

Deformation-dependent Tamura-Udagawa-Lenske multistep direct model

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The multistep direct TUL model has been extended in order to account for nuclear deformation. The new formalism was tested in calculations of neutron emission spectra from the $^{232}\text{Th}(n, xn)$ reaction. These calculations include vibration-rotational coupled channels for the inelastic scattering to low-lying collective levels, “deformed” multistep direct (MSD) for inelastic scattering to the continuum, multistep compound, and Hauser-Feshbach with advanced treatment of the fission channel. Prompt fission neutrons were also calculated. The comparison with experimental data shows clear improvement over the “spherical” MSD calculations and JEFF-3.1 and JENDL-3.3 evaluations. Similar calculational results have been obtained of neutron emission spectra from the stable deformed nuclei ^{181}Ta and ^{184}W .

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I. INTRODUCTION

An approach to direct inelastic scattering to the continuum, i.e., the dense part of the excitation spectrum of the nucleus, is provided by the quantum-statistical multistep direct theory of preequilibrium direct processes, originally formulated by Tamura, Udagawa, and Lenske (TUL) [1] and extended with respect to statistical and dynamic treatment of nuclear structure by Lenske *et al.* [2]. The statistical assumptions involved lead to a description of the preequilibrium direct process as a sum of n -step DWBA cross sections with average state-independent form factors and a coherent treatment of the propagation of the intermediate channels, each n -step term being folded with a product of n nuclear spectroscopic strength functions. These spectroscopic strength functions specify the nuclear response on the external one-body interaction. It is assumed that the closed channel space, i.e., the multistep compound contributions (MSC) have been projected out and can be treated separately within the multistep compound mechanism [3]. In the TUL model as developed by Lenske *et al.* [2] the spectroscopic strength functions are derived assuming the scattering nucleus to be spherical. This approach, as implemented in the EMPIRE-2.19 code [4,5], predicts well double-differential neutron emission spectra from the quasispherical ^{93}Nb nucleus induced by 14.1 MeV neutrons (see, e.g., EMPIRE-2.19 manual [4], p. 158). However, similar inelastic emission spectra from the deformed nucleus ^{232}Th induced by $E_{\text{inc}} \geq 6.1$ MeV neutrons, are severely underpredicted in the region of direct inelastic scattering to

the continuum. To address this deficiency the above TUL approach has been extended to account for nuclear deformation and incorporated into the EMPIRE-3.0 [6] code which has been applied in calculations of double-differential neutron emission spectra from the $^{232}\text{Th}(n, xn)$ reaction and, in addition, from the $^{181}\text{Ta}(n, xn)$ and $^{184}\text{W}(n, xn)$ reactions. The extended formalism is outlined in Sec. II. Section III gives details of calculations. Computed results are compared with experimental data [7–9,29–31] and existing evaluations in Sec. IV. Finally, Sec. V contains the conclusions.

II. TUL FORMALISM

In the TUL model, as developed by Lenske *et al.* [2], the averaged n -step cross section for inelastic scattering is obtained as

$$\begin{aligned} \frac{d^2\sigma^{(n)}}{dEd\Omega} &= \sum_{\lambda_1 \dots \lambda_n} \int dE_1 \dots dE_n \delta(\Sigma E_i) \prod_i S_{\lambda_i}(E_i) \\ &\times |(\chi_E^{(-)} | F_{\lambda_n}(E_n) G^{\text{opt}}(E_{n-1}) \dots \dots \\ &\times G^{\text{opt}}(E_1) F_{\lambda_1}(E_1) | \chi_0^{(+)} |)^2, \end{aligned} \quad (1)$$

where $\chi^{(\pm)}$ are distorted waves, F_λ averaged form factors with multipolarity λ , G^{opt} the Green function for the optical model potential, and $S_\lambda(E)$ is the particle-hole transition strength function for an excitation energy E , from the ground state or a reference state, and transferred angular momentum λ . The one-step cross section is

$$\frac{d^2\sigma^{(1)}}{dEd\Omega} = \sum_\lambda S_\lambda(E) \left(\frac{d\sigma}{d\Omega} \right)_\lambda \quad (2)$$

