Microscopic modeling of direct and pre-equilibrium emission mechanisms for nucleon induced reactions

NT Program INT-17-1a
Toward Predictive Theories of Nuclear Reactions Across the Isotopic Chart

20 March, 2017

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Outline

- Introduction: microscopic models for applications.
- Folding model: direct inelastic scattering and pre-equilibrium emission.
- Applications:
  - Nucleon induced reaction - rearrangement corrections.
  - Pre-equilibrium contribution to (n,xn) reactions.
  - Spin-parity distributions and ^{238}U (n,nγ) cross-sections.
  - Inferring ^{239}Pu (n,2n) cross-sections form (n,2nγ) measurements: impact of a microscopic description of pre-equilibrium.
- Conclusions, a few questions, future works and perspectives.

Context

Basic science questions: better understanding of nuclear structure and reaction, cross sections for astrophysical models

Applications for security, nuclear energy, waste managment, medical applications etc.

$\Downarrow$

Nuclear reactions observables for a **wide range** of **nuclear masses** and **incident energies**.

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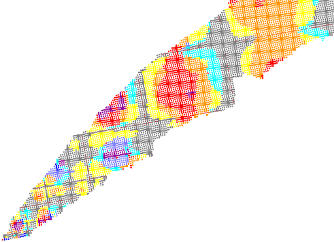
All needed nuclear reaction observables cannot be measured.

Fine precision required: (n,n') or (n,2n) for actinides.

First principles $\leadsto$ reaction observables for light and a few medium mass nuclei at low incident energy.

$\Rightarrow$



Select the relevant parts of the dynamical many-body problem.

Use available experimental knowledge.

$\Downarrow$

Modeling

$\swarrow$ $\searrow$

Phenomenological   Microscopic

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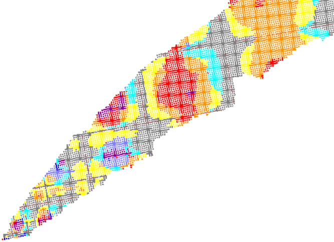

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Modeling

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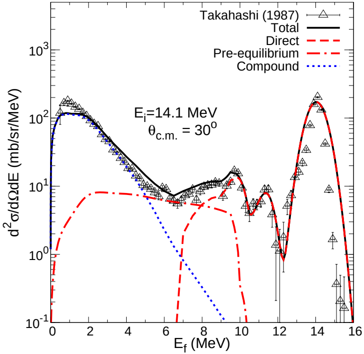
Phenomenological **Microscopic**

Our goal: *improve modeling of nucleon induced reactions up to actinides*

Modeling reaction mechanisms - example of inclusive (n,xn) cross section

Reaction mechanisms

- **Direct** reactions : elastic, inelastic to discrete states and to giant resonances;
- Large energy transfer: **pre-equilibrium** emission;
- **Compound nucleus** formation then evaporation;



Phenomenological approach

- Optical potential, level densities;
- β_l for discrete states, response functions for G.R. (inferred from electron, hadron scatterings exp.);
- Pre-equilibrium : exciton model (coupling constants from global fit);

^{208}Pb (n,xn)

Talys 1.8 (default)

Two-components exciton model

[A.J. Koning, M,C. Duijvestijn, Nucl. Phys. A 744, 15 (2004)]

Direct models models well constrained: β_l, %EWSR well known.

Modeling reaction mechanisms - example of inclusive (n,xn) cross section

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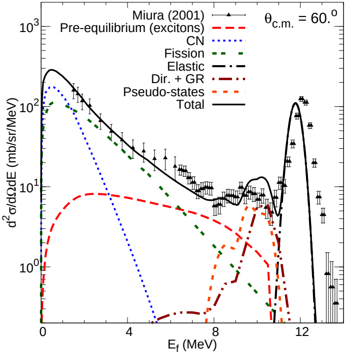

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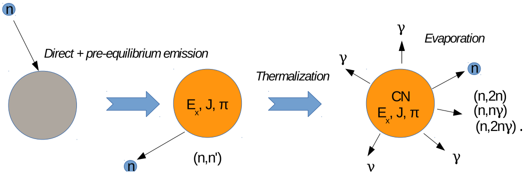
^{238}U (n,xn)
Emission from fission fragments.
Talys 1.4 (adjusted)
Direct reaction models not well constrained:
Evaluations for actinides :
+ **pseudo-states** (see ENDFBVII and others).

Connections between mechanisms



Direct + pre-equilibrium:

- Particles emission.
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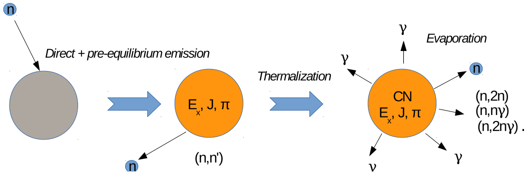

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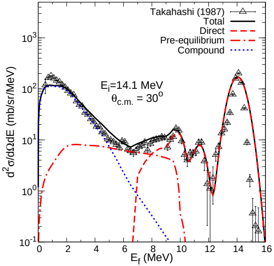
Pre-equilibrium models:

- Account for known doubly-differential cross-sections.
- Junction with direct process arbitrary (continuum).
- J, Π distributions of the residual nucleus: ad-hoc prescriptions for exciton models.



$\Rightarrow J, \Pi$ distributions:

- (n,n'γ) cross sections (indirect determination of the total (n,n') cross sections).
- Surrogate applications.

Microscopic approach to direct and pre-equilibrium reactions

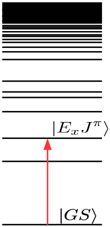
Direct elastic: $\left(K + U^{\text{opt}} - E_i\right) \chi^{+}_{\mathbf{k}_i} = 0$,
$U^{\text{opt}} = \langle GS|V|GS\rangle$.

Direct inelastic scattering to discrete excitations:

$$\frac{d\sigma(\mathbf{k}_i,\mathbf{k}_f)}{d\Omega} \sim \left|\langle \chi^{-}_{\mathbf{k}_f}, E_x J^{\pi} | T | \chi^{+}_{\mathbf{k}_i}, GS\rangle\right|^2$$

$$T = V + VGV + \ldots$$

DWBA: $T \simeq V$.



