponding configuration vector. Second, one configuration corresponds to many nuclear states, which are easily obtained by coupling the angular momentum projections. In other words, a configuration groups all the states built up with the same time conjugated pairs of the basis vectors regardless to the total spin projection of these states. Each configuration corresponds to a different subspace of the basis vectors leading formally to the different solutions of the BCS equations

$$\sum_{i}' 2V_{i\beta}^{\lambda} = \eta \,, \tag{1}$$

$$\sum_{i}' [(\zeta_i - \lambda_\beta)^2 + \Delta_\beta^2]^{-1/2} = 2/G \,, \tag{2}$$

where

$$V_{i\beta}^2 = \frac{1}{2}\left|1 - \frac{\zeta_i - \lambda_\beta}{[(\zeta_i - \lambda_\beta)^2 + \Delta_\beta^2]^{1/2}}\right| . \qquad (3)$$

The prime superscript indicates that the summation runs only over subspace basis vectors (unblocked orbitals). Here the ζ_i are basis vector eigenenergies, η stands for the number of paired nucleons and λ_β and Δ_β are the Fermi energy and correlation function which are to be determined. The latter two are found by minimization of the sum of the two squared BCS equations. The chemical potential and the correlation function have to be found for each configuration (but not for each nuclear state) and determine the total configuration energy which reads

$$E_\beta = \sum_i \zeta_i + \sum_i{}' 2V_{i\beta}^2 \zeta_i - \frac{\Delta_\beta^2}{G} , \qquad (4)$$

where the first summation includes only blocked orbitals.

For some configurations it is not possible to find a real solution for the two BCS equations. In these cases it is assumed that the pairing correlation disappears and the total energy is calculated according to the pure shell model.

The ground state of a neutron (or proton) gas is defined as a combination of N (or Z) basis vectors which gives the lowest possible energy. The excited configurations are classified according to the number of the excitons equal to the dimension of the configuration vector. In order to account for all possible states, we also allow for the configurations which correspond to the excitation of both basis vectors in a time conjugated pair (see Ref.1). The excitons are split into 'holes' and 'particles' depending on the condition if the particular basis vector pair was, or was not involved in the formation of the ground state.

All configurations with a specified number of particles and holes are generated within the assumed set of the basis vectors by means of the permutation enumeration algorithm /5/. For each of them a proper coupling of the spin projections is performed to obtain the nuclear states. The parity of each state is determined as a product of the parities of blocked orbitals (note that two excitons placed in the same orbital couple to M=0 and contribute with positive parity). The state density $\omega(E,M,\pi)$ is found by counting states with the angular momentum projection M and parity π falling

in an interval centered at the excitation energy E. For spherical nuclei the density of n-exciton levels ρ (E,J,π) is calculated according to the well known relation

$$\rho(E,J) = \omega(E,M=J) - \omega(E,M=J+1) \qquad (5)$$

The spin cutoff parameter σ (E) is calculated from the definition

$$\sigma^2(E) = \langle M^2 \rangle - \langle M \rangle^2 = \Sigma_i M_i^2 / \omega(E) \qquad (6)$$

In order to obtain mixed configurations as well, the state densities for neutrons and protons are convoluted before the level density is calculated. The energy of a mixed configuration is taken to be the simple sum of the energies of the two convoluted configurations, since no interaction between protons and neutrons is assumed. With this approximation, the state density for mixed configurations can be written as

$$\omega_{p,h}(E,M) = \sum_{\substack{M_p M_h \\ M_p + M_h = M}} \int_0^E \omega_p(E_p,M_p) \times \omega_h(E - E_p, M_h) dE_p \,. \qquad (7)$$

To reduce edge effects the state densities convoluted in Eq.7 are sorted into 0.1 MeV bins. To reduce fluctuations, the final results are obtained by lumping together states over larger intervals. The spin projection of a mixed configuration is just the sum of the spin projections of the convoluted configurations. Similarly the product of their parities defines the parity of the mixed configuration.

The finite number of orbitals taken into account limits the maximum energy which can be calculated. We take this limit to be the excitation energy of the configuration consisting of only one exciton promoted to the highest orbital. In practice this limit has been increased by 20%, in the hope that the loss of states at these energies is still acceptable.

THE CALCULATIONS

The calculations were carried out in the basis of single particle orbitals derived from the harmonic oscillator well defined by parameters due to Seeger and Howard /6/. Usually 114 neutron and 114 proton orbitals were used in our calculations, except for very heavy nuclei. For each nucleus considered, a value of the pairing strength parameter G was determined from the mass differences. For this purpose the ground state condensation energies E_0^c for the three neigh-

boring nuclei were used instead of the nuclear masses in Eq.1 of Ref.7 giving

$$\epsilon_n=(E^c_{Z,N}-2E^c_{Z,N-1}+E^c_{Z,N-2})/2 \qquad (8)$$

for neutrons and similarly for protons. For odd nuclei the value of G determined for neighboring even nuclei was used.

For the purpose of identification the calculations are denoted by four integer numbers which correspond to the number of neutron particles, neutron holes, proton particles and proton holes respectively. Using this notation, the configuration types (1100), (0011), (1111), (2200), (0022), (2211), (1122) and (2222) for even-even systems and (1000), (0010), (1010), (2100), (0021), (2110), (1021) and (2121) for odd-odd nuclei were considered.

PAIRING INTERACTION EFFECTS

The difference between the total energy of free nucleons and the energy calculated with the pairing interaction included is called the condensation energy and plays a crucial role for our further considerations. It should be noticed that nonvanishing condensation energies are found for some odd systems and that the ground state condensation energy always vanishes for systems in which a shell is closed, even though the correlation function may be different from zero in some of these cases.

Even systems

Let us start with the simplest configuration consisting of one particle and one hole. To create it one pair must be broken and one of the particles be lifted the minimum to the first orbital above the Fermi energy. This way the two orbitals nearest the Fermi energy are blocked and made unavailable for pair scattering. The correlation function is decreased, and if not enough orbitals around the Fermi energy are left unblocked, superconductivity may disappear completely ($\Delta=0$). The condensation energy of the excited state decreases with the suppression of superconductivity and the total energy of the configuration approaches the free gas value. The excitation energy is calculated however with respect to the BCS ground state energy, which is lower by E^c_o compared to the free gas ground state energy. The first excited state is therefore found at an excitation energy higher by $E^c_o - E^c_1$ then the free gas model predictions.

When the excitons are moved away from the Fermi energy, the superconductivity reappears, E_1^c approaches E_0^c and the shift in the excitation energy tends to vanish. This does not imply that the high energy configurations are not affected by pairing correlations. In some cases, especially in the vicinity of closed shells, it is enough that only one exciton blocks an orbital close to the Fermi energy to cause the breakdown of superconductivity. The second exciton can carry high energy so that the high energy configurations may be affected by an energy shift of the value E_0^c .

In Fig.1 the spectra of energy shifts caused by the pairing interaction are shown. An energy shift is defined as the difference between the excitation energies of a configuration calculated with and without the pairing interaction taken into account. In the case of the (1100) configurations in 58Ni a peak around 1.9 MeV is observed, which corresponds to superconductivity breakdown due to blocking. One of the two p3/2 orbitals at the Fermi energy is occupied by a hole in these cases. The energy shifts between 0.1 MeV and 0.6 MeV correspond to configurations with less blocking. In the case of the same (1100) configurations in 116Sn, a more complicated spectrum of shifts is obtained. This is due to the higher density of orbitals around the Fermi energy which allows for solutions of the BCS equations intermediate between the $E_0^c=0$ and $E_1^c = E_0^c$ limits. The peaks in the spectrum correspond to the blocking of subsequent s.p.l. around the Fermi energy. It should be noted that this blocking is never sufficient to destroy the superconductivity since the highest shift is well below E_0^c which amounts to 2.7 MeV. This can not be achieved before the next pair is broken and the four exciton configuration is formed The spectrum of energy shifts then becomes even more complicated, which is easy to understand since with four excitons many more blocking possibilities exist. At this point we would like to stress that the destruction of pairing correlation always results in the energy shift equal to the condensation energy of the ground state and that this value is an absolute limit of the pairing effect. Accordingly, if this limit is reached at say 4 excitons, the configurations with a higher number of excitons will not reveal higher shifts.

It is obvious that there is no hope to reproduce the energy shifts caused by the pairing interaction as a function of excitation energy and/or exciton number alone without making some reference to nuclear structure. This implies that, from the microscopical point of view, state and level density formulae should not be corrected for pairing effects by a simple modification of the excitation energy. In spite of this pessimistic conclusion we have found that the 4,6 and 8 exciton state and level densities calculated in the frame of the free gas model can be brought into perfect agreement with the results obtained including the BCS if a shift of $E_0^c - E_1^c$ is applied. In other words, the pairing effects on the

state and level densities can be accounted for by shifting the free gas results in a way which makes the first excited state in both approaches coincide (Fig.2). This feature is somewhat unexpected after all that has been said concerning the BCS energy shifts. In fact, if one directly compares the state and level densities calculated with and without the pairing interaction, one observes (Fig.3) that the pairing shifts low energy states up and that the BCS density curve starts at a higher energy than the free gas one. It rises more rapidly however and at the end of the energy range considered in our calculations the two curves tend to match. This indicates that the pairing interaction affects mainly the low energy states, while at higher energies the number of states which are shifted up and out from a bin is relatively small and is to some extent compensated by the lower bin states which are shifted up and replace those which were lost. The simple procedure for bringing both curves into agreement by introducing a constant energy shift $E_o^c - E_1^c$ therefore appears to have no physical justification. Its success should be regarded rather as a particular feature of the state or level density shape, which flattens at higher energies. Because of this the densities are not very sensitive to an energy shift in this region. In principle one would expect that the pairing effects could be accounted for by shifting the Fermi gas results by the value of $E_o^c - E_1^c$ averaged over all configurations considered. However this procedure does not give satisfactory compensation of the pairing effects close to the threshold and the final result turns out to be worse than the one which can be achieved with the procedure described above.

The effect of the pairing interaction on the spin cut-off factors appears to be the same as that on the state density. The same procedure for correcting the free gas model results for the pairing interaction is suggested. Since the energy dependence of the spin cut-off factors is rather weak, a constant shift in energy to match the BCS calculated threshold works perfectly well , apart from differences due to fluctuations (Fig.4).

Odd systems

Considerations for the odd systems run along the same lines as for the even ones but the starting point is just the opposite. The ground state of a nucleus with an odd number of neutrons or protons contains a single nucleon at the Fermi energy. This nucleon blocks an orbital important for the pairing correlation, so that Δ and E_o^c decrease or disappear. In the excited states of 1 exciton structure, this nucleon is moved out from the Fermi energy. The orbitals close to the Fermi level are made available for pair scat-

tering and superconductivity is recovered. Accordingly, the condensation energy for the excited state is higher than that for the ground state and the excited state appears at a lower excitation energy compared to the free gas model prediction. Thus, for 1 exciton configurations in odd systems, a negative energy shift is expected. These negative energy shifts were actually obtained in our calculations and are displayed on Fig.5.

The situation becomes more complicated when several exciton configurations are considered. If these excitons are placed far from the Fermi energy, their contribution to the blocking is negligible and negative energy shifts are expected as in the one exciton case. Additional excitons can have however a different effect if the ground state of the nucleus has a nonvanishing condensation energy. In this case, the blocking of orbitals close to the Fermi energy leads to a decrease of the pairing correlation and shifts of positive value appear. Examples of this type are shown in Fig.5. The ground state of the neutron gas in 116In has a condensation energy equal to 2 MeV. The breaking of one pair increases the blocking so that 1.6 MeV of this condensation energy is lost and the first excited state of 2 particle 1 hole structure is found at a higher energy compared to the free gas model.

The qualitative considerations and calculated results discussed above show that, in odd systems, the pairing interaction may lead to positive as well as to negative shift in the excitation energy of a configuration, in contrast with even systems for which only positive shifts are possible. Moreover the ground state condensation energy gives no estimate of the pairing, effects since in odd systems, excited states can possess less blocking than the ground state and therefore superconductivity can be stronger. Fortunately as far as reaction calculations are concerned, we have found that odd system state and level densities may be corrected for the pairing interaction in the same way as even ones. The results obtained in the frame of the free gas model, if shifted to make the first excited states coincide, reproduce the results of our BCS calculation well enough for application purposes.

STATE AND LEVEL DENSITIES

Shell effects and orbital degeneracy make the spectrum of the s.p.l. in spherical nuclei highly nonuniform and this feature is reflected in the state and level densities calculated. In Fig.6 we show state densities calculated for several exciton numbers for the even-even nucleus 56Fe. The well known feature of a rapid increase of the state density

with increasing exciton number is clearly seen. Deviations from the equidistant model manifest themselves in strong fluctuations of the state densities and in the increasing threshold energy for the excitation of configurations with increasing exciton numbers. Fluctuations are pronounced mostly for low exciton numbers and tend to be smoothed out when more degrees of freedom participate in the excitation. In general, the fluctuations are smeared out as the density increases with excitation energy and mass number.

The nuclear deformation is expected to smooth the fluctuations making approaches based on the statistical assumptions (e.g. formula of Williams) more realistic. Therefore, we try to investigate under which conditions the statistical approaches may be considered justified (if at all) and what are their limitations. The calculations were performed for 27Al, 100Mo, and 170Er in the space of the s.p.s. by Seeger and Howard /6/ obtained for different values of the deformation parameter α_2 . The calculated state densities, summed over M, are shown in Figs.7, 8, and 9 for the 1-particle 1-hole configurations of neutrons in three nuclei under consideration. The predictions of the Williams' formula /8/ are given for each case to provide the reference between the results for different deformations and to compare this simple description with the microscopic calculations. For this purpose the s.p.s. density g was set to the standard value A/26 (note that we deal with the neutron gas only).

Using the sets of basis vectors derived from the spherical potential, very strong fluctuations in the state densities are observed for all nuclei. In the case of 27Al we have in fact the well separated groups of states. For 100Mo and 170Er the states are more spread but still, even at the relatively high excitation energies, there are regions where no state exists. Introduction of the small deformation to the nuclear potential (α_2=0.05) leads to the splitting of the spin multiplets of the basis vectors which results in a significant smoothing of the state densities. In a nucleus as light as 27Al it is however not enough to bring the calculated state densities into the form which could be reproduced by any closed form expression. This conclusion remains valid also for much higher deformations α_2 =0.1 and α_2=0.2. In particular, the comparison of the microscopic results with the predictions of the Williams' formula shows an evident nonadequacy of the latter in the low energy region (below 10 MeV) where the preequilibrium emission usually dominates. For the heavier nuclei (Figs.8 and 9) even the small deformation α_2 =0.05 results in the qualitative changes in the calculated results. The gaps are partially filled and a remarkable structure of roughly 5 MeV width appears in the spectra. The peak to valley ratio approaches an order of magnitude at low energies and falls down to 4-6 at the end of the energy range, being higher for 100Mo than

combinations of the above

for 170Er. Increasing the deformation one observes that the valleys in the spectra are gradually filled on the expense of the bumps leading to the step-like curves for $\alpha_2 = 0.1$ and to the relatively smooth ones for $\alpha_2 = 0.2$.

It is surprising, how well the Williams' formula describes the general trend of the state densities for two heavier nuclei, in spite of the very low exciton number and of the fact that no attempt has been undertaken to adjust the s.p.s. density g. For the deformations as high as $\alpha_2 = 0.2$ the Williams' formula may be considered exact, while for the less deformed nuclei the shell structure is expected to show up in a form of the broad structure which is missing in the closed form expression.

