

Evolution of single-particle structure and beta-decay near ^{78}Ni

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Abstract. The extended self-consistent beta-decay model has been applied for beta-decay rates and delayed neutron emission probabilities of spherical neutron-rich isotopes near the r-process paths. Unlike a popular global FRDM+RPA model, in our fully microscopic approach, the Gamow-Teller and first-forbidden decays are treated on the same footing. The model has been augmented by blocking of the odd particle in order to account for important ground-state spin-parity inversion effect which has been shown to exist in the region of the most neutron-rich doubly-magic nucleus ^{78}Ni . Finally, a newly developed form of density functional DF3a has been employed which gives a better spin-orbit splitting due to the modified tensor components of the density functional.

1 Introduction

The region of nuclei near the most neutron-rich ($N-Z/A \sim 0.28$) doubly-magic ^{78}Ni is a unique laboratory for exploring nuclear structure under extreme conditions. New features related to physics of weakly bound open quantum system offer a stringent test for the models of the ground state and β -decay properties. A spherical sub-shell closure at $N=58$ has been experimentally proved recently. It emerges due to reduced neutron binding beyond the major $N=50$ neutron shell, as found by the HFB with SkO functional involving the tensor term [1]. Related weakening of the ^{78}Ni core triggers a crossing of the $p_{2p3/2}$ and $p_{1f5/2}$ levels near $Z \sim 28$. The ground-state spin-parity inversion has been confirmed recently by the magnetic moments measurements in Cu isotopes [2].

Such a drastic change of the single-particle pattern should be properly taken into account in studying the β -decay of very-neutron rich nuclides with $N > 50$ in vicinity of ^{78}Ni . For these nuclides another complication is known: the first-forbidden (FF) decays start to compete with the Gamow-Teller (GT) decays [3].

Recently the half-lives in the $^{82,83}\text{Zn}$ and ^{85}Ga isotopes with $N > 50$ has been measured for the first time at HRIBF ORNL using nearly pure isotopic beams of the studied nuclei and tagging technique with efficiency calibrated γ -detectors [4]. Together with earlier evidence found in Cu isotopes [5], the new data show that even integral characteristic like the beta-decay half-life is rather sensitive to the evolution of single-particle structures due to N and Z dependence of nuclear density functional. First, the new β -decay data confirm that a correlation to the ground-state spin-parity is important indeed. Second, a sensitivity is shown to filling of nearly degenerate

neutron $n_{2d5/2}$ and $n_{3s1/2}$ orbits forming the $N=58$ sub-shell [1]. These unique features of the nuclei close to ^{78}Ni pose a stringent test for the nuclear structure models. In particular, they enable us to extend our Density Functional plus continuum QRPA framework. The density functional DF3a better accounts for tensor components which improves the spin-orbit splitting. The quasi-particle blocking has been employed to fix correct ground state spin-parities of the parent and daughter isobaric companions. On top of that, the first-forbidden decays which are important in the region beyond the closed neutron shell at $N=50$ were included on the same footing as the Gamow-Teller decays.

2 Theoretical background

Our studies are based on a global approach which allows one to calculate simultaneously ground state properties and β strengths functions for all spherical nuclei. The ground state properties are derived self-consistently in the framework of the local energy-density functional (DF) theory. Here we follow an approximate treatment proposed in [3]. This makes use of the fact that, except for the spin-orbit splitting, the ground state properties are insensitive to the spin and spin-isospin components of the DF, while the latter are essential for a reliable description of beta-decays. Hence, the scalar and spin-isospin components of the DF can be approximately decoupled allowing for an independent introduction of the nucleon-nucleon (NN) interaction in the scalar and spin-isospin channels. The β -strength functions are calculated within the continuum quasi-particle random phase approximation (QRPA) of the finite Fermi system theory using the Landau-Migdal spin-isospin NN-

interaction. After inclusion of the first-forbidden transitions this approach has been successfully used to describe the β -decay properties of selected isotopic chains with $Z = 26\text{--}33, 48\text{--}51, 60\text{--}70$ around the magic neutron number $N = 50, 82, 126$ and has been presented in details in Ref. [3].