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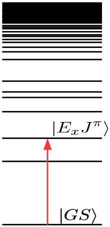

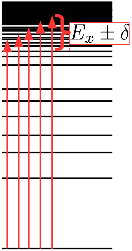

Pre-equilibrium emission: quantum models

$$\frac{d\sigma(\mathbf{k}_i,\mathbf{k}_f)}{d\Omega dE_f} \sim \frac{1}{2\delta}\int_{E_f-\delta}^{E_f+\delta} dE \sum\!\!\!\!\!\!\int_{E_xJ^\pi} \delta(E_i - E_x - E)\left|\langle\chi^-_{\mathbf{k}}, E_xJ^\pi|T|\chi^+_{\mathbf{k}_i}, GS\rangle\right|$$

Target final states: $|E_xJ^\pi\rangle = \sum_{n,ph} c^n_{ph}(E_x)|npnh\rangle$

One-step (DWBA) + 2-body interaction:

$$T \simeq V \quad \Rightarrow \quad |GS\rangle \to c^1_{ph}(E_x)|ph\rangle$$

Microscopic description of target states

Target masses up to actinides, ground state and transition properties
$\Longrightarrow$ **Mean-field and beyond** nuclear structure models, with phenomenological effective interactions (Skyrme, **Gogny** etc.).

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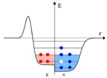
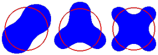
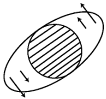




Direct inelastic scattering to
particle-hole excitations,
collective **vibrations/rotations** for many J^{Π}.



Weak perturbation $\Rightarrow$ small amplitude collective motion $\Rightarrow$ **linear response theory**.

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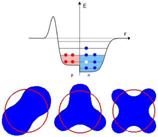

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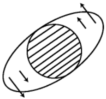

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$$\Downarrow$$

(Quasi-particule) Random phase Approximation

$\Rightarrow$ Nucleus excitation are phonons $\quad |E_x, J^{\pi}\rangle = \Theta^{\dagger}|\tilde{0}\rangle$

RPA $\quad \Theta^{\dagger} = \sum_{ph} X^{J\pi}_{ph}\, a^{\dagger}_{p} a_{h} + Y^{J\pi}_{ph}\, a^{\dagger}_{h} a_{p}$ $\quad$ **p-h** and **h-p** components

QRPA $\quad \Theta^{\dagger} = \sum_{\alpha,\alpha'} X^{J\pi}_{\alpha\alpha'}\, \eta^{\dagger}_{\alpha}\eta^{\dagger}_{\alpha'} + Y^{J\pi}_{\alpha\alpha'}\, \eta_{\alpha}\eta_{\alpha'}$ $\quad$ **2-qp** creation and annihilation

Folding model for direct elastic and inelastic scattering

Direct inelastic scattering: optical potentials and DWBA matrix elements

$$U^{opt} = \langle GS|\ V\ |GS\rangle \qquad \langle \chi^-_{\mathbf{k}_f}, E_x J^\pi|\ V\ \ |\chi^+_{\mathbf{k}_i}, GS\rangle$$

JLM folding model: Brueckner-Hartree-Fock calculation
J.-P. Jeukenne, A. Lejeune, and C. Mahaux. Phys. Rev. C, 16, 1977

- Effective interaction V complex, E,ρ-dependent **+ normalizations**.
- Energy range **1 keV-200 MeV** *E. Bauge, J. P. Delaroche, and M. Girod. Phys. Rev. C, 63, 2001.*
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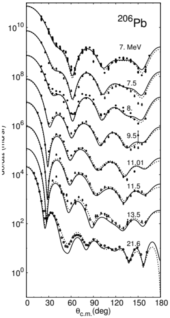
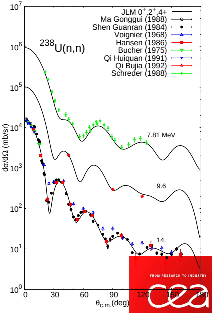


Large range of applications:

Unique structure model: **HF(B)/(Q)RPA** (**Gogny D1S** interaction).

JLM: **parametrization unchanged** for all calculations.

$\Longrightarrow$ **Direct elastic, inelastic, pre-equilibrium** mechanisms, **spherical** and **deformed** targets.



Inelastic scattering to discrete excitations

E_x (MeV)		$B(E3,\uparrow)_{exp}(10^6.e^2.fm^6)$	
Exp.	QRPA	Exp.	QRPA
2.65	3.73	0.611(15)	0.635

QRPA with Gogny force, consitent implementation, spherical and axial def.

S.Péru, H.Goutte, Phys.Rev. C 77, 044313 (2008)

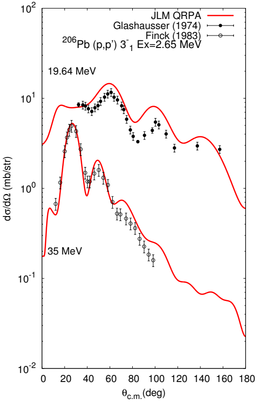
M.Martini, S.Peru, M.Dupuis Phys.Rev. C 83, 034309 (2011)

S.Péru, et al. Phys.Rev. C 83, 014314 (2011)

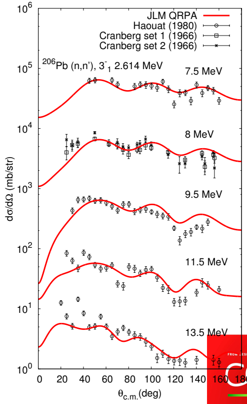
S.Péru, M.Martini, Eur.Phys.J. A 50, 88 (2014)

Consistent description of structure and reactions observables.

