Fundamentals and progress of theoretical models for the evaluation of photonuclear reaction data in CNDC

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CHINA NUCLEAR DATA CENTER

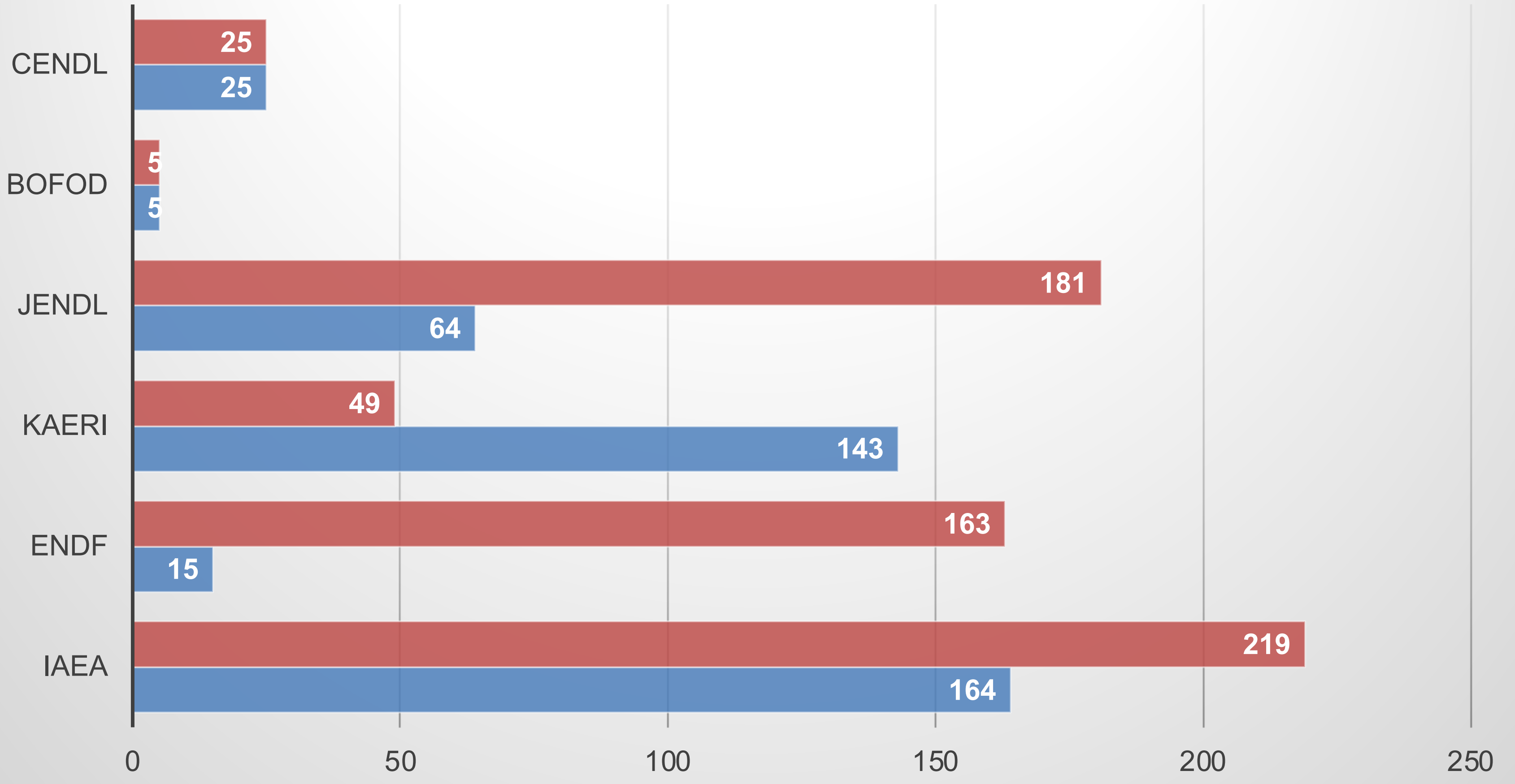
Motivation

1. Photonuclear data are important in application to radiation damage, reactor dosimetry, accelerator shielding, radiation therapy and so on; and recently, the requirements of the high-quality data for more nuclei are increasing from users;

2. The progress of many advanced microscopic nuclear theories could be helpful to obtain a PSF reference database for thousands of nuclei in the nuclide chart and derive reasonable prediction for photoabsorption cross sections et al. consistently; and the new measurements with improved experimental techniques will be good criteria to test them.

3. New measurements in high precision since 1999 are available to make it possible to update the previous recommended photonuclear data and evaluate data for more nuclei and reactions. Shanghai Laser Electron Gamma Source (SLEGS) has officially completed in 2022. The relevant evaluation techniques and codes at CNDC have be improved

Status of photonuclear reaction data



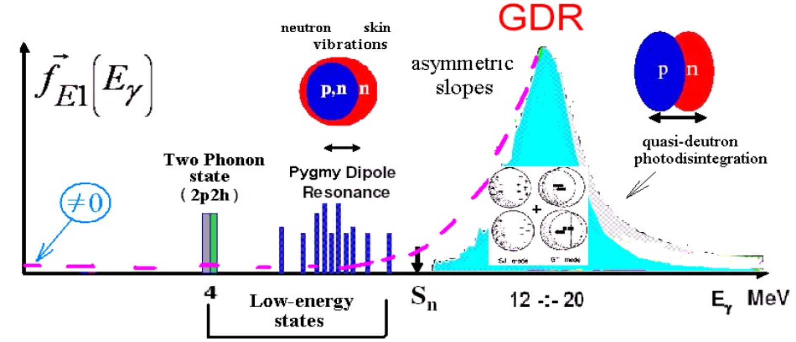
	IAEA	ENDF	KAERI	JENDL	BOFOD	CENDL
2019	219	163	49	181	5	25
1999	164	15	143	64	5	25

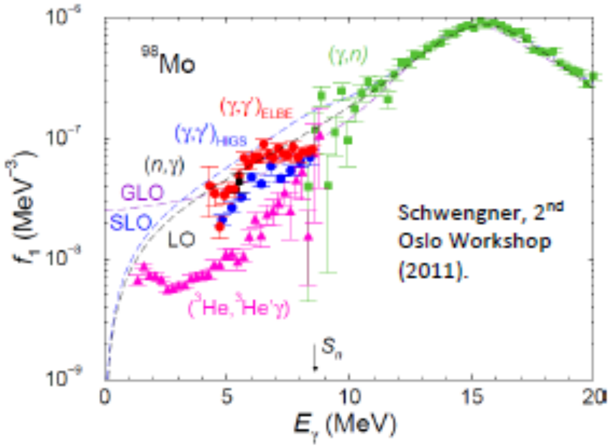
Problem1: PSF divergence at Eg<Sn

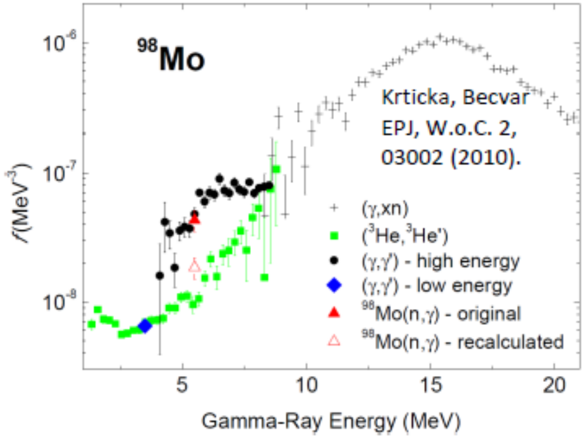
CLOSED-FORM MODELS OF E1 PSF

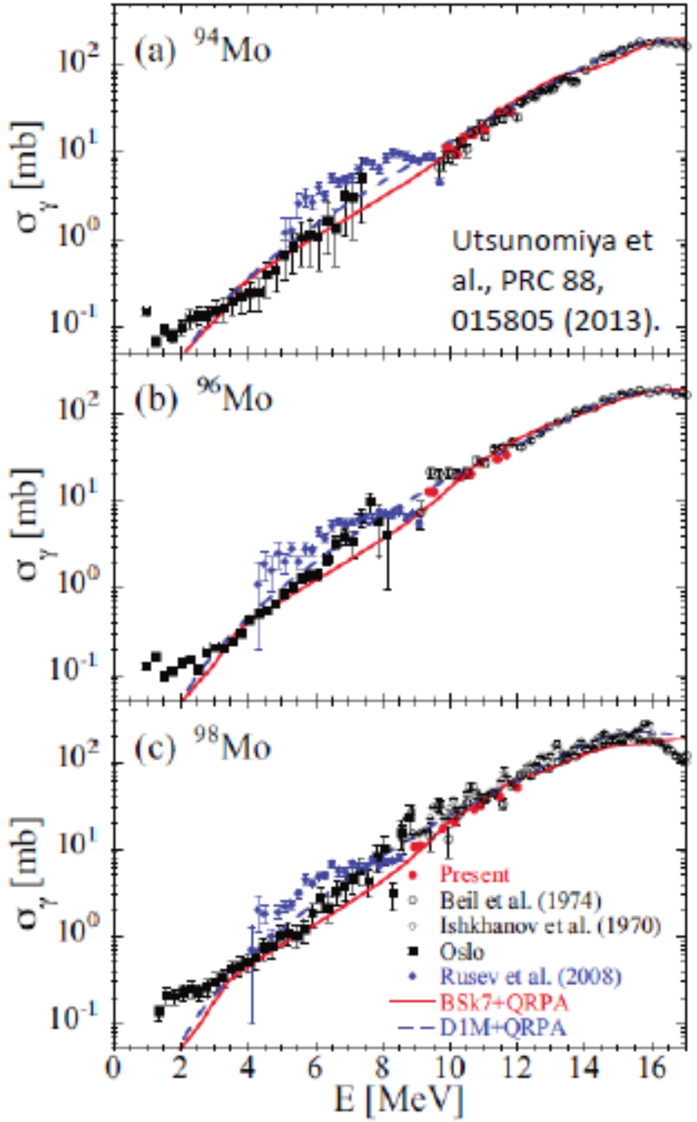
Dipole electric gamma-transitions are dominant ones, if they take place together with transitions of other multipolarities and types

