

Interaction dependence of the nuclear level density calculated using Hartree–Fock–Bogoliubov theory

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Introduction

Motivation

Nuclear data needed for developing a nuclear transmutation system for long-lived fission products (LLFPs)

- We are planning nuclear data evaluations for

4 LLFPs : ^{79}Se , ^{93}Zr , ^{107}Pd , ^{135}Cs

+ nuclei produced via the nuclear transmutation of these LLFPs.

Neutron, proton induced
0~200 MeV energy range

- The nuclear data evaluation is characterized with,

- ✓ Use of new experimental data to be obtained by other project group

- ✓ Development of theoretical methods appropriate/needed for **unstable nuclei**

One of the plan is,



Hauser-Feshbach calculation using a nuclear level density (NLD) derived from a microscopic nuclear structure calculation

For nuclear data evaluation,

- ✓ NLD up to 200 MeV
- ✓ NLD of wide mass range of nuclei are needed

➤ A microscopic method can be used for this purpose is,

- Hartree-Fock-bogoliubov (BCS) + combinatorial (statistical) method

P. Demetriou and S.Goriely, Nucl. Phys. A695 (2001) 95

S.Hilaire, J.P.Delaroche and M.Girod, Eur. Phys. J. A 12 (2001) 169

S.Goriely, S.Hilaire and A.J.Koning, Phys. Rev. C 78 (2008) 064307

➤ The microscopic calculation depends on used Hamiltonian
Effective nuclear interaction
Gogny, BSk, MSk ...

To investigate how NLD depends on the effective nuclear interaction
is an way to know about the reliability of NLD

In this study,

- ✓ NLD were calculated from HFB +statistical method using Skp, SLy4, SkM* Skyrme forces
- ✓ Hauser-Feshbach calculation using these NLD were performed
- ✓ Difference of NLD and resulting (n,2n) cross section are discussed

Framework

- Hartree-Fock-Bogoliubov theory + statistical method

- ✓ Grand partition function

BCS approximation with constant-G approach

P. Demetriou and S.Goriely, Nucl. Phys. A695 (2001) 95

$$Z(\alpha_n, \alpha_p, \beta) = \text{Tr}(e^{-\beta H + \alpha_p \hat{N}_p + \alpha_n \hat{N}_n})$$

$$= \prod_{i \in q=p,n} \exp \left(-\beta \left[(\epsilon_i - \lambda_q) \rho_i + \frac{1}{2} G \rho_i^2 - \frac{\Delta_q^2}{4E_i} - E_i f_i \right] \right) (1 + e^{-\beta E_i})$$

Renormalization term omitted

ϵ_i, λ_q are those obtained from finite temperature HFB calculation

$$\alpha_q = \beta \lambda_q$$

$\Delta_q = G \sum_{i \in q} u_i v_i$ G is determined from HFB pairing energy

$$\beta = 1/T$$

$$f_i = (1 + \exp(\beta E_i))^{-1}$$

- ✓ State density

$$\omega(E, N_n, N_p) \sim \frac{1}{(2\pi)^{3/2}} \frac{e^{S(T)}}{(\det D)^{1/2}}$$

entropy

$$S(T) = - \sum_i (f_i \ln f_i + (1 - f_i) \ln(1 - f_i))$$

- ✓ Thermal excitation energy

$$U(T) = E(T) - E(T = 0)$$

E(T): Total energy of the system obtained from the finite temperature HFB calculation

● Effective nuclear interaction

➤ Skyrme forces: Skp, SLy4, SkM*

✓ Pairing force

$$V_{\text{pair}}^{(n,p)}(\mathbf{r}) = \underline{V_0^{(n,p)}} \left(1 - \frac{1}{2} \frac{\rho_0(\mathbf{r})}{\rho_c} \right) \delta(\mathbf{r} - \mathbf{r}')$$

- Surface-volume mix type
- $\epsilon_{\text{cut}}=60$ MeV

✓ Pairing strength parameters

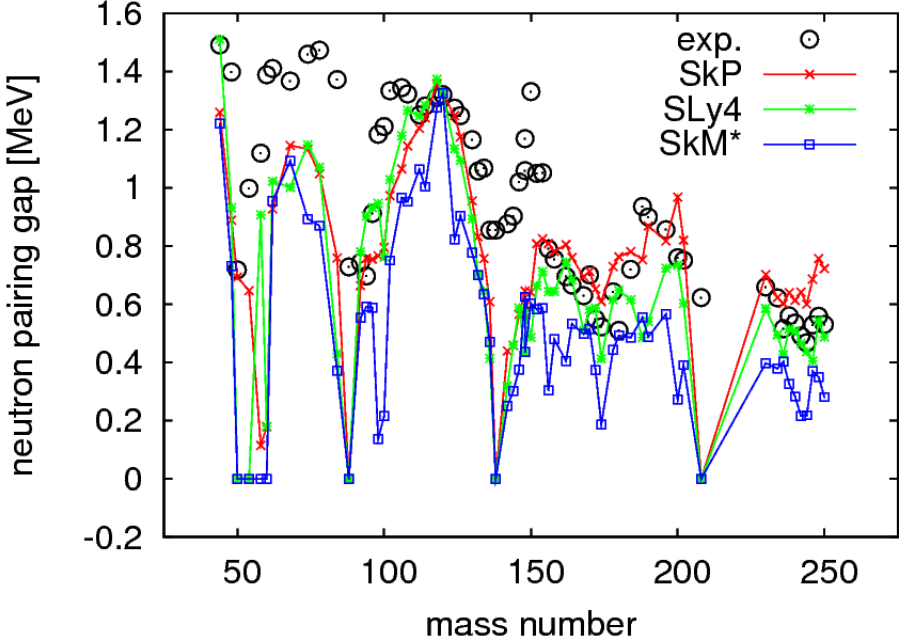
$V_0^{(n)}$ and $V_0^{(p)}$ are determined to reproduce the experimental pairing gaps of ^{120}Sn and ^{138}Ba

Unit: [MeV]