^{206}Pb(p,p') 3_1^-



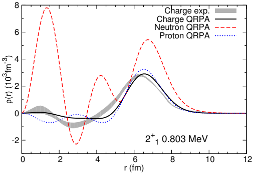
^{206}Pb(n,n') 3_1^-



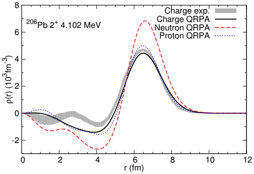
Inelastic scattering to discrete excitations: $^{206}Pb\ 2_1^+$

E_x (MeV)		$B(E2,\uparrow)_{exp}(10^4.e^2.fm^4)$	
Exp.	QRPA	Exp.	QRPA
0.803	1.51	0.1000(20)	0.099

YRAST 2_1^+ $\rho_{tr}(r)$



Isoscalar surface vibration $\rho_{tr}(r)$



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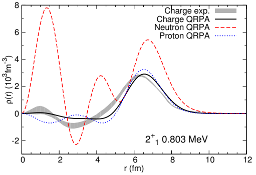

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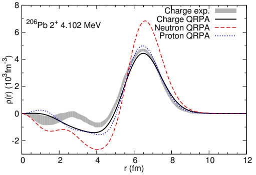
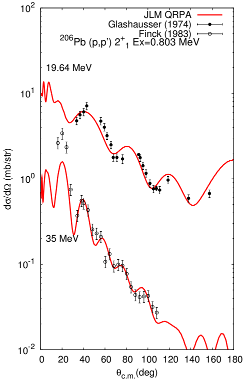
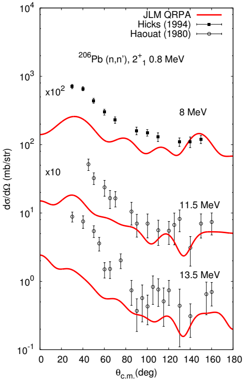


(p,p')



(n,n')



Transition potential: rearrangement

Inelastic process: $\rho_{GS} \rightarrow \rho_{GS} + \delta\rho$:
$\Rightarrow$ Dynamical corrections to $V(\rho_{GS})$

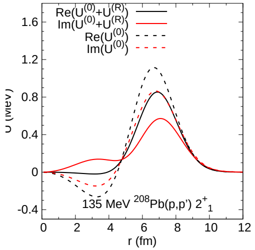
Transition potential:

$$\langle E_x, J^\pi | V | GS \rangle \equiv \rho_{\text{tr}}^{gs \leftarrow E_x} \left\{ V(\rho_{GS}) + \rho_{GS} \frac{\delta V(\rho)}{\delta(\rho)} \right\}$$

T. Cheon, et *al.*, Nucl. Phys. A437, 301 (1985).

$$U^{(0)} \equiv V(\rho_{GS})\rho_{\text{tr}}$$

$$U^{(R)} \equiv \rho_{GS} \frac{\delta V(\rho)}{\delta(\rho)} \rho_{\text{tr}}$$



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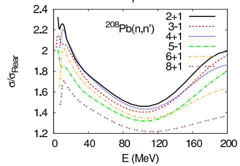
Ratio $\sigma^{(0)}/\sigma^{(0+R)}$:



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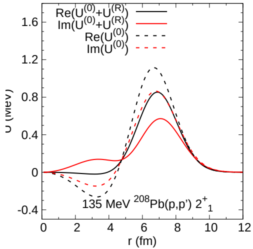
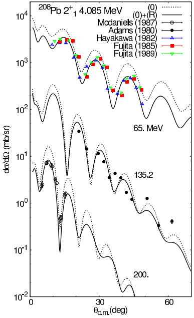
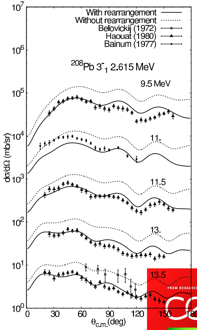


(p,p')



(n,n')



Microscopic approach to direct and pre-equilibrium reactions

Pre-equilibrium emission $E_{in} < 20$ MeV: one-step direct

$$\frac{d\sigma(\mathbf{k}_i,\mathbf{k}_f)}{d\Omega dE_f} \sim \frac{1}{2\delta} \int_{E_f-\delta}^{E_f+\delta} dE \; \sum\!\!\!\!\!\!\int_{E_xJ^\pi} \delta(E_i - E_x - E) \; \left| \langle \chi_{\mathbf{k}}^- \,,\; E_xJ^\pi \,|\, V \,|\, \chi_{\mathbf{k}_i}^+ \,,\, GS \,\rangle \right|^2$$

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Target final states: mix of n-phonons states $(n = 1\ 2\ ...)$

$$|F = E_x J^\pi\rangle = \sum_{n,\{k\}} c^F_{n,\{k\}}(E_x) \prod_i^n \Theta^\dagger_{\{k\}} |\tilde{0}\rangle = c^F_{1,N} \Theta^\dagger_N |\tilde{0}\rangle + c^F_{2,\{N,N'\}} \Theta^\dagger_N \Theta^\dagger_{N'} |\tilde{0}\rangle +$$

One-step + 2-body interaction + Quasi-boson: $|\tilde{0}\rangle \rightarrow c^F_N(E_x)\Theta^\dagger_N|\tilde{0}\rangle$

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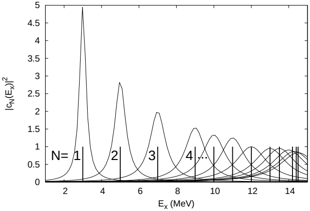

Statistical hypothesis:

$$\langle\, c^F_N(E_x)\, c^F_{N'}(E_x)\, \rangle_E = \delta_{N,N'} \left| C^F_N(E_x) \right|^2$$

$$\left| c^F_N(E_x) \right|^2 = \frac{\Gamma_N}{2} \frac{1}{(E_x - E_N)^2 + \frac{\Gamma_N^2}{4}}$$

Γ_N = damping widths: phenomenological prescription.

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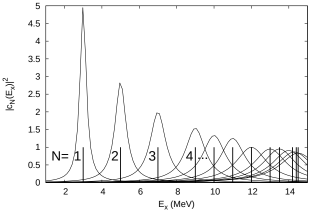
$$\frac{d\sigma(\mathbf{k}_i,\mathbf{k}_f)}{d\Omega dE_f} \sim \frac{1}{2\delta} \int_{E_f-\delta}^{E_f+\delta} dE \sum_N \frac{\Gamma_N}{2} \frac{1}{(E_i - E - E_N)^2 + \frac{\Gamma_N^2}{4}} \left| \langle \chi_{\mathbf{k}}^- , N^{RPA} \mid V \mid \chi_{\mathbf{k}_i}^+ , \tilde{0} \rangle \right|^2$$

Target final states: mix of n-phonons states ($n = 1\ 2 \ldots$)

$$|F = E_x J^\pi\rangle = \sum_{n,\{k\}} c^F_{n,\{k\}}(E_x) \prod_i^n \Theta^\dagger_{\{k\}} |\tilde{0}\rangle = c^F_{1,N} \Theta^\dagger_N |\tilde{0}\rangle + c^F_{2,\{N,N'\}} \Theta^\dagger_N \Theta^\dagger_{N'} |\tilde{0}\rangle +$$

