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Problem with gradual absorption in MSD/MSC calculations

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Abstract. Replacing classical exciton model with the better founded Multistep Direct (MSD) and Multistep Compound (MSC) mechanisms has been impeded by incapability of the latter models to describe central part of the neutron emission spectra at incident neutron energies of about 14 MeV and above. We have ascribed this deficiency to the decrease of absorption to the MSC mechanism resulting from the concept of gradual absorption. We were able to obtain very good reproduction of experimentally measured neutron spectra using MSD/MSC calculations when this option was turned off. Such treatment is, however, at odds with the fundamental distinction between MSD and MSC mechanisms that should proceed through the chain of open (P-space) and closed (Q-space) configurations respectively. By blocking gradual absorption we allow the first stage of MSC to be fully populated from the incident channel that at higher incident energies is impossible. We discuss various attempts of addressing the problem that, so far, remains open. In addition, we present an evidence for much tighter spin distribution of particle-hole states than normally assumed.

1 Introduction

In most of the nuclear reaction codes used nowadays (e.g. CoH3 [1], TALYS [2], CCONE [3] and EMPIRE [4]) equilibration of the composite nucleus produced by absorption of a projectile by a target nucleus is described using various versions of the phenomenological exciton model. All of them, inspired by the seminal paper by Griffin [5], assume that such equilibration starts with a two-body interaction of a projectile with a target's nucleon that leads to excitation of a particle and creation of a hole left by this particle. Such doorway state consists, therefore, of the projectile and the pair of excited nucleon and the respective hole. These excitons may further interact with nucleons in the Fermi sea to produce more excited particle-hole (p-h) pairs eventually leading to the fully equilibrated compound nucleus. In the exciton model the cross section for formation of the first (doorway) state is usually taken equal to optical model absorption cross section. The phenomenological exciton models, properly grasp a physical process of equilibration and preequilibrium emission and generally perform quite well in practical applications. They do miss, however, high energy component of the neutron spectra that is expected to be related to direct scattering to the collective structures in the continuum. This fact was one of the motivations for developing more rigorous quantum approaches that maintain original Griffin's idea of evolution through the chain of classes with increasing complexity but use more fundamental physics concepts to describe the process.

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The two most recent quantum approaches to the preequilibrium mechanism are FKK [6] and the Heidelberg formulation ([7, 8]). Both approaches make use of splitting exciton configurations into those belonging to the P-space (i.e. containing at least one unbound particle) and those belonging to the Q-space in which all particles are bound. This distinction leads to the two distinct reaction mechanisms - Multi Step Direct (MSD) and Multi Step Compound (MSC) respectively. The two mechanisms are connected as a two-body interaction between nucleons may bring P-space configuration to the Q-space and vice versa (the latter being less probable). Naturally, the split necessitates partition of the incoming flux between Q and P spaces. The consequences of such partition are major subject of this paper. Our considerations are based on the model calculations in which we change assumptions regarding the partition between Q and P spaces.

2 The model

We use the nuclear reaction code EMPIRE [4] which in addition to the Heidelberg formulation of MSC and Tamura, Udagawa, Lenske [9, 10] formulation of MSD includes also exciton model (PCROSS) option. This allows for direct comparison of classical and quantum formulations of preequilibrium emission maintaining the same other parts of the calculations (such as Coupled Channels in the incident channel and compound nucleus decay). The TUL approach is coded in the ORION and TRISTAN codes, both incorporated in the EMPIRE.

The original EMPIRE implementation of the Heidelberg MSC is detailed in Ref. [11]. Taking into account it has been published over 30 years ago we summarize below salient points of the formulation and implementation. The MSC cross-section leading from the incident channel a to the exit channel b reads

$$\frac{d\sigma_{ab}}{dE} = (1 + \delta_{ab}) \sum_{n,m} T_n^a \Pi_{n,m} T_m^b \,, \tag{1}$$

where kinematic and angular-momentum factors are omitted. The summation is over all classes n and m. The transmission coefficients T_n^a coupling channel a and class n are given as

$$T_n^a = \frac{4\pi^2 U_n^a}{(1 + \pi^2 \sum_m U_m^a)^2} \,, \tag{2}$$

where $U_n^a = \rho_n^b \langle W_{n,a} \rangle$ is defined by the average bound level density ρ_n^b of class n, and by average matrix elements $W_{n,a}$ connecting channel a with the states in class n. The inverse of the transport matrix Π_{nm} reads