	SkM*	SLy4	SkP
$V_0^{(n)}$	-244	-291	-217
$V_0^{(p)}$	-258	-277	-231

✓ Neutron pairing gaps

66 even-even nuclei
that have experimental values of D_0



Experimental values of the pairing gaps are deduced from the three-point mass differences

$$\Delta^{(3)}(N + 1)$$

✓ Level density

$$\rho(U, J) = (1 - f_{dam}(U))K_{vib}(U)\rho_{sph}(U, J) + f_{dam}(U)K_{vib}(U)\rho_{def}(U, J)$$

$$\rho_{sph}(U, J) = \frac{2J+1}{2(2\pi)^{1/2}\sigma^3} \exp\left(-\frac{J(J+1)}{2\sigma^2}\right) \omega(E, N_n, N_p)$$

$$\rho_{def}(U, J) = \frac{1}{2} \sum_{K=-J}^J \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{J(J+1)}{2\sigma_{\perp}^2} - \frac{K^2}{2}\left(\frac{1}{\sigma^2} - \frac{1}{\sigma_{\perp}^2}\right)\right) \omega(E, N_n, N_p)$$

$f_{dam}(U)$: damping function for smooth transition between ρ_{sph} and ρ_{def}

✓ Phenomenological vibrational collective enhancement

IAEA-TECDOC-1506: Reference Input Parameter Library-2, IAEA, 2005

$$K_{vib}(E_x) = \exp[\delta S - (\delta U/t)]$$

$$\delta S = \sum_i (2\lambda_i + 1) [(1 + n_i) \ln(1 + n_i) - n_i \ln n_i]$$

$$\delta U = \sum_i (2\lambda_i + 1) \omega_i n_i,$$

$$n_i = \frac{\exp(-\gamma_i/2\omega_i)}{\exp(\omega_i/t) - 1}$$

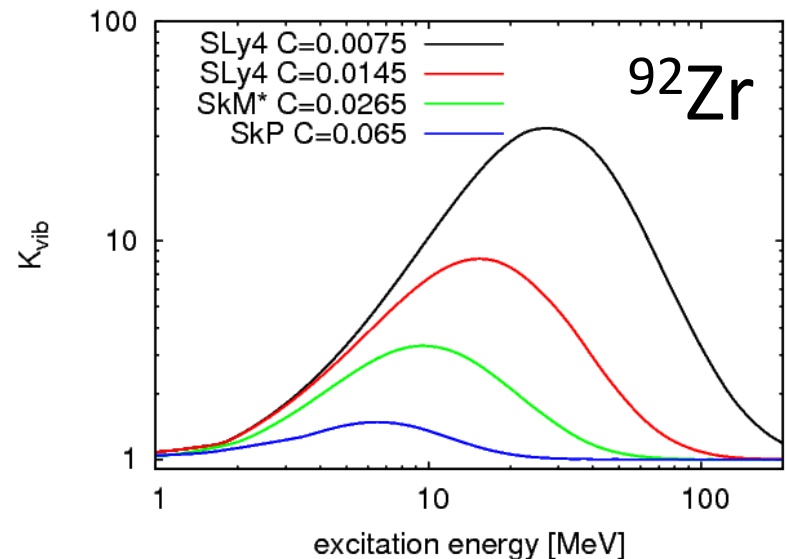
$$\gamma_i = \underline{C} A^{1/3} (\omega_i^2 + 4\pi^2 t^2)$$

damping width parameter

$$\omega_2 = 65 A^{-5/6} / (1 + 0.05 \delta W)$$

$$\omega_3 = 100 A^{-5/6} / (1 + 0.05 \delta W)$$

✓ Damping width parameter C of K_{vib} is optimized for each force by fitting D_0 of well deformed nuclei



- Hauser-Feshbach calculation using the microscopic NLD

CCONE code O. Iwamoto, J. Nucl. Sci. and Technol. 44 (2007) 687.

➤ Hauser-Feshbach statistical model

- ✓ Optical model potential: Koning-Delaroche
- ✓ Gamma strength function: Enhanced generalized Lorentzian (EGLO) model
- ✓ Nuclear level density

Present work

- Hartree-Fock-Bogoliubov theory + statistical method with Skp, SLy4, SkM* forces

For comparison,

- Hartree-Fock-Bogoliubov theory + combinatorial method taken from RIPL-3

S.Goriely, S.Hilaire and A.J.Koning, Phys. Rev. C 78 (2008) 064307

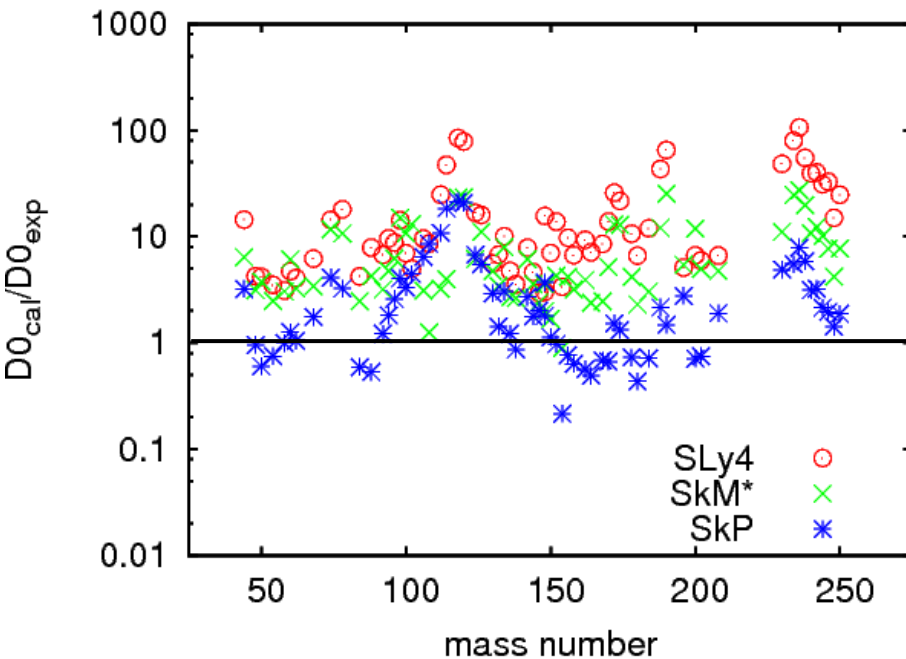
- Fermi Gas model with Mengoni-Nakajima level density parameter