SPIN DISTRIBUTION

The validity of the statistical law describing the spin distribution of nuclear levels must be reviewed when applied to levels with fixed exciton numbers. The formula which reads

$$R(J) = \frac{(2J+1)}{2(2\pi)^{1/2}\sigma^3} \exp(-(J+1/2)^2/2\sigma^2) \quad (9)$$

is derived under the assumption of a Gaussian distribution of spin projections M. While it is very likely to be true when the number of levels is high enough, this assumption may not hold for levels with low exciton number for which the density of states is too low for a statistical treatment. Bearing this in mind we have analysed more than 1000 spin distributions for different configurations, energies and nuclei. We have found out that Eq.9 does very well for configurations containing at least 4 excitons (Fig.10). When there are only few levels in the energy interval the agreement is random as would be expected (Fig.11).

Let us focus our discussion on the spin cut-off parameter σ which contains all information concerning the spin distribution. Like the level and state densities, the spin cut-off parameter reveals strong fluctuations with excitation energy. These are caused by the nonuniform distribution of the s.p.l. spin projections. Our discussion of fluctuations in the state densities applies here as well. Therefore, we will concentrate our attention on the energy, mass and exciton number dependence of spin cut-off parameter disregarding the fluctuations.

Two types of energy dependence of the spin cut-off parameter are observed. The first has a 'logarithm like' shape (Fig.12), while is essentially constant or slightly line-

arly increasing with energy in the second (Fig.12). These features are connected with the spin structure of the s.p.l. in the vicinity of the Fermi energy.

It must be stressed that the energy variations of the spin cut-off parameter for levels with fixed exciton numbers are solely due to the sequence of shell model levels. These variations cannot be traced back to the energy dependence of the spin cut-off factor of total level density (as used in the compound model) because the nature of the latter dependence is absolutely different. Actually, if one looks at the compound levels from the the stand point of the exciton model then the density of compound states is dominated by the configurations with exciton numbers as high as energetically possible (see Fig.6) because of the very fast increase of the state density with exciton number. Since higher exciton number configurations not only have higher densities but also higher spin cut-off factors, the increase of σ for compound nucleus levels is caused mainly by the increase in the number of excitons with increasing excitation energy. This dependence is obviously much stronger than the one due to the s.p.l. alone.

Due to the rather weak energy dependence of the spin cut-off parameter, we can disregard it for the time being to investigate the influence of the exciton and mass numbers. For this purpose, an energy average of the spin cut-off factors was performed for each configuration type in all nuclei considered. Averaged spin cut-off factor can be approximated by

$$\sigma^2(n)=cnA^{2/3}+0.1A^{2/3}+4 \qquad ;c=0.22 \qquad (10)$$

When the intercepts in exciton and mass number dependences are disregarded, formula 10 reduces to

$$\sigma^2(n)=cnA^{2/3} \qquad (11)$$

To account for the global energy trend, a certain energy dependence can be associated with the factor c. In view of the relatively large spread of the points it seems justified to assume linear dependence given by the form

$$c=0.24+0.0038E \qquad (12)$$

There is a slight odd-even effect, which we have disregarded up to now. We have observed that $<\sigma^2>$ for configurations of the type (1010) are about 5 units higher than $<\sigma^2>$ for the (1100) and (0011) configurations, in spite of the equal number of excitons in each of them. This difference reduces to

further conversion with code CONV
ICAR5.LST is listing of the program

are presented on a diskette together with source file of the code.

2 units if 4 exciton configurations are considered (e.g. (2110) and (1111)) and essentially disappears for 6 exciton cases. This odd-even effect is due to the difference in the average spin of the s.p.l. below and above the Fermi level. Since higher spin s.p.l. are found at higher energies, particle type excitons carry in general more angular momentum than holes. Therefore the spin of configurations containing more particle type excitons than holes will be, in general, higher than the spin of the configuration in which the number of both types of excitons is equal. Small deviations at low exciton numbers due to the odd-even effect lead to a shift of the most probable spin by less then one unit which should not affect cross section calculations significantly. However, if composite particle emission or composite particle induced reactions are considered, configurations containing very different numbers of particles and holes may be created (e.g. emission of alpha particle from an 8 exciton configuration leaves the residual nucleus in a pure 4 hole configuration (0202)). In these cases, the predictions of Eq.10 and of Eqs.11,12 will not be accurate enough. A more general formula should contain separate terms for particles and holes, to account for the difference in the average spin projection of the s.p.l. below and above the Fermi level.

For reaction calculations we suggest the use of Eq.10 or Eqs.11,12 for the determination of spin the cut-off parameter. In any case, these formulae must be applied only above the threshold energy for a given type of configuration. Using either one of these two descriptions, one should bear in mind that their predictions are expected to give the general trend rather than exact values. For most practical applications, their accuracy seems to be satisfactory however. Our experience shows that one and two exciton configurations can also be treated, on the average, with the closed forms for spin cut-off factor. Exception has to be made for refined precompound calculations which will perhaps require direct use of combinatorial results.

For the sake of completeness we have to devote some attention to the yrast lines for few quasiparticle configurations. This problem has been addressed already in Ref.9, where we have pointed out that one has to deal with a separate yrast line for each exciton number. In Fig.13, the results of the present calculations for some configurations types in 58Ni are shown. One observes that the restriction imposed by yrast lines are most pronounced for low exciton numbers. Above the threshold energy the yrast lines can be roughly approximated by

$$E_{yrast} = ae^{bJ} \qquad (13)$$

where 'a' and 'b' are mass and exciton dependent constants. The behaviour of 'b' is rather smooth but 'a' reveals a strong dependence on the structure of the s.p.l. around the Fermi level which makes a global parametrization of Eq.13 very difficult. The yrast lines are also affected by the Pauli principle which differentiates yrast lines for mixed configurations from those containing only a single type of nucleon. The latter appear to be shifted to lower spins by one or two units.

PARITY DISTRIBUTION

The parity distribution may in principle have a strong impact on the results of statistical model calculations as well as on precompound emission. This is especially true if the population of discrete levels with known spin and parity is of interest.

We have performed combinatorial calculations to investigate this problem in 56Fe and 136Ba. A few typical results of these calculations are presented in Figs.14 and 15. As expected, very strong fluctuations are observed in the case of 56Fe. For the two-exciton configurations oscillations between nearly only positive and nearly only negative parity levels are observed throughout the whole energy range, also on the average, the amplitude of the fluctuations decreases with increasing energy. For 8 exciton levels, the fluctuations are still very striking, at least up to 30 MeV. The results have evidently oscillating character around the equal probability value of 0.5. In fact considering all generated levels, the ratio of positive to negative parity levels is 1 with an uncertainty usually less than 5%. In the case of 136Ba, the results are similar but the fluctuations are far less pronounced. The higher density of s.p.l. with a more uniform parity distribution leads to a nearly constant and equal parity distribution for the levels containing 4 or more excitons. For lower exciton numbers, the fluctuations are still significant though much weaker than for 56Fe.

BOUND STATE DENSITIES

In this section we deal with the configurations which are subject to the restriction that none of the particle type excitons is allowed to occupy any orbital lying above the nucleon binding energy. The particular interest devoted to those states is connected with the multistep compound mechanism as introduced by Feshbach Kerman and Koonin /10/.

Two examples of the combinatorial calculations for the densities of bound states are shown in Fig.16. Some features of the bound state densities are exactly the same as those we have discussed before in the context of unconditional state densities. The fluctuations and the threshold energy, understood as the minimal energy required to excite a given type of configuration, have the same origin and there is no need to discuss them again. There is also no difference as far as the pairing effects are concerned. In the following we will point out therefore only the aspects which result from the condition imposed on the bound states.

Analysing Fig.16, one observes that at a certain energy, the bound state densities begin to deviate from the unconditional exciton state densities and eventually decrease with increasing energy. This effect is more pronounced for low exciton numbers which is related to the energy at which deviations appear. For higher exciton numbers the effects of the restriction of having all particles bound appear at higher excitation energies. In fact, for the 8 exciton configurations in heavy nuclei, they are hardly seen in the energy range covered in our calculations. This suggests, that for configurations containing at least 8 excitons and at energies below about 30 MeV, the restriction can be disregarded in multistep compound calculations not only as far as the state densities are concerned but also with respect to the spin and parity distributions.

Let us now consider implications of the binding condition on the spin distribution. In Fig.17, we compare the spin cut-off factors for bound states with those obtained if all configurations are taken into account. Similar to the state densities the spin cut-off factors also fall below the values calculated when no restriction had been made. To explain this result, we have to recall that the increase of the spin cut-off factor for levels with a fixed exciton number is related to the high spin orbitals which become available when the excitation energy increases. This is however not the case if only bound states are considered. The boundary condition excludes configurations with particles promoted to orbitals above the binding energy and therefore highly excited states can be formed only by deep hole excitations. This involves low spin orbitals close to the well bottom. The high energy bound states are therefore low spin states and this is reflected in the behavior of the spin cut-off factor. Neglecting this energy dependence spin cut-off parameter for bound states may be parametrized by means of Eq.11 with c taking a value around 0.26.

CONCLUSIONS

We have investigated the densities of few quasiparticle states in the frame of the shell-model with the pairing interaction accounted for in terms of the BCS theory. In the method applied, the pairing is explicitly related to the exciton configuration. We consider this the main advantage compared to all other approaches since it allows for a deeper understanding of the pairing interaction effects. The spin, parity and shell effects are also accounted for directly instead of being smeared out by a statistical treatment. Therefore, the results of our combinatorial calculations are well suited for the description of the structure observed at the high end of the particle spectra in high energy resolution experiments, as attempted in Refs.11, and 12. Although we believe that our results constitute a considerable improvement in the accuracy of the description of state densities with a fixed number of excitons, it is worthwhile summarizing several shortcomings inherent in the method. The main ones are the following:

- The neglect of all residual interactions but pairing. In particular, no interaction between protons and neutrons is taken into account.

- The use of the version of the BCS model which does not conserve the number of quasiparticles.

- The use of the blocking method to introduce configuration dependence into the BCS model.

- The use of a constant pairing strength parameter G for all orbitals.

- The inclusion of all orbitals in the summation range in the BCS equations.

- The approximate treatment of promoted pairs.

In addition to these, all uncertainties contained in the basic set of s.p.l. are directly propagated into the results of the combinatorial calculations.

By means of applying the BCS theory to each configuration we could investigate microscopically the role of the pairing correlation in few quasiparticle states. We have found that, in even systems, the pairing shifts the excited states to higher energy and that the ground state condensation energy plays a key role by determining the limit for this shift. For odd systems, we have found that also negative energy shifts are possible. In spite of the complicated nature of the pairing effects, which are related to the nuclear structure and are therefore configuration dependent, it was shown

that the pairing can be reasonably accounted for by a constant energy shift of the Fermi gas results. The value of the required shift is determined by the difference in the excitation energy of the first excited states in the two approaches. This procedure is sufficiently accurate if energy distributions are smooth or the structure can be disregarded.

Our results show that the closed formulae for state densities, as derived from the equidistant model, fail to reproduce the state densities for spherical nuclei, especially at low excitation energies e.g. in the region where preequilibrium emission dominates. This failure is connected mainly with the shell structure in the s.p.l. and may lead to large gaps in the spectra of states with a fixed number of excitons. In even systems these gaps may be further increased due to the pairing interaction. In addition the closed formulae give no provision for the strong fluctuations typical of low exciton numbers, which are the most important for preequilibrium emission. Nuclear deformation is found to remove these discrepancies only partially. In general, closed formulae may be considered accurate enough only for strongly deformed medium-heavy and heavy nuclei.

As far as the spin distribution of few exciton levels is concerned, we have found that the assumption of a Gaussian distribution of spin projections holds for exciton numbers exceeding 3. For lower exciton numbers some deviations are observed. We point out also that the energy dependence of the spin cut-off is related to the s.p.l. sequence and is different from the energy dependence of the spin cut-off factor for the total level density, which is mainly caused by the increasing number of quasiparticles involved in the excitation. Our approximate formulae for the spin cut-off factors are given by Eq.10 or Eqs.11,12 and can be easily applied in preequilibrium calculations. Their average validity can be extended to 2 and 3 exciton configurations if fluctuations are disregarded. We note however that the formulae were derived for the cases containing an approximately equal number of particles and holes and this condition has to be observed in their applications.

An analysis of the parity distribution reveals strong fluctuations in the ratio of the two parities. The fluctuations are reduced with the increase of the deformation, exciton number and mass of the nucleus. No dominance of either parity over a large energy range was observed in contradiction with previous results /13,14/.

The conclusions concerning state densities and pairing effects which we have obtained are found to be valid also for states subject to the restriction of having all excitons bound. An exception must be made for the global trend of the energy dependence in the state density and spin cut-off fac-

blocked orbitals (note that two excitons placed in the same orbital couple to M=0 and contribute with positive parity). The state density $\omega(E,M,\pi)$ is found by counting states with the angular momentum projection M and parity π falling

tor. At a certain energy, the restriction imposed shows up in both quantities causing them to fall below the results obtained when this condition is not imposed. For low exciton numbers this effect is observed at energies slightly surpassing the neutron or proton binding energy. Configurations with higher exciton numbers are less sensitive to the 'binding condition' which, in these cases, turns out to be important only at high excitation energies.

In particular cases it is feasible to perform combinatorial calculations of states with low exciton numbers and to use such realistic state densities in the exciton or hybrid model as well as in the multistep compound approach. Doing this one can not only test the validity of the models more reliably but also investigate the extend to which the structure in the high energy part of the particle and gamma spectra can be interpreted in terms of the preequilibrium models. If this turns out to be successful preequilibrium models might also become a tool for nuclear structure studies.

This work was supported by Ente Nazionale Energie Alternative Contract No. 12498.

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lations, except for very heavy nuclei. For each nucleus considered, a value of the pairing strength parameter G was determined from the mass differences. For this purpose the ground state condensation energies E_o^c for the three neigh-

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free gas value. The excitation energy is calculated however with respect to the BCS ground state energy, which is lower by E_o^c compared to the free gas ground state energy. The first excited state is therefore found at an excitation energy higher by $E_o^c - E_1^c$ then the free gas model predictions.

FIGURE CAPTIONS.

Fig.1 The spectrum of energy shifts induced by the pairing interaction for several even configurations: (1100) in 58Ni and 116Sn and (2200) in 116Sn.

Fig.2 A comparison of the state densities calculated including the pairing interaction (solid lines) with the results of the noninteracting gas model (dashed lines) for (2222) and (1111) configurations in 56Fe. Results of the noninteracting gas model were shifted to make the energy of first excited state coincide with the value obtained when pairing is taken into account.

Fig.3 A comparison of the densities of (2222) configurations in 56Fe, calculated including the pairing interactions (solid line) with the results of calculations in the frame of the noninteracting gas model (dashed line).

Fig.4 The spin cut-off factors for (2200) and (1111) configurations in 56Fe calculated including the pairing interaction (solid lines) and without the pairing interaction (dashed lines). The results of the noninteracting gas model were shifted to make the energy of first excited state coincide with the value obtained when the pairing interaction is included.

Fig.5 The spectrum of energy shifts induced by the pairing interaction for two odd configurations: (0010) in 86Rb and (0021) in 134Cs.

Fig.6 The state densities for some specified configurations in 56Fe calculated with the pairing interaction taken into account.

Fig.7 The densities of 1-particle 1-hole neutron states in 27Al calculated in the space of s.p.s. by Seeger-Howard for different values of the deformation parameter α_2 (histograms). Solid line represents predictions of the formula by Williams with g=A/26.

Fig.8 The same as Fig.7 but for 100Mo.

Fig.9 The same as Fig.7 but for 170Er.