One-step + 2-body interaction + Quasi-boson: $|\tilde{0}\rangle \rightarrow c^F_N(E_x)\Theta^\dagger_N|\tilde{0}\rangle$



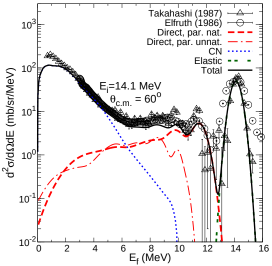
Statistical hypothesis:

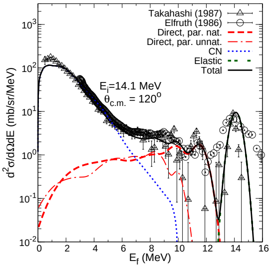
$$\langle\, c^F_N(E_x)\, c^F_{N'}(E_x)\, \rangle_E = \delta_{N,N'} \left| C^F_N(E_x) \right|^2$$

$$\left| c^F_N(E_x) \right|^2 = \frac{\Gamma_N}{2} \frac{1}{(E_x - E_N)^2 + \frac{\Gamma_N^2}{4}}$$

Γ_N = damping widths: phenomenological prescription.

One-step direct (n,n') - ^{208}Pb(n,xn)





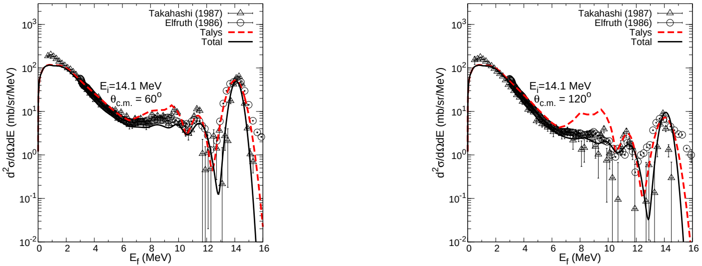
JLM with RPA excitations (natural parities)

JLM: no spin flip possible.

$V_{JLM} \Rightarrow V_{CDM3Y}$ non-natural parity transitions ($0^+ \to J^\pi$ with $\pi = -(-)^J$)

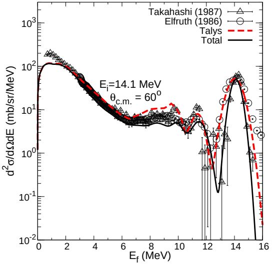
CDM3Y: real, ρ-dependent, include two-body spin-orbit and tensor interactions.

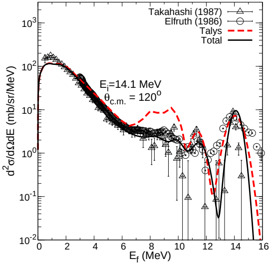
One-step direct (n,n') - ^{208}Pb(n,xn)



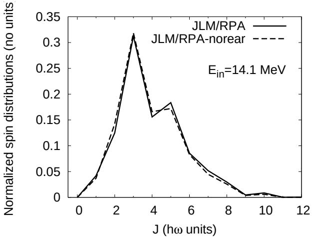
Comparison to calculations from Talys 1.8 (default settings).

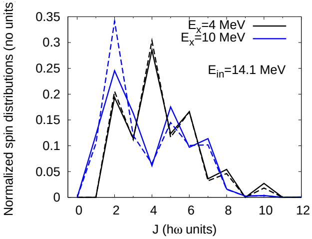
One-step direct (n,n') - ^{208}Pb(n,xn)





(n,n') from RPA states: **spin-parity distributions** / impact of **rearrangement**.





Nuclear structure
GS and excitations

HF(B)+(Q)RPA,
Gogny force

$\Downarrow$

- Densities, radii, deformations
- Radial transition densities, $B(E_L)$
- Response functions, EWSR

$\Longrightarrow$

In-medium: n-n two-body interaction

JLM, from nuclear matter

semi-microscopic

normalizations fixed

+ two-body S.O. and tensor for unnatural parity transitions.

$\Downarrow$

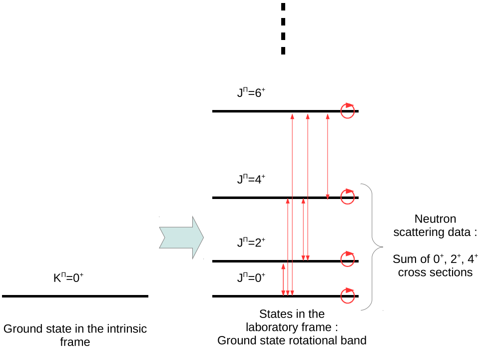
Nucleon induced **direct reactions** for **spherical nuclei**:

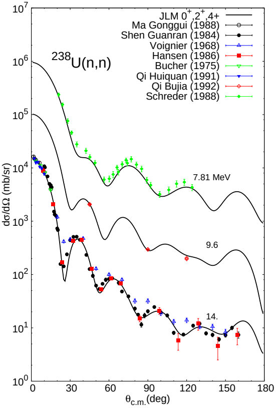
- Elastic scattering
- Inelastic scattering to discrete states
- First step of pre-equilibrium emission

$\Rightarrow$ **Application to n + actinides** $\longrightarrow$ axial deformation.

Neutron induced reactions on actinides

JLM model + HFB axial densities : $L = 0, 2, 4...$ multipoles.





Excitation spectrum of a nucleus with a static axial deformation

QRPA with axial deformation, good quantum numbers:

- Projection K , of the total angular momentum $\vec{J}$ on the symmetry axis Oz,
- Parity π.

Target excitations in the **i**ntrinsic frame : $|\alpha K \Pi\rangle = \Theta^{+}_{\alpha K \Pi} |\tilde{0}_I\rangle$.