$$(\Pi^{-1})_{nm} = \delta_{nm}(2\pi\rho_n^b)(\Gamma_n^{\downarrow} + \Gamma_n^{ext}) - (1 - \delta_{nm}) 2\pi\rho_n^b \overline{V_{n,m}^2} 2\pi\rho_m^b \tag{3}$$

with the mean squared matrix element $\overline{V_{n,m}^2}$ coupling states in classes n and m, the average spreading width $\Gamma_n^{\downarrow}$ of states in class n, and the average total decay width Γ_n^{ext}in class n. The spreading width $\Gamma_n^{\downarrow}$ is expressed trough the mean squared matrix element $\overline{V_{n,m}^2}$

$$\Gamma_n^{\downarrow} = 2\pi \sum_m \overline{V_{n,m}^2} \rho_m^b \,. \tag{4}$$

Under the chaining hypothesis $\overline{V_{n,m}^2}$ couples only neighboring classes. The decay width Γ_n^{ext} is determined by the sum of the transmission coefficients T_n^a over all open channels

$$\Gamma_n^{ext} = (2\pi\rho_n^b)^{-1} \sum_a T_n^a \,. \tag{5}$$

Following Ref. [11] the microscopic quantities $\langle W_{n,a} \rangle$ and $\overline{V^2_{n,m}}$ are expressed in terms of the macroscopic ones. To define $\langle W_{n,a} \rangle$ EMPIRE uses Eq. (2) and equates it to the optical model transmission coefficient. The matrix element $\overline{V^2_{n,m}}$ is related to the imaginary part of the optical model potential $W(\epsilon)$ using Eq. (4) with

$$\Gamma_n^{\downarrow} = 2W(\epsilon) = 2 \times 0.03\epsilon^2, \tag{6}$$

where ϵ is the excitation (in MeV) of a single exciton with respect to the Fermi level. This equation has to be averaged over all particle-hole configurations in a given class n. We note that Eq. (6) removes essential free parameter (mean free-paths or squared matrix element M^2) which arbitrary scales predictions of the exciton model. It is replaced by the factor 0.03 in Eq. (6) as proposed in Ref. [12]. Although some uncertainty can be assigned to this factor it cannot be varied as liberally as M^2 in case of the exciton model.

Introducing P and Q-spaces does not exclude possibility of unbound configurations to become bound as a result of the two-body interaction. In fact, Eq. (1) allows for feeding higher MSC classes directly from the MSD chain. The sum (over m) corresponds to the population of various classes directly from the open channel space in addition to the transitions along the MSC chain. To this end EMPIRE employs phase-space approach proposed in Ref. [13]. It requires that the incoming flux split between the first MSD and MSC classes in proportion to the respective state densities and to the average value of the squared matrix elements coupling unbound to unbound ($\langle V^2_{uu} \rangle$) and unbound to bound states ($\langle V^2_{ub} \rangle$). With $R = \langle V^2_{ub} \rangle \mid \langle V^2_{uu} \rangle$, denoting the optical model transmission coefficient by T_{om}, the density of bound and unbound states in class n by ρ_n^b and ρ_n^u respectively, and their sum by ρ, the transmission coefficient populating the first MSC class may be written as

$$T_1 = T_{om} \frac{\langle V^2_{ub} \rangle \rho_1^b(E)}{\langle V^2_{ub} \rangle \rho_1^b(E) + \langle V^2_{uu} \rangle \rho_1^u(E)} = T_{om} \frac{R}{(R-1) + \frac{\rho_1(E)}{\rho_1^b(E)}} \tag{7}$$

The same reasoning may be applied to the flux remaining in the open space, which may enter the MSC chain in subsequent steps of the reaction. Assuming R to be independent of the class number the transmission coefficient T_n populating the n^{th} MSC class is written as

$$T_n = \left(T_{om} - \sum_{i=1}^{n-1} T_i \right) \frac{R}{(R-1) + \frac{\rho_n(E)}{\rho_n^b(E)}}. \tag{8}$$

By default, values of the matrix elements in Eq. (7) are set to be equal, i.e., R=1 is assumed.