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with $(\frac{d\sigma}{d\Omega})_\lambda$ an average DWBA cross section. The two-step cross section is expressed as

$$\frac{d^2\sigma^{(2)}}{dE d\Omega} = \sum_{\lambda_1 \lambda_2} \int dE_1 S_{\lambda_1}(E_1) S_{\lambda_2}(E - E_1) \times |\langle \chi^{(-)}(E) | F_{\lambda_2} G^{\text{opt}}(E - E_1) F_{\lambda_1} | \chi^{(+)}(0) \rangle|^2. \quad (3)$$

Here the total response of the intrinsic system at an energy loss E is contained in the first and second step transition strength functions. The folding accounts for the partitions of the total energy E into first- and second-step parts such that E is conserved.

A. Spherical nuclei

The transition strength function for the external one-body operator $U_\lambda = v(r)Y_\lambda$ is calculated as

$$S_\lambda(E) = -\text{Im} \frac{1}{\pi} \langle \Phi_0 | U_\lambda^\dagger G_\lambda^{\text{intr}}(E + i\Gamma/2) U_\lambda | \Phi_0 \rangle = \text{Im} \frac{1}{\pi} \chi_\lambda(E + i\Gamma/2) \quad (4)$$

with χ_λ the response function for the operator U_λ , Γ the spreading width [4], $|\Phi_0\rangle$ the nuclear ground state or a reference state and $G_\lambda^{\text{intr}}(E)$ the intrinsic nuclear Green function or propagator with multipolarity λ . The latter contains the information about the nuclear structure. Configuration mixing of 1p-1h excitations, and correlations in the reference state, due to the residual 1p-1h interaction, are treated within the framework of the random phase approximation (RPA) which corresponds to summing the complete series of 1p-1h interaction diagrams. By taking into account also pairing correlations the excitations are given in terms of two-quasiparticle (2qp) rather than 1p-1h configurations. In 2qp RPA (QRPA) the intrinsic Green function is then given in terms of the uncorrelated 2qp Green function by a Bethe-Salpeter (B-S) equation [10]:

$$G_\lambda^{\text{intr}}(E) = G_\lambda^{\text{QRPA}}(E) = G_\lambda^{2qp}(E) + V G_\lambda^{2qp}(E) G_\lambda^{\text{QRPA}}(E) \quad (5)$$

with V the 1p-1h residual interaction. For spherical nuclei the uncorrelated 2qp Green function is given as [11]

$$G_\lambda^{2qp}(E) = - \sum_{\alpha \leq \beta} [c_{j_\beta}^\dagger \otimes c_{j_\alpha}]^\lambda | \Phi_0 \rangle \langle \Phi_0 | [c_{j_\alpha}^\dagger \otimes c_{j_\beta}]^\lambda \times \left(\frac{1}{E_\alpha + E_\beta - E - i\eta} + \frac{1}{E_\alpha + E_\beta + E - i\eta} \right) \times (u_\alpha v_\beta + v_\alpha u_\beta), \quad (6)$$

where the spin-spherical tensors $c_{j_\beta}^\dagger$ and c_{j_α} operating to the right, are particle and hole creation operators for the spherical sp states $n_\beta l_\beta j_\beta$ and $n_\alpha l_\alpha j_\alpha$, respectively. v_α^2 and v_β^2 the BCS occupation probabilities, $u_\alpha^2 = 1 - v_\alpha^2$, and E_α, E_β the quasiparticle energies.

Assuming a separable residual particle-hole interaction of the form $V^{\text{sep}}(1, 2) = \sum_\lambda \kappa_\lambda U_\lambda(1) U_\lambda(2)$, with κ_λ being a coupling constant, and using Eqs. (4) and (5), the QRPA

correlated response function for the operator U_λ may be written as

$$\chi_\lambda^{\text{QRPA}}(E) = \chi_\lambda^{2qp}(E) + \kappa_\lambda \chi_\lambda^{2qp}(E) \chi_\lambda^{\text{QRPA}}(E) \quad (7)$$

with $\chi_\lambda^{2qp}(E) = \langle \Phi_0 | U_\lambda^\dagger G_\lambda^{2qp}(E) U_\lambda | \Phi_0 \rangle$ the uncorrelated 2qp response function.