Nuclear states excited by E1 field









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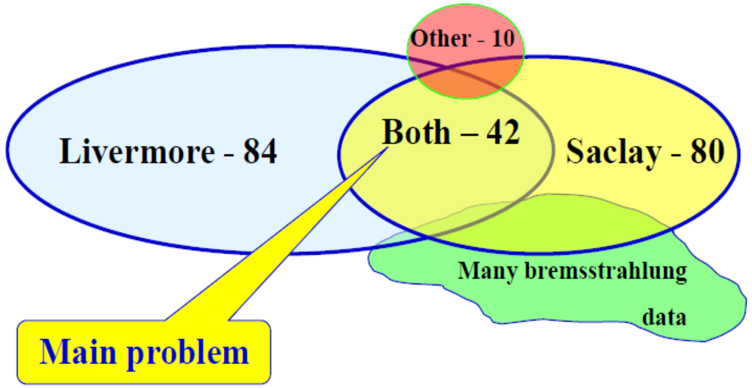
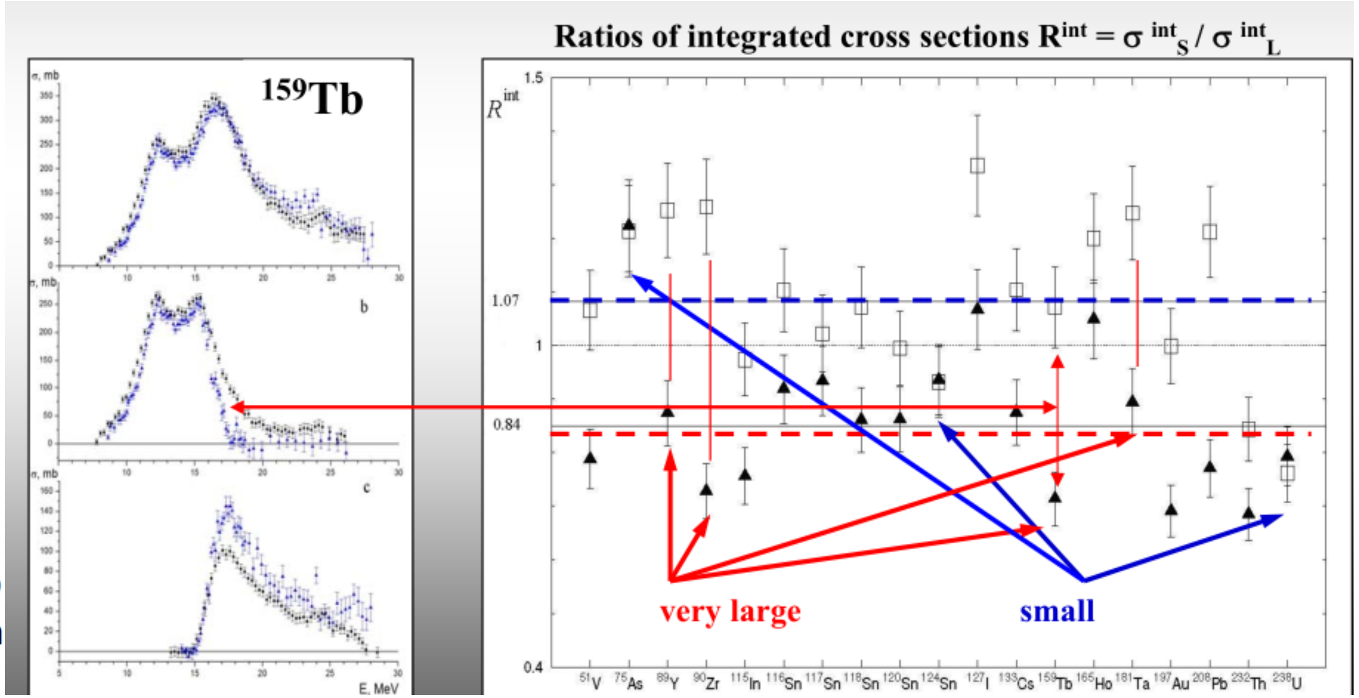
Problem2 : Discrepancies in (g,xn) c.s

Present situation of photoneutron cross sections data
in the GDR region

- Most of the photoneutron cross section measurements were performed using quasi-monochromatic annihilation – QMA photons using positron in flight annihilation at two major facilities:
  - Saclay (France)
  - Lawrence Livermore National Laboratory (USA)
- Large discrepancies in (γ,xn) c.s. measured at the two facilities:
  - (γ, 1n) c.s. are generally noticeably larger at Saclay than at Livermore
  - (γ, 2n) c.s. are generally larger at Livermore than at Saclay.



No systematic way to resolve the discrepan
<u>New and reliable measurements are required!</u>



Squares - ■ - ratios for (γ, 1n) reactions – are larger than 1.0:

<R> ~ 1.07.

Long standing problem
LLNL vs. Saclay

Triangles - △ - ratios for (γ, 2n) reactions – are smaller than 1.0:

<R> ~ 0.84.

Evaluation process of Photonuclear reaction data in CNDC

EXFOR data
↓
Experimental analysis for (G,abs)
↓
GDR parameter calculation
↓
(G,abs) calculation (GDR + QD)
↓
Input to GLUNF and MEND-G
↓
Experimental analysis for partial photon-neutron emission reactions and (n,p), (n,alpha) …
↓
GLUNF for Be-9
MEND-G for medium-heavy nuclei
↓
ENDF/B-6 output and format check

- Standard Lorentzian (SLO) Brink(1955)& Axel(1962)
- Enhanced Generalized Lorentzian (EGLO) *Kopecky& Uhl(1993)*
- Hybrid model (GH) *Goriely (1998)*
- Modified Lorentzian model (MLO) Plujko et al (1999)
- Generalized Fermi liquid model (GFL) *Mughabghab&Dunford (2000)*
- Triple (triaxial) Lorentzian model (TL) *Junghans et al (2008)*
- Simplex Modified Lorentzian Model (SMLO) Plujko et al (2008)

- Semi-classical thermodynamic approach
- Hartree-Fock ground state (QRPA)
- Relativistic mean field ground state (RQRPA)
- Theory of finite fermi systems

Phonological GDR parameters

1. RIPL-3 recommend GDR parameters
2. CNDC GDR parameters
3. Results comparison

Spherical nuclei

$$E_r \equiv E_0 = aA^{-1/3} + bA^{-1/6}\ \text{MeV},$$
$$\Gamma_r = cE_r^{\delta}\ \text{MeV},$$
$$S_r \equiv \frac{\pi}{2}\sigma_r\Gamma_r = 60\ d\ NZ/A\ \text{mb}\cdot\text{MeV},$$

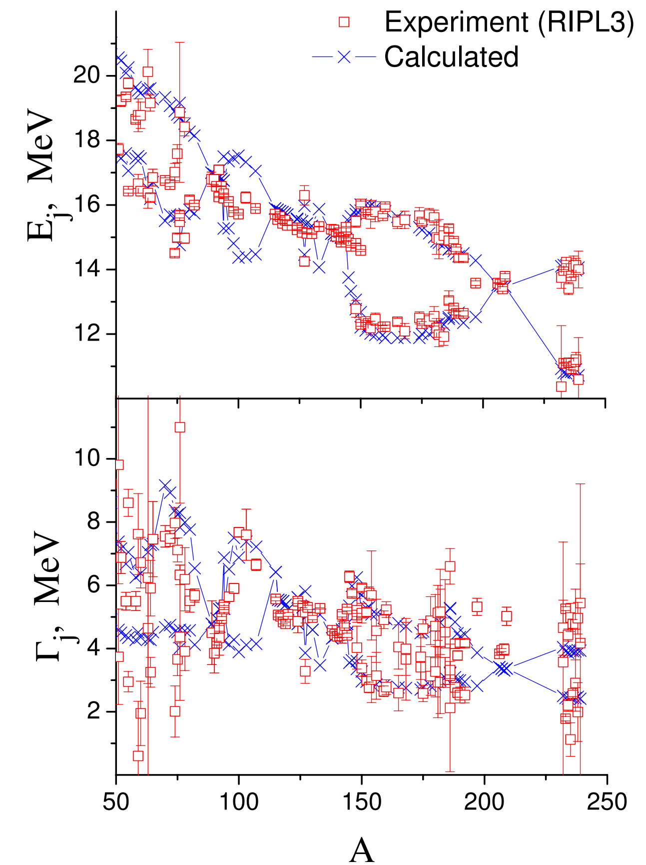
$$SLO:$$
$$a = 27.47 \pm 0.01,\quad b = 22.063 \pm 0.004,$$
$$c = 0.0277 \pm 0.4\cdot 10^{-4},\quad d = 1.222 \pm 0.002\ ;$$
$$MLO:$$
$$a = 28.69 \pm 0.01,\quad b = 21.731 \pm 0.004,$$
$$c = 0.0285 \pm 0.4\cdot 10^{-4},\quad d = 1.267 \pm 0.002.$$