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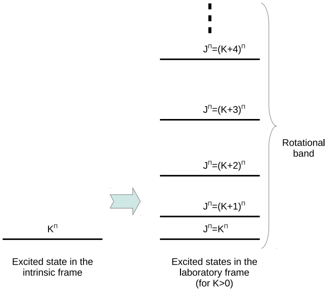
Target states in the **l**aboratory frame : projection on total angular momentum
$\Longrightarrow$ **r**otational bands, on for each intrinsic excitation, $J \geq K$



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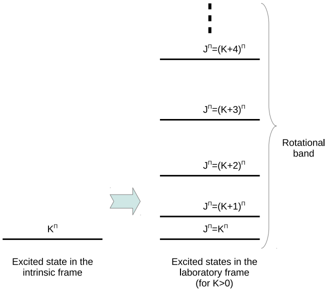
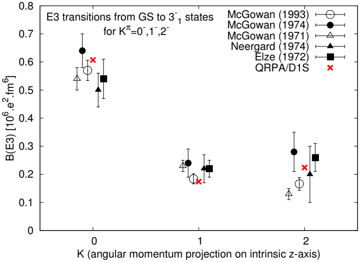


E3 transition probabilities



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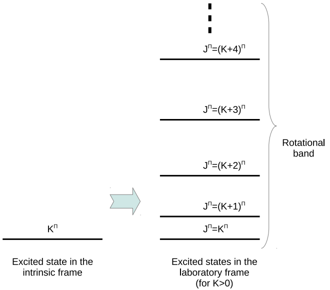
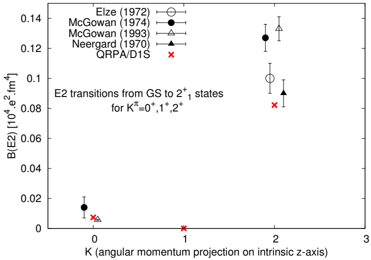


E2 transition probabities



Excitation spectrum of a nucleus with a static axial deformation

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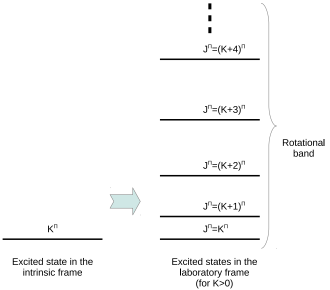
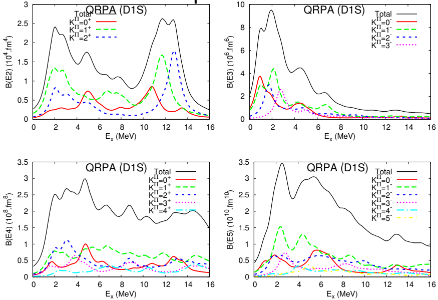


E2-E5 response functions



11-18 MeV (n,xn) ^{238}U spectra

Direct emission component:

$$\frac{d\sigma(\mathbf{k}_i,\mathbf{k}_f)}{d\Omega dE_f} = \frac{1}{2\delta}\int_{E_f-\delta}^{E_f+\delta} dE \sum_{N=K^\pi, J\geq K} \frac{\Gamma_N}{2} \frac{1}{(E_i-E-E_N)^2+\frac{\Gamma_N^2}{4}} \frac{d\sigma_N}{d\Omega}$$

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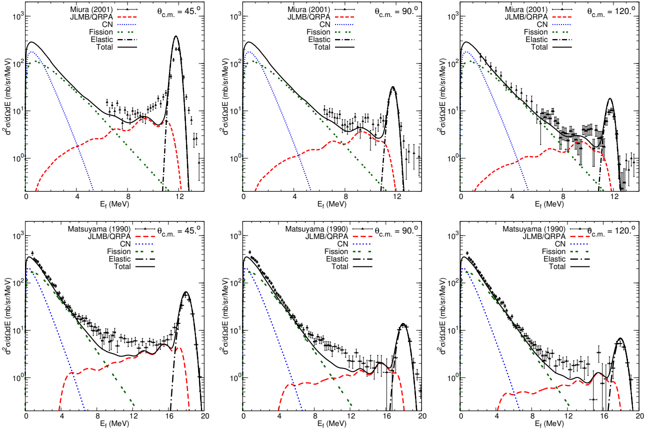
$\theta = 30^\circ$ $\theta = 60^\circ$ $\theta = 120^\circ$

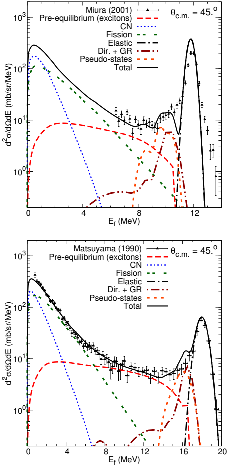


11.8 MeV

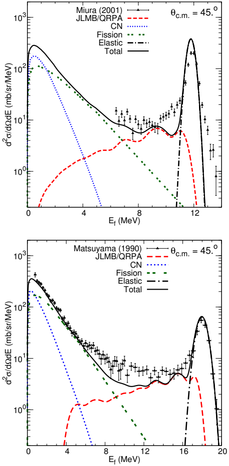
18. MeV

Comparison to previous more phenomenological calculations

Excitons + collective model + pseudo states

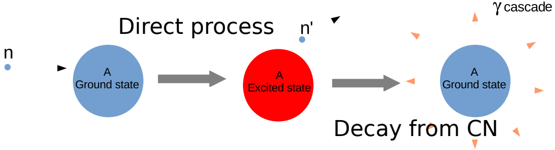


JLMB/QRPA

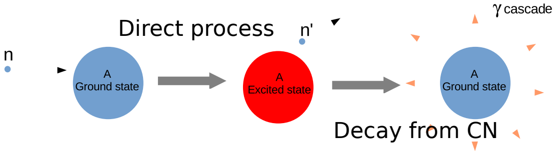


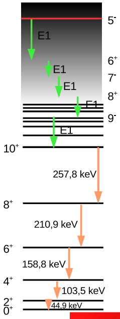
$\Rightarrow$**need n.n.p states and 2-step process for $E_{in} \simeq 10$ MeV**