A.Mengoni, Y.Nakajima, J. Nucl. Sci. Technol. 31 (1994) 152

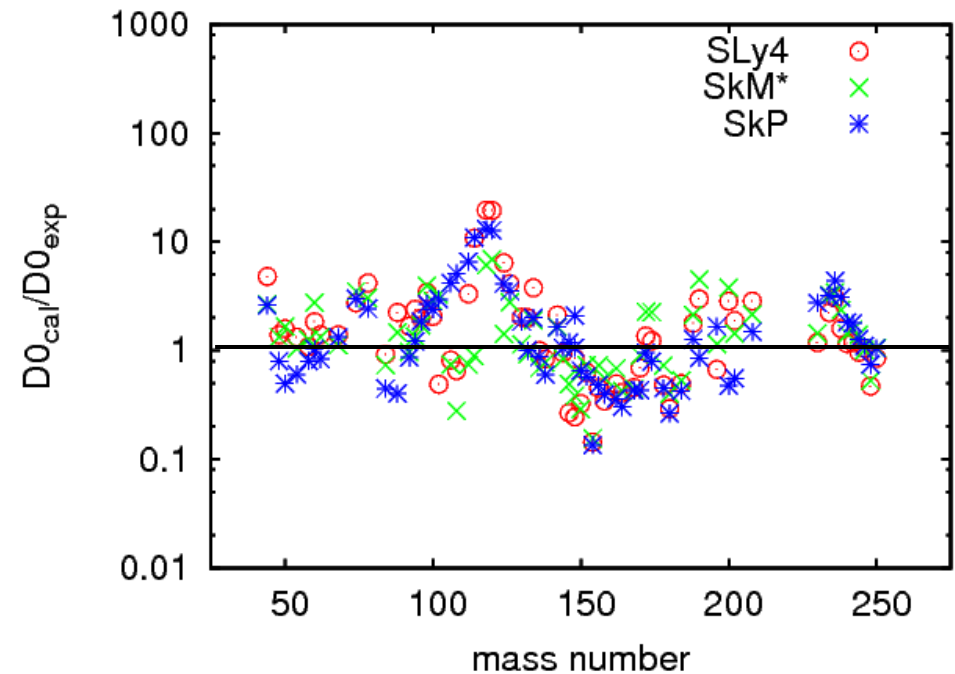
Results

- S-wave neutron resonance spacing D_0 for 66 even-even nuclei

✓ Without K_{vib}

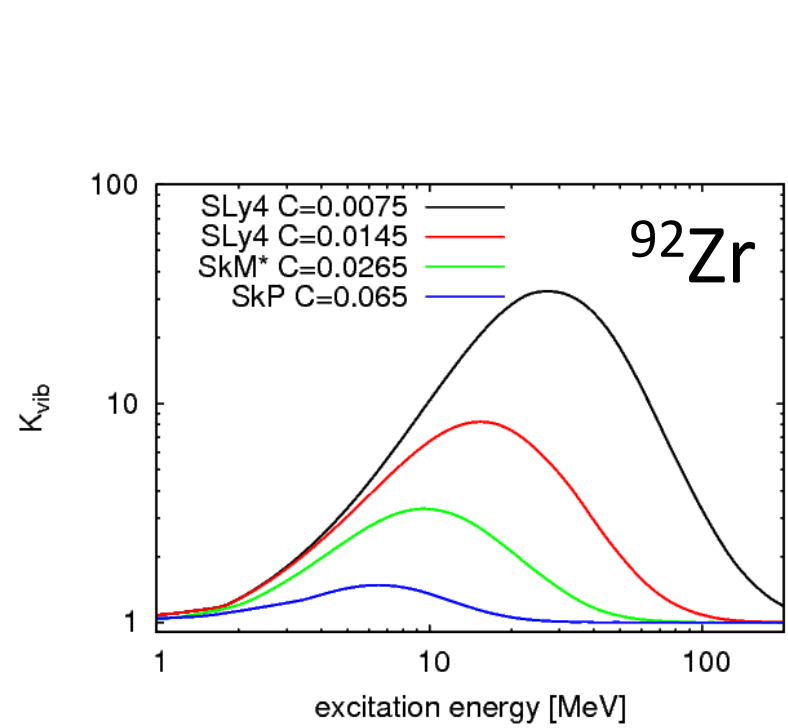
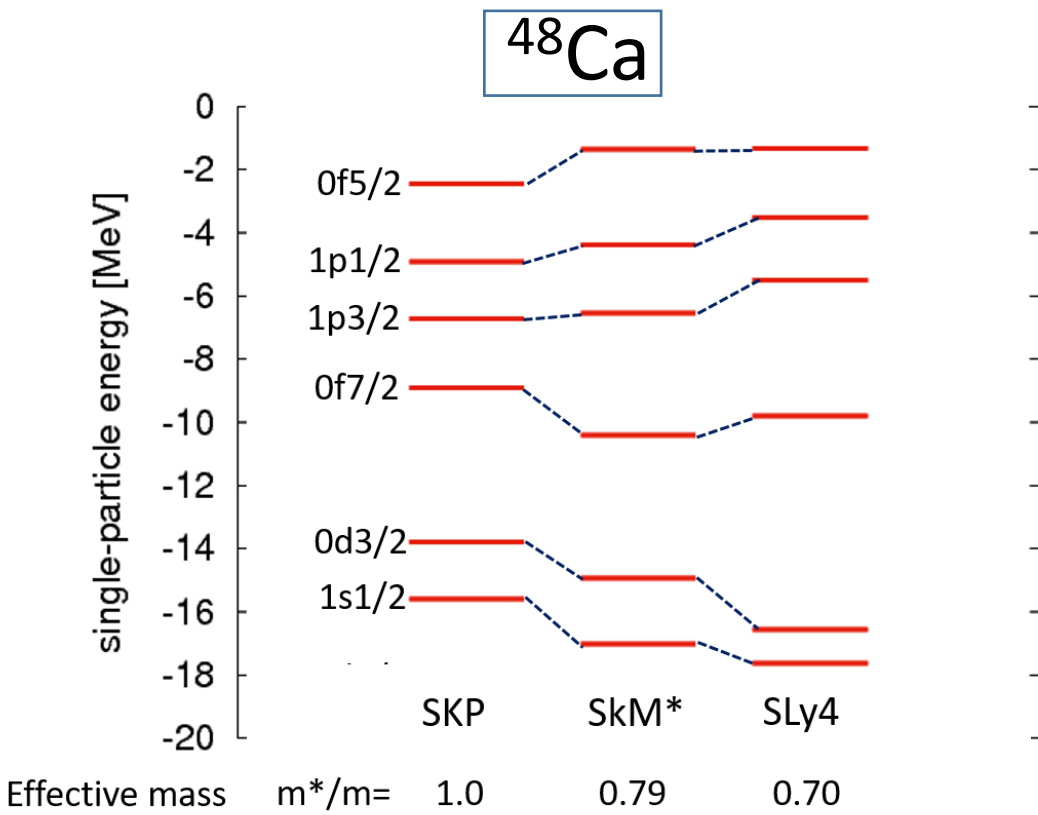