B. Extension to deformed nuclei

In case of a deformed Hamiltonian the sp (and qp) wave functions are not eigenfunctions of the angular momentum squared L^2 . If, however, symmetry exists with respect to the deformation axis both parity π and angular momentum projection K onto this axis are still conserved. When the deformed sp wave function is expanded into spherical components the wave function in the nominator of Eq. (6): $[c_{j_\beta}^\dagger \otimes c_{j_\alpha}]^\lambda | \Phi_0 \rangle$ is substituted by

$$\sum_{j_\alpha j_\beta L} s_{k_\beta}^{j_\beta} s_{k_\alpha}^{j_\alpha} [c_{k_\beta}^\dagger \otimes c_{k_\alpha}^\dagger]^\lambda | \Phi_0 \rangle, \quad (8)$$

where $s_{k_\alpha}^{j_\alpha}$ is the fractional occupation number for the spherical j_α component of the deformed sp wave function with azimuthal quantum number k_α and $K = k_\alpha - k_\beta$ (see also [12]). From expression (8) it is clear that the ‘‘deformed’’ Green function is not diagonal with respect to angular momentum and the uncorrelated 2qp multipole response function for the external one-body field $U_{\lambda,K} = v_{\lambda,K}(r)Y_\lambda^K$ is then

$$\chi_{\lambda\lambda',K}^{2qp}(E) = \langle \Phi_0 | U_{\lambda,K}^\dagger G_{\lambda\lambda',K}^{2qp}(E) U_{\lambda',K} | \Phi_0 \rangle. \quad (9)$$

The QRPA correlated response function is obtained in the schematic RPA from the B-S equation for each K [13]:

$$\chi_{\lambda\lambda',K}^{\text{QRPA}}(E) = \chi_{\lambda\lambda',K}^{2qp}(E) + \sum_{\lambda''} \kappa_{\lambda\lambda'',K} \chi_{\lambda\lambda'',K}^{2qp}(E) \chi_{\lambda''\lambda',K}^{\text{QRPA}}(E). \quad (10)$$

The multipole spectroscopic strength function:

$$S_\lambda(E) = -\text{Im} \frac{1}{\pi} \langle \Phi_0 | \sum_{\lambda',K} U_{\lambda',K}^\dagger G_{\lambda\lambda',K}^{\text{QRPA}}(E + i\Gamma/2) U_{\lambda,K} | \Phi_0 \rangle = -\text{Im} \frac{1}{\pi} \sum_K \chi_{\lambda,K}^{\text{QRPA}}(E + i\Gamma/2) \quad (11)$$

is however still diagonal with respect to angular momentum λ [13] and from Eq. (10) it follows that $\chi_{\lambda,K}^{\text{QRPA}}$ is calculated as

$$\chi_{\lambda,K}^{\text{QRPA}}(E) = \chi_{\lambda\lambda,K}^{2qp}(E) + \sum_{\lambda'} \kappa_{\lambda\lambda',K} \chi_{\lambda\lambda',K}^{2qp}(E) \chi_{\lambda\lambda',K}^{\text{QRPA}}(E). \quad (12)$$

Equation (12) differs from Eq. (7) as it includes also couplings between different transfer spins in the second term of the right-hand side. As Eq. (12) is valid for each separate particle-hole excitation with definite parity, only angular momenta with the same parity are coupled to each other.