Axial deformed nuclei

$$E_{r,1} = E_{r,2}/\left[0.911\frac{a_0}{b_0} + 0.089\right],$$
$$E_{r,2} = E_0\frac{1}{b_0}\left[1 - 1.51\cdot 10^{-2}(a_0^2 - b_0^2)\right],$$
$$\Gamma_{r,1} = 0.026E_{r,1}^{1.91},\quad \Gamma_{r,2} = 0.026E_{r,2}^{1.91},$$
$$\sigma_{r,1} = \sigma_0/3,\quad \sigma_{r,2} = 2\sigma_0/3,$$

$$R(\theta) = R_0'\left(1 + \alpha_2 P_2(\cos\theta)\right) = R_0'\left(1 + \beta_2 Y_{20}\right),$$
$$R_0' = R_0/\lambda,\qquad \lambda^3 = 1 + \frac{3}{5}\alpha_2^2 + \frac{2}{35}\alpha_2^3,$$

$$a_0 \equiv R(\theta = 0)/R_0 = (1 + \alpha_2)/\lambda,$$
$$b_0 \equiv R(\theta = \pi/2)/R_0 = (1 - 0.5\alpha_2)/\lambda.$$



Phonological GDR parameters

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$$E_r = a_1(1 + a_6 I^2)/A^{1/3} + a_2(1 + a_7 I^2)/A^{1/6},$$
$$\Gamma_r = a_3 E_r^{a_4} - a_8 E_r \beta_2,$$
$$\sigma_r = \frac{2}{\pi} a_5 \cdot \sigma_{TRK}/\Gamma_r.$$

$$I = (N - Z)/A, \qquad \sigma_{\mathrm{TRK}} = 60NZ/A$$

$$E_{r,2} = E_r \frac{1}{b_0}[1 - 1.51 \cdot 10^{-2}(a_0^2 - b_0^2)],$$
$$E_{r,1} = E_{r,2} / \left[0.911 \frac{a_0}{b_0} + 0.089\right],$$
$$\Gamma_{r,2} = b_2 E_{r,2}^{b_3} - E_{r,2} b_6 \beta_2, \qquad \Gamma_{r,1} = b_4 E_{r,1}^{b_5} - E_{r,1} b_7 \beta_2,$$
$$\sigma_{r,2} = \sigma_r |1 - b_8 + b_1 \beta_2|, \qquad \sigma_{r,1} = \sigma_r |b_8 - b_1 \beta_2|.$$

$$a_0 = (1 + \alpha_2)/\lambda$$
$$b_0 = (1 - 0.5\alpha_2)/\lambda$$
$$\lambda^3 = 1 + \frac{3}{5}\alpha_2^2 + \frac{2}{35}\alpha_2^3$$

TABLE IV. Parameters and χ^2-values of systematics within MLO1, MLO2, MLO3, EGLO, GFL, SLO, GH and SMLO models.

	MLO1	MLO2	MLO3	EGLO	GFL	SLO	GH	SMLO	SLO*	MLO1*
a_1	42.722	41.504	42.563	43.1769	39.2025	39.7783	38.4423	42.0152	27.47	28.69
a_2	16.0865	16.7204	16.1593	16.0834	18.8849	17.6336	18.6947	16.4032	22.063	21.731
a_3	0.0111	0.0124	0.0122	0.0048	0.0104	0.012	0.01	0.0062	0.0277	0.0285
a_4	1.0375	1.0157	1.0071	1.1963	1.0186	1.0095	1.0114	1.1682	1.9	1.9
a_5	0.0452	0.0477	0.0457	0.0309	0.0395	0.0459	0.0384	0.0364	1.222	1.267
a_6	-9.0294	-10.4079	-10.3748	-5.00	-6.6123	-11.7035	-10.4802	-10.5713	0	0
a_7	8.8811	9.6039	10.3457	4.1809	4.4196	9.7693	7.6594	10.3444	0	0
a_8	0.0039	0.0049	0.0043	0.0017	0.0023	0.0051	0.0039	0.0014	0	0
b_1	-0.8837	-0.903	-0.8877	-0.7608	-0.8142	-0.8966	-0.8669	-0.7962	0	0
b_2	0.2753	0.5083	0.395	0.0086	0.2809	0.5838	0.5052	0.0629	0.026	0.026
b_3	1.0789	0.8666	0.9495	2.2425	1.1868	0.7884	0.9247	1.5836	1.91	1.91
b_4	0.0855	0.0503	0.0758	0.1945	0.4745	0.0757	0.1551	0.1821	0.026	0.026
b_5	1.4629	1.5903	1.4809	1.4222	0.9907	1.4819	1.3278	1.2703	1.91	1.91
b_6	-0.184	-0.1789	-0.1604	-0.1539	-0.3373	-0.1666	-0.2366	-0.1882	0	0
b_7	0.0815	-0.0221	0.036	1.0276	0.3179	0.1194	0.2426	0.2623	0	0
b_8	0.2448	0.2307	0.2474	0.2914	0.2475	0.229	0.2303	0.304	0.333	0.333
χ^2	9.8769	12.8526	10.7246	9.742	10.1275	15.9214	15.6991	9.5161	25.8048	19.0095

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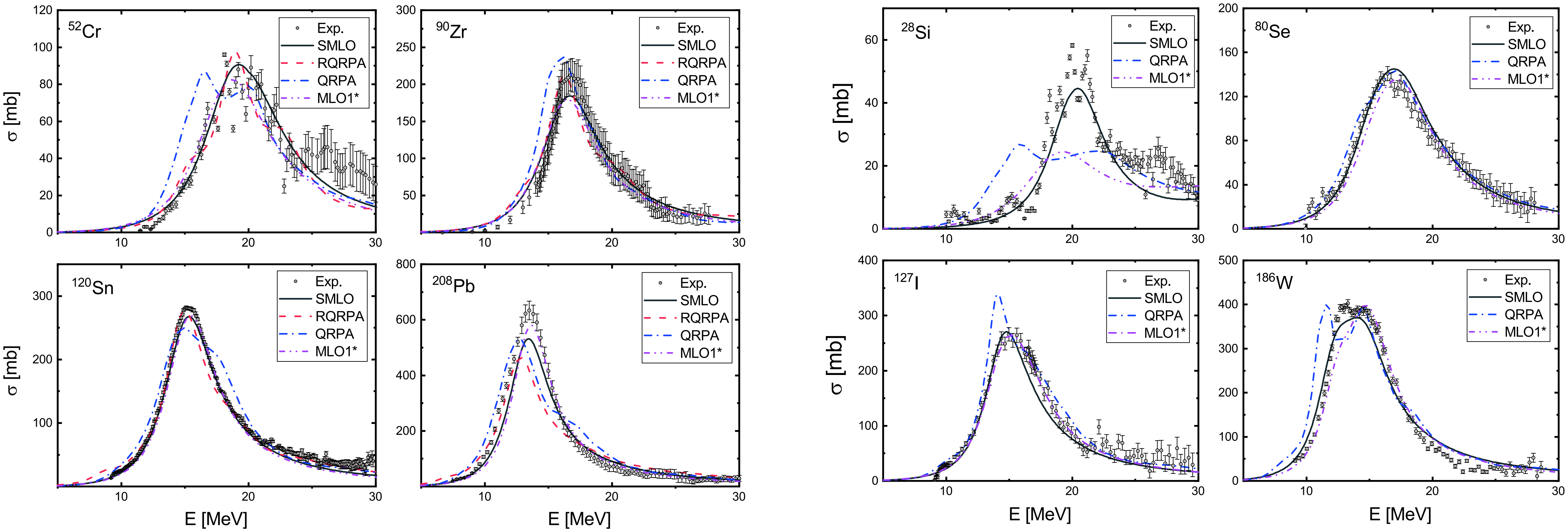

