frescoPRC

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The tool frescoPRC has been created to easily generate inputs for the nuclear reaction program FRESCO[1] [3] that describe the scattering of neutrons by even and odd actinides using a dispersive optical model with effective couplings between bands presented in [1]. In said article, calculations were done with the nuclear reaction program OPTMAN [2] but its use is limited compared to others more popular like FRESCO, so it could be useful for the nuclear physics community to be able to do this kind of calculations in a more widely used program. The tool frescoPRC uses as input the parameters that define the dispersive optical potential given in Table I of [1]. In addition to this, the effective parameters of the target, presented in the Table IV of [1] for ^{238}U and in Table VI for ^{239}Pu, as well as the energy scheme of the target are part of frescoPRC's input. Beside this, the energy of the neutron and some integration parameters also have to be included in the tool's input.

Volume	Surface	Spin-orbit	Coulomb
V_0 = 50.41 + 0.0292 (A - 238) MeV		V_{spo} = 5.64 MeV	C_{coul} = 1.36 MeV
λ_{HF} = 0.00977 MeV^{-1}	-	λ_{so} = 0.005 MeV^{-1}	
C_{viso} = 17.5 MeV			
A_v = 11.91 MeV	W_0 = 17.70 MeV	W_{spo} = -3.1 MeV	
B_v = 81.86 MeV	B_s = 10.85 MeV	B_{so} = 160 MeV	
E_a = 55 MeV	C_s = 0.01331 MeV^{-1}		
α_v = 0.355 MeV$^{1/2}$	C_{wiso} = 29.0 MeV		
r_{HF} = 1.2490 - 0.00171 (A - 238) fm	r_s = 1.1701 + 0.0041 (A - 238) fm	r_{so} = 1.1214 fm	
a_{HF} = 0.638 + 0.002190 (A - 238) fm	a_s = 0.617 fm	a_{so} = 0.59 fm	
r_v = 1.2657 fm			r_c = 1.12894 fm
a_v = 0.6960 - 0.00021 (A - 238) fm			a_c = 0.547 fm

Table I: Dispersive optical-model parameters for dispersion of neutrons by actinides presented in [1].

Target	β_{20}	β_{40}	β_{60}
^{238}U	0.231	0.062	-0.0096
^{239}Pu	0.236	0.086	-0.0310

Table II: Static axial deformation parameters for ^{238}U and ^{239}Pu given in [1].

[1] More specifically, it has been created to be compatible with the version *frxy6j* of FRESCO modified to be able to define states grouped by bands.

Bands	Deformation parameters
β-band	$[\beta_2]_{\text{eff}} = 0.1039$
γ-band	$[\gamma_{20}]_{\text{eff}} = 0.0476$
Octupole band	$[\beta_{30}]_{\text{eff}} = 0.2684$
γ-band (non-axial)	$[\gamma_{22}]_{\text{eff}} = 0.3030$

Table III: Effective deformation parameters for ^{238}U. This numerical values do not coincide with ones presented in the table IV of [1] because they are multiplied by β_{20} to meet OPTMAN's convention. With this said, effective parameters in table IV of [1] are actually $\beta_{20} \times [\beta_\lambda]^{\text{eff}}$.

Bands	Deformation parameters
Octupole band (axial)	$\alpha(1/2, 1/2) \times [\beta_{30}]_{\text{eff}} = 0.2627$
γ-band (non-axial)	$\alpha(5/2, 1/2) \times [\gamma_{22}]_{\text{eff}} = 0.1059$

Table IV: Effective deformation parameters for ^{239}Pu. Like in Table III, this numerical values are different from ones presented in table VI of [1] because they are multiplied by β_{20} to meet OPTMAN's convention. In addition, the non-axial band is a γ-band instead of a octupole band because there is not change of parity in the transition from G.S band to the non-axial band.