III. EMPIRE CALCULATIONS

The updated TUL formalism has been implemented in the EMPIRE-3.0 code [6] and applied in calculations of double-differential neutron emission spectra from $n+^{232}\text{Th}$. Results of such calculations in which deformed sp states were obtained from a spherical Nilsson Hamiltonian plus a quadrupole deformation, have been presented in a previous paper [14]. In this paper we present and discuss results of similar calculations in which inelastic neutron scattering to the quasicontinuum ($E_{\text{exc}} \geq 1.19$ MeV) has been treated using more realistic deformed Woods-Saxon sp levels and wave functions as generated by the WSBETA code [15] (see also [16]).

In WSBETA the sp states are obtained by diagonalizing the (spherical or deformed) Woods-Saxon Hamiltonian in an axially symmetric harmonic oscillator basis. The resulting deformed wave functions are then presented as linear combinations of axially symmetric harmonic oscillator eigenfunctions in cylindrical coordinates. As the MSD module TRISTAN of the EMPIRE code assumes H.O. eigenfunctions in spherical coordinates the WSBETA results were converted into spherical symmetry representation according to the relations of Talman [17] (see also [18]).

The “optimal” parametrization of the Woods-Saxon potentials for neutrons and protons, intrinsic in the WSBETA code, was used. In this parametrization the systematics of the experimental data on both spherical and deformed odd-mass nuclei have been taken into account simultaneously (see for more details [15] and references therein). The deformations $\beta_2 = 0.213$, $\beta_4 = 0.066$, and $\beta_6 = 0.013$ are taken from the dispersive CC neutron optical model potential for ^{232}Th of Soukhovitskii *et al.* [19]. The calculated Fermi energies (BCS values) are -5.76 MeV and -6.65 MeV for neutrons and protons, respectively, rather close to the experimental values of -5.6 and -6.4 MeV.

While the aforementioned diagonalization procedure in an harmonic oscillator basis is a reliable method to obtain bound states, positive-energy solutions, at the other hand, depend strongly upon the dimension N of the basis, in that sense that increasing N in general results in lowering of the energy eigenvalues. Below the barriers consisting of the centrifugal and spin-orbit terms and the Coulomb barrier for protons, however, the (positive-) energy eigenvalues remain constant for a range of N values, approximating the sp resonance energies, and therefore may be considered as relatively stable [15]. The diagonalization method in WSBETA does not allow for calculating resonance widths.

The MSD treatment, involving one- and two-step calculations, has been applied for incident neutron energies above 4.5 MeV, where its contribution is sizable. The spherical part of the afore mentioned optical model potential of Soukhovitskii *et al.* was used, as quoted in the RIPL library (RIPL 608) [21], in the calculation of the initial and final distorted waves and the propagation of the intermediate channel. The off-diagonal couplings in the “deformed” Bethe-Salpeter equation (12) were included in the MSD calculation. The convergence turned out to be rather fast. For the quadrupole response, for example, only angular momentum $\lambda = 0, 2$, and 4 need to be included (see also [13]). The off-diagonal terms appeared to contribute

only a few percent to the MSD cross sections. The inelastic-scattering cross sections to excited levels in the discrete region ($E_{\text{exc}} < 1.19$ MeV) and the neutron transmission coefficients for the neutron channel were obtained with the coupled-channel code ECIS03 [20] incorporated in EMPIRE-3.0. The same CC optical model potential of Soukhovitskii *et al.* was used. 19 levels, five from the ground-state rotational band and the few lowest from the $K^\pi = 0^+$ (730.5 keV) β -vibration, $K^\pi = 2^+$ (785.5 keV) γ -vibration, and $K^\pi = 0^+$ (1078.7 keV) anomalous quadrupole vibrational bands as well as the $K^\pi = 0^-$ (714.25 keV) octupole vibrational band [22], were coupled simultaneously within the vibration-rotational model [20,23]. It was found that inclusion of additional members of the above bands in the coupling does not change the results of calculations noticeably in comparison with the original coupling scheme [19]. The dynamical deformations of the phonons involved were taken from literature or obtained by adjustment to the data. Preequilibrium compound neutron emission was calculated in the Heidelberg multistep compound (MSC) approach [3]. The total preequilibrium neutron emission spectra was obtained as an incoherent sum of both MSD and MSC contributions. Equilibrium compound decay was treated within the Hauser-Feshbach statistical model [24] with fission decay probabilities obtained in the optical model for fission [25]. The total neutron emission spectra also include prompt fission neutrons [26].