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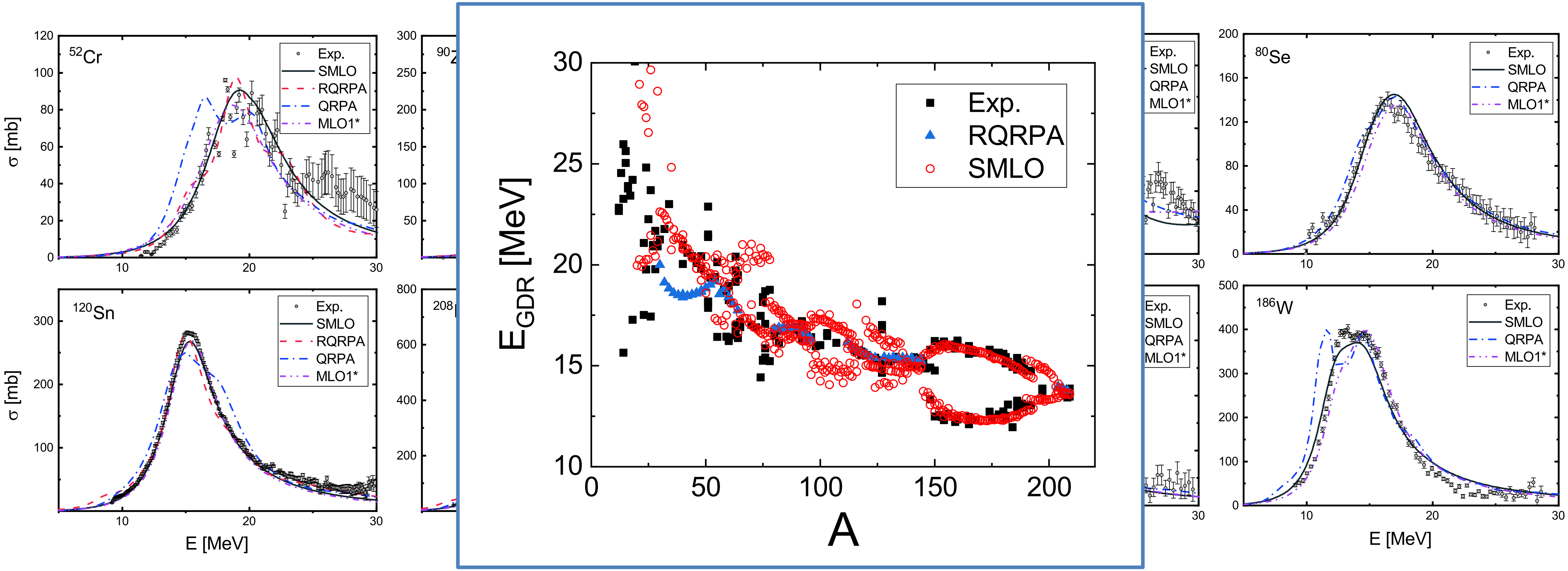


Microscopic GDR parameters

1. RHB calculate the ground state properties of nuclei
2. RQRPA calculate the GDR for the spherical nuclei
3. DIRQFAM calculate the GDR for deformed nuclei
4. Results comparison

RHB

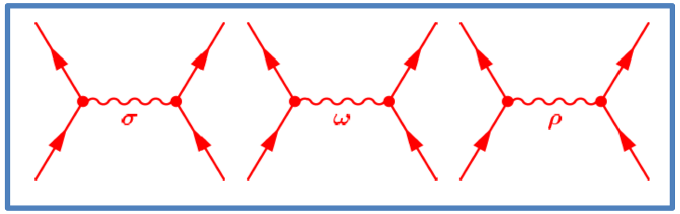
$$\begin{pmatrix} \hat{h} & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}^* \end{pmatrix} \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix} E_k$$

$$\hat{h} = \frac{\delta E'}{\delta \hat{\rho}} = ap + V + \beta(m - S)$$

$$\hat{\Delta} = \frac{\delta E}{\delta \hat{\kappa}} = \frac{1}{2}\sum_{cd} V_{abcd}^{pp} \kappa_{cd}$$

$$V(\mathbf{r}) = g_\omega \omega(\mathbf{r}) + g_\rho \vec{\tau}\vec{\rho}(\mathbf{r}) + eA(\mathbf{r})$$

$$S(\mathbf{r}) = g_\sigma \sigma(\mathbf{r})$$



Binding energy, radius, single particle level

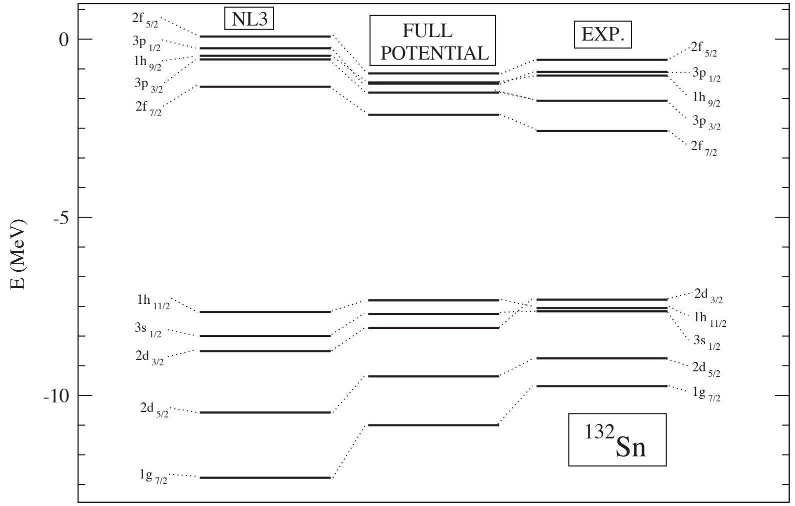


Fig. 43. Same as in Fig. 42, but for the neutron single-particle states in ^{132}Sn (from Ref. [172]).

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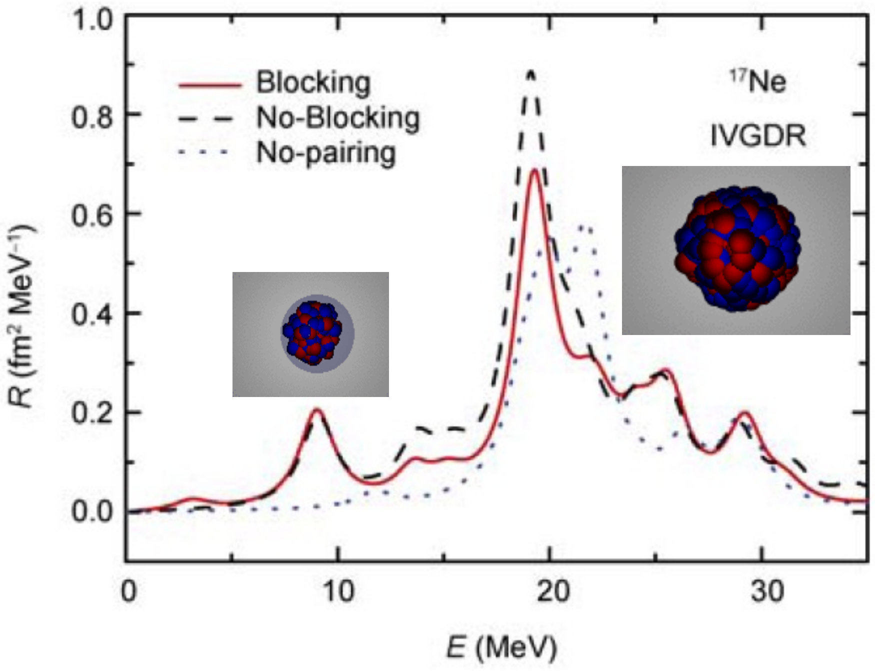
RQRPA

$$\begin{pmatrix} A^J & B^J \\ B^{*J} & A^{*J} \end{pmatrix} \begin{pmatrix} X^{\nu,JM} \\ Y^{\nu,JM} \end{pmatrix} = \omega_\nu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^{\nu,JM} \\ Y_{\nu,JM} \end{pmatrix}$$

$$A^J_{\kappa\kappa'\lambda\lambda'} = H^{11(J)}_{\kappa\lambda}\delta_{\kappa'\lambda'} - H^{11(J)}_{\kappa'\lambda}\delta_{\kappa\lambda'} - H^{11(J)}_{\kappa\lambda'}\delta_{\kappa'\lambda} + H^{11(J)}_{\kappa'\lambda'}\delta_{\kappa\lambda} + \frac{1}{2}(\xi^+_{\kappa\kappa'}\xi^+_{\lambda\lambda'} + \xi^-_{\kappa\kappa'}\xi^-_{\lambda\lambda'})V^{ppJ}_{\kappa\kappa'\lambda\lambda'} + \zeta_{\kappa\kappa'\lambda\lambda'}V^{phJ}_{\kappa\lambda'\kappa'\lambda}$$

$$B^J_{\kappa\kappa'\lambda\lambda'} = \frac{1}{2}(\xi^+_{\kappa\kappa'}\xi^+_{\lambda\lambda'} - \xi^-_{\kappa\kappa'}\xi^-_{\lambda\lambda'})V^{ppJ}_{\kappa\kappa'\lambda\lambda'} + \zeta_{\kappa\kappa'\lambda\lambda'}(-1)^{j_\nu - j_{\nu'} + J}V^{phJ}_{\kappa\lambda\kappa'\lambda'}$$