3 Gradual absorption issue

The findings presented below are off-spin of the work on neutron induced reactions on ^{181}Ta for the forthcoming edition of the evaluated nuclear data library ENDF/B-VIII.1. Quasi-mono-isotopic ^{181}Ta comes with a benefit of relatively wealthy experimental coverage. There are several measurements of double-differential neutron emission spectra with incident neutrons between 5 and 20 MeV and different angles of outgoing neutrons. Such data are particularly sensitive to the reaction models involved in the calculations. Typically, the exciton model supplemented with the DWBA inelastic calculations to the arbitrarily set collective levels in the continuum would be used. The DWBA calculations are needed to describe the high energy part of the emission spectra. Our choice was to employ MSD/MSC mechanisms outlined in the previous section as they are founded on more solid physical ground being derived rigorously from the assumption of the Gaussian orthogonal ensemble. The MSC options used in the calculations were the following:

- Transmission coefficients calculated using matrix elements determined in the incident channel
- Spreading width to next class calculated using matrix element determined from the optical model imaginary part
- 2p-1h initial configuration with neutrons = 1.2, protons = 0.80 ($\sigma_{nn}/\sigma_{np} = 4$)
- Ratio of unbound-bound to unbound-unbound matrix elements set to 1.0
- 4-stage MSC calculations followed by the Hauser-Feshbach
- Single-particle level density set at $A/13$

There is, however, a problem that has been known for years - MSC/MSD calculations tend to underestimate central part of the neutron spectra as shown in Figs. 1 - 2. At incident neutrons of 5.19 MeV it is irrelevant since the MSD/MSC contribution is negligible. With increasing incident energy we see that MSD/MSC calculations (red lines) fall short of experimental data in the central part of the spectra. The discrepancy gets worse with increasing incident energy. The discrepancy is also larger for the backward angles where the relative contribution of the MSC mechanism is bigger than at MSD-dominated forward angles (not shown here because of the space limitations.) Therefore, the MSC mechanism seems likely to be responsible for the deficiency.

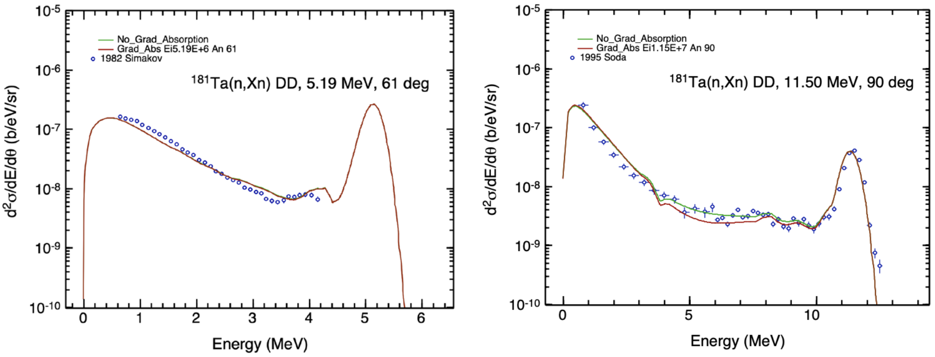

Figure 1. Effect of including gradual absorption on neutron emission spectra from ^{181}Ta hit by 5.19 and 11.5 MeV neutrons. Green lines refer to no-gradual-absorption while red ones take it into account.

Table 1. Population of MSC classes $Q(n)$ in ^{181}Ta at different incident neutron energies when using gradual-absorption. The last column (Σ) shows sum of Q1 trough Q4 that represents fraction of the incoming flux that gets involved in the MSC mechanism.

E (MeV)	Q1	Q2	Q3	Q4	Σ
5	0.60	0.35	0.04	0.001	0.991
11	0.26	0.38	0.27	0.08	0.99
14	0.19	0.30	0.30	0.16	0.95
20	0.11	0.18	0.24	0.23	0.76

Analyzing the implementation of the MSC we came to the conclusion that gradual absorption is responsible for the deficiency of the combined MSD/MSC calculations. Figs. 1 - 2 show that if the gradual absorption is turned off, i.e. total absorption flux is assumed to