The basis of our ground state calculations is the phenomenological density functional DF3a: a modification of the Fayans functional [6] consisting of a normal and a pairing part. The functional is augmented by a two-body spin-orbit and tensor velocity-dependent effective nucleon-nucleon interaction. The inclusion of the latter ensures a reliable description of the single-particle structure near the very neutron-rich doubly-magic nuclei ^{78}Ni and ^{132}Sn . In the present model we allow for quasi-particle blocking prescription. It gives one a possibility to fix (before the variation) the ground state spin-parities of the parent and daughter isobaric companions.

The excited states are determined by the continuum QRPA equations of the finite Fermi system (FFS) theory. A minimal set of the energy variables is used including the β -transition energy, $Q\beta$ and $Q\beta x_n$ -windows. A redundant variable E_x is not needed.

We consider like-particle ($T = 1$) ground-state pairing, as well as effective NN-interaction in the particle-hole (ph) and particle-particle (pp) channels. An exact treatment of the particle-hole continuum has been performed.

For the spin-isospin effective NN-interaction in the ph channel a finite-range $\delta + \pi + \rho$ forms is assumed. The competition between the one-pion attraction (characterized by $g_{\pi} Q < 0$, where g_{π} is the πN -coupling constant and the quenching factor Q is defined below) and the spin-isospin contact repulsion, defined by the Landau-Migdal parameter $g' > 0$, influences the β -decay half-lives [3].

The $T = 0$ spin-isospin component of the effective NN-interaction in the pp channel is assumed to have a delta-function form with a strength parameter g'_{ξ} similar to the one which describes like-particle ($T = 1$) pairing. We note that the inclusion of isovector and isoscalar effective NN-interactions is essential to guarantee the $SO(8)$ symmetry of the pnQRPA equations and to avoid unrealistic odd-even staggering of total β -decay half-lives. It was shown in [3] that for $g'_{\xi} = 0.2\text{--}0.3$ (i.e. rather far from the instability point in the pp channel), the CQRPA-like equations of the FFS allows a reasonable description of nuclear spin-isospin modes in even and odd- A nuclei

The “low energy” spin-isospin response (at excitation energies ω below the Fermi energy, $\omega < \epsilon_F$) is quenched due to a universal in-medium renormalization beyond the QRPA-type correlations caused by higher order np-nh configurations, delta-resonance admixtures, etc. The quenching is accounted for by re-scaling the spin-dependent components of the weak-interaction multipole operators by the same energy-independent factor $Q^{1/2} = (g_A/G_A)$. Importantly, it was assumed that the spin-isospin polarisation operator and one-pion component of the residual interaction are quenched consistently by the same constant factor Q . As in [3], the quenching factor

$Q = 0.81$ is used. Together with the Landau-Migdal parameter $g' = 1.0$ and the effective pion coupling constant $f_{\pi} = -1.38$ (both normalized to the constant $C_0 = 300 \text{ MeV} \cdot \text{fm}^3$) this set of the FFS parameters has been proven to give a good description of magnetic moments [7], GT and M1 resonance energies and the β -decay properties of spherical nuclei [3].

For the calculation of the β -decay half-lives we have considered allowed and first-forbidden transition. The latter are treated microscopically in terms of the reduced multipole operators depending on the space and spin variables [3]. The corresponding β strength functions have been calculated as function of the β -decay transition energy ω relative to the parent nucleus ground state by solving the CQRPA equations. First-forbidden transitions, if favoured by selection rules and phase space, reduce the total half-lives, as it happens for the nuclei with the neutrons numbers bigger than $N = 28, 50, 82$ and 126 [3].