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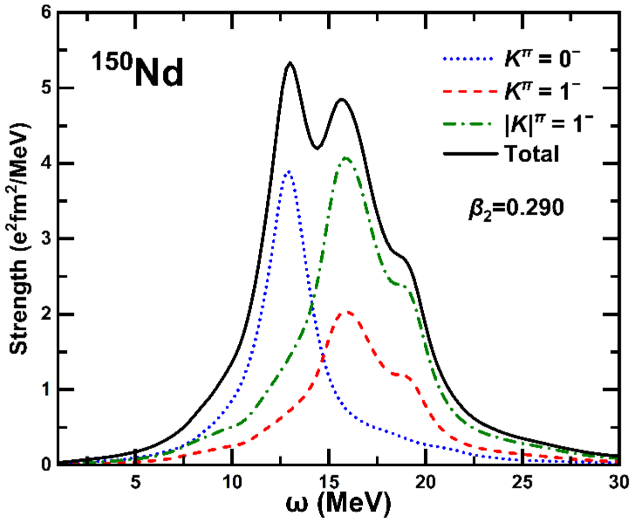
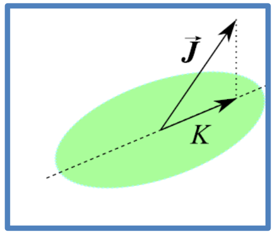


$$(E_\mu + E_\nu - \omega_\gamma) X_{\mu\nu}(\omega_\gamma) = -\left(F^{20}_{\mu\nu}(\omega_\gamma) + \delta H^{20}_{\mu\nu}(\omega_\gamma) \right),$$
$$(E_\mu + E_\nu + \omega_\gamma) Y_{\mu\nu}(\omega_\gamma) = -\left(F^{02}_{\mu\nu}(\omega_\gamma) + \delta H^{02}_{\mu\nu}(\omega_\gamma) \right),$$



$$\omega_\gamma = \omega + \gamma i.$$

N_{shells}	Memory [GB]	Time [s]
10	0.42 (0.75)	0.24 (0.36)
12	0.68 (1.46)	0.49 (0.82)
14	1.11 (2.75)	0.99 (1.75)
16	1.77 (5.68)	1.82 (3.32)
18	2.83 (8.39)	3.23 (5.71)
20	4.40 (13.9)	5.52 (9.54)
22	6.65 (22.2)	8.97 (15.5)
24	11.1 (34.2)	14.1 (26.0)

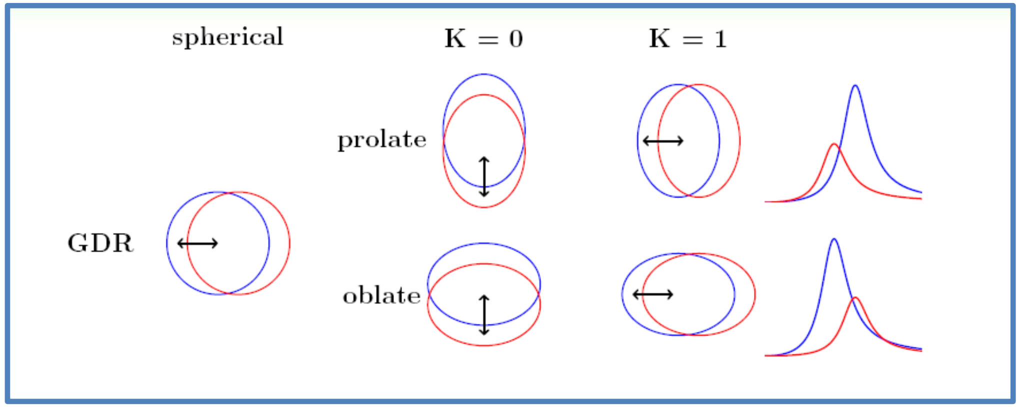


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figure from D. Pena Arteaga

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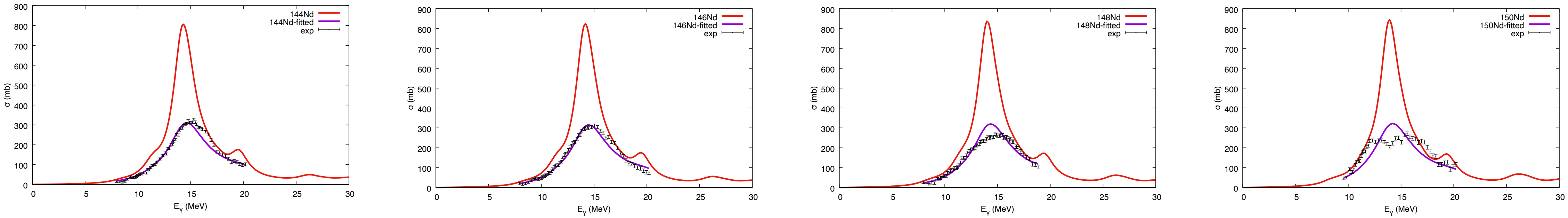
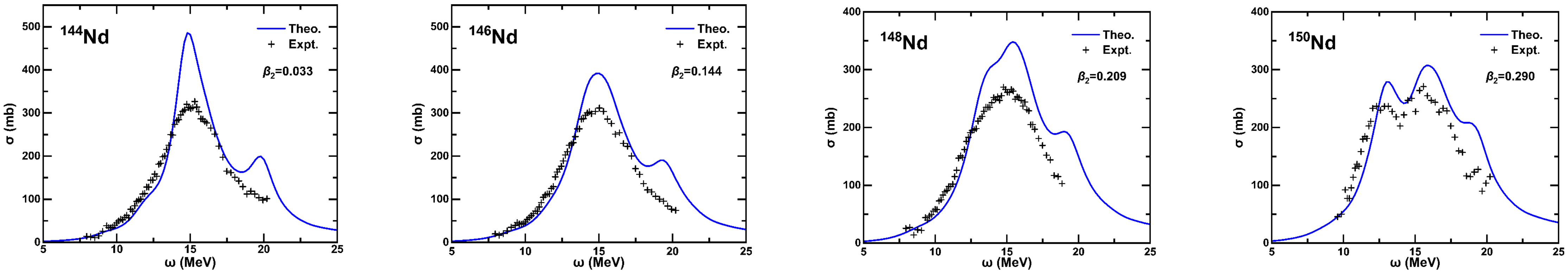
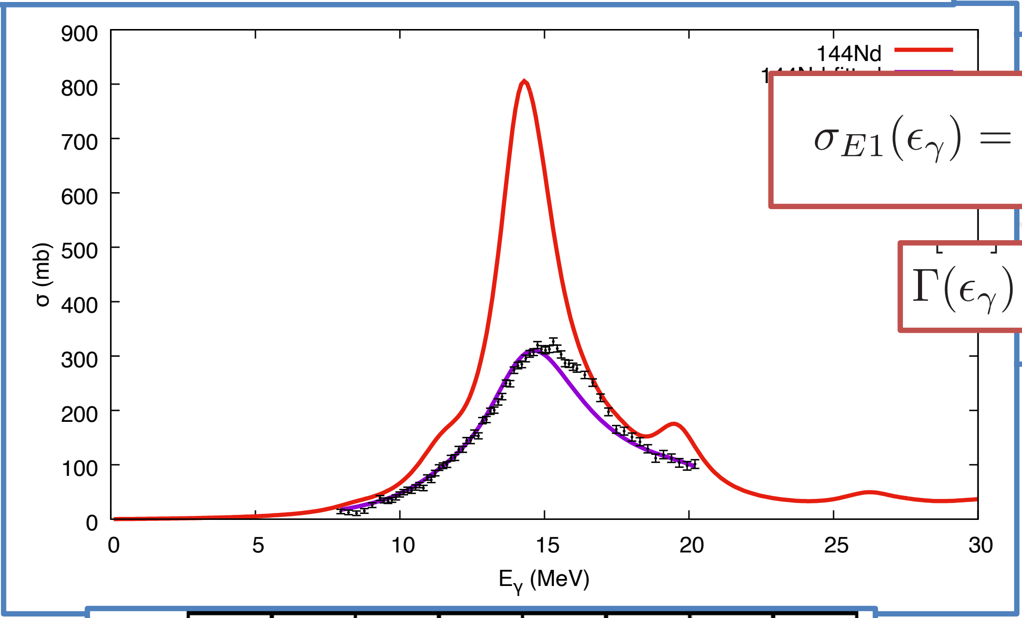
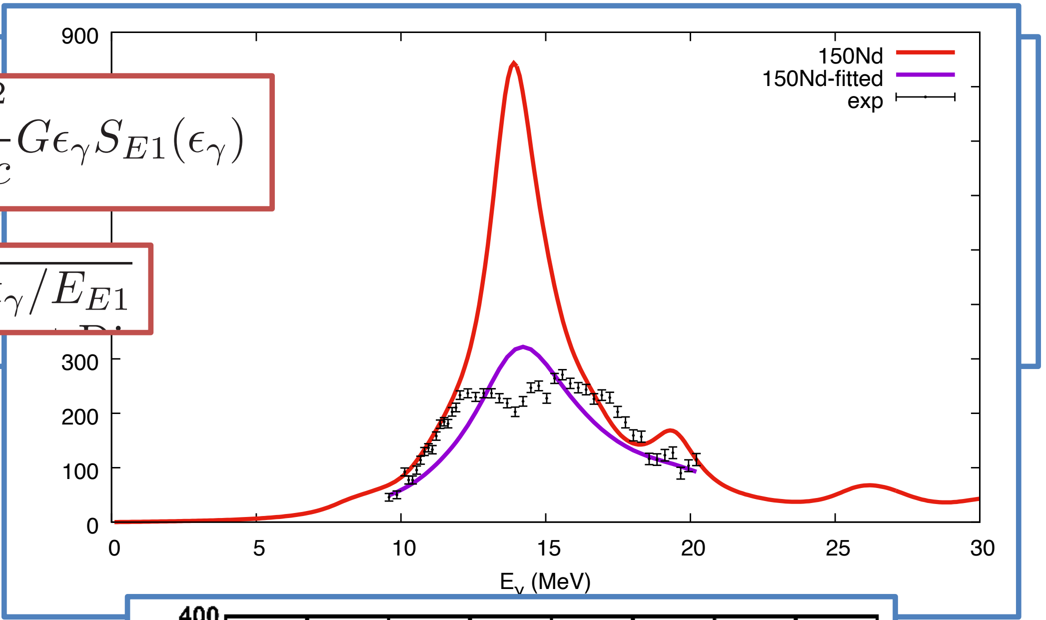




