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FRAGMENTATION OF SINGLE-PARTICLE STATES IN DEFORMED NUCLEI

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1. In the study of the structure of states of intermediate and high excitation energy in atomic nuclei of much importance is the single-particle fragmentation, that is the distribution of the single-particle strength over many nuclear levels. In the independent-particle and quasiparticle models[1] the single-particle strength is concentrated on a single level. In the extreme statistical model it is chaotically distributed over all nuclear levels. In the earlier period of the study of resonance nuclear reactions and the construction of neutron strength functions Lane, Thomas and Wigner[2] introduced a model of intermediate coupling for describing fragmentaion. Since that time one represented the fragmentation in the form of the Breit-Wigner curve[3,4].

To describe fragmentation, in refs.[5,6] it was suggested to employ the mechanism of interaction of quasi-particles with phonons which is very important in the calculation of the energy and the structure of low-lying non-rotational states of atomic nuclei (see refs.[1,7,8]). The idea of the model based on the account of the quasiparticle-phonon interaction was formulated in ref.[9], and in ref.[10] an approximate method of solving its equations was developed. In ref.[11] the model was generalized to the case of introduction of spin-multipole forces, in ref.[12] it was applied to doubly even deformed nuclei, while in ref.[13] to spherical nuclei. The first results of our investigations on single-particle fragmentation are presented in ref.[14]

In the present paper we study the fragmentation of several single-particle states in ^{239}U and ^{169}Er. We investigate the single-particle fragmentation as a function of the position of the single-particle level with respect to the Fermi level and the particular features of the particle and hole state fragmentation. We also suggest a new method of calculation of neutron strength functions and calculate the s- and p- wave strength functions.

2. We consider a model for describing fragmentation in the case corresponding to an odd-mass deformed nucleus. The model Hamil onian is taken to comprise an average field described by the nonspherical Saxon-Woods potential, interactions leading to superconducting pairing correlations, and multipole-multipole interactions. We should remember that in the case of the nonspherical Saxon-Woods potential the strength of each subshell of the spherical basis is distributed over several single-particle states. This fragmentaion is illustrated, e.g., in ref./15/.

We give numerical results for the nuclei ^{239}U and ^{169}Er. The Saxon-Woods potential parameters and the interaction constants are taken from refs./7,8/. In ref./16/ the same parameters are used to calculate the level density. It should be noted that in our calculations there is not a single free parameter since all the parameters were fixed earlier in studying the low-lying states of deformed nuclei.

The wave function of an odd-A deformed nucleus state is written in the form

$$\Psi_i(K^\pi) = C_\rho^i \frac{1}{\sqrt{2}} \sum_\sigma \Big\{ \alpha^+_{\rho\sigma} + \sum_{\nu,g} D^{gi}_{\rho\nu\sigma} \alpha^+_{\nu\sigma} Q^+_g + \sum_{\nu g g_2} F^{g g_2 i}_{\rho\nu\sigma} \alpha^+_{\nu\sigma} Q^+_g Q^+_{g_2} \Big\} \Psi_0, \quad (1)$$

where Ψ_0 is the wave function of the ground state of a doubly even nucleus, i is the number of the level, $\alpha^+_{\nu\sigma}$ and Q^+_g the quasiparticle and phonon creation operators, $(\rho\tau)$ and $(\nu\sigma)$ the characteristics of single-particle states, $\sigma = \pm 1$, $g = \lambda\mu i$, $\lambda\mu$ the multipolarity and its projection, j is the number of the root of the secular equation for a phonon. The normalization condition for the wave function (1) reads

$$(C^i_\rho)^2 \Big\{ 1 + \sum_{\nu g} (D^{g i}_{\rho\nu})^2 + 2 \sum_{\nu g_1 g_2} (F^{g_1 g_2 i}_{\rho\nu})^2 \Big\} = 1 . \qquad (2)$$

The quantity $(C^i_\rho)^2$ defines the contribution of the single-quasi-particle component to the wave function normalization.