Fig.10 The calculated spin distributions of 4 and 8 quasiparticle levels (histograms) compared with

this pessimistic conclusion we have found that the 4,6 and 8 exciton state and level densities calculated in the frame of the free gas model can be brought into perfect agreement with the results obtained including the BCS if a shift of $E_o^c - E_1^c$ is applied. In other words, the pairing effects on the

the predictions of Eq.9 when σ is taken as a free parameter (lines). The nuclei and configuration types are shown in the figure. For each case, the energies of the levels considered are contained in the 1 MeV interval centered at the depicted energy.

Fig.1

Fig.11 The same as Fig.10 but for the 2 quasiparticle levels in Cr and Pb.

Fig.1

Fig.12 The energy dependence of the calculated spin cut-off factor of the (2222) configurations in 56Fe and 116Sn.

Fig.1

Fig.13 The yrast lines for several configuration types in 58Ni.

Fig.1

Fig.14 The fractions of positive parity states in the (2222) and (0011) configurations in 56Fe as a function of the excitation energy.

Fig.1

Fig.15 The fractions of positive parity states in the (2200) and (1100) configurations in 136Ba as a function of the excitation energy.

Fig.

Fig.16 The bound (dashed lines) and unconditional (solid lines) state densities for the (2222) and (0022) configurations in 58Ni as a function of the energy.

Fig.

Fig.17 The same as Fig.16 but for the spin cut-off factor.

energy. This nucleon blocks an orbital important for the pairing correlation, so that Δ and E_0^C decrease or disappear. In the excited states of 1 exciton structure, this nucleon is moved out from the Fermi energy. The orbitals close to the Fermi level are made available for pair scat-

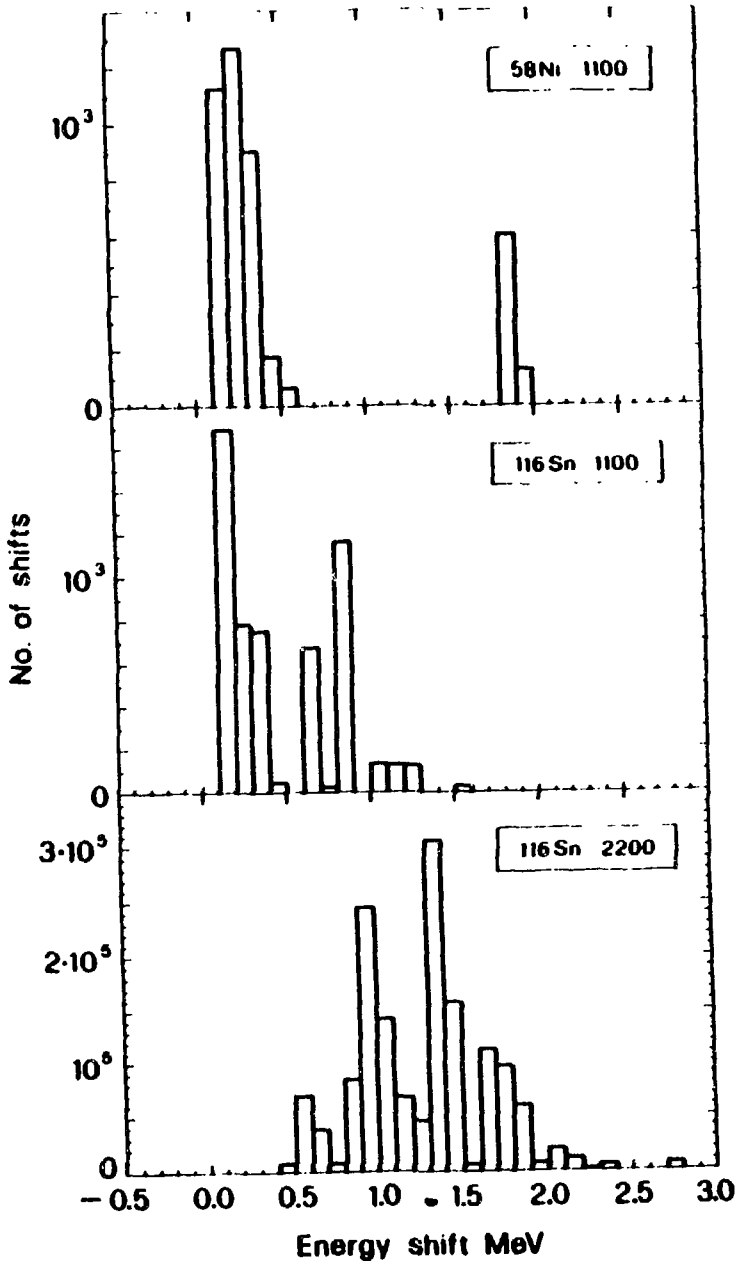


Fig.1

the s.p.l. In spherical nuclei highly nonuniform
feature is reflected in the state and level densities calculated. In Fig.6 we show state densities calculated for several exciton numbers for the even-even nucleus 56Fe. The well known feature of a rapid increase of the state density

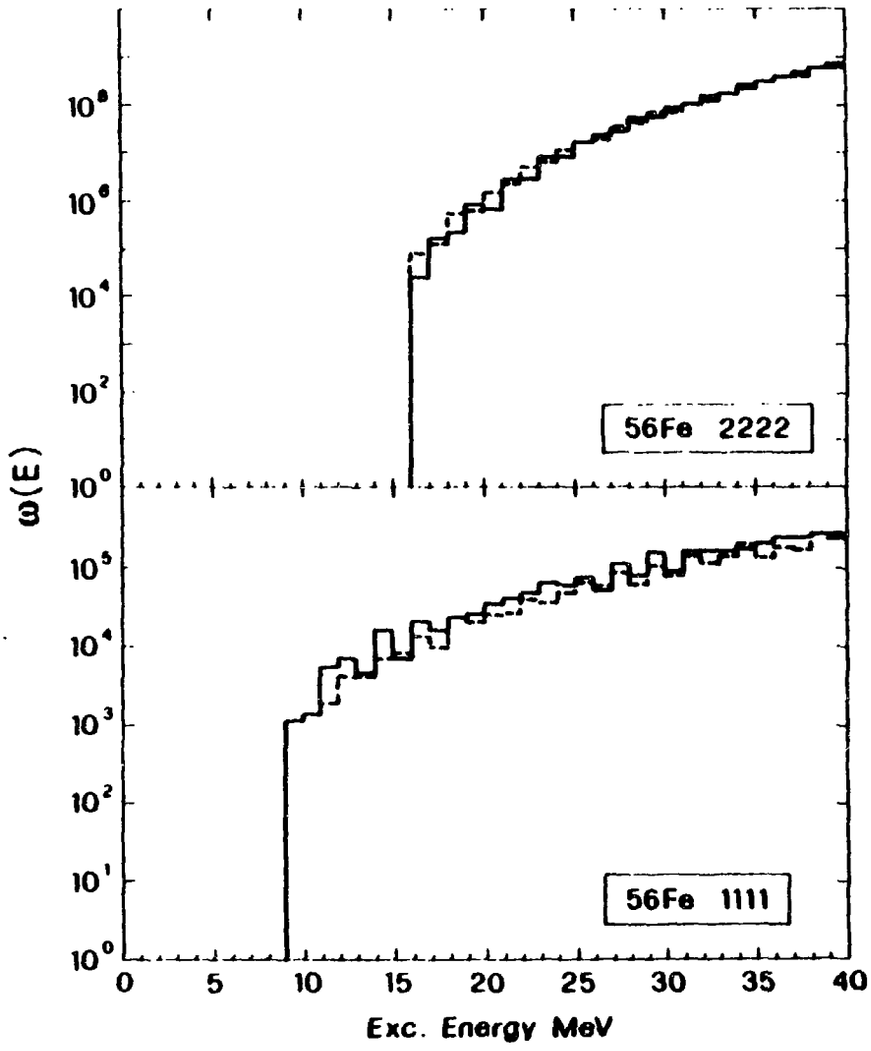
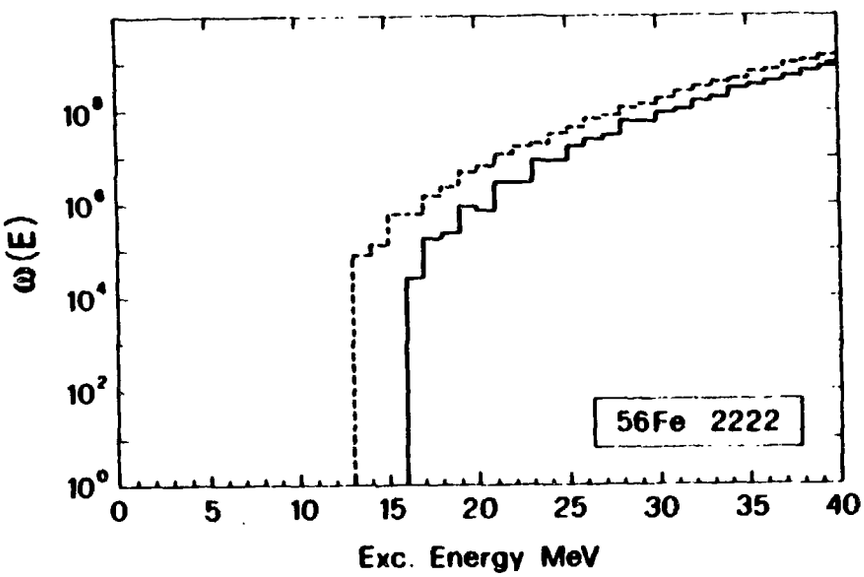


Fig.2

changes in the calculated results. The gaps are partially filled and a remarkable structure of roughly 5 MeV width appears in the spectra. The peak to valley ratio approaches an order of magnitude at low energies and falls down to 4-6 at the end of the energy range, being higher for 100Mo than



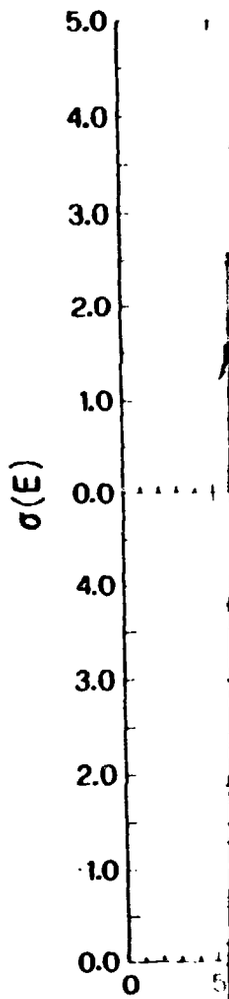


Fig.3

ing the fluctuations.

Two types of energy dependence of the spin cut-off parameter are observed. The first has a 'logarithm like' shape (Fig.12), while is essentially constant or slightly line-

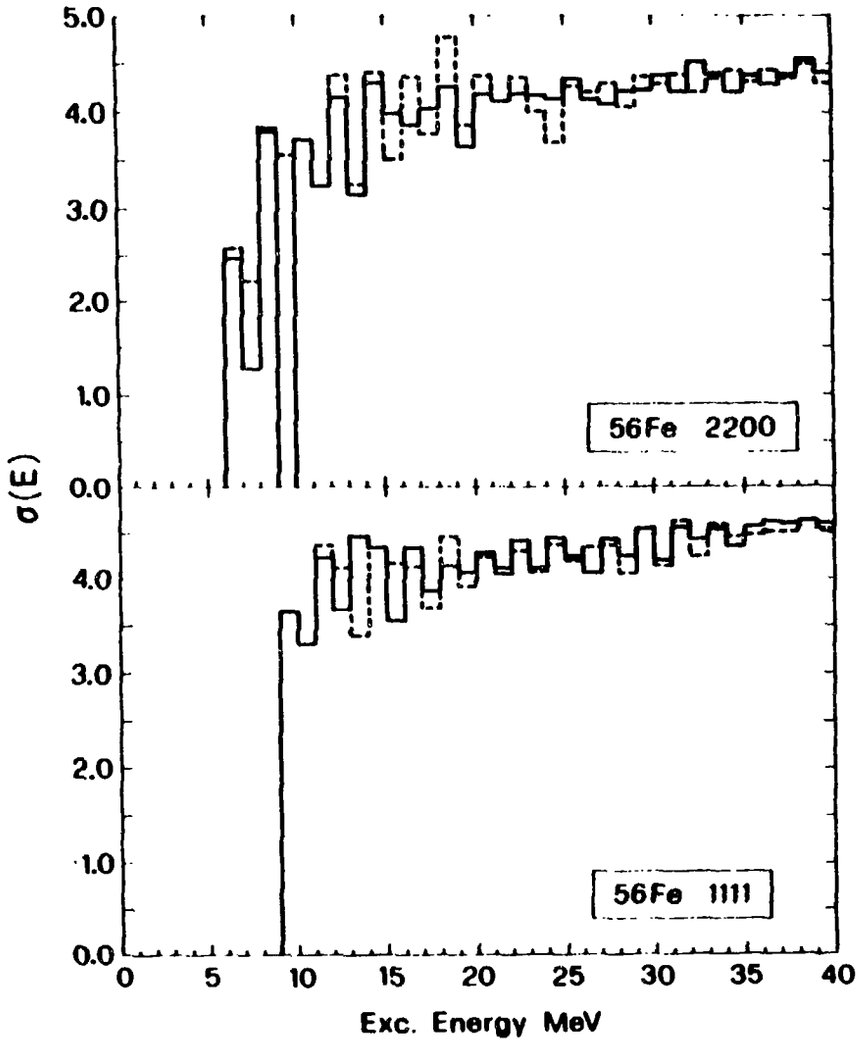


Fig.4

There is a slight odd-even effect, which we have disregarded up to now. We have observed that $\langle \sigma^2 \rangle$ for configurations of the type (1010) are about 5 units higher than $\langle \sigma^2 \rangle$ for the (1100) and (0011) configurations, in spite of the equal number of excitons in each of them. This difference reduces to