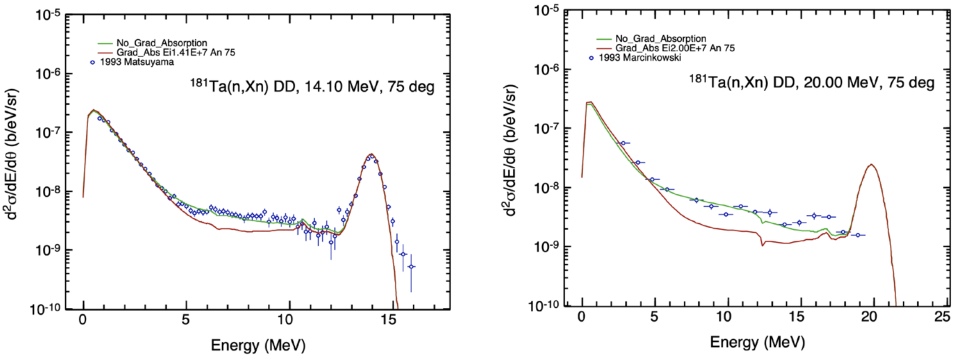

Figure 2. The same as Fig. 1 but at 14.1 and 20 MeV.

populate Q_1 space, it is possible to reproduce experimental data in the entire incoming and outgoing energy range (green lines). In a sense, it is close to the exciton model that does not make a distinction between P and Q spaces. The insight to the problem is given in Table 1 that, following Eq. (8), lists fractions of the absorption cross section that Q_n classes are populated due to the P-space coupling. With gradual absorption turned off the first Q class is fully populated and the fractions for all Q_1 classes would be one. With introduction of the gradual absorption population of the Q_1 is lower than one and decreases with increasing incident energy. The maximum of the population moves to higher class number as incident energy is increasing. As preequilibrium emission decreases with the class number introducing gradual absorption decreases the MSC contribution. In addition, the sum of Q_n populations is lower than one, which implies that remaining part of the absorption cross section is going straight to the compound nucleus mechanism lowering MSC contribution even further. These two effect are responsible for bringing MSC cross sections down.

The fact that turning off gradual absorption improves agreement with experimental neutron spectra is encouraging but there remains an essential theoretical problem since this assumption is unphysical. There is overwhelming evidence that MSD mechanism is necessary to describe neutron emission spectra. This implies a necessity to consider P and Q spaces in the preequilibrium decay. Having done this, we need to note that it is highly improbable, if not impossible, to create a bound(!) 2p-1h state at higher incident energies (say above 10 MeV). We admit that we've made this conclusion on the bases of pure phase-space considerations but Kawano came to the same inference using microscopic calculations [14]. Thus there seems to be an inconsistency between the theory (or rather its implementation) and the experimental evidence. While we do not question any of the two, we will analyze possible flaws in the implementation.

The implementation is far from ideal and there are several possibilities that come to mind while looking for possible solution to the gradual absorption problem. We remind that the two essential reasons for a problem are (i) shifting initial MSC population to higher classes and (ii) loosing part of the flux that avoids Q space. Therefore, below we focus on addressing these two issues.

Number of classes considered in the MSD. The scope of the ORION and TRISTAN codes are limited to the first two Q classes, which are not enough to allow all the flux to be dumped to the Q space. EMPIRE, however, applies Eq. (8) independently of the MSD calculations, so the MSC feeding from the P space continues. It is simply assumed that there is no MSD emission from higher classes. We were not in a position to test an effect of such emission but intuitively it seems that it would not make substantial difference since importance of MSD emission decreases with increasing number of excitons and the emission energy range remains about the same being defined by the distribution of the collective strength in the RPA response functions.

Number of classes considered in the MSC This number (4) could be easily extended but it would not affect calculations up to 14 MeV where the sum in Table 1 is close to one. It would slightly improve situation at 20 MeV but it is clear that the major player is the shift in the initial MSC population.

Change ratio of unbound->bound to unbound->unbound ($R = 1$) Making transitions from P space to Q space more likely than those within P space would solve the problem but we would need ratio of $R = 2.5$. Is there any plausible explanation for such disparity? Could there be some collectivity effects favoring creation of a bound particle-hole pair by the particle in the continuum in such a way that it itself becomes bound? Even if this were possible at lower incident energies it would not work at higher ones.

Backward transition P2 => Q1 This would be the most obvious way of shifting back MSC distribution but it is practically impossible to convert 3p-2h with unbound particle into 2p-1h bound configuration.