By means of the variational principle in refs. /9,10/ one obtained a system of equations for determining the energies η_i and the functions C^i_ρ, $D^{g i}_{\rho\nu}$ and $F^{g_1 g_2 i}_{\rho\nu}$. In the real cases, when a large number of single-particle states and phonons is taken into account, in order to solve the system of equations it is necessary to diagonalize matrices of the order of 10^4 and higher. In ref. /10/ an approximate method of solving this system of equations is suggested which takes into account all coherent terms and pole noncoherent terms. We call it here the two-phonon approximation. Its accuracy is investigated by the example of a restricted basis. The comparison of the components of the wave functions for the exact and approximate solutions shows that their large components are close to each other while their very small components may differ strongly.

In studing fragmentation we also use the one-phonon approximation, when in the wave function (1) it is put $F^{g_1 g_2 i}_{\rho\nu} = 0$. In this approximation

$$(C^i_\rho)^2 = \Big\{ 1 + \sum_{\nu g} \frac{(\Gamma^g(\rho\nu))^2}{\varepsilon(\nu) + \omega_g - \eta_i} \Big\}^{-1} , \qquad (3)$$

that is, $(C^i_\rho)^2$ is expressed in terms corresponding to all the poles quasiparticle plus phonon. Here $\varepsilon(\nu)$ and ω_g are the quasiparticle and phonon energies, $\Gamma^{g}(\rho\nu)$ contains single-particle matrix elements and the phonon characteristics, it is given in ref./10/.

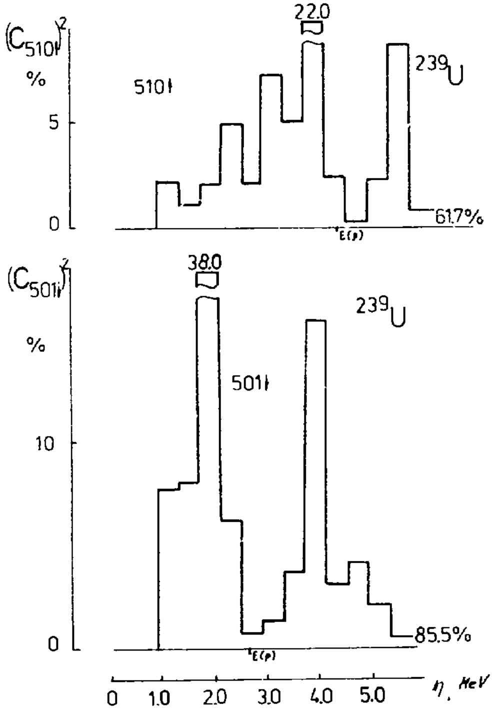
The numerical calculations have been performed on the JINR computor CDC-6200. A total of 15 multipolatities $\lambda\mu$, which for ^{239}U are given in a table, and 10-70 roots for the phonon secular equations have been used. It is seen from the table that the wave function (1) has a large number of different components and, therefore, can describe the complex structure of states. The solution of the secular equations in the two-phonon approximation requires much computor time, therefore, up to now one has obtained only somewhat more than 100 solutions and the appropriate wave functions.

Our investigations have shown that the wave functions calculated in the two-phonon approximation contain a large number of non-zero components. However, in some cases we have obtained an overestimated value for the main component which is a shortcoming of the approximation used. The energies and the wave functions calculated in the one- and two-phonon approximations differ strongly from each other. In the one-phonon approximation the fragmentation of the states quasiparticle plus phonon is badly described and for many solutions the main component exceeds 99%. However, the distribution of the strength of the single-quasiparticle state is almost the same for both the approximations. For example, in ^{239}U for the 631↓ state on the first level 90.1% of the strength is concentrated in the one-phonon approximation and 85.6% in the two-phonon one. The total 631↓ strength related to all the levels of 1.9 MeV energy is 93% in the one-phonon approximation and 92.5% in the two-phonon one. For the 620↑ state (without the solution corresponding to the one-quasiparticle fundamental pole) the total strength on the levels up to 1.9 MeV is 16% in the one-phonon and 14% in the two-phonon approximations. Therefore, when we need obtain several hundreds of solutions we shall use the one-phonon approximation.