✓ Using K_{vib} with damping width parameter optimized for each force



- ✓ For Skp force, NLD calculated without K_{vib} is not bad compared to SkM* and SLy4
- ✓ Vibrational collective enhancement is essential for NLDs calculated using SkM* and SLy4
- ✓ By using the optimized K_{vib} , all forces deduce similar D_0

● Single-particle levels

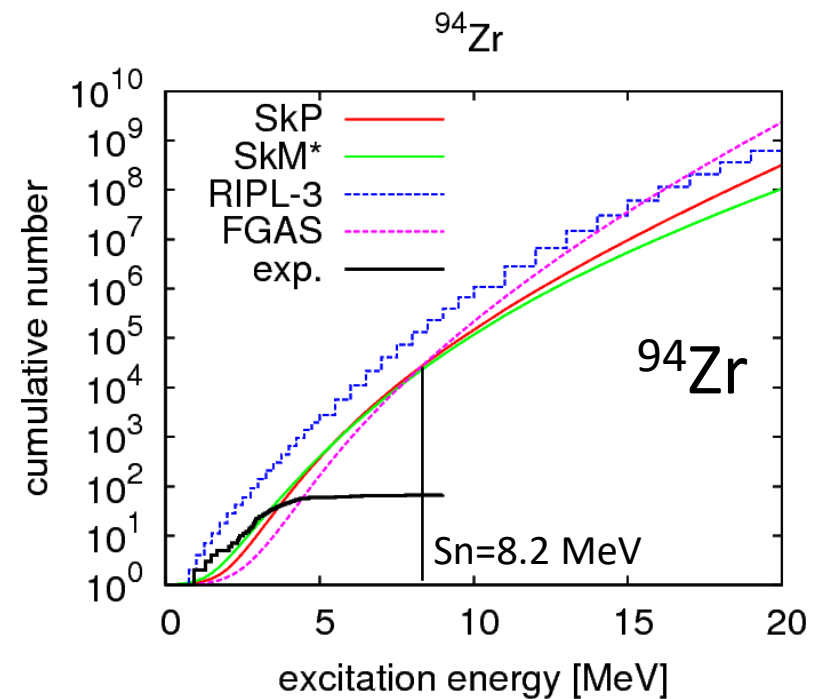
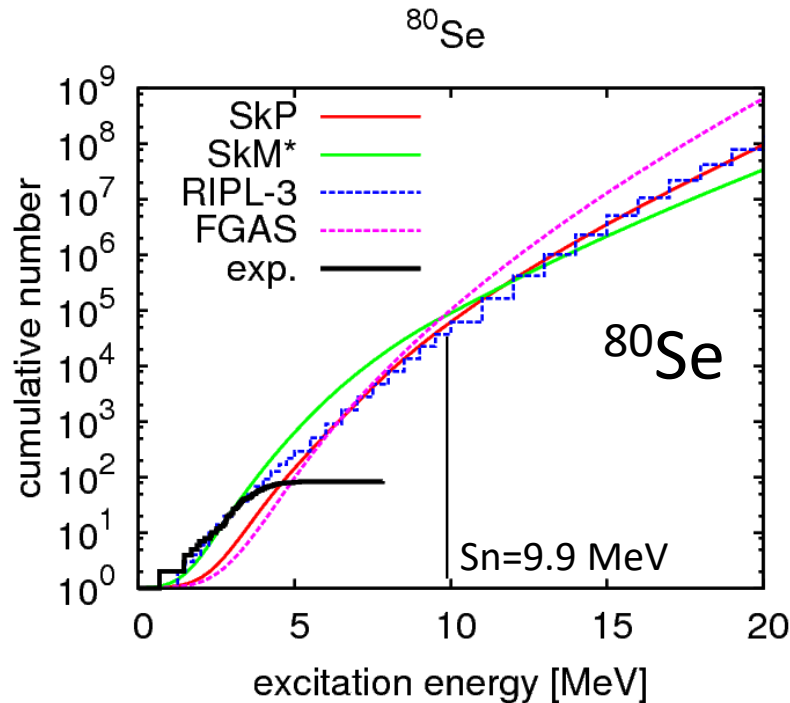


- ✓ Vibrational collective enhancement should be treated explicitly in NLD calculated using effective mass ~ 0.7 Skyrme forces
- ✓ Effect of the vibrational collective enhancement may be implicitly included in effective mass ~ 1 forces