Spreading width in MSC Adjusting M^2 or mean free path is a standard way of adjusting classical preequilibrium calculations to experimental data. In the EMPIRE implementation of MSC this would mean to decrease the factor of 0.03 in Eq. (6). While the "universal" value of 0.03 allows for some degree of freedom our tests showed that even very drastic lowering of this factor does not save calculations at incident neutrons of 20 MeV. It confirms our previous conclusion that the shift in the initial MSC population is by far the most important.

Handling of spin and parity Spin and parity distributions in MSD emission are treated very approximately (see next section). Those in MSC are following compound nucleus coupling rather than Y-factors as defined in FKK. Spin and parity effects, however, are important for population of specific levels, especially isomers, but have very limited effect on reactions cross sections such as inelastic. It is very unlikely that better treatment of spin and parity would make for a difference we are looking for.

Summarizing above discussion we are not able to propose a satisfying solution for maintaining the gradual absorption in the MSD/MSC calculations in spite of physical necessity of keeping it. Favoring P-Q transitions with respect to P-P would be probably less controversial than assuming full absorption to the Q_1 class (as in all classical preequilibrium models) but this surmise would have to be tested at higher incident energies where the effect of the gradual absorption will suppress MSC contribution to a larger extent.

4 Spin distribution in preequilibrium emission

Evaluation of the chain of platinum isotopes provided another hint regarding preequilibrium emission. This time related to the spin distribution of states populated in the final nucleus. There are metastable states and unstable ground states in residues of (n,p) reaction on three Pt isotopes (194, 195 and 196). Experimental data are available for all of these six reactions (ground state and meta for each isotope). Since the population of isomeric states depends primarily on the spin of the levels and spin distribution of the continuum in residual nuclei such data provide valuable source of information about spin distribution of the levels in continuum which are populated in the (n,p) reactions. In the Pt calculations the exciton model has been used since MSC (even without gradual-absorption) was underestimating experimental (n,p) data. We note also that current MSD model in EMPIRE does not include charge-exchange reactions so it could not be used. It turned out that compound nucleus contribution to (n,p) reactions on Pt isotopes around 14-15 MeV is negligible and preequilibrium is a leading mechanism.

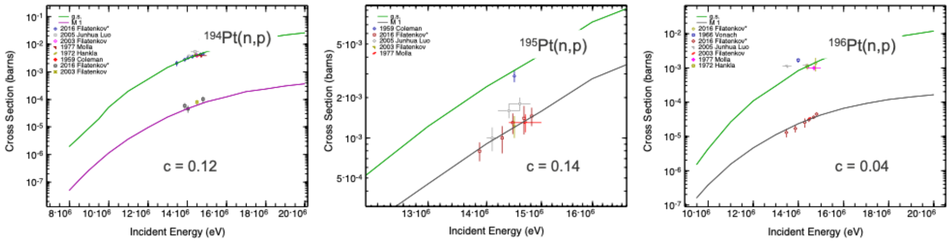

Figure 3. Calculated isomeric (grey or purple lines) and ground-state (green lines) cross sections for three isotopes of Pt compared with the experimental data. Values of c factors (Eq. 9), as used in the calculations, are shown in the plots.

The continuum population by exciton model is distributed proportionally to the spin distribution of 1p-1h states shifted by the spin of the target ground state as the exciton model code PCROSS does not consider explicitly angular distribution. Choice of the 1p-1h spin distribution reflects dominant contribution of the first step of the exciton model, which leaves the residual nucleus in the 2-exciton state. The spin-cutoff parameter determining the width of spin distribution of exciton states is usually taken in the form [15]

$$\sigma^2 = m \times c \times A^{2/3}, \tag{9}$$

where m is a number of excitons, c is a factor estimated to be 0.24 in combinatorial calculations [15] and A is the mass of a nucleus.

After adjusting model parameters to fit total (n,p) cross sections (see Fig. 3), it turned out that isomeric and ground state cross sections are calculated poorly, which clearly indicates problem with the spin distributions. In order to reproduce trusted experimental data the c factor in Eq. (9) had to be decreased down to 0.12, 0.14 and 0.04 for ^{194}Pt, ^{195}Pt and ^{196}Pt targets respectively. It implies that preequilibrium mechanism populates states of lower spin which is consistent with the $l = 0, 1$ angular momenta transfer dominating MSD emission (we may consider exciton model as a classical substitute for MSD). This observation is confirmed by the microscopic calculations reported in Ref. [16] that also call for a much smaller spin-cuttoff parameter than suggested by Eq. (9).