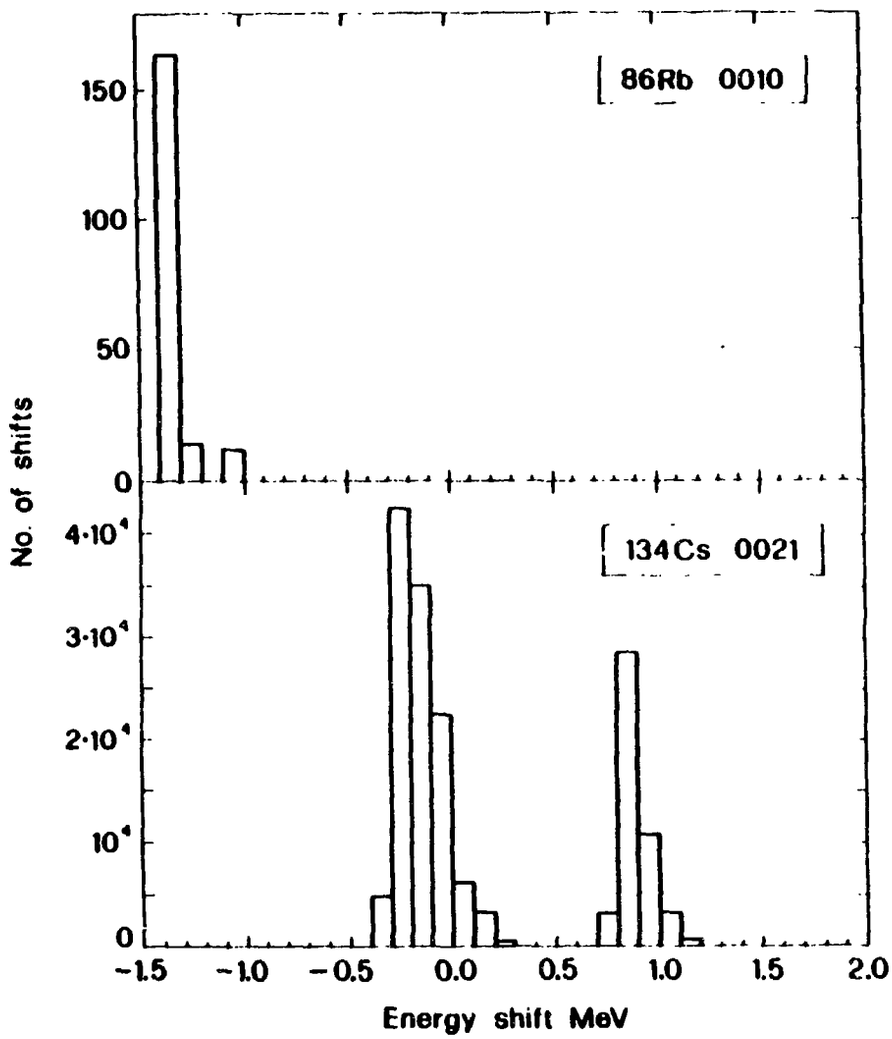


Fig.5

roughly approximated by

$$E_{yrast} = ae^{bJ} \qquad (13)$$

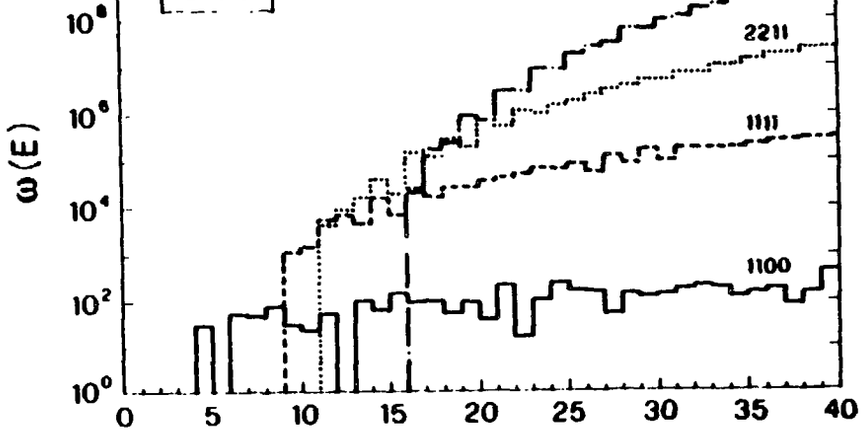


Fig.6

subject to the restriction that none of the particle type excitons is allowed to occupy any orbital lying above the nucleon binding energy. The particular interest devoted to those states is connected with the multistep compound mechanism as introduced by Feshbach Kerman and Koonin /10/.

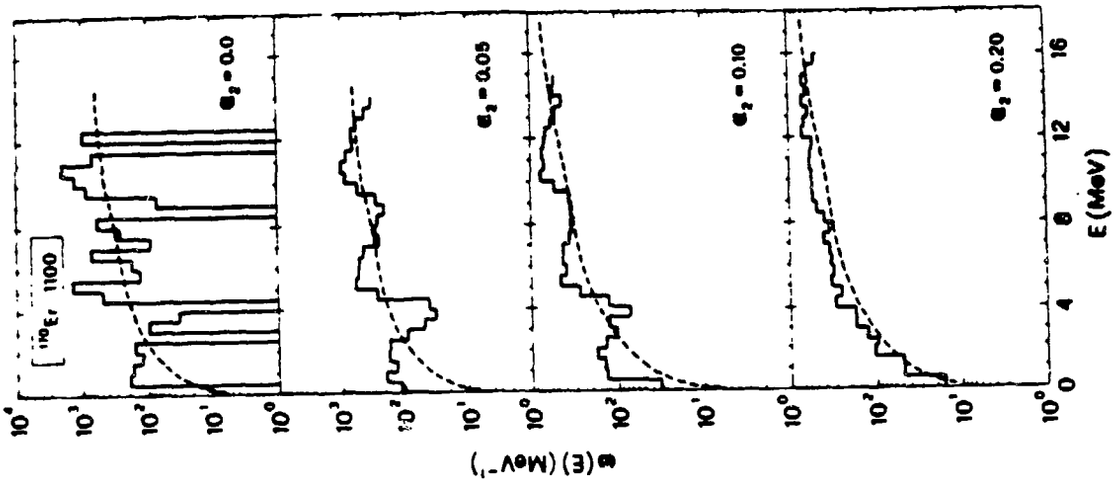


Fig.9

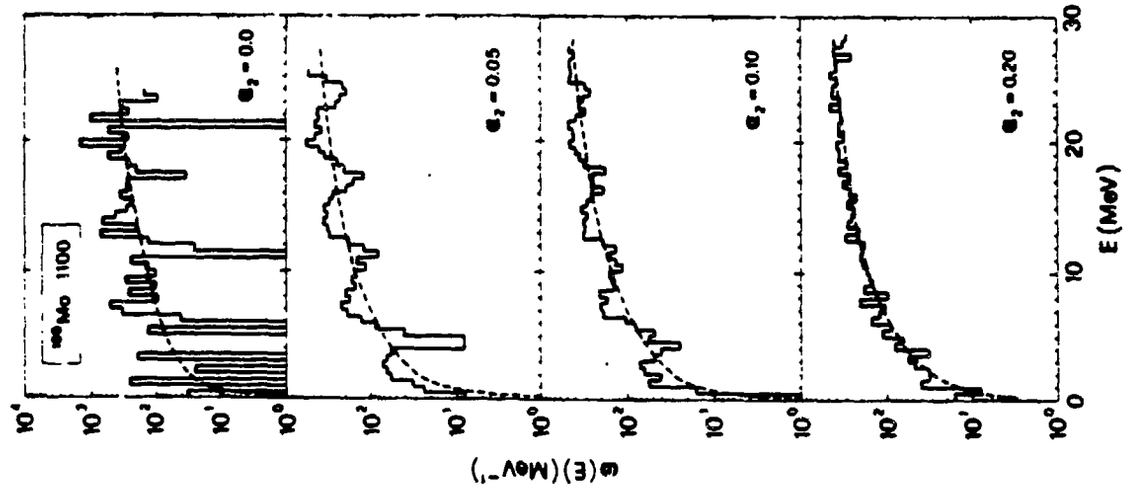


Fig.8

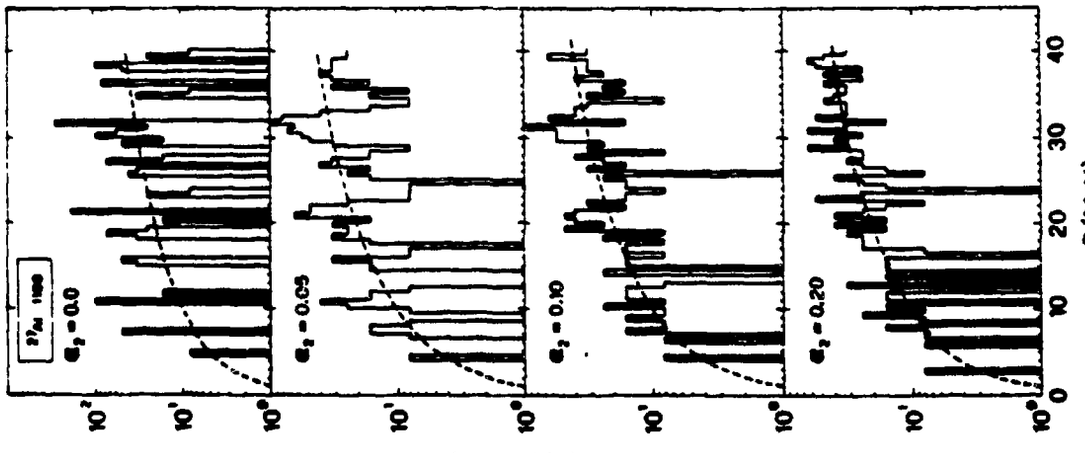


Fig.7

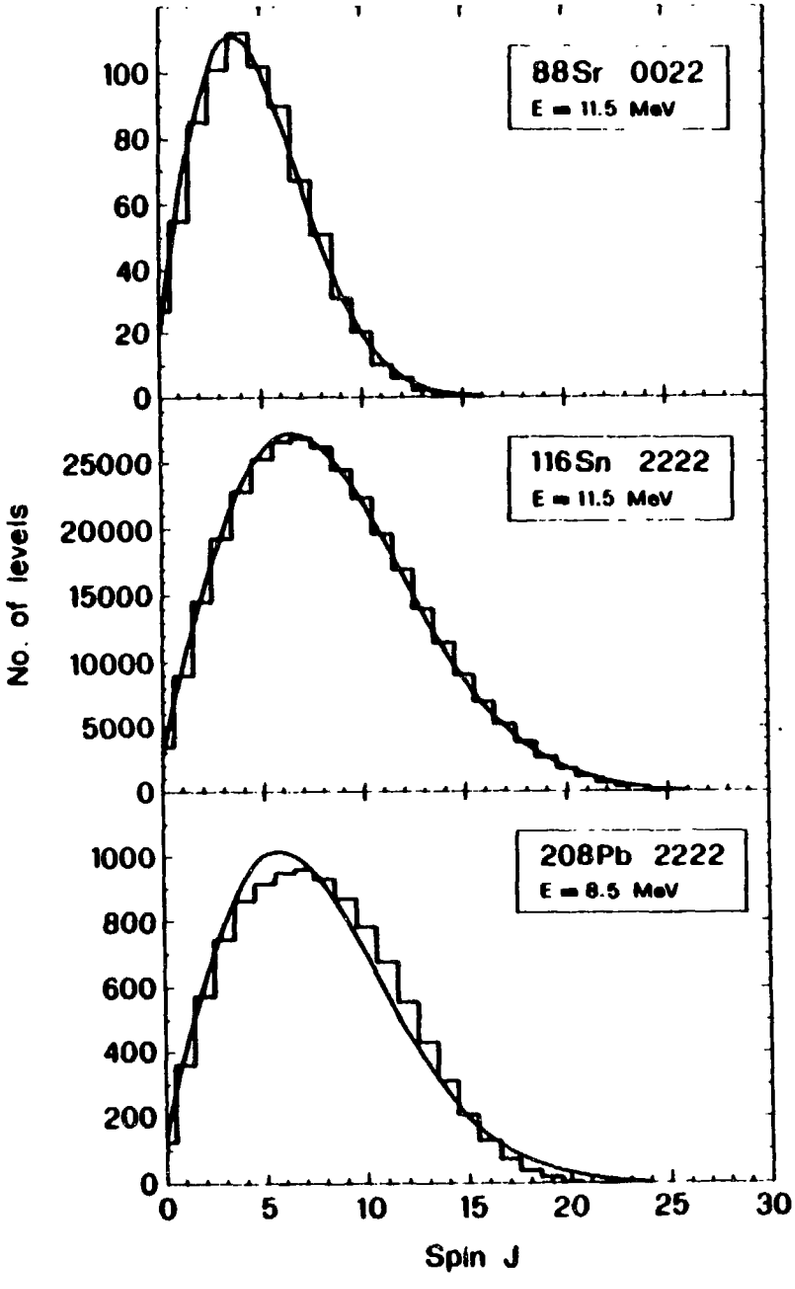

88Sr 0022
E = 11.5 MeV
116Sn 2222
E = 11.5 MeV
208Pb 2222
E = 8.5 MeV
No. of levels
Spin J
0
5
10
15
20
25
30
100
80
60
40
20
25000
20000
15000
10000
5000
1000
800
600
400
200

Fig.10

higher energy and that the ground state [illegible] plays a key role by determining the limit for this shift. For odd systems, we have found that also negative energy shifts are possible. In spite of the complicated nature of the pairing effects, which are related to the nuclear structure and are therefore configuration dependent, it was shown

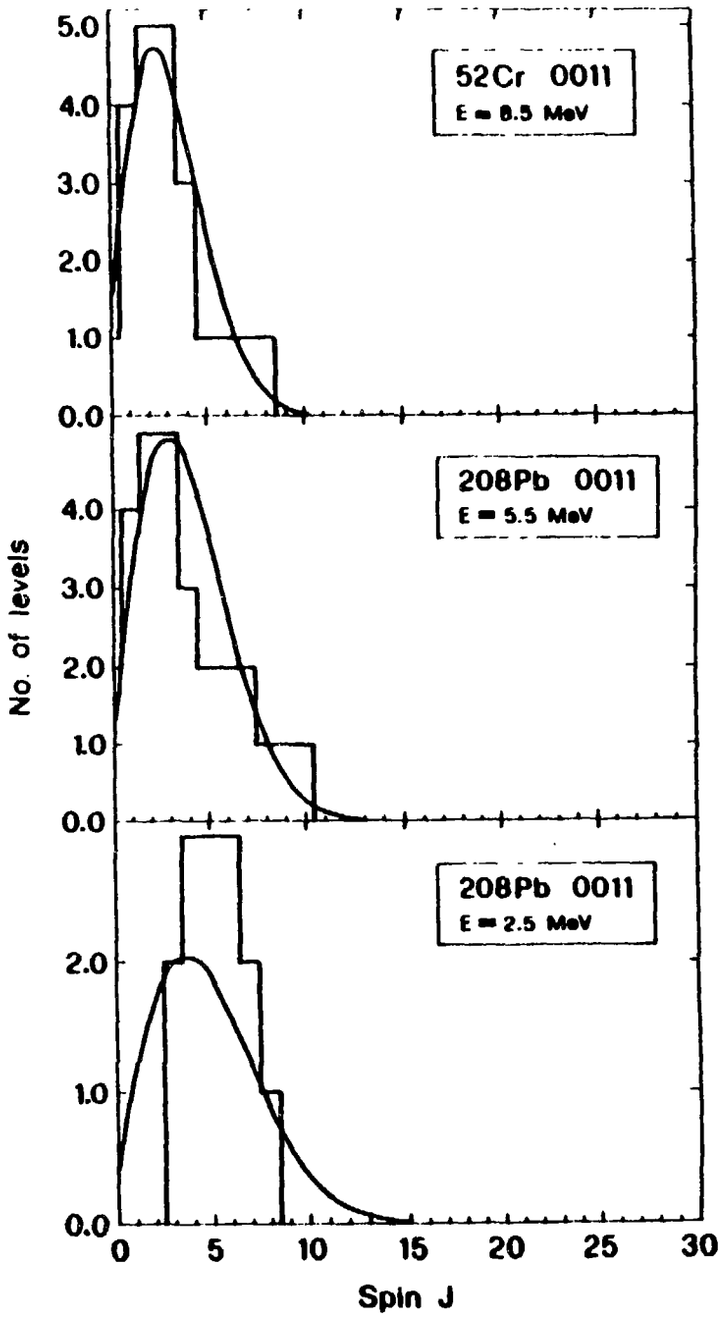


Fig.11

The conclusions concerning state densities and pairing effects which we have obtained are found to be valid also for states subject to the restriction of having all excitons bound. An exception must be made for the global trend of the energy dependence in the state density and spin cut-off fac-

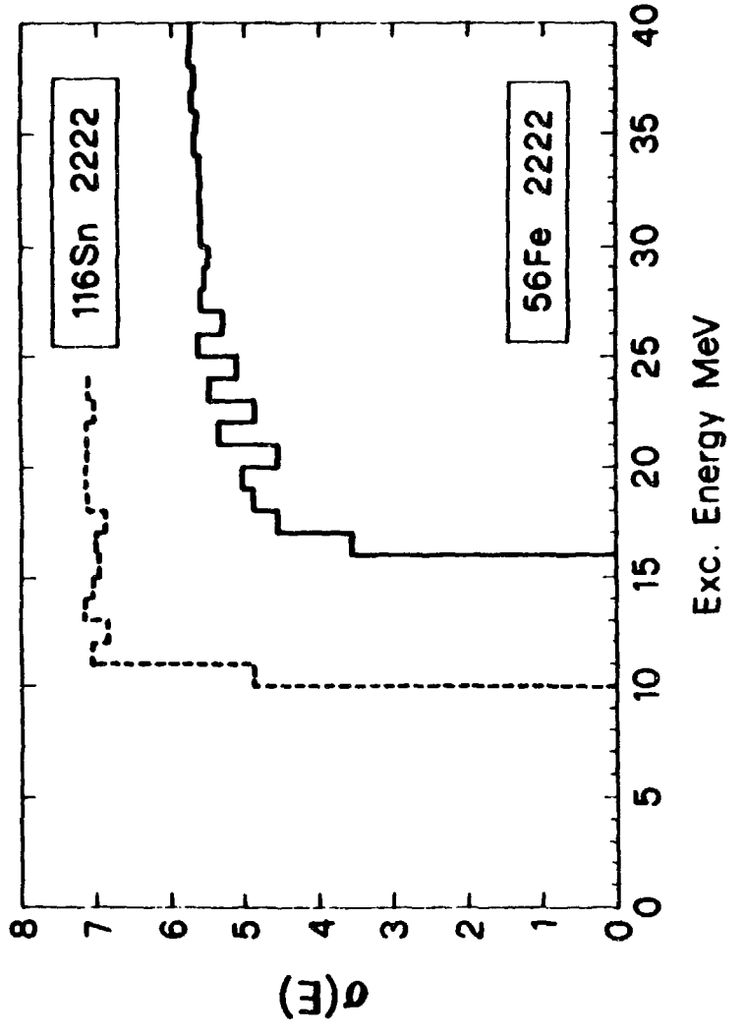


Fig.12

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10. H.Feshbach, A.Kerman and S.Koonin; Ann. of Phys. 125(1980)429.