- Cumulative number of levels

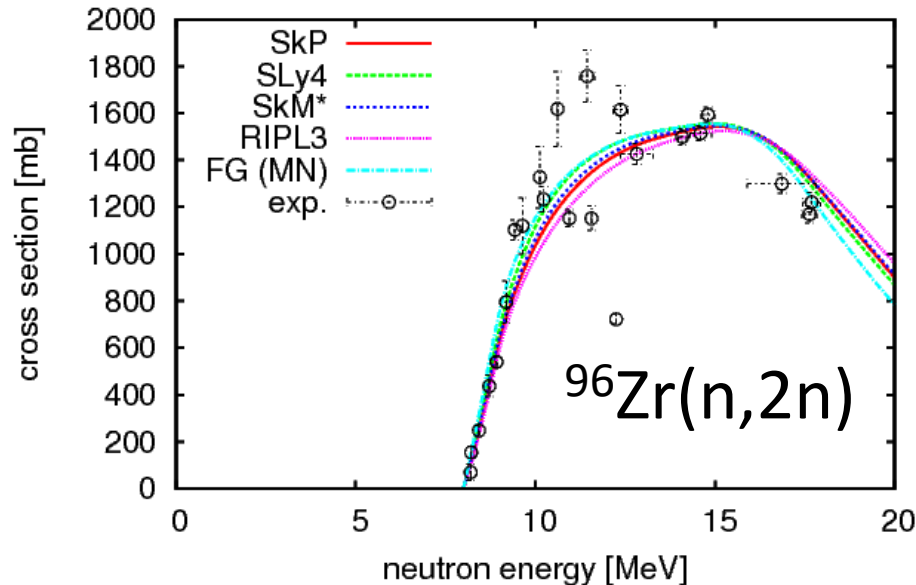
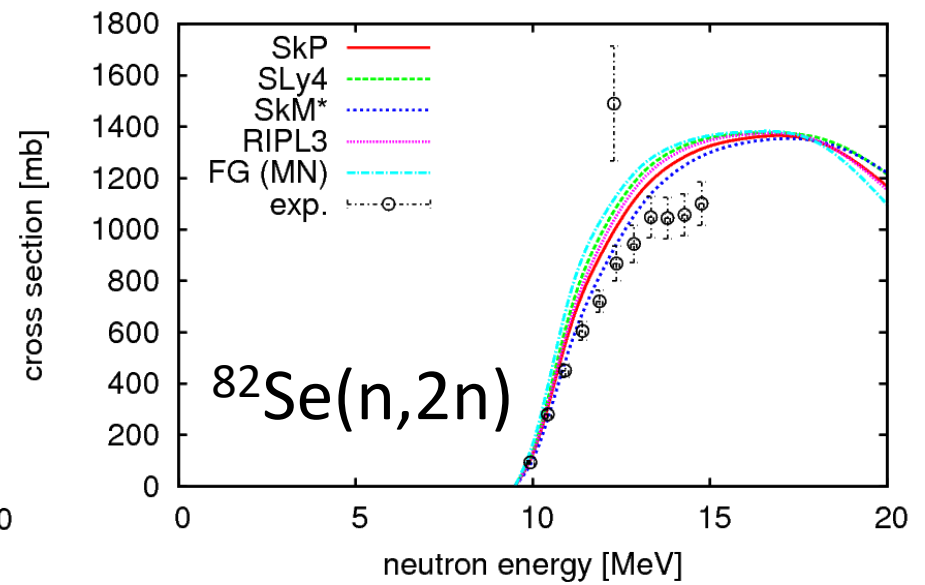
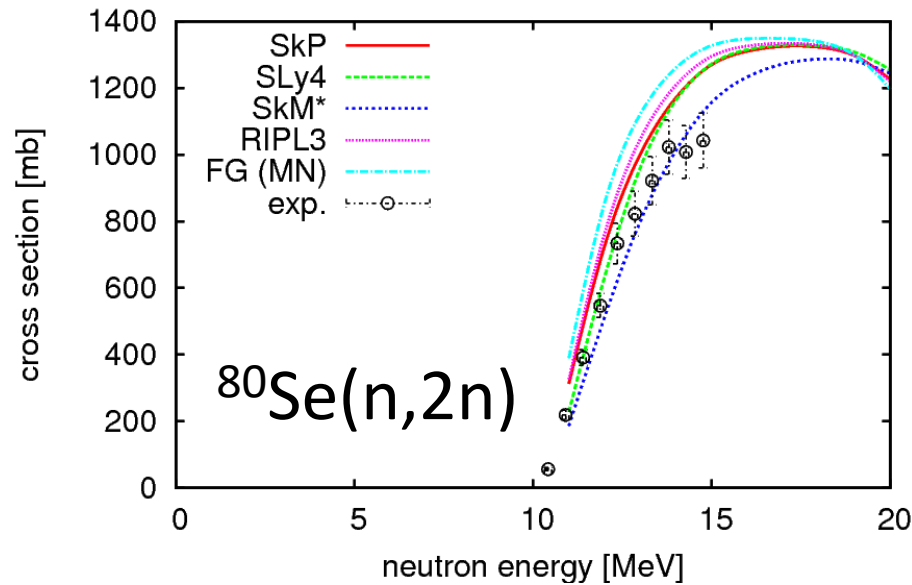
FGAS: Fermi Gas without constant temperature cal.
 RIPL-3: S.Goriely, S.Hilaire and A.J.Koning, PRC78 (2008) 064307

Compound nuclei of LLFPs (^{79}Se , ^{93}Zr)