5 Conclusions

We have shown that MSD/MSC calculations of neutron induced reactions on ^{181}Ta suffer from underestimation of the neutron emission spectra in the middle of the emissive energy range that gets worse with increasing incident energy. This deficiency can not be cured with a simple change of model parameters and appears to be a more fundamental problem. We have identified the gradual absorption as a source of the discrepancy since assuming full absorption of the incoming flux to the Q_1 class works very well for neutron spectra emitted from n + ^{181}Ta. On the other hand, it is obvious that at incident neutron energies exceeding 50 MeV (optical depth of the real potential plus neutron binding energy) there is just no possibility of creating a bound 2p-1h configuration and all the incoming flux has to go through the P-space chain before it can eventually populate Q-space leading to the compound nucleus formation. Therefore, some form of gradual absorption must be built into our calculations. We were not able to pinpoint any detail of the MSC implementation that could save phase-space based partition of the incoming flux in the practical calculations. Thus, ignoring the gradual absorption is the most convenient way to go but the very nature of the problem remains open for investigation. One of the possibilities would be creation of the applicable model in which MSD and MSC chains are treated coherently within the same framework and the gradual absorption comes out naturally. Neutron spectra above 20 MeV would be necessary to validate such a model.

We have also confirmed findings of Ref. [16] calling for substantially lower spin-cutoff parameters for spin distributions of exciton states in final nuclei. This does not necessarily invalidate Eq. (9) that simply counts a number of possibilities that m particles occupying single-particle levels can couple to a given total angular momentum. The direct reactions, however, follow their own rules and couple residual states that are compatible with the ground state spin and the direct reaction l-value transfer.

Finally, we bring up an issue of developing applicable MSD formulation that would account for P-Q coupling and charge-exchange reactions. Ideally, such formulations should also allow for more than 2 classes and explicit angular momentum coupling.

References

[1] T. Kawano, Springer Proceedings in Physics **254**, 27 (2021), CNR2018: International Workshop on Compound Nucleus and Related Topics, LBNL, Berkeley, CA, USA, September 24 – 28, 2018, J. Escher, Y. Alhassid, L.A. Bernstein, D. Brown, C. Fröhlich, P. Talou, W. Younes (Eds.)

[2] A. Koning, D. Rochman, Nuclear Data Sheets **113**, 2841 (2012), special Issue on Nuclear Reaction Data

[3] O. Iwamoto, N. Iwamoto, S. Kunieda, F. Minato, K. Shibata, Nuclear Data Sheets **131**, 259 (2016), special Issue on Nuclear Reaction Data

[4] M. Herman, R. Capote, B. Carlson, P. Obložinský, M. Sin, A. Trkov, H. Wienke, V. Zerkin, Nuclear Data Sheets **108**, 2655 (2007), special Issue on Evaluations of Neutron Cross Sections

[5] J.J. Griffin, Phys. Rev. Lett. **17**, 478 (1966)

[6] H. Feshbach, A. Kerman, S. Koonin, Ann. of Phys. **125**, 429 (1980)

[7] H. Nishioka, J.J.M. Verbaarschot, H.A. Weidenmüller, S. Yoshida, Ann. Phys. **172**, 67 (1986)

[8] H. Nishioka, H. Weidenmüller, S. Yoshida, Annals of Physics **183**, 166 (1988)

[9] T. Tamura, T. Udagawa, H. Lenske, Phys. Rev. **C26**, 379 (1982)

[10] H. Wienke, R. Capote, M. Herman, M. Sin, Phys.Rev. C **78**, 064611 (2008)

[11] M. Herman, G. Reffo, H. Weidenmüller, Nucl. Phys. **A536**, 124 (1992)

[12] C. Mahaux, P. Bortignon, R. Broglia, C. Dasso, Phys. Rep. **120**, 1 (1985)

[13] A. Marcinkowski, J. Rapaport, R. Finlay, C. Brient, M. Herman, M. Chadwick, Nuclear Physics A **561**, 387 (1993)

[14] T. Kawano, Phys. Rev. C **59**, 865 (1999)

[15] M. Herman, G. G. Reffo, Phys. Rev. C **36**, 1546 (1987)

[16] M. Kerveno, M. Dupuis, A.. Bacquias, Phys. Rev. C **104**, 044605 (2021)