As fission complicates the analysis, in addition (n, xn) spectra from the nonfissile deformed nuclei ^{181}Ta , at $E_{\text{inc}} = 14.1$ MeV, and ^{184}W , at $E_{\text{inc}} = 11.5$ MeV, have been calculated. The CC optical neutron potentials RIPL 1488 [27] and RIPL 423 [28] from the RIPL-2 database were used, respectively. The static deformations included in these potentials were employed in generating the deformed Woods-Saxon sp levels with the WSBETA code, which determine the response functions for the deformed MSD calculation. As for the discrete level region, only the ground state rotational band members were included in the CC calculation.

IV. RESULTS AND DISCUSSION

The calculated cross sections versus incident neutron energy of the competing $^{232}\text{Th}(n, 2n)$ and $^{232}\text{Th}(n, f)$ processes nicely agree with the experimental data (not shown in this paper but see [14]). The left-hand plots in Fig. 1 present the EMPIRE-3.0 calculations of the double-differential neutron emission spectra from the $^{232}\text{Th}(n, xn)$ reaction, with above deformed Woods-Saxon sp states versus the ones obtained from the spherical Nilsson potential (default in the released 2.19 version of EMPIRE), together with the experimental data for selected forward emission angles at incident neutron energies 11.9 [7], 14.1 [8], and 18 MeV [9], respectively. The EMPIRE-3.0 calculations accounting for nuclear deformation in MSD, well reproduce the data in the direct quasicontinuum region ($\sim 5 \geq E_{\text{exc}} \geq 1.19$ MeV) while the “spherical” calculations underpredict the same data by a factor ~ 3 – ~ 6 . The right-hand plots show the corresponding double-differential neutron emission spectra from the JENDL-3.2 and JEFF-3.1 evaluations and the recent IAEA evaluation [26] adopted for