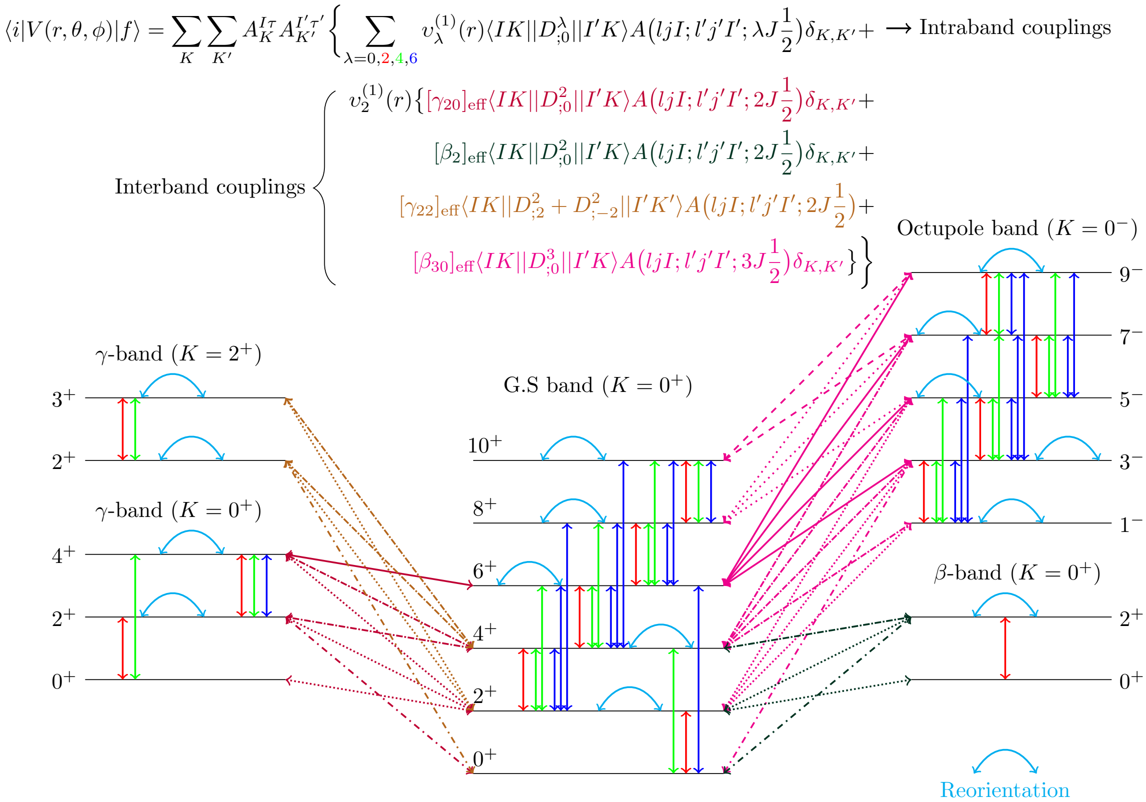

Figure 1: Coupling scheme for n+^{238}U (energy levels are not in scale) showing intraband and interband couplings due to different terms in the coupling matrix elements expression B.12 from [1].

frescoPRC's input line by line is :

- Record 1: Z, A, E_f FORMAT (F5.1,F6.1,F7.4)

  Atomic number, mass number and Fermi energy of the target in MeV.

- Record 2: n_{stat} FORMAT (I2)

  Number of coupled levels considered in the calculation.

- Record 3: E_{stat}, J_{val}, KBAND, NBAND, COEFF FORMAT (E12.5,F5.2,F4.2,I3,F7.5)

  One line per level considered. The level is characterised by an energy E_{stat} in keV, an angular momentum J_{val} and a projection KBAND. NBAND is a integer that is common to all states in a same band [**all states from G.S band must have NBAND=1 while any other integer identify an excited band**] and its sign determines the parity of the band. For states of G.S band COEFF is β_{20} and for states of excited bands COEFF is $\beta_{20} \times [\beta_\lambda]^{\rm eff}$ where $[\beta_\lambda]^{\rm eff}$ is the effective deformation parameter (e.g. parameters from Tables III and IV for ^{238}U and ^{239}Pu).

- Record 4: J_{max}, h_{cm}, r_{match}, NGRID, NENERG FORMAT (I3,F6.2,F7.2,I4,I3)

  r_{match} is the matching radius in fm, h_{cm} is the integration step for coupled equations in fm, J_{max} is maximum value of angular momentum for a coupled-channels sets and NENERG is the number of energies for which the calculation is performed (incident neutron's energies). External form factors (fort.4) are calculated from r=0 to r=r_{match} with a total number of points NGRID (NGRID > 1).

- Record 5: E_{inc} FORMAT (5E12.5)

  Incident neutron's energies in MeV.

- Record 6.1: V_0^a, V_0^b, $\lambda_{\rm HF}$, $C_{\rm viso}$, $V_{\rm spo}$, $\lambda_{\rm spo}$, C_{coul} FORMAT (7E12.4)
- Record 6.2: A_v, B_v, W_0, B_s, $W_{\rm spo}$, $B_{\rm so}$ FORMAT (6E12.4)
- Record 6.3: E_a, α_v, C_s, $C_{\rm wiso}$, A_d FORMAT (5E12.4)
- Record 6.4: $r^a_{\rm HF}$, $r^b_{\rm HF}$, $a^a_{\rm HF}$, $a^b_{\rm HF}$, r_v, a^a_v, a^b_v FORMAT (7E12.4)
- Record 6.5: r^a_s, r^b_s, a_s FORMAT (3E12.4)
- Record 6.6: $r_{\rm so}$, $a_{\rm so}$, r_c, a_c FORMAT (4E12.4)

  Records from 6.1 to 6.6 are dispersive optical-model parameters given in Table I. Parameters that depend on the mass number A are characterised by two components with superscripts a and b (e.g. $V_0 = V_0^a + V_0^b(A - A_d)$).

- Record 7: β_{20}, β_{40}, β_{60} FORMAT (3E12.4)

  Static deformation parameters (e.g. Table II for ^{238}U and ^{239}Pu).