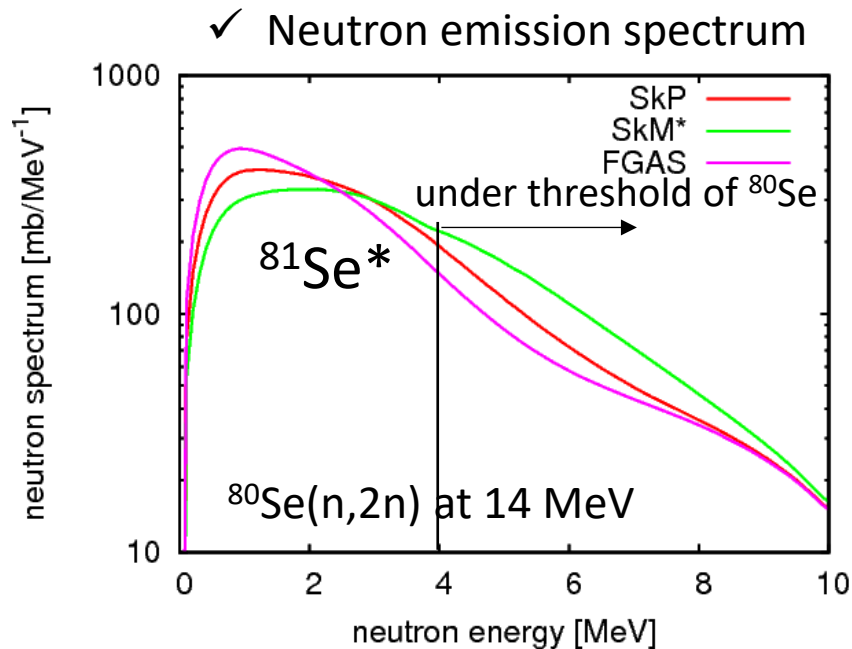
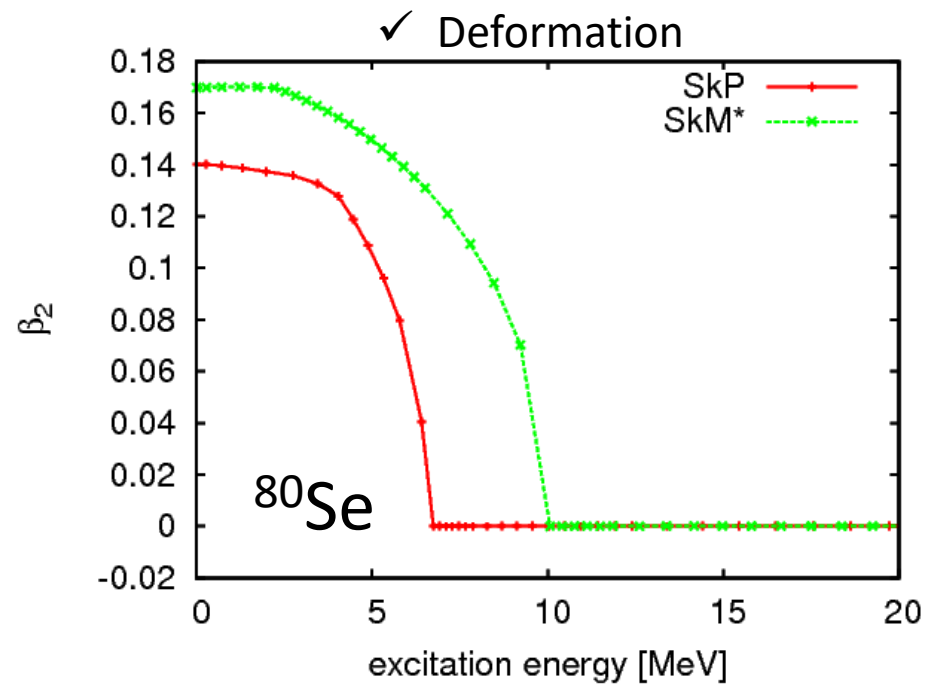
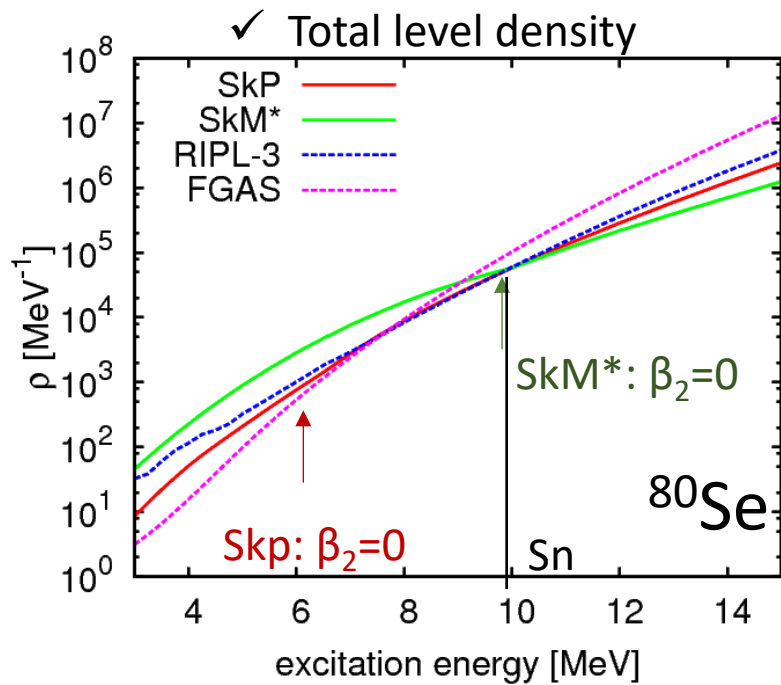


- ✓ NLDs cross around the neutron threshold.
- ✓ NLD around and above neutron threshold are influenced by the disappearance of deformation and vibrational collective enhancement.
- ✓ How these differences affect the cross section calculated using Hauser-Feshbach ?