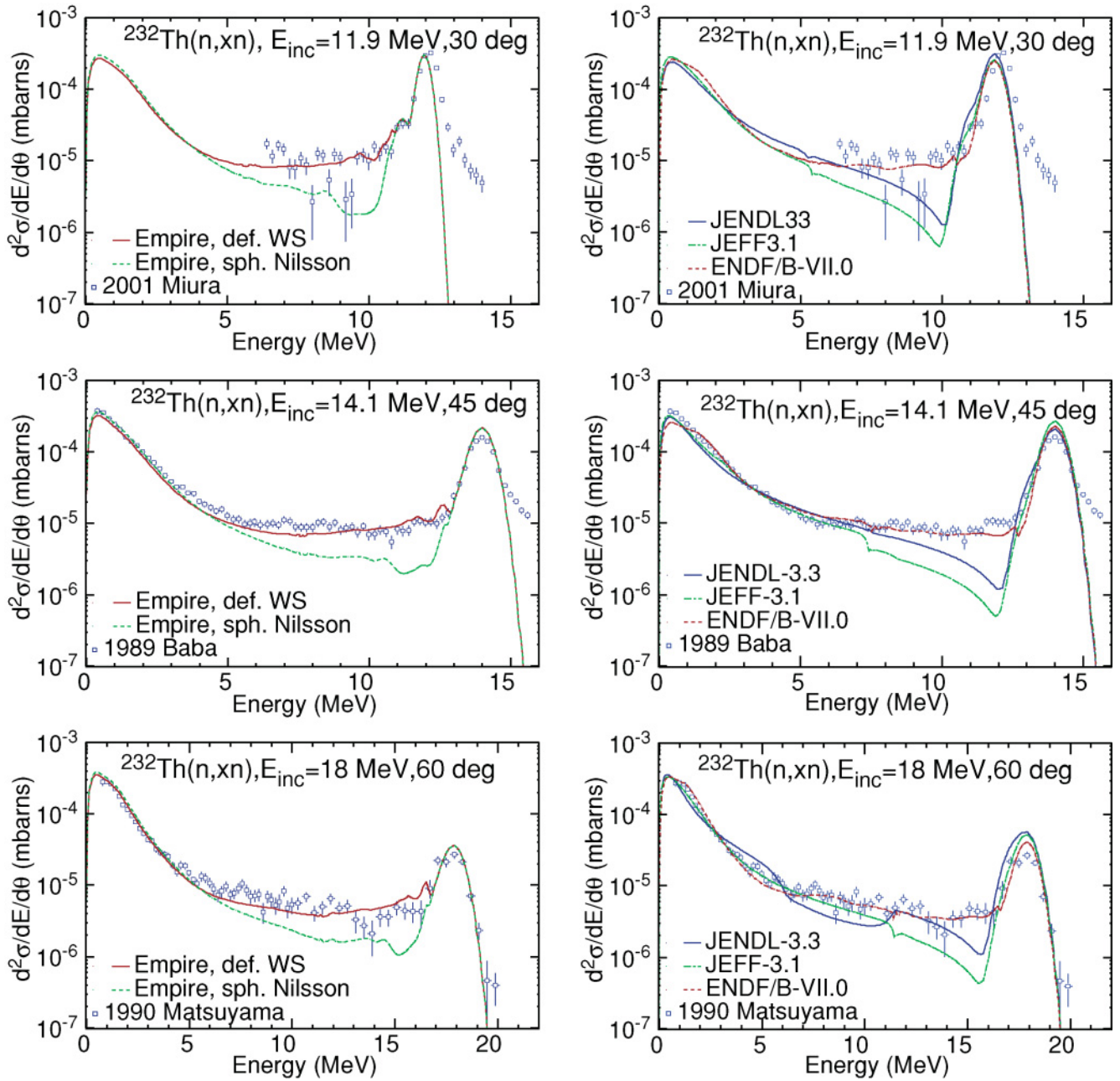


FIG. 1. (Color online) $^{232}\text{Th}(n, xn)$, $E_{\text{inc}} = 11.9, 14.1$ and 18 MeV results with deformed Woods-Saxon MSD (solid) and spherical Nilsson MSD (dotted) (left), ENDF-B-7.0 (dotted), JEFF-3.1 (dashed) and JENDL-3.3 (solid) data (right).

the ENDF/B-VII.0 library [32]. The “deformed” EMPIRE results show overall better agreement with the measurements than the corresponding JENDL-3.2 and JEFF-3.1 evaluations and similar agreement as the IAEA evaluation. It should be stressed that, except for adjustment of dynamic deformations used in the coupled-channel calculations and the fission input taken over from the previous exercise [25,26], the present results were obtained without any additional parameter fitting, i.e., there was no adjustment of the MSD part of the calculations, the part that forms the essence of this paper. In the IAEA evaluation for ^{232}Th the missing strength in the continuum region of the neutron spectrum was filled

up with DWBA to a large number of fictitious collective levels embedded in the continuum. Similar approach has also been used in other ENDF/B-VII evaluations for important actinides, such as $^{235,238}\text{U}$ and ^{239}Pu [32,33]. Subsequent validation proved that the thus obtained improvements of inelastic scattering data largely improved data performance in integral benchmarking [34]. Obviously our “deformed” MSD approach allows to achieve similar result on a physically sound basis.

The use of the sp eigenenergies and wave functions, derived, in our present work, from realistic deformed Woods-Saxon potentials, results in a slight but noticeable improvement of