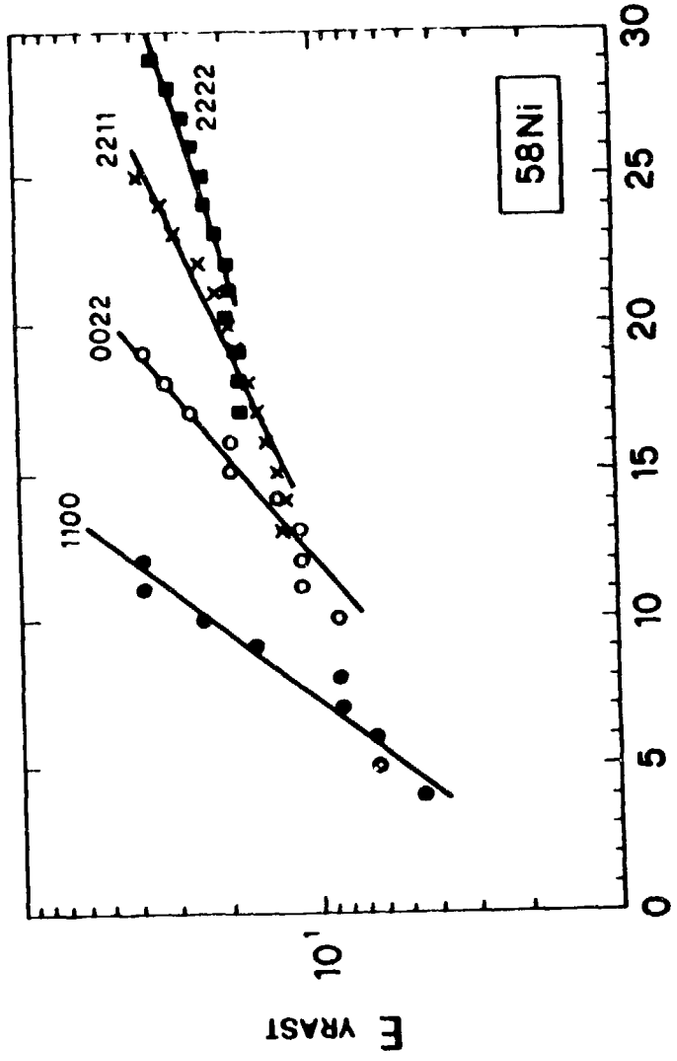

Fig.13

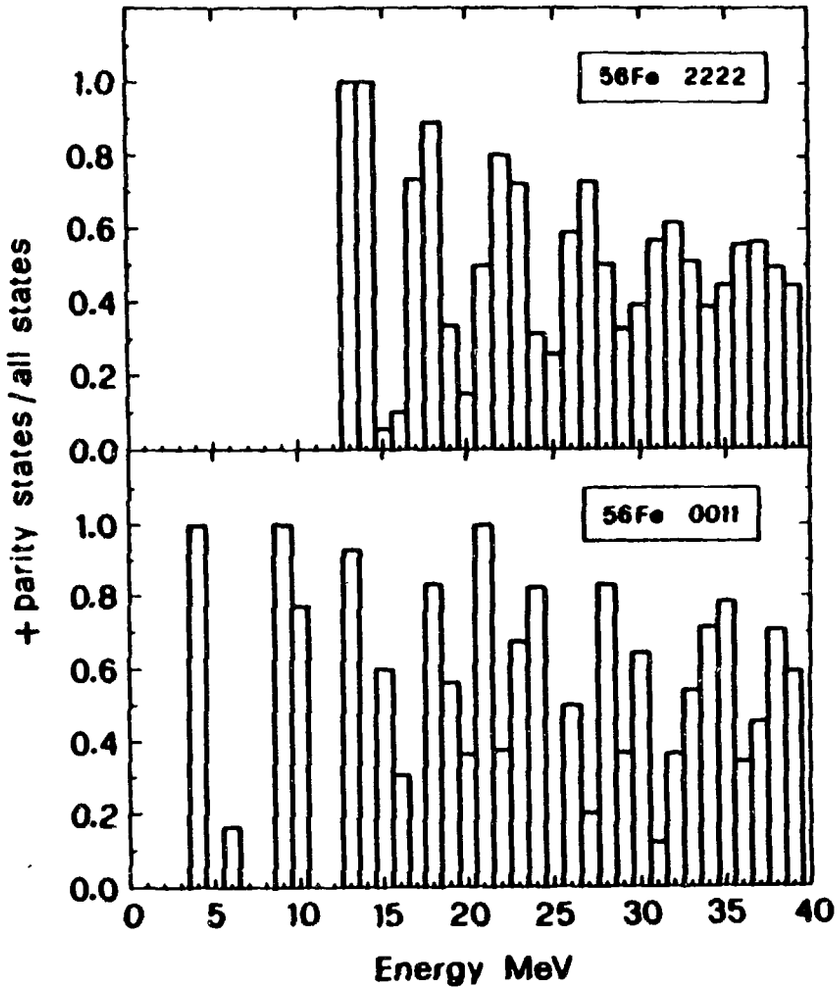
56Fe 2222
56Fe 0011
+ parity states / all states
1.0
0.8
0.6
0.4
0.2
0.0
0
5
10
15
20
25
30
35
40
Energy MeV

Fig.14

Fig.8 The same as Fig.7 but for [illegible]

Fig.9 The same as Fig.7 but for 170Er.

Fig.10 The calculated spin distributions of 4 and 8 quasiparticle levels (histograms) compared with