3. We consider the fragmentation of the single-particle states in ^{239}U and ^{169}Er. We study the strength distribution as a function of the position of the single-particle level with respect to the Fermi level and the shape of this distribution.

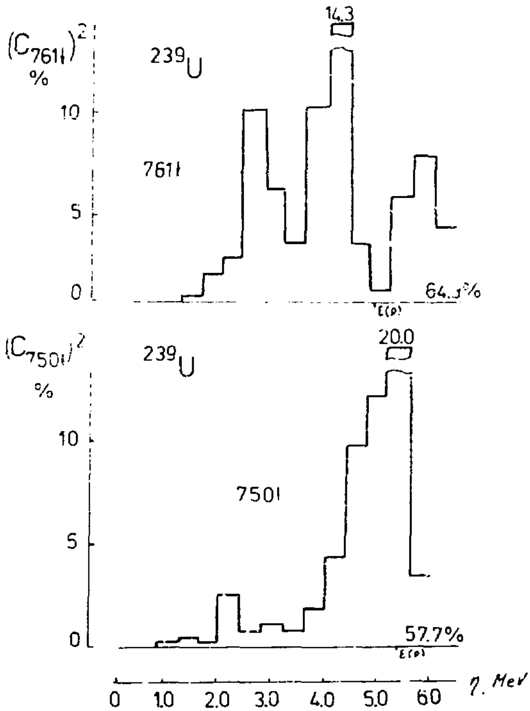
Part of the results on fragmentation is given in figs.1-3. The quantities $(C_\rho^i)^2$ are calculated in the one-phonon approximation from expression (3), are represented as a sum over the states lying in the energy interval ΔE = 0.4 MeV, are denoted as $(C_\rho)^2 = \sum_{i-\Delta E} (C_\rho^i)^2$ and are given in percent. On the abscissa axis common for both the states are the excitation energies reckoned from the ground state energy which for ^{239}U is $\eta_{622\downarrow}$=0.4MeV and for ^{169}Er $\eta_{521\downarrow}$ = 0.68 MeV. The figures give the quasiparticle energies $\varepsilon(\rho)$ and the total contribution of the $(C_\rho)^2$ values up to the maximum energy of the appropriate histogram.

The first results on single-particle fragmentation in ^{239}U are given in refs./14,17/. In ref./17/ one gives the fragmentation of the ground 622↓ state while in ref./14/ the fragmentation of the four 631↓, 620↑, 600↑ and 640↑ states with $K^\pi = 1/2^+$. It is shown that if a single-particle state is located near the Fermi surface then more than 90% of the strength is concentrated on the lowest level with a given K^π and the remaining 10% are spreaded



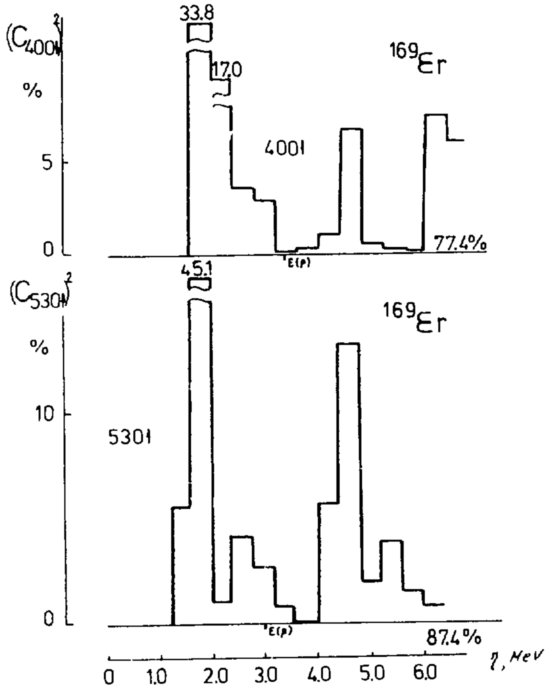
22.0
$(C_{510l})^2$
%
510l
^{239}U
5
0
61.7%
E(p)
38.0
$(C_{501l})^2$
%
^{239}U
501l
10
0
85.5%
E(p)
0
1.0
2.0
3.0
4.0
5.0
η, MeV