- Record 8: PythonFlag FORMAT (1I)

  if PythonFlag=1 then graphs for elastic, absorption and total cross section will be generated using Python at the end of the run (matplotlib library and the bash script *runall.sh* are required). Set PythonFlag to any other integer to do not generate any graph.

Calculations for ^{238}U and ^{239}Pu using level schemes presented in Tables IV and VI of [1] are presented in Figures 2 and 3 comparing FRESCO and OPTMAN results[2].

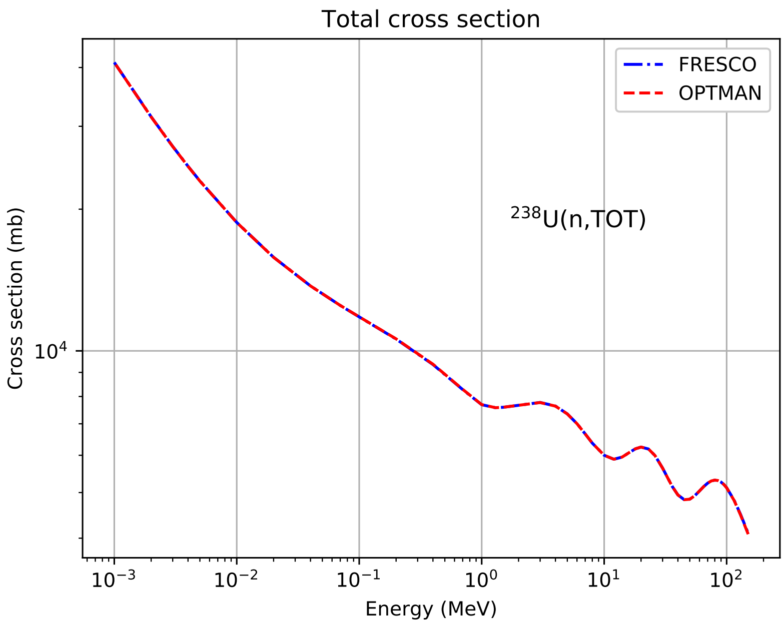

Figure 2: Total cross section for n+^{238}U using parameters from Tables III and I calculated with FRESCO and OPTMAN.

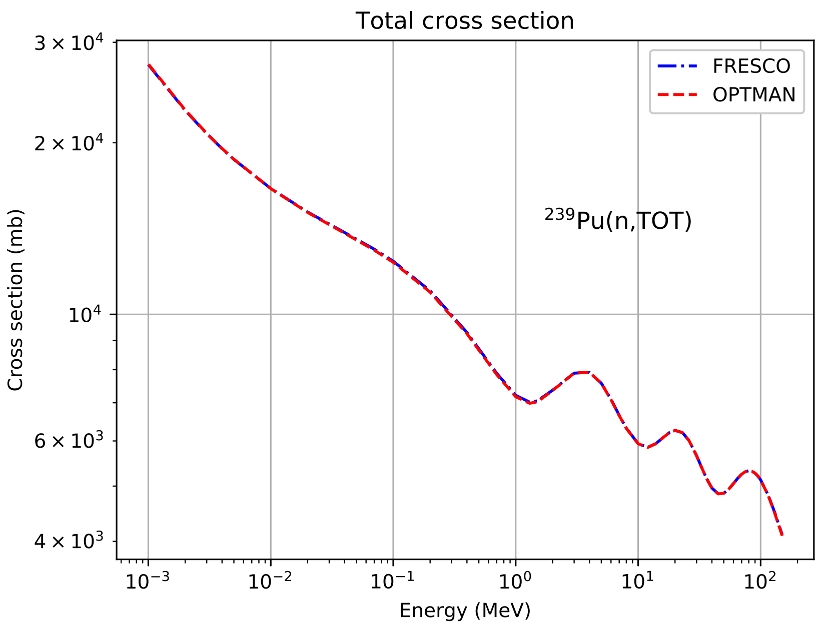

Figure 3: Total cross section for n+^{239}Pu using parameters from Tables IV and I calculated with FRESCO and OPTMAN.

[2]In order to compare results from both programs, OPTMAN's results are for the case of MEAPP=1 [i.e., no potential dependency on level energy losses], so small differences for low energies are expected for MEAPP=0.

References

[1] E. Sh. Soukhovitskiĩ, R. Capote, J. M. Quesada, S. Chiba, and D. S. Martyanov. "Nucleon scattering on actinides using a dispersive optical model with extended couplings". *Phys. Rev. C* 94 (6 2016), 064605. DOI: 10.1103/PhysRevC.94.064605.

[2] E.Sh. Soukhovitskiĩ, G.B. Morogovskiĩ, R. Capote Noy, S. Chiba, and J. M Quesada. *Program OPTMAN Version 14 (2013), User's Guide Coupled-Channel Optical Model Code Based on Rigid- or Soft-Rotator Models, Compatible with the Empire Nuclear Data Evaluation System.* International Atomic Energy Agency (IAEA), 2013.

[3] Ian J. Thompson. *FRESCO, coupled reaction channels calculations.* http://www.fresco.org.uk/.