- Differences in (n,2n) cross section

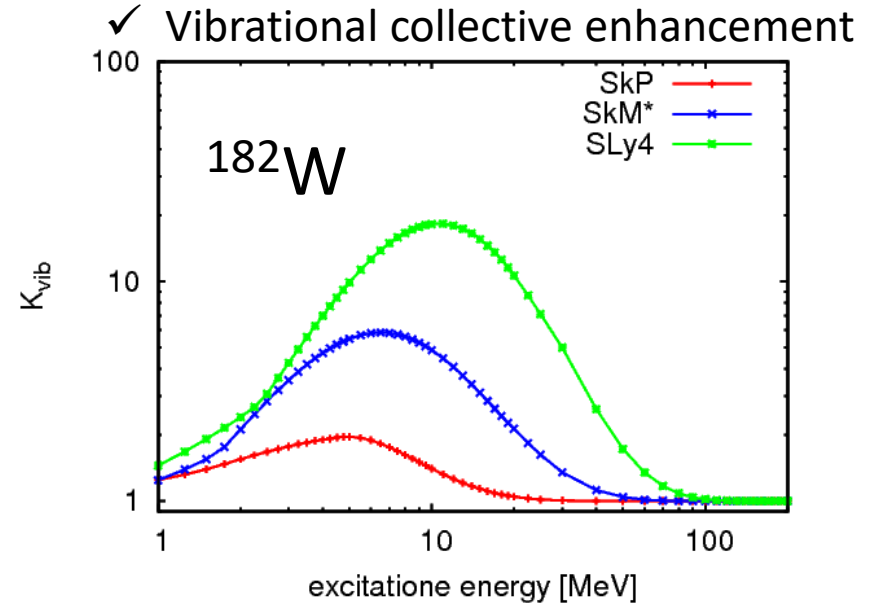
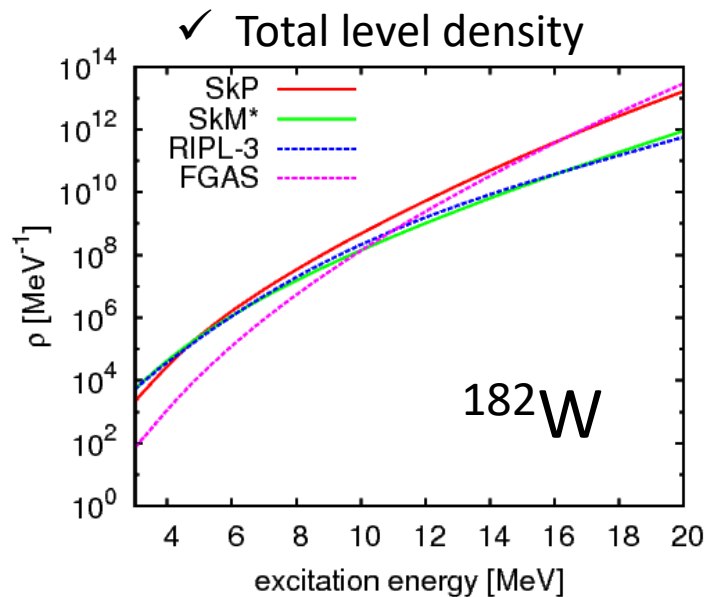
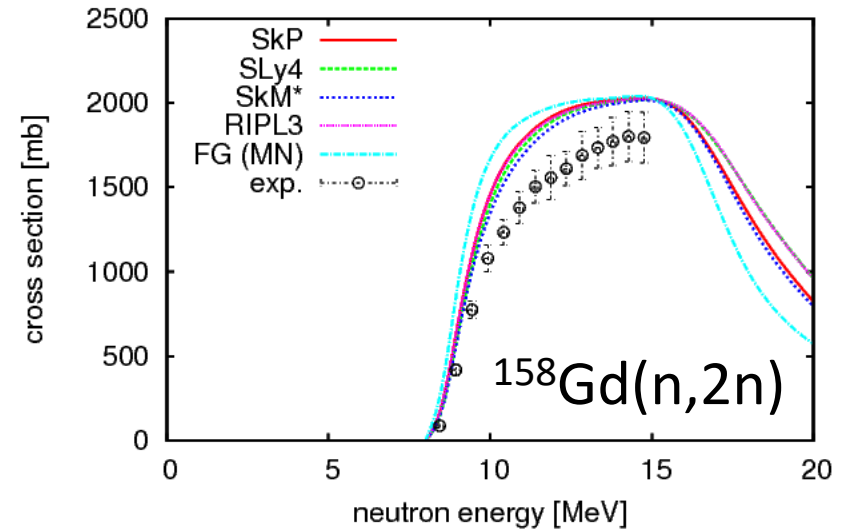
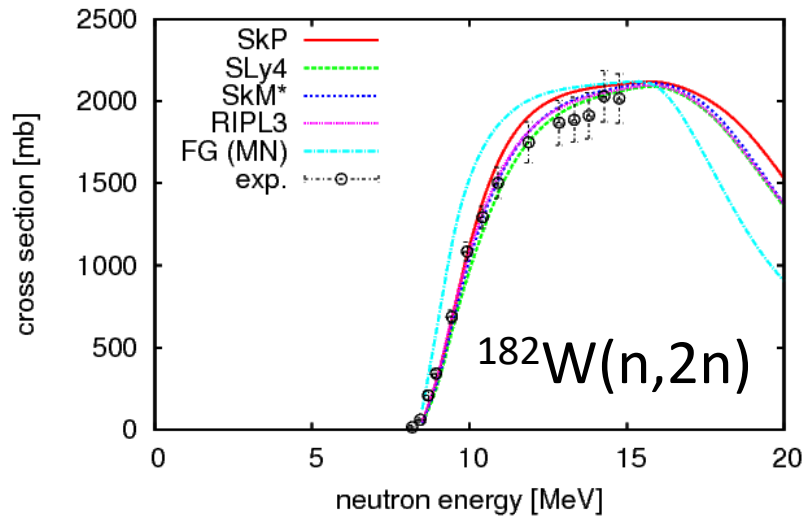


- ✓ (n,2n) cross section even have sensitivity to the difference of NLD
- ✓ Significant difference is found in ^{80}Se
- ✓ What is the reason for this differences ?