Fig. 1



14.3
$(C_{761l})^2$
%
^{239}U
10
761l
5
0
64.3%
E(p)
20.0
$(C_{750l})^2$
^{239}U
%
10
750l
5
0
57.7%
E(p)
0
1.0
2.0
3.0
4.0
5.0
6.0
η, MeV

Fig. 2



$(C_{4001})^2$
%
33.8
17.0
^{169}Er
4001
5
0
E(p)
77.4%
45.1
$(C_{5301})^2$
%
^{169}Er
10
5301
0
E(p)
87.4%
0
1.0
2.0
3.0
4.0
5.0
6.0
η, MeV

Fig. 3

over a wide energy interval. As the single-particle level moves away from the Fermi surface, the strength concentrated on the lowest level decreases, and the distribution itself expands in favour of higher excitation energies. Figs.1 and 2 give the fragmentation of the four $K^{\pi}=1/2^{-}$ states in ^{239}U . According to the level scheme,the hole 501↓ and 510↑ states lie lower the Fermi surface energy by 2.5 and 4 MeV.The particle 761↓ and 750↑ states lie above the Fermi surface energy by 5.2 and 5.7 MeV.Fig.2 shows that the fragmentation of the 761↓ and 750↑ states having close single-particle energies strongly differ from each other, that is,the shape of the distribution function depends on single-particle wave functions.Fig.3 shows histograms for the two hole 400↑ and 530↑ states in ^{169}Er lying lower the Fermi surface energy by 3.17 and 3.19 MeV.

The histogram for the 501↓ state clearly exhibits two maxima, one near the quasiparticle energy $\mathcal{E}(\rho)$,the other at higher excitation energy.Two maxima are also seen in the histograms for the 620↑ and 640↑ states in ^{239}U given in ref./14/ and for the 530↑ state in ^{169}Er .In a more or less explicit form the second maximum exhibits in almost all the calculated states. The appearance of the second maximum in the distribution functions is a new and somewhat surprising result.

The distribution functions have long tails in favour of high excitation energies.Even for the 521↓ state,which is a Fermi level in ^{169}Er ,up to the neutron binding energy B_n = 6 MeV only 94.7% of the strength of this state is exhausted. Figs.1 and 3 show that up to 6 MeV, 60-85% of the strength of the hole states is exhausted. For the particle 600↑ state in ^{239}U lying above the Fermi surface by 4.3 MeV only 60% of its strength is exhausted up to a neutron binding energy B_n = 4.8 MeV. It is seen from fig.2 that the strength of the 761↓ and 750↑ states, the single-particle energies of which lie somewhat above B_n, only 60% is exhausted up to an excitation energy of 6 MeV.

Thus, the strength distribution for the single-particle states in deformed nuclei displays the following particular features:

i) at high excitation energies, in addition to the first maximum, there appears a second one, ii) the distribution function is nonsymmetric with respect to its largest value due to its slower fall in favour of high energies, iii) the shape of the distribution function is mainly defined by the position of the single-particle level with respect to the Fermi surface, but it depends on the wave function of the single-particle state, iv) the strength distribution has a long tail which, even for the single-particle states lying near the Fermi surface, expands essentially father behind the neutron binding energy.

It should be noted that in our calculations of fragmentation there is a strong fluctuation from one energy interval to another and, especially, from level to level. Strong fluctuations are, to a large extent, due, firstly, to the use of the one-phonon approximation and, secondly, to the roughness of the model in the present formulation which disregards some collective branches such as spin-multipole, Gammov-Teller and giant resonances. In ref./14/ it is indicated that it is interesting to clarify how the giant resonances affect fragmentation.