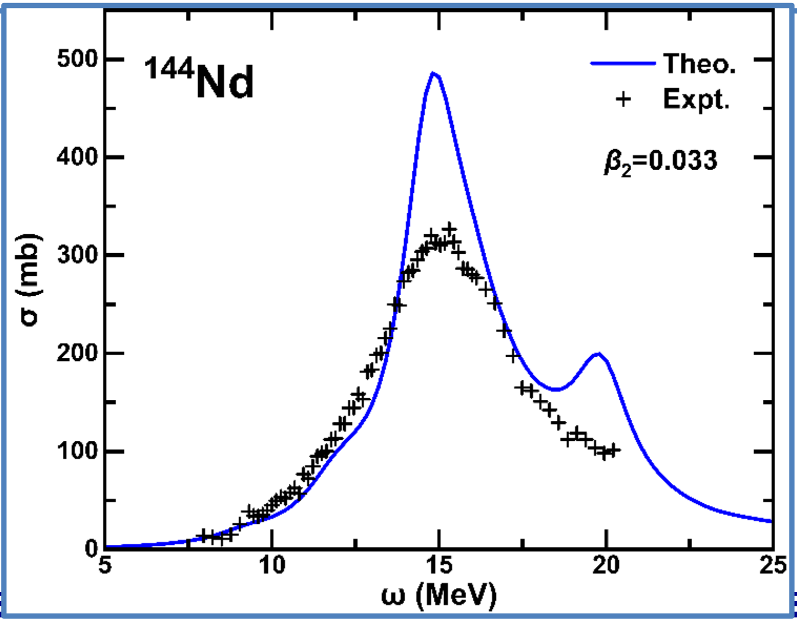
Microscopic GDR parameters



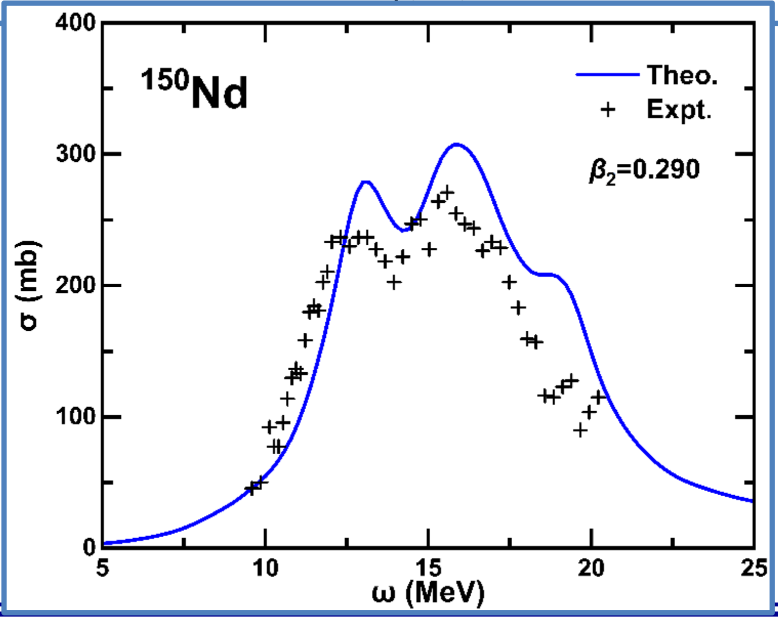


$$\sigma_{E1}(\epsilon_\gamma) = \frac{16\pi^3}{9}\frac{e^2}{\hbar c} G\epsilon_\gamma S_{E1}(\epsilon_\gamma)$$

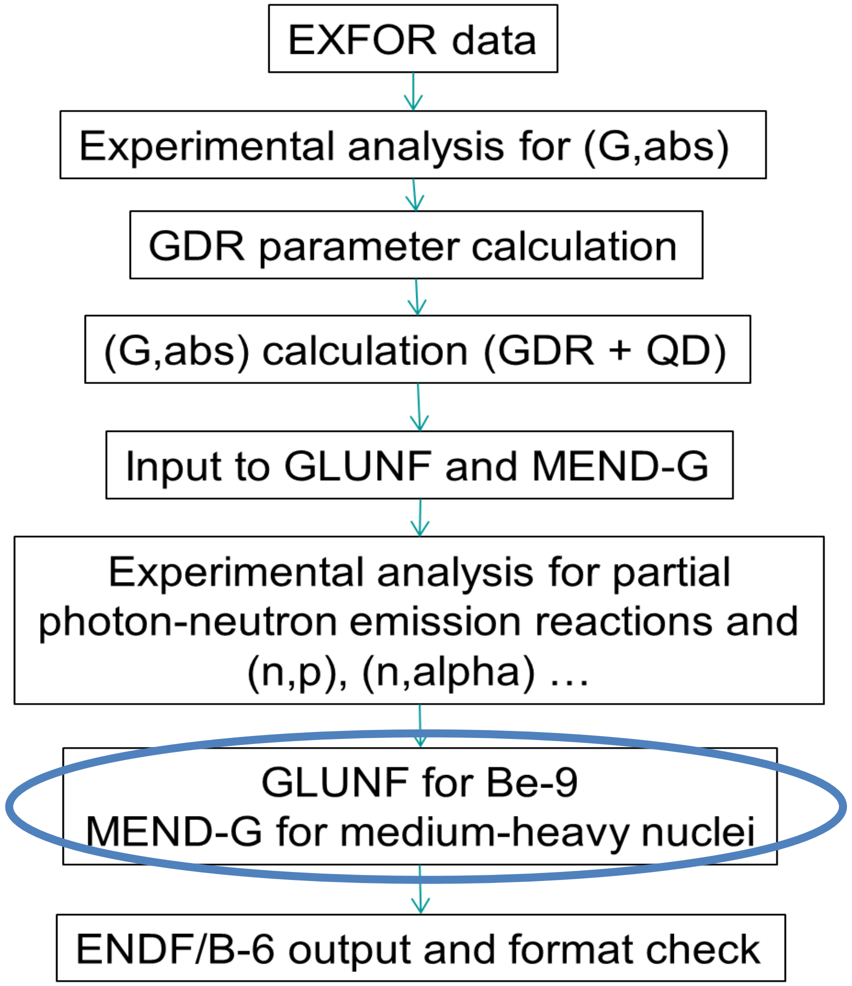
$$\Gamma(\epsilon_\gamma) = \Gamma\sqrt{\epsilon_\gamma / E_{E1}}$$



$$\omega_\gamma = \omega + \gamma i.$$



Photoneutron cross section



1. 7 models including the microscopic RQRPA, SLO, MLO et al. are utilized to estimate the photon strength function and derive the gamma absorption,

2. Quasi-deuteron dissociation model (QD) is included to describe the (g,abs) in the larger energy region;

3. Optical models for n,p,alpha,d,t,He-3 (KD potential for n, p)

4. Equilibrium emission model (Gilbert-Cameron-Cook-Ignatyuk, Su Zongdi modification)

5. Pre-equilibrium emission model (2p-2h state)

6. The emission particles include n,p,alpha,d,t,He-3; First to eighteenth emission processes are considered, more than 570 million reaction channels are involved in GMEND below 200MeV

Photoneutron cross section

	Particles emitted	Total num. of reactions
1	**n,p,α,d,t,He-3**	6
2	n,p,α,d,t,He-3	6^2=36
3	n,p,α,d,t,He-3	6^3=216
4	n,p,α,d,t,He-3	6^4=1296
5	**n,p,α,d**	**6^4X4=5184**
6	n,p,α,d	6^4X4^2=20736
7	n,p,α,d	6^4X4^3=82944
8	n,p,α	6^4X4^3X3=248832
9	n,p,α	6^4X4^3X3^2=746496
10	n,p,α	6^4X4^3X3^3=2239488
11	n,p	6^4X4^3X3^3X2=4478976
12	n,p	6^4X4^3X3^3X2^2=8957952
13	n,p	6^4X4^3X3^3X2^3=17915904
14	n,p	6^4X4^3X3^3X2^4=35831808
15	n,p	6^4X4^3X3^3X2^5=71663616
16	n,p	6^4X4^3X3^3X2^6=143327232
17	n,p	6^4X4^3X3^3X2^7=286654464
18	**n,p**	**6^4X4^3X3^3X2^8=573308928**