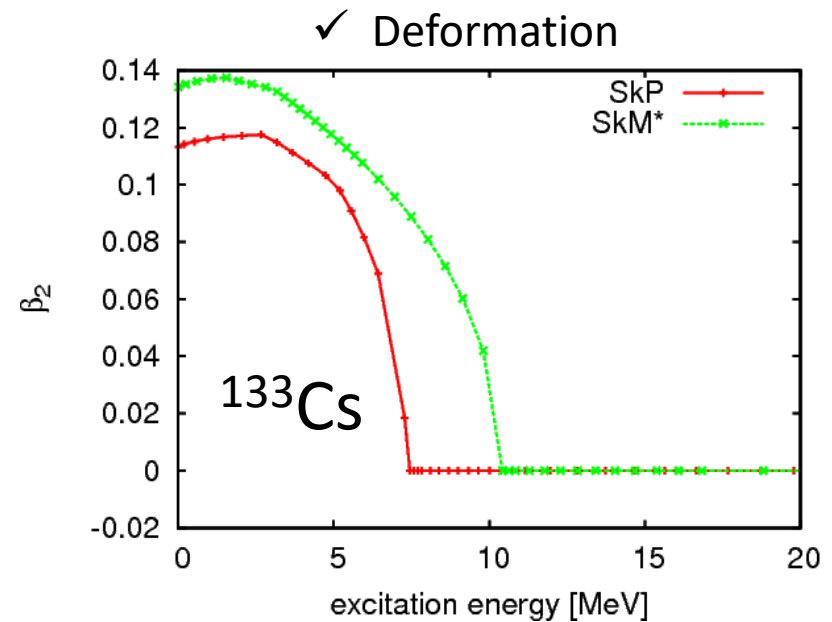
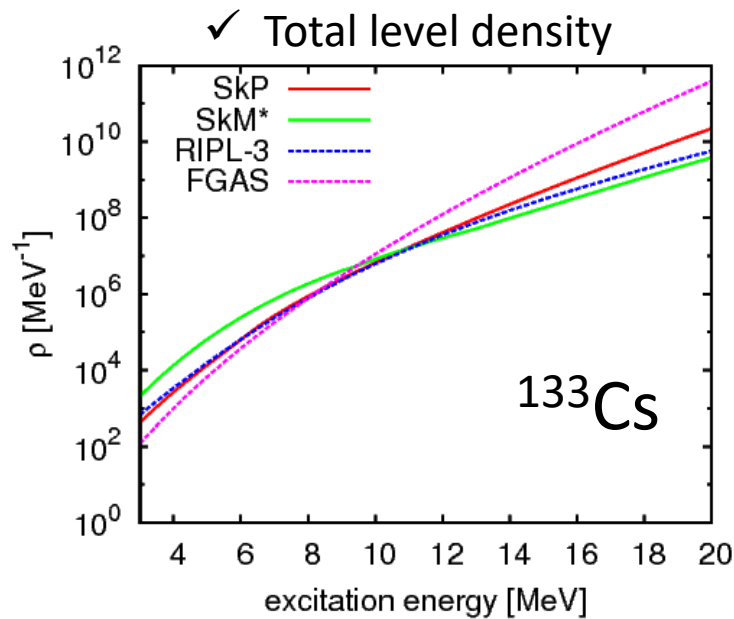
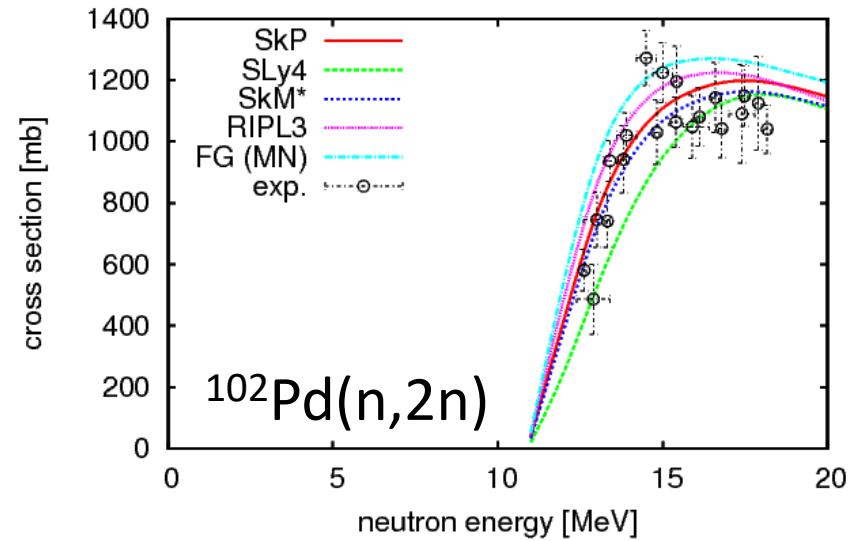
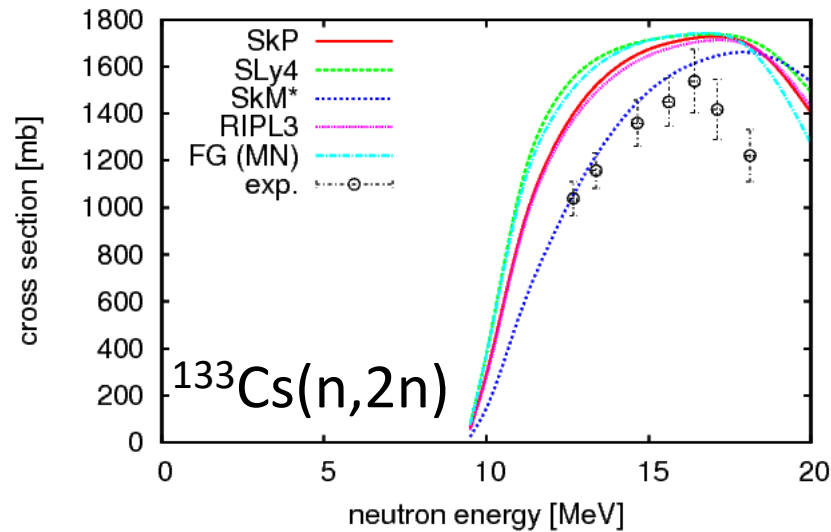
- ✓ (n,2n) cross section has sensitivity to the slope of the target nucleus NLD
- ✓ If the deformation change occurs around the neutron threshold, (n,2n) cross section is significantly reduced

● (n,2n) cross section of well deformed nuclei



- ✓ If the deformation does not change below 20 MeV, difference is small
- ✓ On the other hand, difference in K_{vib} has noticeable effect on (n,2n) cross section

- Differences in (n,2n) cross section of nuclei around LLFPs



✓ Difficulty in describing the deformation change is a source of large uncertainty

Summary

- NLD were calculated from HFB +statistical method using Skp, SLy4, SkM* Skyrme forces
 - ✓ The vibrational collective enhancement is essential for effective mass ~ 0.7 forces
 - ✓ NLD obtained from Skp, SLy4, SkM* forces deduce similar D_0 if the optimized vibrational collective enhancements are combined
- Hauser-Feshbach calculation using these NLD
 - ✓ $(n,2n)$ cross section have sensitivity to the slope of the target nucleus NLD
 - ✓ If the deformation change occurs around the neutron threshold, $(n,2n)$ cross section is significantly reduced
→ Large difference among used forces
 - ✓ Difference in the damping of K_{vib} for each forces is also visible in $(n,2n)$ cross section