3 Beta-decay rates

3.1 Global models

Below we compare the experimental half-lives and delayed neutron emission total P_n -values with the ones from the global models [8-12], as well as our present DF3a+CQRPA model for the Gamow-Teller and FF decays augmented by blocking.

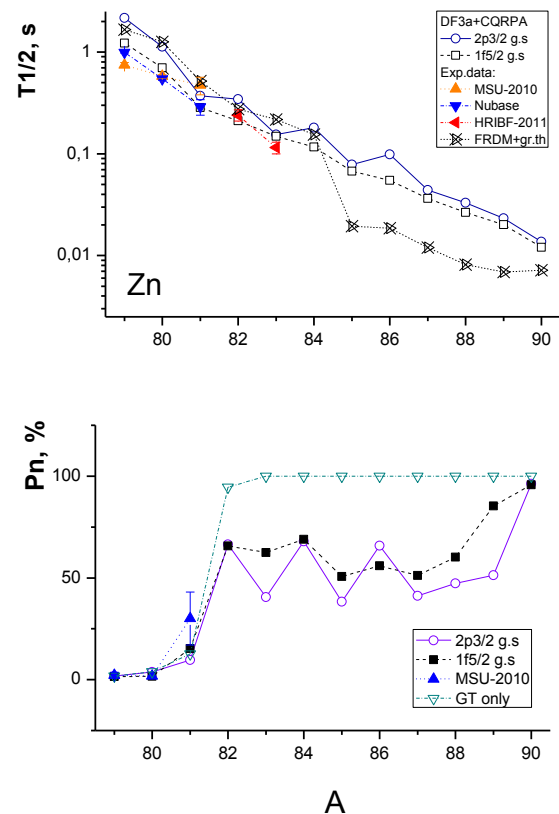


Fig.1. Beta-decay half-lives for Ga isotopic chain calculated in the FRDM (GT), FRDM (GT+FF) and DF3a + CQRPA (GT+FF) models.

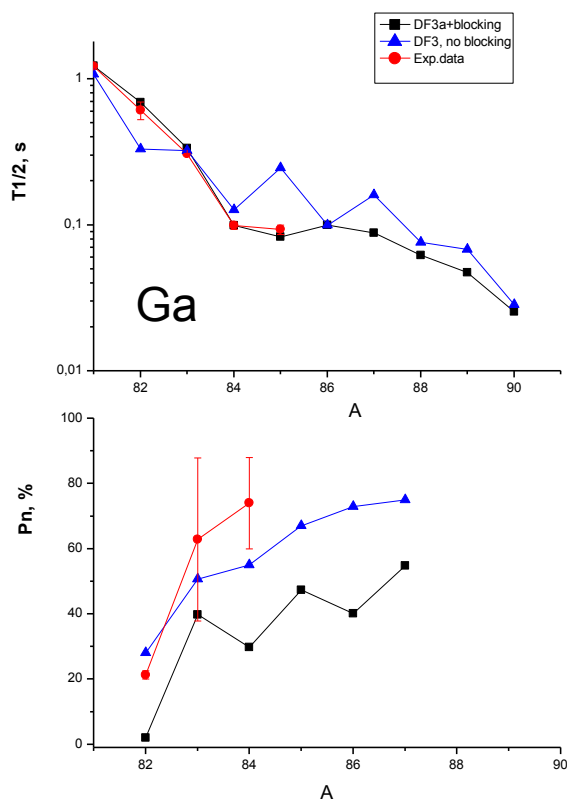


Fig.2. Beta-decay half-lives and P_n -values for Ga isotopic chain calculated in the DF3a+CQRPA (GT+FF) with a) blocking and b) no blocking.