Modeling ^{238}U (n,n'γ) reactions

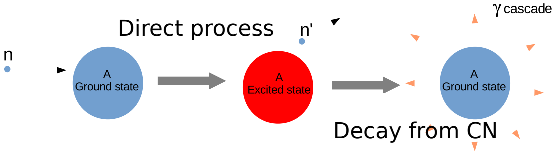


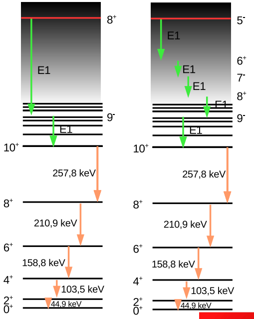
Modeling ^{238}U (n,n'γ) reactions



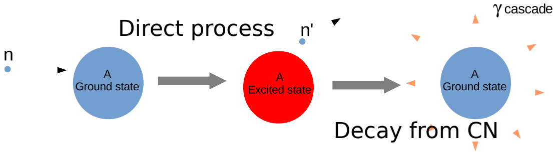


Modeling ^{238}U (n,n'γ) reactions

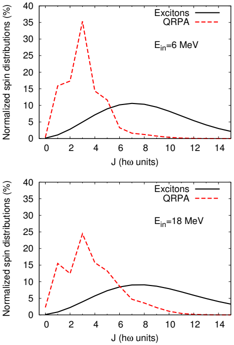


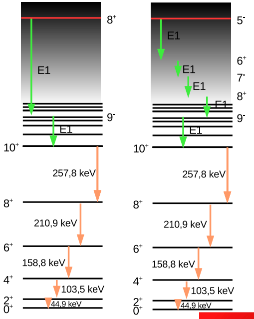


Modeling ^{238}U (n,n'γ) reactions

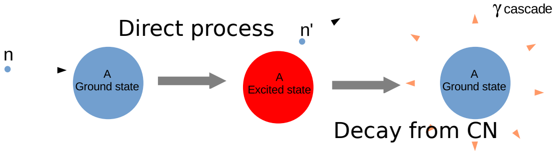


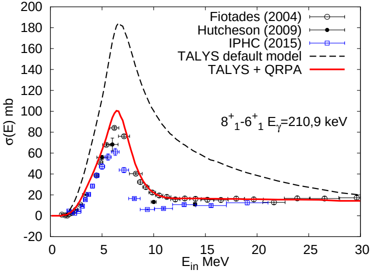
Residual nucleus: E_x, J^π



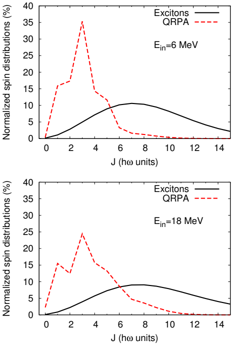


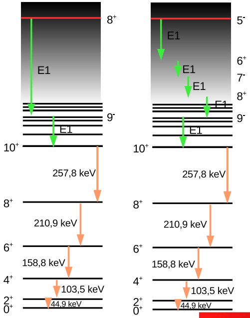
Modeling ^{238}U $(n,n'\gamma)$ reactions





Residual nucleus: E_x, J^π

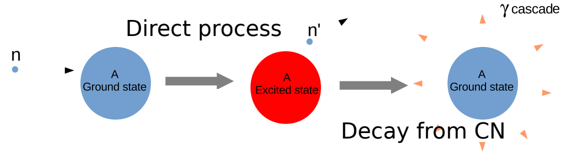


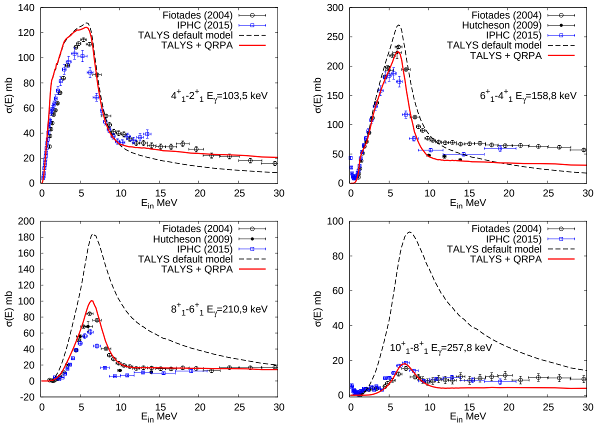


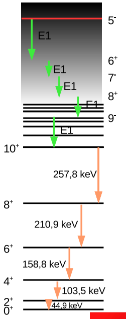
Neutron Time of flight facility
GELINA@IRMM(Geel)

M. Kerveno et *al.*, IPHC, Strasbourg, France.

Modeling ^{238}U (n,n'γ) reactions



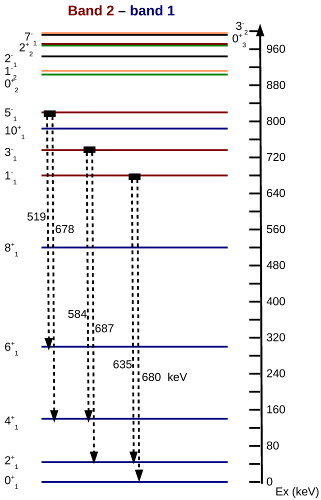


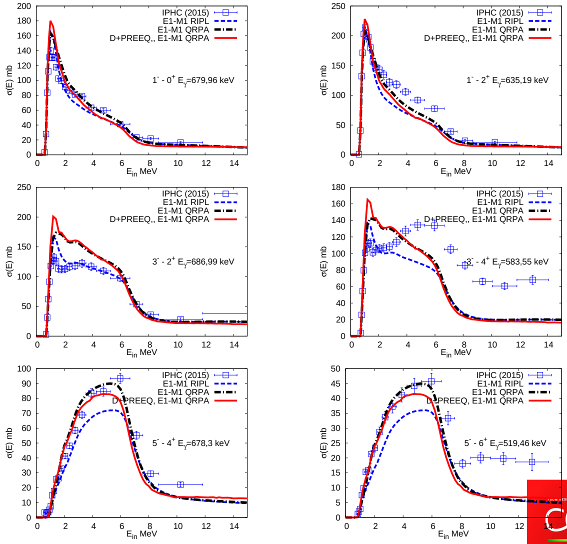


Inter-band transitions

Direct + Preequilibrium from JLM+QRPA

E1-M1 response functions: RIPL $\longrightarrow$ QRPA : S. Goriely PL002, I387 (S. Hilaire).