4. We use the obtained results on single-particle fragmentation for the calculation of neutron strength functions. The neutron strength function is defined as

$$S_\ell = \frac{\langle \Gamma_n^\ell \rangle}{\langle D \rangle} \quad , \tag{4}$$

where Γ_n^ℓ is the reduced neutron width, D the spacing between the levels with given I^π. Using the wave functions of neutron resonances (1) we get the following expression for the S-wave strength function

$$S_0 = \frac{15(keV)}{\Delta E(keV)} A^{-4/3} (a^{\rho}_{0 1/2})^2 u_\rho^2 \sum_{\Delta E} (C_\rho^i)^2 , \tag{5}$$

where ΔE is the energy interval inside which a summation of $(C_\rho^i)^2$ over the excited states is performed; u_ρ^2 is the Bogolubov canonical transformation coefficient calculated with the correlation function and the chemical potential for the ground state of the target-nucleus. According to [8], the single-particle wave function φ_ρ is represented as an expansion in the spherical basis

$$\varphi_\rho = \sum_{n\ell j} a^\rho_{n\ell j} \varphi_{n\ell j} \quad , \quad a^\rho_{\ell j} = \sum_n a^\rho_{n\ell j} \; . \tag{6}$$

The expression for the p-wave strength function consists of three terms

$$S_1 = S_1(1/2^- 1/2) + S_1(3/2^- 1/2) + S_1(3/2^- 3/2) , \tag{7}$$

where the first term is relative to the $I^\pi K$ = 1/2$^-$ 1/2 states, the second one describes the contribution from the appropriate rotational components for which $I^\pi K$ = 3/2$^-$ 1/2, and the third term gives the contribution from the K^π = 3/2 states. They look like

$$S_1(1/2^- 1/2) = \frac{15(keV)}{\Delta E(keV)} A^{-1/3} (a^\rho_{1 1/2})^2 u_\rho^2 \sum_{\Delta E} (C_\rho^i)^2 , \tag{8}$$

$$S_1(3/2^- - 1/2) = \frac{30(keV)}{\Delta E(keV)} A^{-1/3} (a^f_{1 1/2})^2 u_f^2 \sum_{\Delta E} (C_f^i)^2, \quad (9)$$

$$S_1(3/2^- - 3/2) = \frac{30(keV)}{\Delta E(keV)} A^{-1/3} (a^f_{1 1/2})^2 u_{f_2}^2 \sum_{\Delta E} (C_f^i)^2, \quad (10)$$

where f is relative to the $K^{\pi} = 1/2^-$ states, f_2 to the $K^{\pi} = 3/2^-$ states.

According to our calculations for ^{239}U

$$S_c^{cal} = 1.2 \times 10^{-4}, \quad (11)$$

which is in satisfactory agreement with the experimental value $S_c^{exp} = 1 \times 10^{-4}$. The main contribution in S_c^{cal} comes from the fragmentation of the 600↑, 880↓ and, partially, 611↓ states.

The situation of the S_c^{cal} calculations in ^{149}Er is more complicated and interesting. In the single-particle wave functions, in ref.[8], there is no contribution from the $4S_{1/2}$ subshell which is in the continuous spectrum. Therefore, the related calculations yield

$$S_c^{cal} = 0.05 \times 10^{-4}, \quad (12)$$

which is in disagreement with the experimental value $S_c^{exp} = 1.5 \times 10^{-4}$. The main contribution comes from the fragmentation of the 400↑ state which is weakened due to the multiplier $u_p^2 = 0.02$. Note that the u_p^2 effect on S_c was first noticed in ref.[18]. Employing the single-particle wave functions calculated by Gareev and Jamalejev in the framework of the method from ref.[19], in which the $4S_{1/2}$ subshell is taken into account, we get

$$S_c^{cal} = 1 \times 10^{-4}, \quad (12')$$

the main contribution being due to the 640↑ state fragmentation. The S_0^{cal} results depend on the averaging interval ΔE , in the ^{169}Er case an essential expansion of ΔE results in an increase of the value (12') by a factor of 1.5-2.0. Inclusion of the $4S_{1/2}$ subshell leads to a good agreement between the calculated and experimental strength function.