First, the new experimental half-lives for Zn and Ga isotopic chains ([4], figures 1, 2) show the semimicroscopic global models fail to describe the ground state properties in the most neutron rich region of nuclear chart. Description of spherical sub-shell closure at $N=58$ [1] is beyond their performance. It emerges due to reduced neutron binding above the major $N=50$ neutron shell as predicted by the HFB with SkO functional involving the tensor term [1] and confirmed also in the DF3a calculations. The neutron-proton interaction weakening the ^{78}Ni core triggers a crossing of the $p_{2p3/2}$ and $p_{1f5/2}$ levels near $Z\sim 28$. The newly measured half-lives together with magnetic moments [2] and new P_n -branching measurements [5] present the available experimental data sensitive enough to validate this theoretical picture which is far from being trivial.

Second, the new half-lives for very-neutron rich Zn and Ga isotopes have questioned the global β -decay calculations in this region which do not properly account for ground state spin-parity inversion and the first-forbidden transitions. The ‘‘Gross Theory’’ [8], parameterization underestimate both old and new Zn, Ga data significantly (not shown in figures 1,2). Thus, it can not provide a reliable r-process modeling in specific region of ^{78}Ni . The pnQRPA based on empirical ground state description [9] reveals rather regular A -dependence in $Z\sim 28$, $N=50-60$ region. It has been normalized directly to the available half-lives at $N\sim 50$. The forbidden decays were not included, however even within the GT approximation the new experimental half-lives for $^{82,83}\text{Zn}$

and ^{85}Ga are underestimated by [9] (not shown in figures 1, 2).

As can be seen from figure 1, the new data for Ga isotopes rule out the standard FRDM [10] and FRDM+Gross-Theory [11] extrapolations which have been previously used in the r-process modeling. Similar to the pnQRPA model by [9], the models by [10,11] however miss the important ingredient of the $T=0$ particle-particle interaction. (Obviously, this effect cannot be replaced by re-fitting of the particle-hole interaction). A strong spurious odd-even staggering seen in the FRDM calculations for Zn and Ga isotopes at $N>50$ (figures 1, 2) is a signature of skipping the NN-interaction in the pp-channel.

Notice, the FRDM half-lives [2] calculated in the GT approximation (figure 1) are systematically lower than the data for $A<85$. After including the FF decays within the FRDM+Gross-Theory [11], the total half-lives for $^{81-84}\text{Zn}$ and $^{82-87}\text{Ga}$ become longer than the ones of pure GT decay approximation. The result cannot be explained by reasonable arguments. For $A>85$ a rapid drop of the half-lives is observed. It is worth to mention that FRDM half-lives re-calculated assuming a spherical approximation for $31<Z<39$, and $52<N<60$ in [12] overestimate the data. All the above mentioned features of the calculations [10-12] contradict the present data for $^{84,85}\text{Ga}$. Thus, testing the validity of global models predictions is important, as they are widely used in network r-process calculations when no experimental data exist.

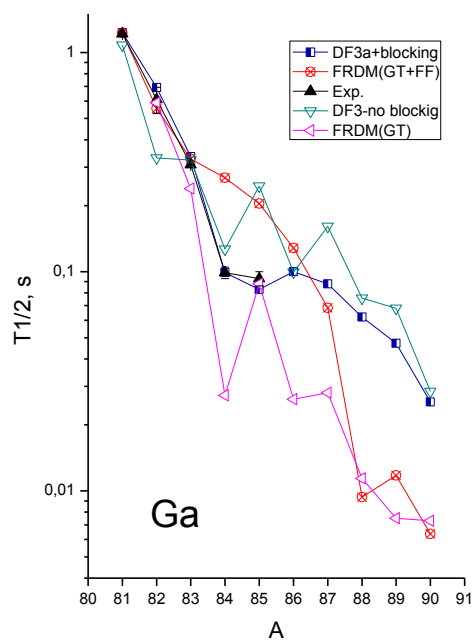


Fig.3. Experimental beta-decay half-lives for Ga isotopic chain calculated in the DF3a+CQRPA (GT+FF) with blocking and with no-blocking in comparison to the FRDM (GT) and FRDM + Gross Theory (GT+FF).