Odd actinides - early developments

Direct excitation process in ^{239}Pu:

Transitions: $\left|\frac{1}{2}^{+}\right\rangle \;\rightarrow\; \left|j^{\pi}\right\rangle$

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$$a_{\frac{1}{2}^+}|0^+\rangle \;\rightarrow\; a_{\frac{1}{2}^+}|N\rangle \;.$$

$|N\rangle \Rightarrow$ phonons calculated in ^{240}Pu $\Rightarrow$ **weak-coupling** approximation.
Main features of collective responses in A and $A \pm 1$ are expected to be similar

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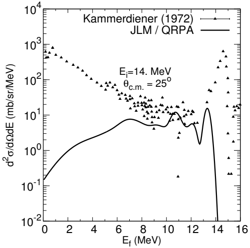
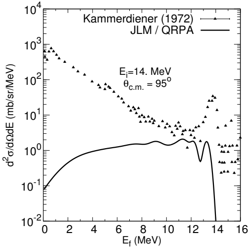
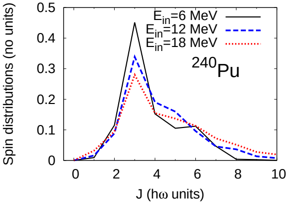
14. MeV ^{239}Pu(n,xn)

C

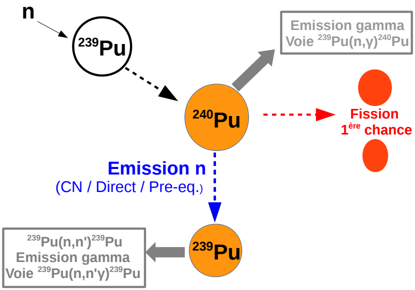


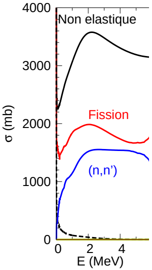




Missing neutron contributions: **fission fragments**.

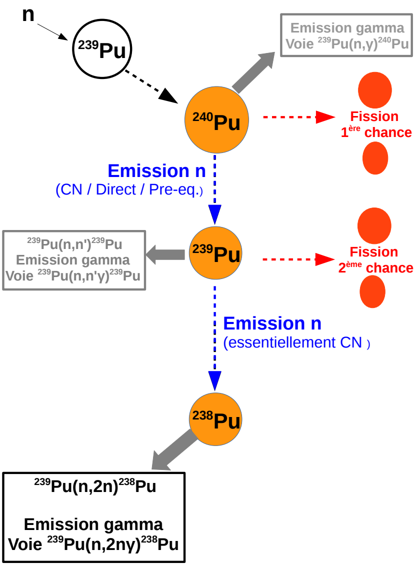
^{239}Pu (n,2n) : reaction mechanisms

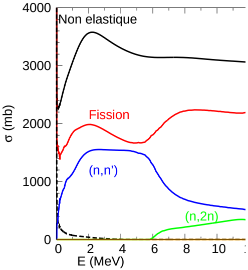




BRC (P. Romain, B. Morillon, H. Duarte).

^{239}Pu (n,2n) : reaction mechanisms





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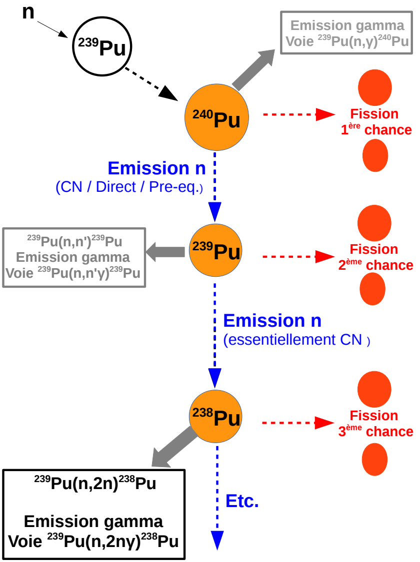

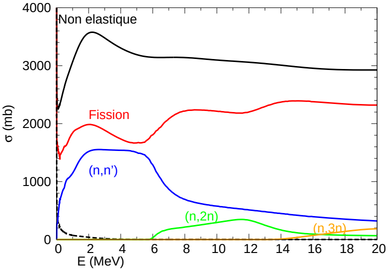

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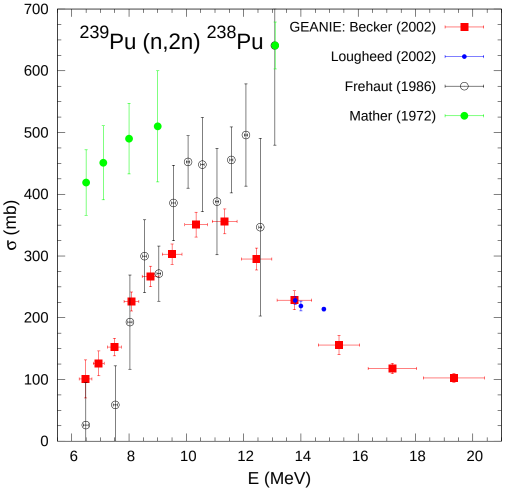
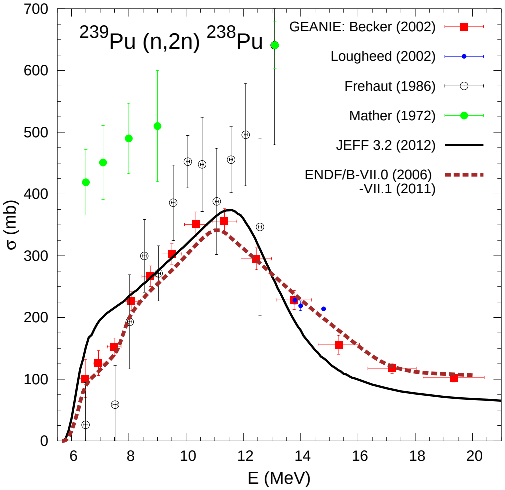
Measurements and evaluations ^{239}Pu (n,2n) ^{238}Pu



GEANIE/GNASH (Bernstein 2002) : (n,2n) extrapolated (using GNASH code) from partial (n,2nγ) measured cross sections (GEANIE : Germanium array).

Measurements and evaluations ^{239}Pu (n,2n) ^{238}Pu



Large discrepancies between various evaluations :
for E_{in} in the 6.5 - 8 MeV range
for $E_{in} > 11$ MeV.

GEANIE measurements

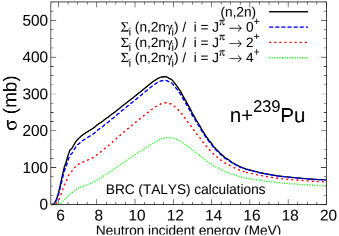
LANL 1999

height measured transitions

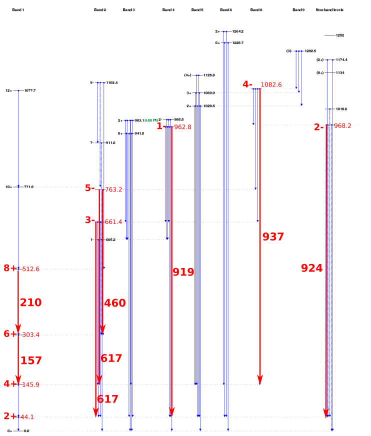
(seven cross sections) (n,2nγ)

Difficulties

- $E < 6.5 < MeV$ (n,2n) without γ emission.
- Internal conversion : $2^+_1 \rightarrow 1^+_1$ γ-ray conversion : 735.
- γ from fission fragments, sample activity.
- exemple: the $4^+_1 \rightarrow 2^+_1$ γ-ray yields was overwhelmed by a fission-product γ-ray.