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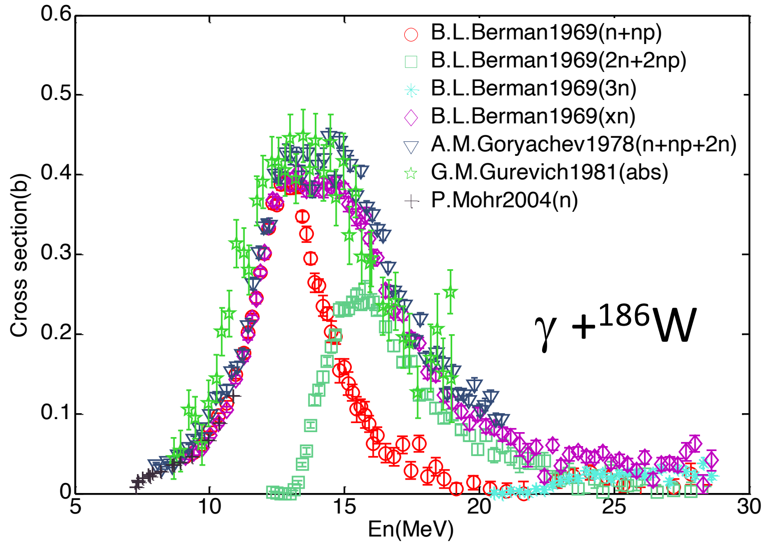
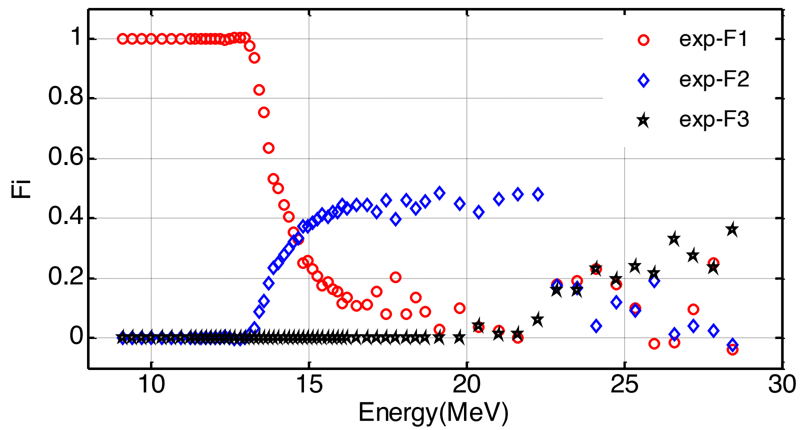
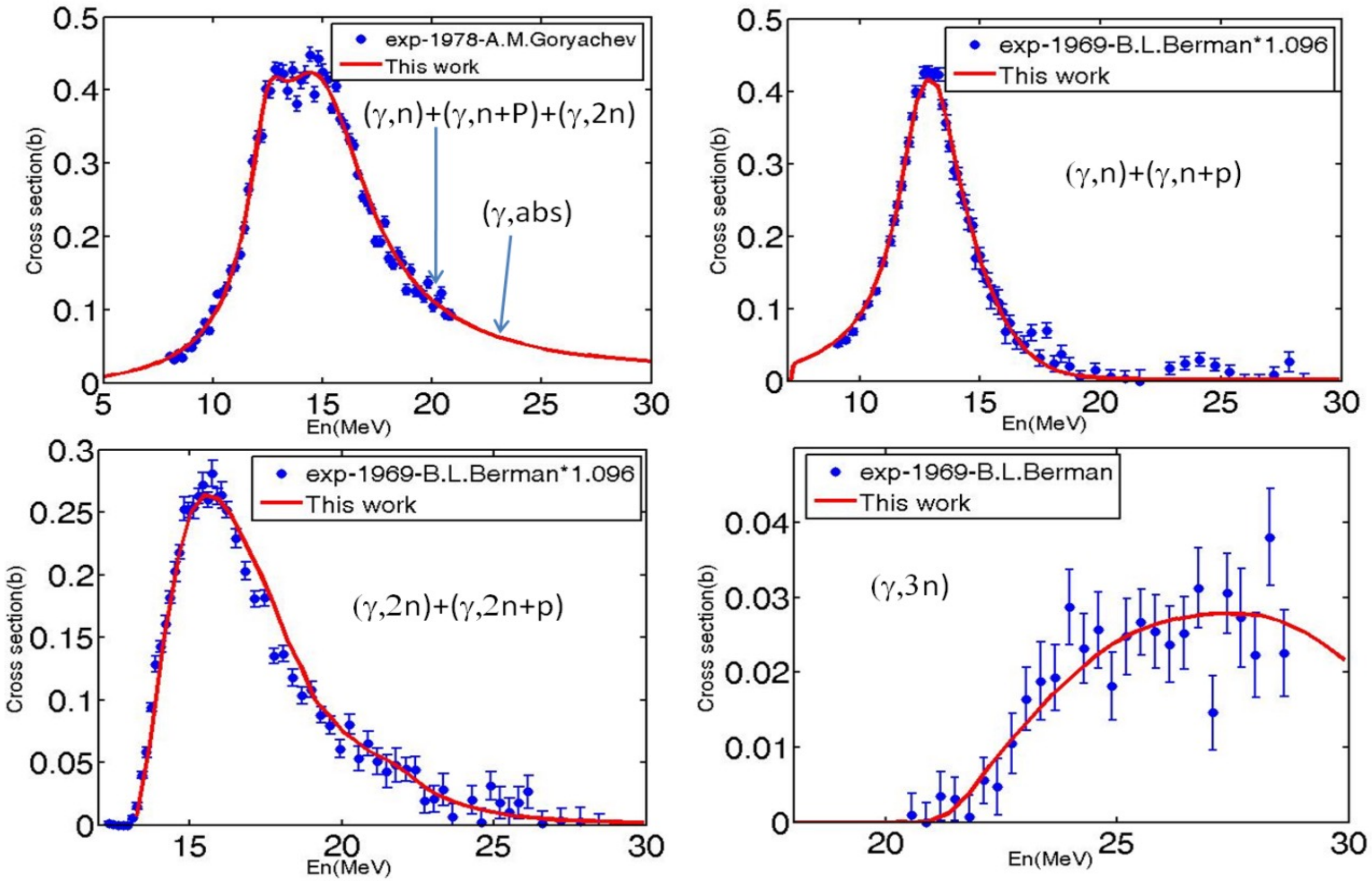
MEND-G calculation



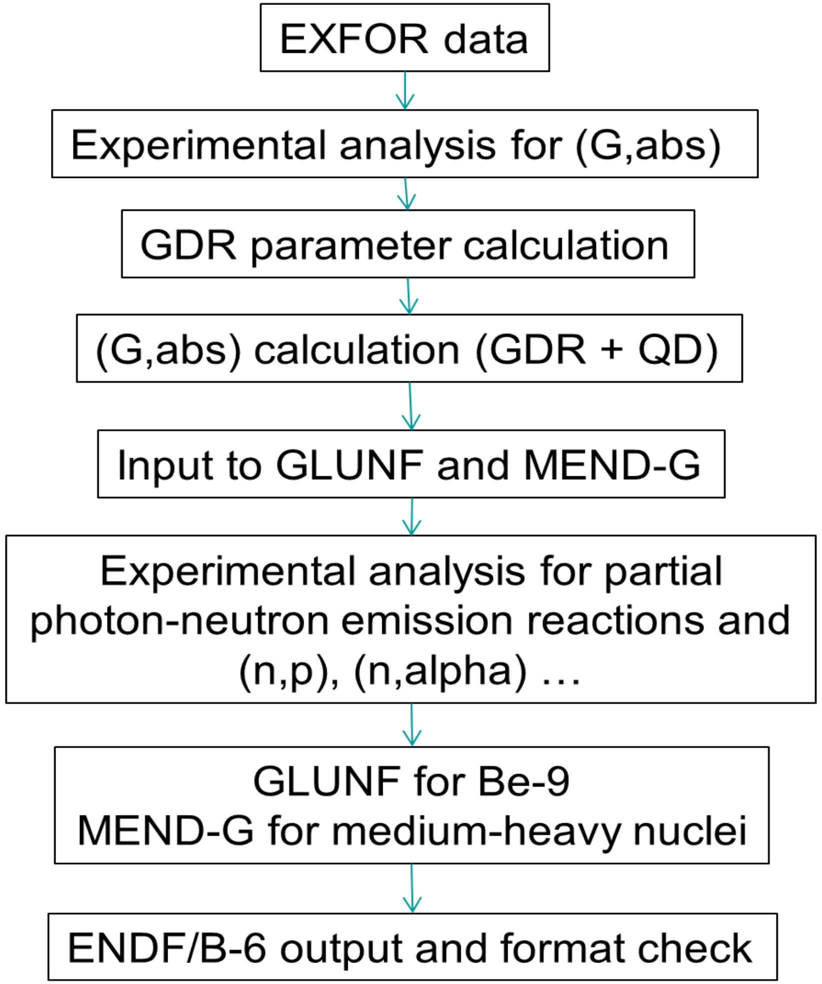
$$F_x = \sigma(\gamma, xn)/\sigma(\gamma, Sn)$$
$$= \sigma(\gamma, xn)/[\sigma(\gamma, 1n) + 2\sigma(\gamma, 2n) + 3\sigma(\gamma, 3n) + \ldots]$$