The S_0^{cal} calculations with two sets of the single-particle wave functions are of great interest since the transition from the (12) value to the (12') value seems to be a transition from the minimum to the maximum of the strength function. Inclusion of the $4S_{1/2}$ subshell results in a 20 times increase of S_0^{cal}. In spherical nuclei such an increase may be still larger.

The calculation of the p-wave strength function in ^{239}U has been performed for two sets of the single-particle wave function. These are just the wave functions from ref.[9] which do not include the $4p_{1/2}$ and $4p_{3/2}$ subshell contribution and the wave functions calculated by Gareev and Jamalejev in which these subshells are taken into account. The calculations with the wave functions[9] yield

$$S_1^{cal} = 0.23\times10^{-4}. \tag{13}$$

The calculations with the wave functions containing the subshells $4p_{1/2}$ and $4p_{3/2}$ give the following value

$$S_1^{cal} = 2.7\times10^{-4}, \tag{13'}$$

which is in agreement with the experimental values $S_1^{exp}=2.2\times10^{4}$. Inclusion of the subshells $4p_{1/2}$ and $4p_{3/2}$ leads to an increase of S_1^{cal} by a factor of 12. Such a relatively small increase is due to the contribution in (13) from the single-particle 50'↑

state fragmentation which remains rather large in spite of its weakening due to $u_p^2 = 0.02$.

The calculation of the p-wave function in ^{169}Er with the single-particle wave functions from ref.[8] yield the following value

$$S_1^{cal} = 1.2 \times 10^{-4}, \qquad (14)$$

which somewhat exceeds the experimental value $S_1^{exp} = 0.7 \times 10^{-4}$. The largest contribution in (14) comes from the fragmentation of the 501↑ state, that is, from the same state which gives the main contribution in (13).

In the present paper we have suggested a fundamentally new semi-microscopic method of calculation of the neutron strength functions based on the account of the quasiparticle-phonon interaction. The s and p-wave neutron strength functions for ^{239}U and ^{169}Er calculated by this method are in satisfactory agreement with experiment. Note that there is a good description of the quantities S_0 and S_1 in these nuclei in the framework of the phenomenological approach by a suitable choice of the optical model potential parameters. We would like to stress that all the calculations of the neutron strength function available by the present time have been performed phenomenologically on the basis of the Breit-Wigner formula in the framework of the optical model (see ref.[20]).

5. The calculation of the single-particle fragmentation provides new possibilities of studying the structure of the states of intermediate excitation energy for the description of which the language of the strength functions of different kind should be used. There have appeared first experi -

mental papers[21] on the study of the single-particle fragmentation.

The calculations of single-particle fragmentation in odd-A deformed nuclei allows one, e.g., to find the dependence of the ℓ-wave strength functions on excitation energy. To this end, when calculating fragmentation we should take into account in the wave function (1) the terms quasiparticle plus two phonons and generalize it by introducing summation over ρ for a simultaneous account of several single-particle states. The $(d p)$ reactions exhibit the behaviour of the ℓ-wave strength functions for particle states at different excitation energies. At the neutron binding energy and still slightly higher these functions coincide with the neutron strength functions. The $(d t)$ reactions yield some information on the ℓ-wave strength function behaviour for hole states at different excitation energy.

Of great interest is the study of single-particle fragmentation in spherical nuclei and the calculation of the neutron strength functions. It is important not only to obtain good values of the neutron strength functions in the range of their maxima, but also to explain their behaviour in the range of their minima. These problems are the focus of our attention.

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Table

The $\lambda\mu$ values and the number of the terms of the wave function (1) in ^{239}U.

$\lambda\mu$	Number of terms of the type	
20 22 30 31 32 33 41 43 44 54 55 65 66 76 77	$\alpha^{+}_{\nu\sigma} Q^{+}_{g}$	$\alpha^{+}_{\nu\sigma} Q^{+}_{g} Q^{+}_{g_2}$
j = 1,2,... 10	870	9×10^4
j = 1,2,... 35	1×10^4	1.1×10^6
j = 1,2,... 70	5×10^4	5×10^6

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