3.2 DF3a+CQRPA model

Our calculations for Zn and Ga isotopic chains are shown in figures 2 and 3. The DF3a plus blocking model extended to account for spin-parity inversion in ^{78}Ni region shows the half-lives in agreement with both old and new data. This approach is also consistent with the systematics of the spin and parity of the ground state of Cu isotopes (understood as driven by the proton-neutron interaction when filling the $n1g9/2$ shell [5]). We found that the calculation blocking the ground state configuration to a $1f5/2$ proton single-particle state was able to reproduce the ^{85}Ga half-life value (see figure 2). No other modifications or local adjustments were made.

The no-blocking option resulted in odd-even staggering which is not supported by the data. This gives us a confidence in our theoretical extrapolation of the half-lives, in particular for Zn, Ga beyond $N=54$. Important feature of our calculation is a remarkable stabilization of the half-lives in Ga isotopic chain when neutrons are filling the $n2d5/2$ orbital. A subsequent drop of the half-lives may be related to filling of the neutron $3s1/2$ orbital and opening of the $(n3s1/2, p2p1/2)$ FF-transitions. Thus, the β -decay half-lives in Ga chain reveal a sensitivity to forming of the $N=58$ subshell.

The role of the FF transitions is decisive, as their energies and intensities define mostly the total half-lives after crossing the $N=50$ shell. Even the ordering of both proton and neutron shells is important, it is principal whether the $(n2d5/2, 1f5/2)$ or $(n3s1/2, p2p3/2)$ and $(n3s1/2, p2p1/2)$ first-forbidden transitions undergoes first. Displayed in figure 4 is a systematic calculation of the β -decay energies of most intensive GT and FF transitions. It clearly demonstrates an existence of generic low-energy GT and high-energy FF pattern for the whole Ga isotopic chain.

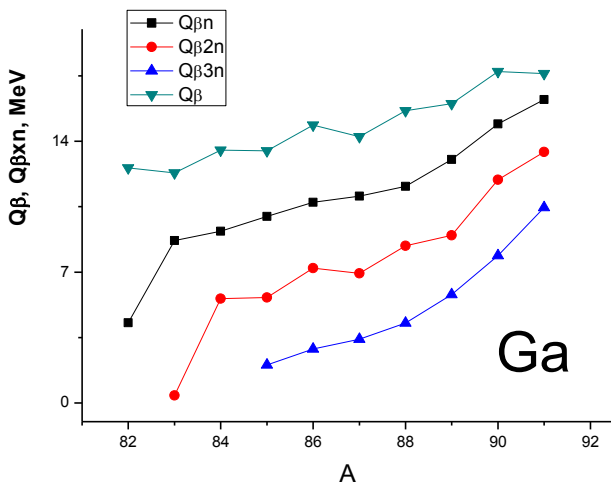


Fig.5. Q_β and $Q_{\beta xn}$ windows for delayed multi-neutron emission in Ga isotopes calculated with DF3a functional.

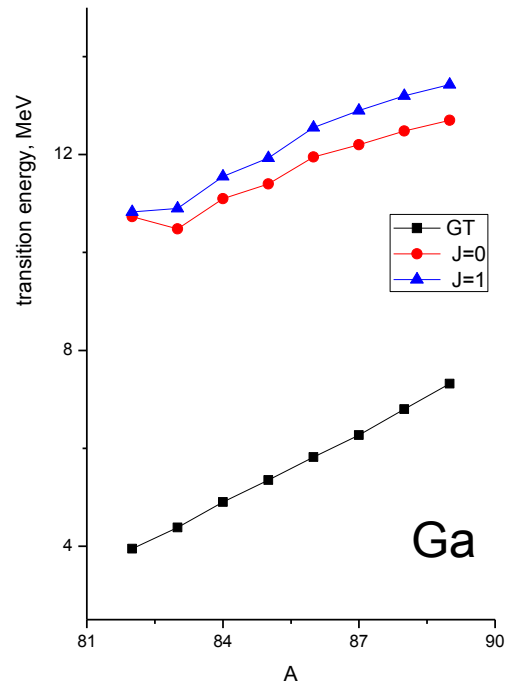


Fig.4. A-dependence of the transition energies for the most intensive GT and FF decays.