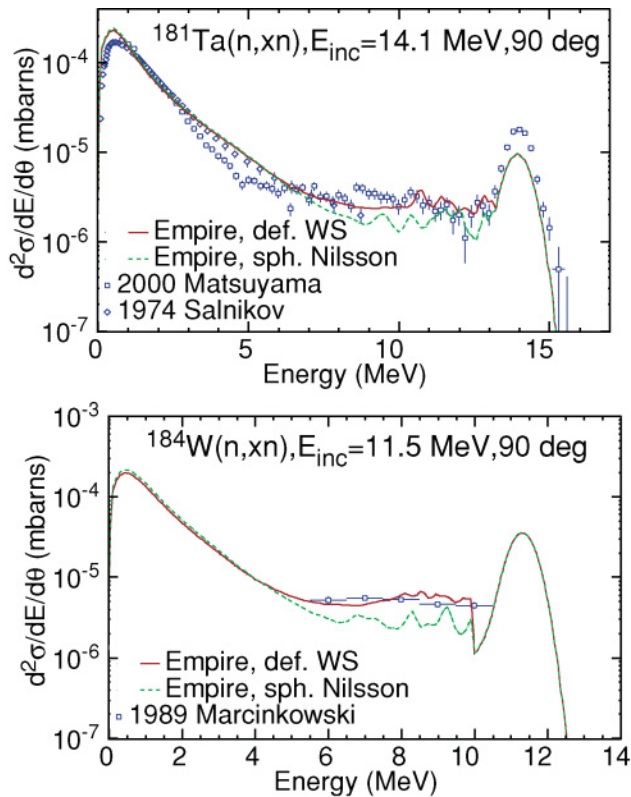


FIG. 2. (Color online) Results of EMPIRE calculations with deformed Woods-Saxon MSD (solid) and spherical Nilsson (dotted) for $^{181}\text{Ta}(n, xn)$ (above) and $^{184}\text{W}(n, xn)$ (below).

the descriptions of the emission spectra, particularly at higher incident neutron energies (14.1 and 18 MeV), compared to the ones presented in Ref. [14], which were obtained using sp states derived from the simple deformed Nilsson potential.

Recently Dupuis *et al.* [12] have reported results of MSD calculations of neutron-emission spectra from ^{238}U , at incident neutron energies 11.8, 14.2, and 18 MeV. The inelastic scattering to the continuum was obtained using microscopic DWBA to deformed Hartree-Fock-BCS states. Their results show some missing strength in the high-energy region of the spectra, in contrast with our MSD results. It should be noted that they did not use a residual p-h interaction which accounts for collectivity. In the TUL approach, however, configuration mixing due to p-h correlations is treated with the (Q)RPA

method. Furthermore, Dupuis *et al.* only consider the one-step (DWBA) process, while in our MSD calculations also two-step processes are included which describe two-phonon excitations.

The neutron emission spectra from (n, xn) reactions at the nonfissile deformed nuclei ^{181}Ta and ^{184}W , calculated with deformed and spherical response functions, are presented in Figs. 2(a) and 2(b), respectively, together with the $E_{\text{inc}} = 14.1$ MeV $^{181}\text{Ta}(n, xn)$ data of Matsuyama *et al.* [29] and Salnikov *et al.* [30], and the $E_{\text{inc}} = 11.5$ MeV $^{184}\text{W}(n, xn)$ data of Marcinkowski *et al.* [31]. Also here the results obtained with the deformed response functions show a clearly better agreement with the data than those obtained with the spherical ones in the energy range where MSD is important. However, the differences between both calculational results are somewhat smaller than those between the $^{232}\text{Th}(n, xn)$ ones.

V. CONCLUSIONS

The multistep direct TUL model, as developed by Lenske *et al.* [2] has been extended in order to account for nuclear deformation of the target nucleus. The new formalism has been implemented in the EMPIRE-3.0 code. Deformed response functions have been derived from realistic Woods-Saxon sp states obtained with the WSBETA code [15].

Calculations of double-differential neutron emission spectra from the $^{232}\text{Th}(n, xn)$, $^{181}\text{Ta}(n, xn)$ and $^{184}\text{W}(n, xn)$ reactions, based upon this formalism, show a substantially improved agreement with experimental data in the MSD dominated range and, as for $^{232}\text{Th}(n, xn)$, also in comparison with corresponding JENDL-3.2 and JEFF-3.1 evaluations and in similar agreement with measurements as the latest IAEA evaluation. This improvement is attained by advancing physical contents of the model rather than by forcing parameter values or patching the model.

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