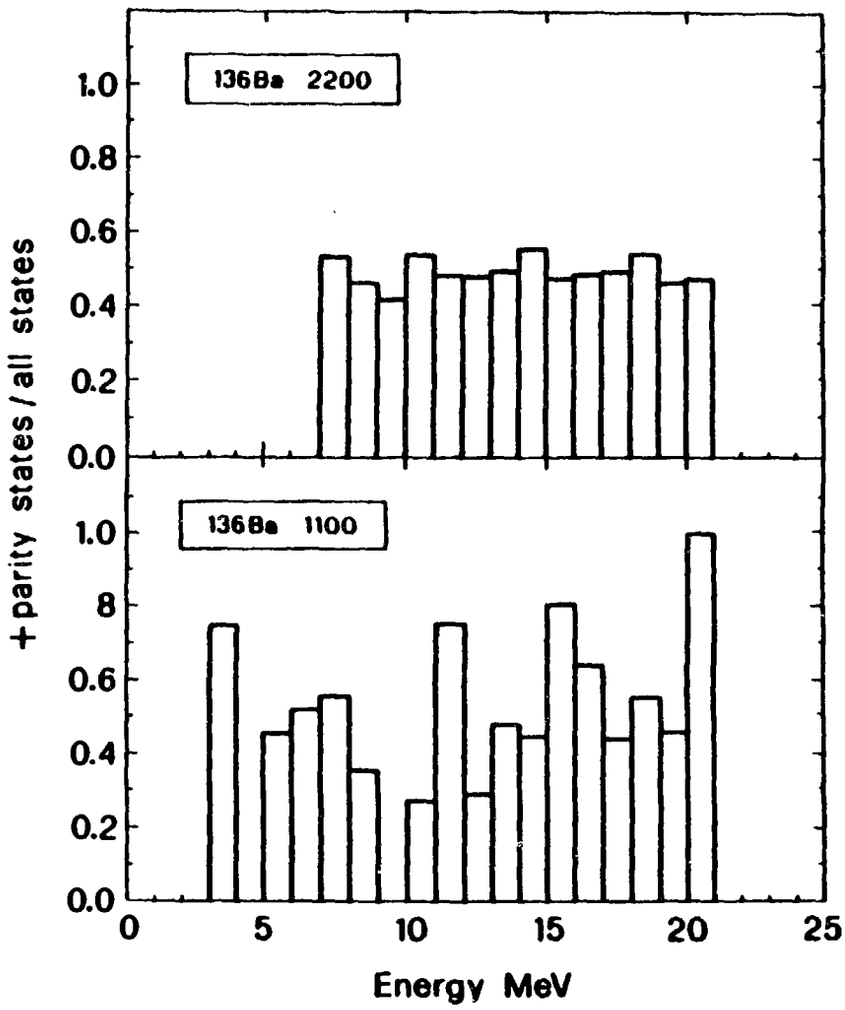

Fig.15

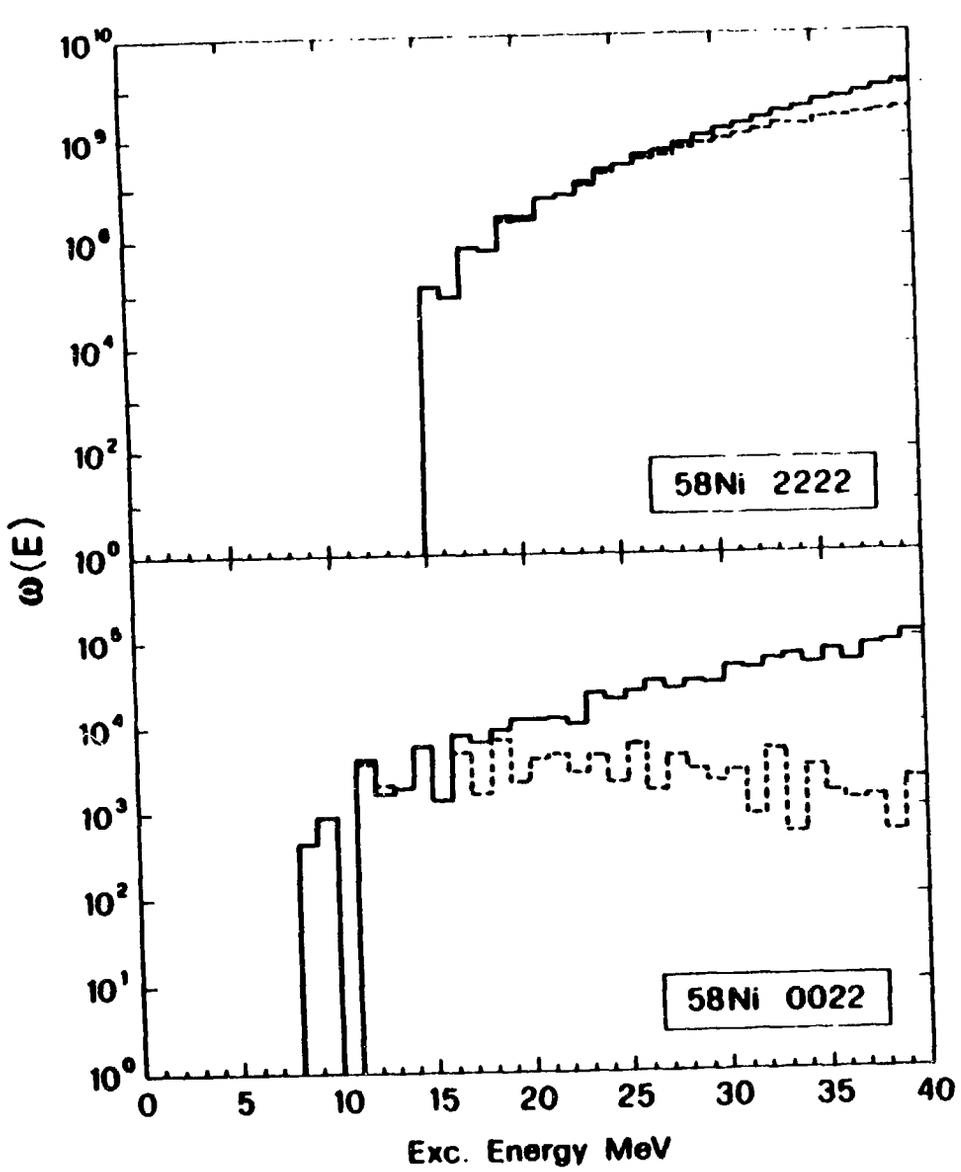

Fig.16

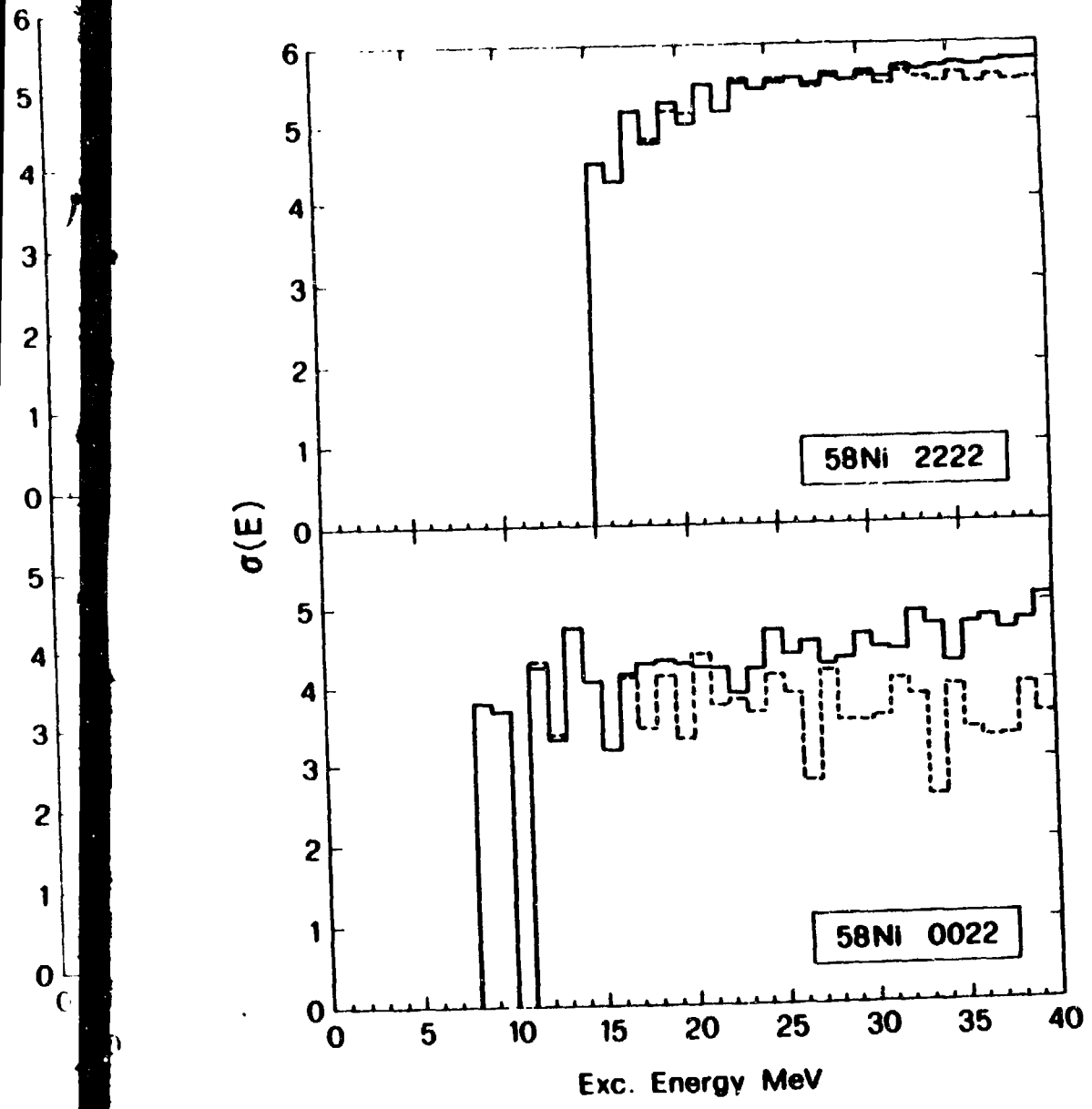

Fig.17

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ENEA

COMITATO NAZIONALE PER LA RICERCA E PER LO SVILUPPO
DELL'ENERGIA NUCLEARE E DELLE ENERGIE ALTERNATIVE

CHAIN OF CODES FOR THE COMBINATORIAL CALCULATION OF LEVEL DENSITIES

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Testo pervenuto nel marzo 1987

SUMMARY

A chain of codes has been developed to calculate state and level densities characterized by fixed exciton numbers. Shell-model orbitals are used as a basis for the calculations and the different configurations possible are generated by use of combinatorial calculations. The pairing interaction is accounted for in the frame of the BCS theory. The spin and parity distributions are provided. For deformed nuclei only state density is calculated.

CONTENTS

1.0 INTRODUCTION

It is well known, that the state density with fixed exciton number is the most uncertain ingredient in various preequilibrium models used so far to calculate nuclear reactions. The presently available level density approaches are affected by uncertainties which are too large with respect to the need of accuracy recognized in many cross section calculations for basic studies and technology. In particular pairing effects and parity distributions are not yet completely settled and call for improvement.

This chain of codes is thought to provide the possibility of direct counting of the levels with fixed number of excitons so that at least part of the usually made assumptions (equidistant single particle levels, saddle point approximation, no residual interactions) can be dropped. To this end combinatorial calculations seem to be best suited. The codes described in this report generate all possible configurations for selected number of excitons within the set of shell-model orbitals. For each configuration the energy, spin projection M and parity is determined. The configurations generated, each of them representing several states, are sorted according to the excitation energy to obtain state densities.

The chain consists of two main codes ICAR and CONV ~~which perform entirely the calculations and of an additional one RESULT for further~~ processing of the results.

Code ICAR executes the combinatorial calculations for neutron or proton type of excitons. The calculations can be done with or without pairing interaction. Calculations can be restricted to bound states only to obtain densities used in statistical multi step compound model of Feshbach, Kerman and Koonin.(1) An option for the calculation of the pairing strength parameter G from the experimental mass differences is provided. ICAR can be used also for the determination of the BCS properties of the ground state and of the first excited state only. Results of ICAR for neutron and proton gas are convoluted by CONV code to obtain mixed configurations containing neutron and proton type of excitons. Performing this convolution no interaction between neutrons and protons is assumed.

~~RESULT code is devoted to final analysis of results obtained with ICAR and CONV~~.

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(1) H.Feshbach, A.Kerman and S.Koonin; Ann. of Phys. 125(1980)429.

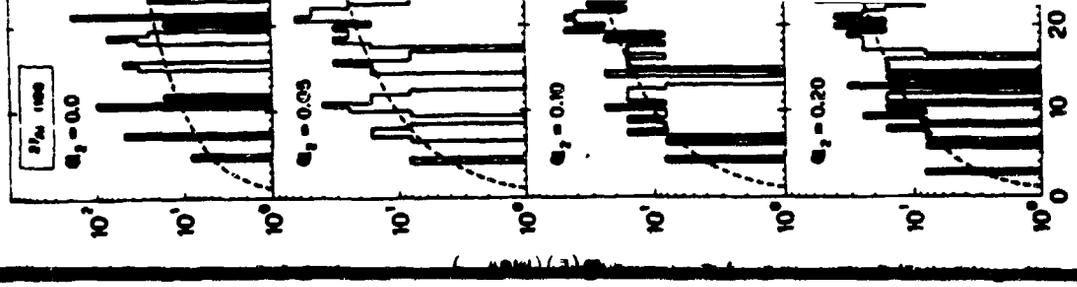

Fig.

2.0 THE MODEL

We define an exciton of 'particle' type as the unpaired particle above the Fermi energy and exciton of 'hole' type as the unpaired particle below the Fermi energy. For this purpose the Fermi energy is defined as the energy of the last occupied orbital in the ground state of the nucleus. In order to take into account states with two excitons in the same orbital two nucleons are allowed to occupy the same orbital without loosing their 'exciton' character e.g. being treated as an noninteracting pair.

Each configuration of n excitons represents a set of nuclear states and may be described by n numbers denoting subsequent occupied orbitals. If orbitals (each of which can hold two particles) are enumerated from the bottom of the well and the Fermi level is i_F, each configuration β of n_h hole and n_p particle excitons can be written as

$$C^{\beta}_{n=n_p+n_h} = (i^h_1,..,i^h_h,\ i^p_1,..,i^p_{n_p}) \qquad (1)$$

where $1 \leq i^h_j \leq i_F$ and $i_F < i^p_j \leq n_{max}$

n_{max} being number of orbitals accounted for. To fulfill the Pauli principle the same pointer may appear only twice (this representing noninteracting pair). In addition permutation of pointers must be avoided since due to the indistinguishibility of particles each permutation represents the same set of states.

Total energy of each configuration is determined basing on the superconductivity theory. The simplified version by Wahlborn[2] is used. Configuration dependence is introduced into the BCS by the blocking method. Accordingly for each generated configuration a set of two BCS equation is solved.

$$\sum_i{}' \ 2\,V^2_{i\beta} = n \qquad (2)$$

$$\sum_i{}' \ \frac{1}{\sqrt{(\epsilon_i - \lambda_\beta)^2 + \Delta^2_\beta}} = \frac{2}{G} \qquad (3)$$

---

2. S.Wahlborn; Nucl. Phys. 37(1962)554.

where

$$V_{i\beta}^2 = \frac{1}{2}\left(1 - \frac{\epsilon_i - \lambda_\beta}{\sqrt{(\epsilon_i - \lambda_\beta)^2 + \Delta_\beta^2}}\right) \qquad (4)$$

here ϵ_i are shell-model orbital energies, η stands for number of paired nucleons and λ_β and Δ_β are the Fermi energy and correlation function which are to be determined. The prime superscript indicates that summation in eqs.2 and 3 is taken over all unblocked orbitals only. λ_β and Δ_β are found by minimization of the sum of two squared BCS equations. Each configuration enters BCS equations trough the blocking, which removes orbitals occupied by unpaired nucleons from the summations in eqs.2 and 3. Thus for each configuration solution of BCS equations should be in principle repeated. For spherical nuclei the advantage of orbital energy degeneracy is taken. When next considered configuration differs from the preceding one only by the displacement of the exciton within the same subshell, solution of BCS equations is not needed.

The total configuration energy according to BCS model reads:

$$E_\beta = \sum_j \epsilon_j + \sum_i{}' \left(1 - \frac{\epsilon_i - \lambda_\beta}{\sqrt{(\epsilon_i - \lambda_\beta)^2 + \Delta_\beta^2}}\right)\epsilon_i - \Delta_\beta^2 / G \qquad (5)$$

where the first summation includes only blocked orbitals. Excitation energy is calculated in turn as the difference between total energy of a configuration and total energy of the ground state.

For some configurations it is not possible to find real solutions for the two BCS equations. In these cases it is assumed that pairing correlation disappears and total energy is calculated according to the free gas model.

The total spin projection M is obtained summing over the spin projections m_i of all blocked orbitals. Because of the double degeneracy of orbitals one configuration, as defined by eq.1, corresponds to the set of nuclear states. Accordingly all possible combinations of m_i signs giving rise to the total M are accounted for and values up to M=30 are considered. Parity of each state is determined as a product of the parities of the blocked orbitals. To avoid edge effect, at first, results are sorted into 0.1 MeV energy bins, providing n-exciton state densities $\omega_n(E,M)$, which will be later convoluted. Final results are averaged over 1 MeV

intervals to reduce fluctuations. Spin cut-off factors are calculated from the definition

$$\sigma_n^2 = \langle M^2 \rangle = \sum M^2 * \omega_n(E,M)/\omega_n(E) \qquad (6)$$

where $\omega_n(E)$ stands for state density summed over spin projections M. For spherical nuclei also n-exciton level density $\rho_n(E,J)$ is calculated according to well known relation

$$\rho_n(E,J) = \omega_n(E,M=J) - \omega_n(E,M=J+1) \qquad (7)$$

In order to obtain also mixed configurations, state densities for neutrons and protons are convoluted, before level density calculation. The energy of mixed configuration is taken to be a simple sum of energies of the two convoluted configurations, since no interaction between protons and neutrons is assumed. Under this approximation state density for mixed configurations can be written:

$$\omega_{p,h}(E,M) = \sum_{\substack{M_p,M_h \\ M_p+M_h=M}} \int_0^E \omega_p(E_p,M_p) * \omega_h(E-E_p,M_h)\,dE_p \qquad (8)$$

Spin projection of the mixed configuration is just a sum of spin projections of the configurations convoluted. Similarly parity product defines parity of the mixed configuration.

The finite number of orbitals taken into account limits the maximum energy which can be calculated. This limit is defined by the excitation energy of the configuration consisting of only one exciton promoted to the highest orbital. In practice this limit is increased by 20%, hoping that loss of states at this energies is still acceptable.

3.0 ICAR CODE

Code ICAR performs state and level density calculations for a specified type of nucleons. Calculations can be executed in terms of free gas model or in the frame of BCS formalism to account for the pairing interaction. In both cases it is possible to restrict calculations to orbitals lying below binding energy e.g. to calculate density of bound states in the spirit of multistep compound model.

At the beginning code calculates properties of the ground state, such as correlation function, chemical potential, total energy and condensation energy. Next all possible configurations of n excitons within the adopted orbitals are generated by means of combination enumeration algorithm due to Liu and Tang as modified by Payne and Ives[3]. For each configuration BCS equations are solved by means of minimization routine MINSQ taken from Harwell library. Then the energy of configuration is calculated. Parities and spin projections M of the states represented by the configuration are determined. Each state is so characterized by its energy, spin projection and parity and is stored, giving rise to the increase of the proper element of DMN(E,M,π) matrix. Because of the symmetry of spin projection distribution states with positive and negative values of M are stored in the same element of DMN matrix.

When all configurations are generated the code prints out the spectrum of CHI**2 values for BCS solutions which were abnormally terminated. The spectrum of energy shifts is also provided. These are the differences between the configuration energy calculated in terms of BCS and the energy of the same configuration in free gas model. Results of state and level density calculations along with the spin cut-off factors are printed first for positive and next for negative parities. Finally the energy averages and energy dependence analysis of spin cut-off is given. At the end a summary of the results is printed.

Code ICAR provides also additional options which allow for the determination of the pairing strength parameter G and for quick runs limited to the calculation of the properties of the ground and first excited state. These options are to be run interactively at the terminal and when they are selected computer will ask selfexplanatory questions for the required input data. If G search option is chosen code will calculate the difference of condensation energies among three neighbouring nuclei, as defined by Nemirovsky and Adamchuk[4], and return it as 'pairing energy' which is to

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3. W.H.Payne and F.M.Ives; Amc. Trans. of Math. Soft. 5,2(1979) p.163

be compared against experimental value (Ref.4 for example). If no good agreement is obtained a new value of G should be entered for further iterations untill desired order of accuracy is reached.

Results for state density calculations are written unformatted onto file/unit 21.This file must be allocated before execution and kept since it is used afterwards by CONV code to convolute neutron and proton state densities to obtain mixed neutron and proton configuration density.

To facilitate final analysis of the calculations, results are written onto the file/unit 23 (formatted). Allocation of this data set should be done in the way which ensures end-of-file position of the file to avoid overwriting of the previous results. Data set 23 is to be processed with code RESULT.

The calculation time depends very strongly on the number of excitons considered and on the number of orbitals taken into account. Dependence on the mass number of the nucleus is less pronounced. Typical running times for 114 orbitals with pairing interaction accounted for are: 7 sec. for 2 excitons, 200 sec. for 3 excitons and around 3000 sec. for 4 excitons, when a spherical nucleus is considered. For deformed nuclei these values are to be increased approximately by a factor of 4.

3.1 LIST OF FUNCTIONS AND SUBROUTINES IN ICAR CODE

SMAT -returns chemical symbol of a nucleus.

CONFIG -controls configuration generation, BCS solution and energy determination; calculates parity and spin projection of the states. Configurations with only one exciton in an orbital are considered.

CONFIP -the same as CONFIG but considerations are restricted only to the excitons remaining after the exclusion of those placed in the same orbital, which are treated in the main code.

FCN -calculates squares of two BCS equations.

ENER -calculates energy of the configuration.

PNXCB -generates exciton configurations.

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4. P.E.Nemirovsky and Yu.V.Adamchuk; Nucl. Phys. 39(1962)551

MINSQ -minimizes sum of squares of two BCS equations.

VD01A -internal subroutine called by MINSQ

In addition to the routines listed above the code contains a number of plot routines which are described in the listing of the code.

3.2 INPUT FOR ICAR CODE

IA,IZ,LVN,LVP,GI,NP,NH,KIND,KRO,KX8,BE,EOG,IPLO unformatted

IA -A of nucleus

IZ -Z of nucleus

LVN -number of neutron orbitals to be used in calculations (typically 114)

LVP -number of proton orbitals to be used in calculations (typically 114)

GI -pairing force strength parameter multiplied by A .