4 Delayed multi-neutron emission

The total delayed neutron emission branchings in Zn and Ga chains are not very different for the blocking and no-blocking calculations. More important is an observed reduction of the total P_n -values relative to the ones obtained in pure GT approximation (figures 1, 2). This effect was explained in [3] by the role of the FF decays proceeding outside the $Q_{\beta n}$ -window. In Ga isotopes the blocking approximation also results in stronger reduction of the total P_n -values.

As the beta-decay energy releases are high in $Z>28$, $N>50$ region, the delayed multi-neutron emission can be expected for majority of studied isotopes. As seen from figure 5, the DF3a calculation predicts 2n or even 3n-emission for Ga isotopes with $N>54$. The corresponding P_{1n} - P_{3n} delayed emission probabilities are displayed in figure 6. The A-behaviour of the P_{xn} -values is not monotonic reflecting the difference in the amount of the GT and FF strengths located within the corresponding xn -phase spaces. Such an appreciable P_{2n} -branching ratio in Ga isotopes could be measured at existing facilities.

It should be stressed that theoretical estimate of the delayed neutron emission branchings is very demanding. First, it relies on the calculations of the Q -windows and neutron separation thresholds. A typical deviation of these quantities from the experimental data is about 0.5-1.0 MeV which may bring a sizable uncertainty to the resulting P_n -values. Second, it is extremely sensitive to the distribution of the beta-strength in the near-thresholds regions. To illustrate this point, the total P_n -values in Ge isotopes (figure 7) were calculated for different assumptions on relaxation of the spin-isospin strength: a) constant spreading width equal to 200 KeV and b) spreading width depending on the transition energy as $\alpha \cdot (Q_\beta - \omega)^2$.

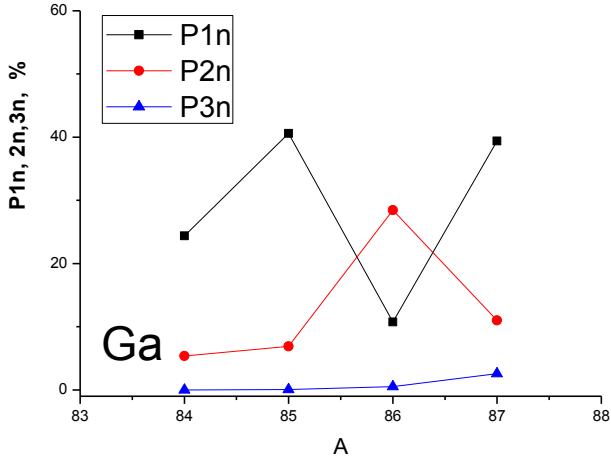


Fig. 6. P1n–P3n - values for Ga isotopes calculated with DF3a functional.