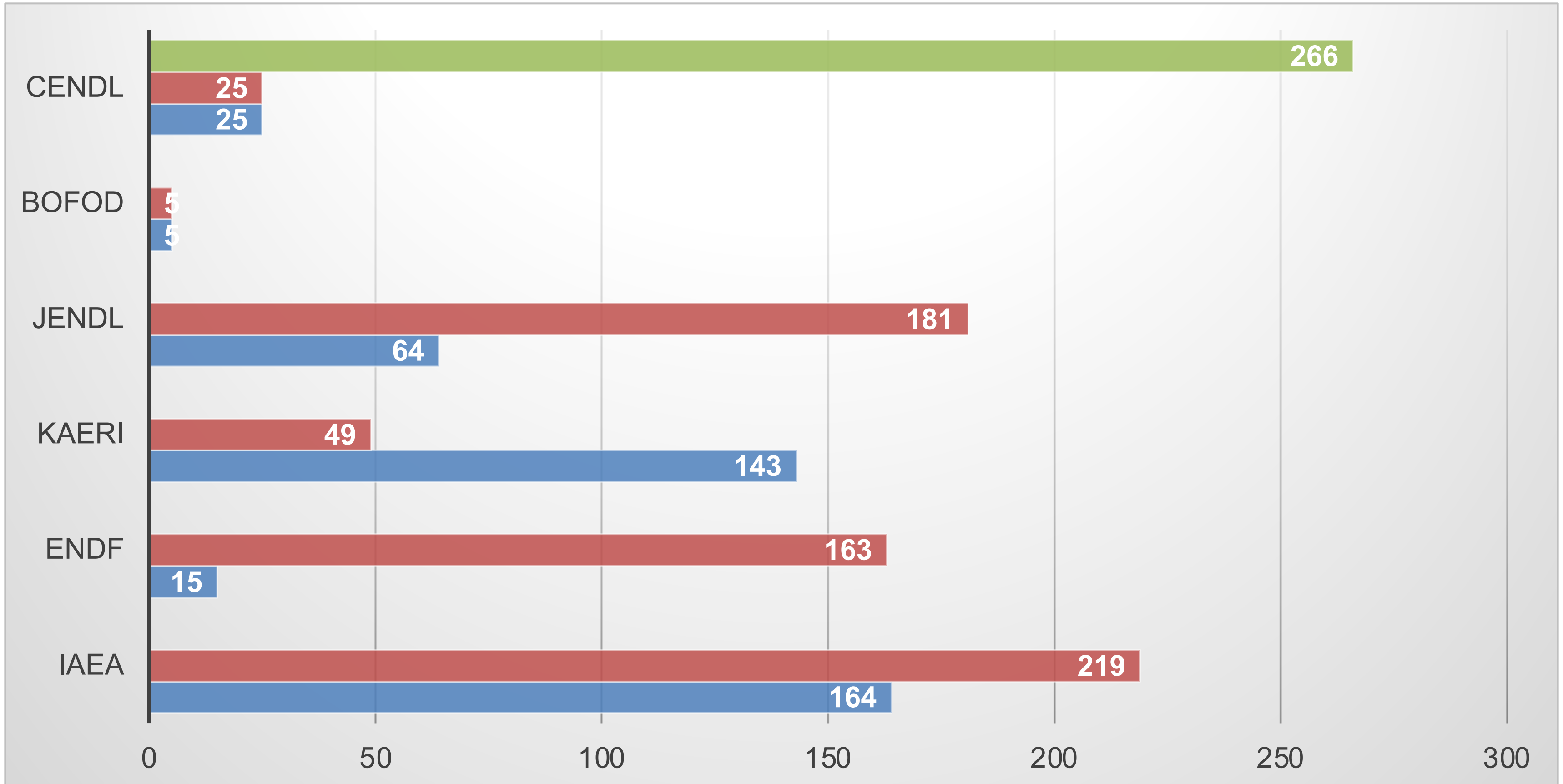
Level density parameter	p \ n	1	2	3
	0	25.999	15.032	19.108
Pairing correlation	p \ n	1	2	3
	0	0.988	0.869	0.89

Conclusion and outlook



1. Collect the latest experimental data and collaborate with **Shanghai Laser Electron Gamma Source (SLEGS)** with measure new nuclear cross section data.
2. Improve the width calculation of DIRQFAM program, microscopic theoretical model can better describe the experiment.
3. Systematically study the effect of energy level density on (g,xn) cross section
4. Release new photonuclear reaction evaluation database of China

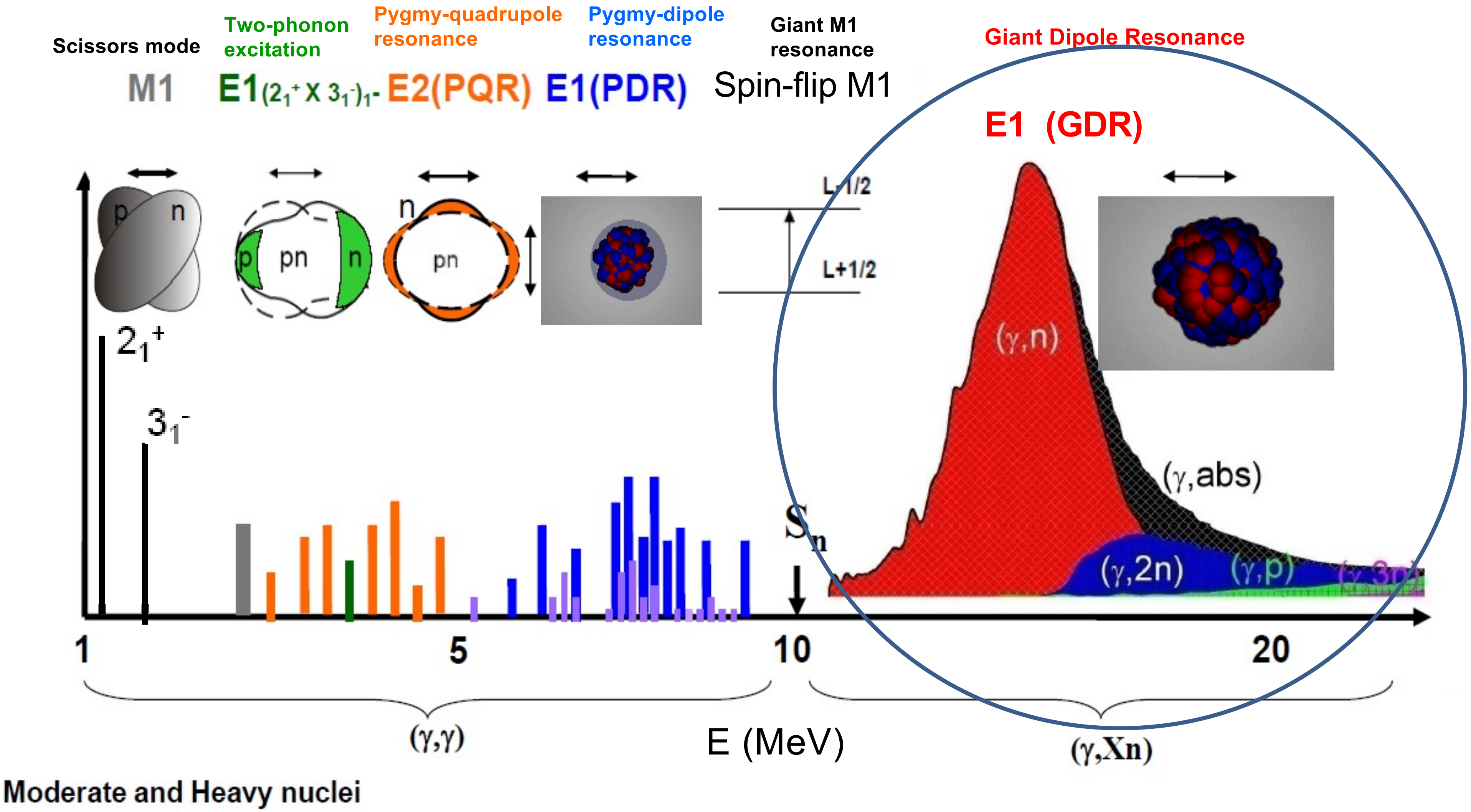
New photonuclear evaluation date of China



	IAEA	ENDF	KAERI	JENDL	BOFOD	CENDL
2023						266
2019	219	163	49	181	5	25
1999	164	15	143	64	5	25

Thank you for your attention !

Photon Strength Function



Theoretical prediction of Pygmy Quadrupole Resonance: N. Tsoneva, H. Lenske, Phys. Lett. B 695 (2011) 174.

N.Tsoneva, ERICE14

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