NP -number of excitons of 'particle type'

NH -number of excitons of 'hole type'

KIND -1 for neutrons

2 for protons

KRO -0 for density calculations

1 for G search and/or for only ground and first excited state calculations

2 grid search for G

KX8 -0 for calculations from shell model orbitals

8 for calculations in equidistant orbitals approximation for which spacing is determined as the energy of the highest orbital considered divided by the number of the orbitals LVN or LVP

BE -if greater than 0 density of bound states is calculated

EOG -if greater than 0 orbitals are taken to be equidistant with EOG spacing

IPLO -0 plots of state density, level density, spin cut-off and BCS energy shifts are drawn for both parities

1 no plots are drawn

2 the same as IPLO=0 but plots of spin distributions for internally selected energies are drawn in addition

Nilsson model orbitals, deduced from the properly deformed potential, must be provided as input file/unit 09. The data set has to be organized as following:

1. card which specifies nucleus and contains Z, N and A numbers (FORMAT(3I10)). This card may be left blank if a general set of s.p. levels is used.

2. card which specifies number of neutron s.p. levels NLVN (FORMAT(I10)). If blank default value of 315 is taken.

3. NLVN cards each of them containing energy, spin projection and parity (1. or -1.) of s.p. neutron level. Cards must be ordered according to increasing energy. (FORMAT(E15.5,F10.1,F5.0)).

4. card which specifies number of proton s.p. levels NLVP (FORMAT(I10)). If blank default value of 286 is taken.

5. NLVP cards each of them containing energy, spin projection and parity (1. or -1.) of s.p. proton level. Cards must be ordered according to increasing energy. (FORMAT(E15.5,F10.1,F5.0)).

4.0 CONV CODE

The code CONV convolutes neutron and proton state densities providing state and level densities as well as spin cut-off factors for mixed configurations. It requires allocation of files/units 21 and 22 which contain results calculated with ICAR code and written by ICAR on file/unit 21. ~~In order to keep CONV results for further processing, file/unit 22 must be allocated (the same as for ICAR).~~

The code checks if the data contained on the allocated files are consistent for convolution. Cases where convolution of different nuclei or of the same type of gas are attempted will be rejected.

CONV has no input except files 21 and 22
Input for CONV is unformatted and consists of only one control variable which ~~should be set to 0~~ if plots are required ~~or to 1~~ if they are to be omitted.

Calculation time for CONV code is of the order of few seconds.

Fig.17

6.0 SAMPLE CALCULATIONS WITH ICAR CODE

The sample calculations for 1 particle 1 hole configurations of neutron type in 93Nb are given. The nucleus is assumed to be spherical, and so energy degenerated orbitals are used. For the set of 114 orbitals used in the present calculations, value of 12.24 was determined for pairing force strength parameter multiplied by mass number A.

The input for the case considered reads:

93 41 114 114 12.24 1 1 1 0 0 0 0 0

The output of calculations begins with the heading and input data which identify a run. The shell model orbitals, as used in calculations, are also printed. Then ground state characteristics are given.

If exciton number is lower than 3, each solution of BCS equations is printed. The table contains position of the particle and hole in respect to the Fermi level (MNEW and MNEH respectively), correlation function (DEL), chemical potential (LAM), CHI**2 for a solution (FF), BCS configuration energy (EC) and energy of the configuration calculated in terms of free gas model (ECF). Here only small part of this table is reproduced.

After generation of configurations is completed, statistic for all the BCS solutions is given. It is followed by a histogramme of energy shifts caused by pairing interaction. The 'energy gap', which is printed after, is the energy at which first state appears in calculations.

Finally two tables of state and level densities for positive parity and next two for negative parity are found. These tables have the same structure. In each line energy, state (or level) density, spin cut-off and number of states (or levels) of given M (or J) are printed. Spin or M dependent densities are ordered according to increasing value of J (or M), starting with the smallest possible value of 0 or 1/2. The second half of the table, containing states of high J or M (15 to 29 or 31/2 to 59/2), is printed below. After each table with level density spin cut-off factor analysis is given. In the case of negative parity it is however preceeded by the table which contains the relative contributions of positive parity states to the total state density for the energies considered.

At the end most important results are summarized on one page.

NUCLEUS 93NB 1100

114 NEUTRON OR 114 PROTON LEVELS TAKEN INTO ACCOUNT
G= 0.13161 CORRESPONDS TO 12.24/A
1 PARTICLES 1 HOLES CONFIGURATIONS

1	11.710	0.500	1.	2	18.159	0.500	-1.	3	18.159	1.500	-1.	4	22.234	0.500	-1.	5	25.135	0.500	1.
6	25.135	1.500	1.	7	25.135	2.500	1.	8	28.355	0.500	1.	9	30.092	0.500	1.	10	30.092	1.500	1.
11	32.220	0.500	-1.	12	32.220	1.500	-1.	13	32.220	2.500	-1.	14	32.220	3.500	-1.	15	35.678	0.500	-1.
16	35.678	1.500	-1.	17	37.684	0.500	-1.	18	37.684	1.500	-1.	19	37.684	2.500	-1.	20	38.020	0.500	-1.
21	39.269	0.500	1.	22	39.269	1.500	1.	23	39.269	2.500	1.	24	39.269	3.500	1.	25	39.269	4.500	1.
26	43.077	0.500	1.	27	43.077	1.500	1.	28	43.077	2.500	1.	29	45.101	0.500	1.	30	45.101	1.500	1.
31	45.101	2.500	1.	32	45.101	3.500	1.	33	45.451	0.500	1.	34	46.296	0.500	-1.	35	46.296	1.500	-1.
36	46.296	2.500	-1.	37	46.296	3.500	-1.	38	46.296	4.500	-1.	39	46.296	5.500	-1.	40	46.317	0.500	1.
41	46.317	1.500	1.	42	50.477	0.500	-1.	43	50.477	1.500	-1.	44	50.477	2.500	-1.	45	50.477	3.500	-1.
46	52.307	0.500	-1.	47	52.307	1.500	-1.	48	52.307	2.500	-1.	49	52.307	3.500	-1.	50	52.307	4.500	-1.
51	52.472	0.500	1.	52	52.472	1.500	1.	53	52.472	2.500	1.	54	52.472	3.500	1.	55	52.472	4.500	1.
56	52.472	5.500	1.	57	52.472	6.500	1.	58	53.286	0.500	-1.	59	53.286	1.500	-1.	60	54.303	0.500	-1.
61	54.303	1.500	-1.	62	54.303	2.500	-1.	63	54.926	0.500	-1.	64	58.150	0.500	1.	65	58.150	1.500	1.
66	58.150	2.500	1.	67	58.150	3.500	1.	68	58.150	4.500	1.	69	58.663	0.500	1.	70	58.663	1.500	1.
71	58.663	2.500	1.	72	58.663	3.500	1.	73	58.663	4.500	1.	74	58.663	5.500	1.	75	58.998	0.500	-1.
76	58.998	1.500	-1.	77	58.998	2.500	-1.	78	58.998	3.500	-1.	79	58.998	4.500	-1.	80	58.998	5.500	-1.
81	58.998	6.500	-1.	82	58.998	7.500	-1.	83	62.109	0.500	1.	84	62.109	1.500	1.	85	62.109	2.500	1.
86	62.436	0.500	1.	87	62.436	1.500	1.	88	62.436	2.500	1.	89	62.436	3.500	1.	90	64.350	0.500	1.
91	64.490	0.500	1.	92	64.490	1.500	1.	93	65.300	0.500	-1.	94	65.300	1.500	-1.	95	65.300	2.500	-1.
96	65.300	3.500	-1.	97	65.300	4.500	-1.	98	65.300	5.500	-1.	99	65.322	0.500	-1.	100	65.322	1.500	-1.
101	65.322	2.500	-1	102	65.322	3.500	-1.	103	65.322	4.500	-1.	104	65.322	5.500	-1.	105	65.322	6.500	-1.
106	65.375	4.500	1.	107	65.375	1.500	1.	108	65.375	0.500	1.	109	65.375	5.500	1.	110	65.375	2.500	1.
111	65.375	6.500	1.	112	65.375	7.500	1.	113	65.375	8.500	1.	114	65.375	3.500	1.				

NUCLEUS IS TREATED AS SPHERICAL
FREE GAS ENERGY= 1649.866
28
FREE GAS FERMI ENERGY= 43.077

GROUND STATE BCS SOLUTION CHI SQ - .3800E-06
NEUTRON GR. STATE
ENERGY= 1648.393 DELTA= 0.92128E+00 LAMBDA= 0.42596E+02
CONDENSATION ENERGY= 1.472
MAXIMUM ENERGY TO BE CONSIDERED IS 22.3

FIRST EXC. STATE OF FREE GAS WITH PAIR EXCITATIONS EXCLUDED 2.024

MNEW=	2	MNEH=	2	DEL=	.37127E-02	LAM=	42.439	FF=	.10281E-07	EC=	3.50 ECF= 2.02
MNEW=	2	MNEH=	4	DEL=	.79251	LAM=	42.694	FF=	.34258E-06	EC=	6.05 ECF= 5.83
MNEW=	2	MNEH=	9	DEL=	.80746	LAM=	42.688	FF=	.35782E-06	EC=	7.29 ECF= 7.08
MNEW=	2	MNEH=	10	DEL=	.81040	LAM=	42.686	FF=	.11089E-08	EC=	7.63 ECF= 7.42
MNEW=	2	MNEH=	13	DEL=	.82170	LAM=	42.681	FF=	.30229E-07	EC=	9.61 ECF= 9.42
MNEW=	2	MNEH=	15	DEL=	.83118	LAM=	42.676	FF=	.54541E-07	EC=	13.05 ECF= 12.88
MNEW=	2	MNEH=	19	DEL=	.83446	LAM=	42.674	FF=	.96963E-08	EC=	15.18 ECF= 15.01
MNEW=	2	MNEH=	21	DEL=	.83641	LAM=	42.673	FF=	.58535E-08	EC=	16.91 ECF= 16.75
MNEW=	2	MNEH=	22	DEL=	.83900	LAM=	42.672	FF=	.58591E-08	EC=	20.13 ECF= 19.97
MNEW=	2	MNEH=	25	DEL=	.84047	LAM=	42.671	FF=	.49650E-06	EC=	23.02 ECF= 22.87
MNEW=	2	MNEH=	26	DEL=	.84227	LAM=	42.670	FF=	.70364E-08	EC=	27.09 ECF= 26.94
MNEW=	2	MNEH=	1	DEL=	.37127E-02	LAM=	42.439	FF=	.10281E-07	EC=	3.50 ECF= 2.02
MNEW=	3	MNEH=	4	DEL=	.79256	LAM=	42.694	FF=	.19572E-07	EC=	6.07 ECF= 5.83
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MNEW=	77	MNEH=	4	DEL=	.84779	LAM=	42.638	FF=	.72268E-07	EC=	26.17	ECF= 26.05
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MNEW=	78	MNEH=	9	DEL=	.86461	LAM=	42.630	FF=	.28381E-07	EC=	27.45	ECF= 27.35
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MNEW=	1	MNEH=	9	DEL=	.80746	LAM=	42.688	FF=	.35782E-06	EC=	7.29	ECF= 7.08
MNEW=	1	MNEH=	10	DEL=	.81040	LAM=	42.686	FF=	.11089E-08	EC=	7.63	ECF= 7.42
MNEW=	1	MNEH=	13	DEL=	.82170	LAM=	42.681	FF=	.30229E-07	EC=	9.61	ECF= 9.42
MNEW=	1	MNEH=	15	DEL=	.83118	LAM=	42.676	FF=	.54541E-07	EC=	13.05	ECF= 12.88
MNEW=	1	MNEH=	19	DEL=	.83446	LAM=	42.674	FF=	.96963E-08	EC=	15.18	ECF= 15.01
MNEW=	1	MNEH=	21	DEL=	.83641	LAM=	42.673	FF=	.58535E-08	EC=	16.91	ECF= 16.74
MNEW=	1	MNEH=	22	DEL=	.83900	LAM=	42.672	FF=	.58591E-08	EC=	20.13	ECF= 19.96
MNEW=	1	MNEH=	25	DEL=	.84047	LAM=	42.671	FF=	.49650E-06	EC=	23.02	ECF= 22.87
MNEW=	1	MNEH=	26	DEL=	.84227	LAM=	42.670	FF=	.70364E-08	EC=	27.09	ECF= 26.94
MNEW=	1	MNEH=	1	DEL=	.37127E-02	LAM=	42.439	FF=	.10281E-07	EC=	3.49	ECF= 2.02

610 MINSQ ENTRIES AVERAGE CHI.SQ. FOR NORMAL SOLUTIONS= .84587E-07
106 ENTRIES WITHOUT REAL SOLUTIONS AVERAGE CHI.SQ.= .37463E-03

CHI.SQ. SPECTRUM OF UNREAL SOLUTIONS

1.0E 2	0
1.0E 1	0
1.0E 0	0
1.0E -1	0
1.0E -2	25
1.0E -3	3
1.0E -4	8
1.0E -5	2
1.0E -6	21
1.0E -7	28
1.0E -8	15
1.0E -9	4

1.0E-10	0
1.0E-11	0
1.0E-12	0
1.0E-13	0
1.0E-14	0
1.0E-15	0
1.0E-16	0
1.0E-17	0
1.0E-18	0
1.0E-19	0
1.0E-20	0
1.0E-21	0
1.0E-22	0

HISTOGRAM OF ENERGY SHIFTS

MEV	BCS-FG
-0.15	0.
-0.05	0.
0.05	1796.
0.15	2528.
0.25	264.
0.35	0.
0.45	0.
0.55	0.
0.65	0.
0.75	0.
0.85	0.
0.95	0.
1.05	0.
1.15	0.
1.25	0.
1.35	0.
1.45	876.
1.55	156.
1.65	0.

AVERAGE ENERGY SHIFT BCS-FG= 0.36

ENERGY GAP= 3.45
TOTAL STATE DENSITY= 5620.0

P O S I T I V E P A R I T Y

ENERGY AND M DEPENDENCE OF LEVEL DENSITIES

0.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
1.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3.5	0.600000E+02	2.68	8.	16.	14.	10.	6.	4.	2.	0.	0.	0.	0.	0.	0.	0.
4.5	0.240000E+02	2.04	4.	8.	6.	4.	2.	0.	0.	0.	0.	0.	0.	0.	0.	0.

5.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0
6.5	0.100000E+03	3.54	10.	20.	18.	16.	14.	10.	6.	4	2.	0.	0	0.	0.	0.	0
7.5	0.400000E+02	3.08	4.	8.	8.	8.	6.	4.	2.	6.	0.	0.	0.	0.	0.	0.	0
8.5	0.960000E+02	3.76	8.	16.	16.	16.	14.	12.	8.	4.	2.	0.	0.	0.	0.	0.	0
9.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0
10.5	0.132000E+03	4.12	10.	20.	20.	20.	20.	16.	12	8.	4.	2.	0.	0.	0.	0.	0
11.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0
12.5	0.640000E+02	2.74	8.	16.	14.	12.	8.	4.	2.	0.	0.	0.	0.	0.	0.	0.	0.
13.5	0.140000E+03	4.95	10.	20.	20.	18.	16.	14.	12.	10.	8.	6.	4.	2.	0.	0.	0
14.5	0.208000E+03	3.60	20.	40.	40.	34.	28.	20.	12.	8.	4.	2	0.	0.	0.	0.	0.
15.5	0.720000E+02	2.15	12.	24.	18.	10.	6.	2.	0.	0	0.	0.	0.	0.	0.	0.	0.
16.5	0.180000E+03	2.81	24.	44.	40.	32.	20.	12.	6.	2	0.	0.	0.	0.	0.	0.	0.
17.5	0.108000E+03	3.26	16.	26.	20.	16.	10.	8.	6.	4.	2.	0.	0.	0.	0.	0.	0.
18.5	0.176000E+03	3.59	22.	40.	32.	24.	18.	14.	12.	8.	4.	2.	0.	0.	0.	0.	0.
19.5	0.148000E+03	4.19	14.	28.	24.	20.	18.	14.	10.	8.	6.	4.	2.	0.	0.	0.	0.
20.5	0.224000E+03	3.07	28.	54.	46.	36.	26.	18.	10.	4.	2.	0.	0.	0.	0.	0.	0.
21.5	0.184000E+03	4.25	16.	32.	30.	26.	22.	18.	14.	12.	8.	4.	2.	0.	0.	0.	0.
22.5	0.216000E+03	3.24	24.	48.	44.	36.	26.	18.	12	6.	2.	0.	0.	0.	0.	0.	0.
23.5	0.252000E+03	4.77	18.	36.	34.	32.	30.	28.	26.	20.	14.	8.	4.	2.	0.	0.	0.
24.5	0.520000E+02	3.81	4.	8.	8.	8.	8.	8.	6.	2.	0.	0.	0.	0.	0.	0.	0.
25.5	0.600000E+02	3.03	6.	12.	12.	12.	10.	6.	2.	0.	0.	0.	0.	0.	0.	0.	0.
26.5	0.180000E+03	5.93	10.	20.	20.	20.	20.	18.	16.	14.	12.	10.	8.	6.	4.	2.	0.