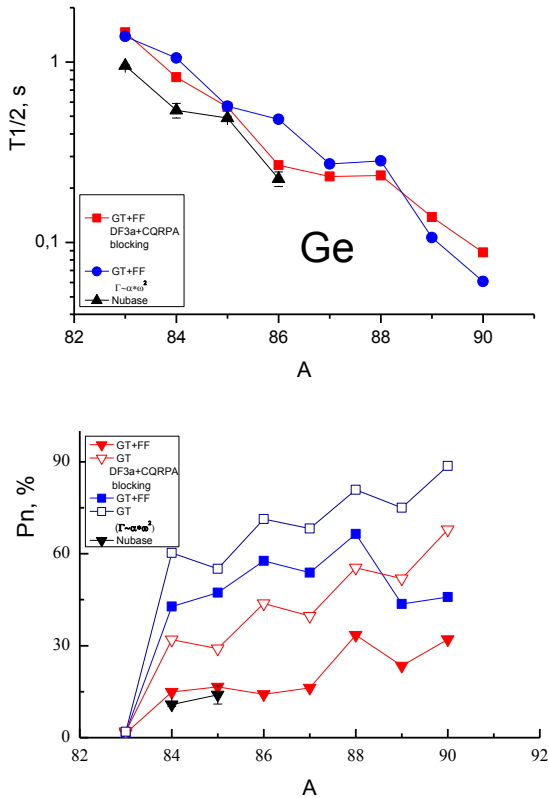


Fig.7. Beta-decay half-lives and total P_n-values for Ge isotopes calculated with DF3a functional.

5 Conclusions

The new experimental β -decay half-lives in ^{78}Ni region reveal a significant deviation from the global models predictions for nuclei crossing the major neutron shell at $N=50$. We have shown that the problem calls for a fully self-consistent treatment. In these nuclei, the beta-decay model has to include microscopically both Gamow-Teller and first-forbidden transitions since neutrons fill positive parity orbitals ($1g9/2$, $2d5/2$ and $3s1/2$) while protons occupy negative parity ones ($1f5/2$, $2p3/2$ and $2p1/2$). A nontrivial nuclear structure feature is a reduced neutron

binding above the major $N=50$ neutron shell due to the tensor term in the DF3a density functional, as well as weakening of the ^{78}Ni core by neutron-proton interaction. This makes the beta decay intensity distribution very sensitive to ordering of both proton and neutron orbitals. First, the appropriate model should comply with correct ground-state spin-parity prescription and the odd proton must be placed to $1f5/2$ orbital. Second, it is important whether the valence neutrons are in the $2d5/2$ or the $3s1/2$ orbitals, as the corresponding FF transitions contribute significantly to the half-lives of nuclei above the $N=50$ shell.

A reasonable agreement of the DF3a+blocking model with both old and new data gives some confidence in our theoretical extrapolation of the half-lives, in particular for Zn, Ga, Ge isotopic chains. For Ga isotopes with $N=54-59$, where only extrapolations are available, our self-consistent model predicts rather unexpected stabilization of the half-lives beyond $N=56$. Importantly, for $N>56$ the DF3a+CQRPA predicts significantly longer lifetimes than the global FRDM+QRPA model. The new experimental half-lives are shorter than the values obtained in the standard FRDM+RPA model, and are essentially reproduced in our DF3a+CQRPA calculations.

Since the DF3a+CQRPA lifetimes strongly deviate from the predictions of the global model they must also have a significant impact on calculations of r-process nucleosynthesis. This was investigated in our previous paper [4]. In the network r-process simulations, the half-lives for $Z=27-32$ and $Z=51$ were replaced by new experimental data and more reliable DF3a+blocking predictions (about 70 nuclides in total). The new important qualitative result was an increased isotopic production for heavier mass nuclei at the third peak [4]. This can be mostly explained from the difference between the FRDM and DF3a half-lives for nuclei of mass above and below the threshold around $N=56$ ($A=85$). The longer DF3a+QRPA half-lives above $A=85$ cause more material to be trapped in the first peak, around $A=80$ in comparison with the standard FRDM simulation. Since less material is acquired in the first peak, fewer neutrons are used up in this region. Consequently, it provides more neutrons available for capture on $A>90$ nuclei boosting a production of heavier species.

The limitations of the global models to calculate refined structure properties of nuclei near shell closures are reflected in discrepancies with new experimental β -decay half-lives. A new generation of self-consistent models, with sound microscopic foundation, is required to provide reliable masses, beta-decay rates, delayed neutron emission probabilities etc for our deeper understanding of the nuclei far from stability and for performing reliable r-process network calculations. Nowadays, fully microscopic approaches are indispensable for numerous decay data applications. One has to mention in this context the predictions for new radioactive beam experiments [13] and forthcoming IAEA delayed neutron evaluation initiative [14].

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