0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0	0.	0.	0.	0.	0	0	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

ENERGY AND SPIN DEPENDENCE OF LEVEL DESITIES

0.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
1.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
2.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3.5	0.800000E+01	2.68	0.	1.	2.	2.	1.	1.	1.	0.	0.	0.	0.	0.	0.	0.	0.
4.5	0.400000E+01	2.04	0.	1.	1.	1.	1.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5.5	0.0	0.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.

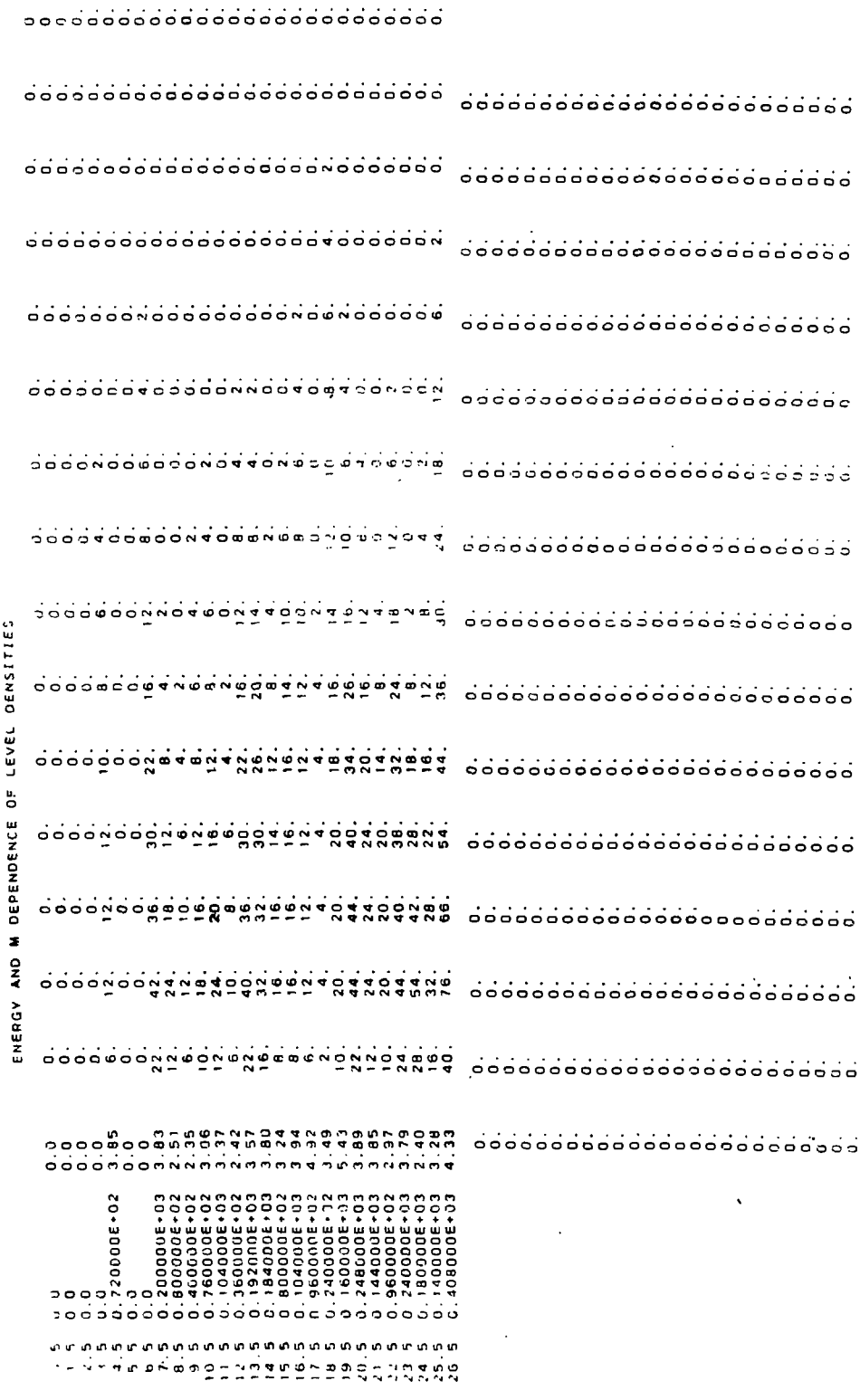
SPIN CUT-OFF ENERGY DEPENDENCE ANALYSIS

SIG Ave.= 3.553 SIG/N= 6.311 SIG/N/A**2/3= 0.307
SIG**2= 2.598+ 0.060*E

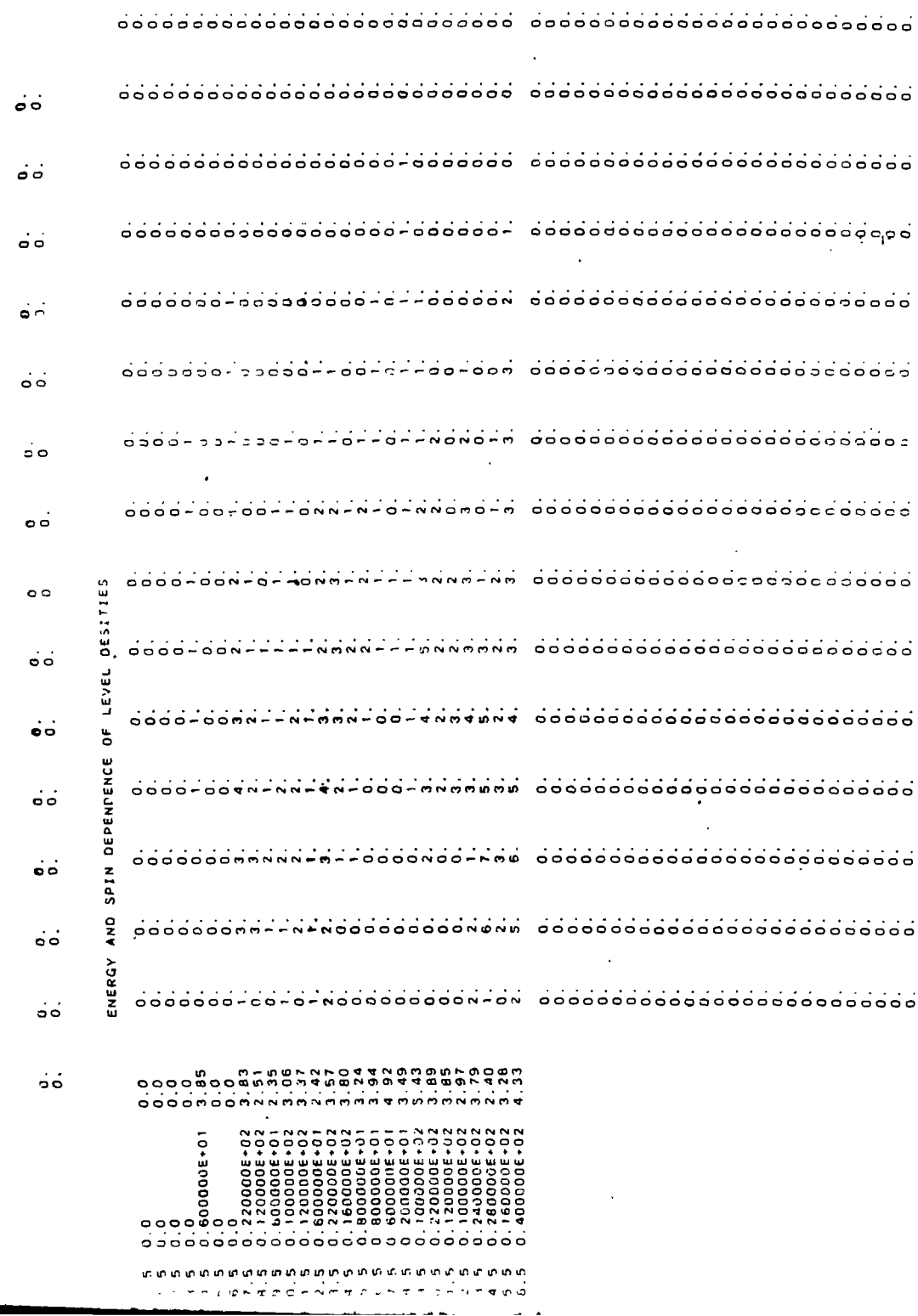
N E G A T I V E P A R I T Y

(1) H.Feshbach, A.Kerman and S.Koonin; Ann. of Phys. 125(1980)429.

2. S.Wahlborn; Nucl. Phys. 37(1962)554.



by eq.1, corresponds to the set of nuclear states. Accordingly all possible combinations of m_i signs giving rise to the total M are accounted for and values up to M=30 are considered. Parity of each state is determined as a product of the parities of the blocked orbitals. To avoid edge effect, at first, results are sorted into 0.1 MeV energy bins, providing n-exciton state densities $\omega_n(E,M)$, which will be later convoluted. Final results are averaged over 1 MeV



0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.

POS. PARITY STATES/ALL STATES

0.5	0.0
1.5	0.0
2.5	0.0
3.5	1.000
4.5	0.250
5.5	0.0
6.5	1.000
7.5	0.167
8.5	0.545
9.5	0.0
10.5	0.635
11.5	0.0
12.5	0.640
13.5	0.422
14.5	0.531
15.5	0.474
16.5	0.634
17.5	0.529
18.5	0.880
19.5	0.481
20.5	0.475
21.5	0.561
22.5	0.692
23.5	0.512
24.5	0.224
25.5	0.300
26.5	0.306

SPIN CUT-OFF ENERGY DEPENDENCE ANALYSIS

SIG AVE.= 3.537 SIG/N= 6.255 SIG/N/A**2/3= 0.305
SIG**2= 3.077+ 0.028*E

NUCLEUS 93NB 1100

114 NEUTRON OR 114 PROTON LEVELS TAKEN INTO ACCOUNT
G= 0.1316 CORRESPONDS TO 12.24/A
NEUTRON GR. STATE
ENERGY= 1648.393 DELTA= 0.92128E+00 LAMBDA= 0.42596E+02
CONDENSATION ENERGY= 1.472

AVERAGE ENERGY SHIFT BCS-FG= 0.36

ENERGY GAP= 3.45
TOTAL STATE DENSITY= 5620.0

MEV	+ST. DENS.	-ST. DENS.	+LEV. DENS.	-LEV. DENS.	+SIGMA	-SIGMA	+/ALL	MEV	SHIFT
0.5	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.0	0.0	0.0	-0.15	0.
1.5	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.0	0.0	0.0	-0.05	0.
2.5	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.0	0.0	0.0	0.05	1796.

required input data. If G search option is chosen [illegible] calculate the difference of condensation energies among three neighbouring nuclei, as defined by Nemirovsky and Adamchuk[4], and return it as 'pairing energy' which is to

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3. W.H.Payne and F.M.Ives; Amc. Trans. of Math. Soft. 5,2(1979) p.163

-3.5	0.60000E+02	0.10000E+01	0.80000E+01	0.10000E+01	2.68	0.0	1.000	0.15	2528.		
4.5	0.24000E+02	0.72000E+02	0.40000E+01	0.60000E+01	2.04	3.85	0.250	0.25	264.		
5.5	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.0	0.0	0.0	0.35	0.		
6.5	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	3.54	0.0	1.000	0.45	0.		
7.5	0.40000E+02	0.20000E+03	0.40000E+01	0.22000E+02	3.08	3.83	0.167	0.55	0.		
8.5	0.96000E+02	0.80000E+02	0.80000E+01	0.12600E+02	3.76	2.51	0.545	0.65	0.		
9.5	0.10000E+01	0.40000E+02	0.10000E+01	0.60000E+01	0.0	2.35	0.0	0.75	0.		
10.5	0.13200E+03	0.76000E+02	0.10000E+02	0.10000E+02	4.12	3.06	0.635	0.85	0.		
11.5	0.10000E+01	0.10400E+03	0.10000E+01	0.12000E+02	0.0	3.37	0.0	0.95	0.		
12.5	0.64000E+02	0.36000E+02	0.80000E+01	0.60000E+01	2.74	2.42	0.640	1.05	0.		
13.5	0.14000E+03	0.19200E+03	0.10000E+02	0.22000E+02	4.95	3.57	0.422	1.15	0.		
14.5	0.20800E+03	0.18400E+03	0.20000E+02	0.16000E+02	3.60	3.80	0.531	1.25	0.		
15.5	0.72000E+02	0.80000E+02	0.12000E+02	0.80000E+01	2.15	3.24	0.474	1.35	0.		
16.5	0.18000E+03	0.10400E+03	0.24000E+02	0.80000E+01	2.81	3.94	0.634	1.45	876.		
17.5	0.10800E+03	0.96000E+02	0.16000E+02	0.60000E+01	3.26	4.92	0.529	1.55	156.		
18.5	0.17600E+03	0.24000E+02	0.22000E+02	0.20000E+01	3.59	3.49	0.864	0.0	0.		
19.5	0.14800E+03	0.16000E+03	0.14000E+02	0.10000E+02	4.19	5.43	0.481	0.0	0.		
20.5	0.22400E+03	0.24800E+03	0.28000E+02	0.22000E+02	3.07	3.89	0.475	0.0	0.		
21.5	0.18400E+03	0.14400E+03	0.16000E+02	0.12000E+02	4.25	3.85	0.561	0.0	0.		
22.5	0.21600E+03	0.96000E+02	0.24000E+02	0.10000E+02	3.24	2.97	0.692	0.0	0.		
23.5	0.25200E+03	0.24000E+03	0.18000E+02	0.24000E+02	4.77	3.79	0.511	0.0	0.		
24.5	0.52000E+02	0.18000E+03	0.40000E+01	0.28000E+02	3.81	2.40	0.424	0.0	0.		
25.5	0.60000E+02	0.14000E+03	0.60000E+01	0.16000E+02	3.03	3.28	0.300	0.0	0.		
26.5	0.18000E+03	0.40800E+03	0.10000E+02	0.40000E+02	5.93	4.33	0.306	0.0	0.		

SIG AVE.= 3.553 SIG/N= 6.311 SIG/N/A**2/3= 0.307
SIG**2= 2.598+ 0.060*E

SIG AVE.= 3.537 SIG/N= 6.255 SIG/N/A**2/3= 0.305
SIG**2= 3.077+ 0.028*E

ENER -calculates energy of the configuration.

PNXCB -generates exciton configurations.

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4. P.E.Nemirovsky and Yu.V.Adamchuk; Nucl. Phys. 39(1962)551

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