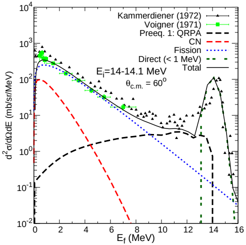


^{238}Pu γ-decay scheme

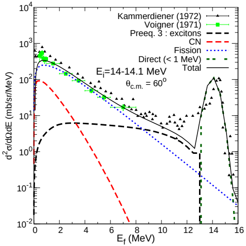


Pre-equilibrium models - ^{239}Pu (n,xn) spetrum

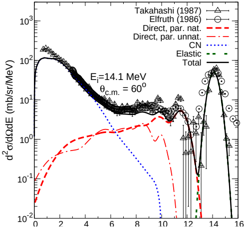
JLM / /one-phonon QRPA



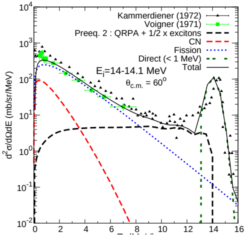
Excitons (two-components, TALYS impl.)



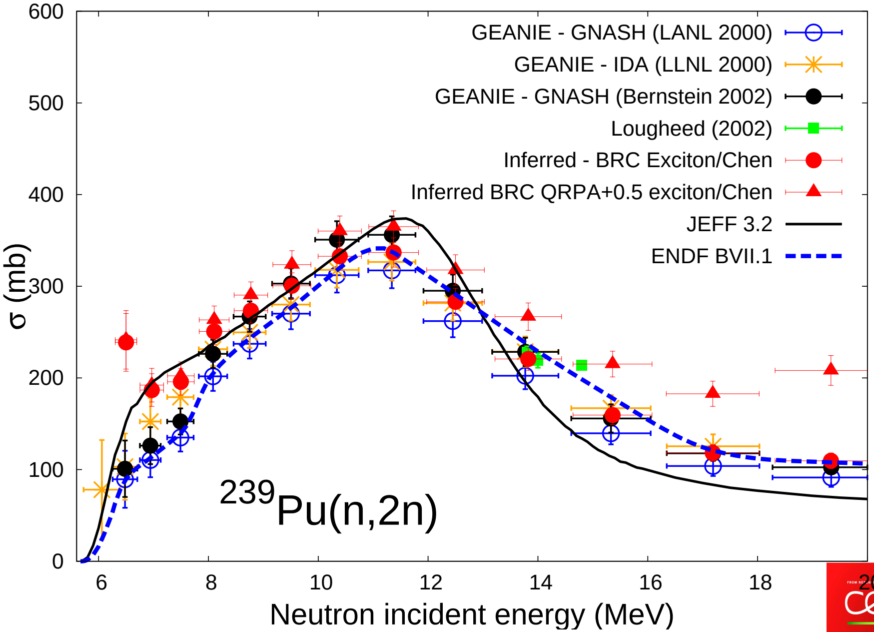
JLM : No unnatural parity excitations. ^{208}Pb(n,xn)



QRPA + $\frac{1}{2}$ Excitons



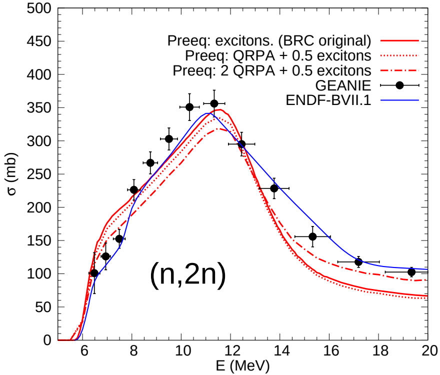
Discussion



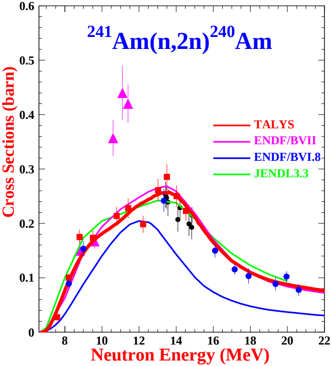
σ (mb)
600
500
400
300
200
100
0
6
8
10
12
14
16
18
20
Neutron incident energy (MeV)
GEANIE - GNASH (LANL 2000)
GEANIE - IDA (LLNL 2000)
GEANIE - GNASH (Bernstein 2002)
Lougheed (2002)
Inferred - BRC Exciton/Chen
Inferred BRC QRPA+0.5 exciton/Chen
JEFF 3.2
ENDF BVII.1
239Pu(n,2n)

Discussion: ^{241}Am(n,2n)

^{239}Pu(n,2n)



^{241}Am(n,2n)



Conclusions and questions

- Direct inelastic and pre-equilibrium (first-step): QRPA one phonon excitations.
- ρ-dependent effective interaction $\rightarrow$ large rearrangement corrections.
- Improve high energy neutron spectra in (n,xn) and (n,n'γ) cross-sections for ^{238}U .

- Future of folding models for low energies ? Which interactions ?
- Folding models / inelastic processes / rearrangement : full-folding models (Melbourne), link with beyond low density expansions NM theories (H. Arellano, Univesity of Chile).

Future works

Work in progress

- Analysis of (n,xn) and (n,xnγ): ^{239}Pu and ^{241}Am, ^{232}**Th and Tungsten (IPHC, GELINA).**
- ^{239}Pu (n,2n) cross section extracted from (n,2nγ) data : new analysis with microscopic direct reaction modeling.

Plans for model improvements

Better interaction, **two-step process with 2-phonon states**, **qp-blocking+QRPA** for **odd-nuclei**, **QRPA charge exchange**, consistent description of structure and reaction

Actinides: microscopic derivation of coupling **non-local potentials**, solving **coupled channels** for a large coupling scheme (**PhD of A. Nasri, CEA, DAM, DIF, Bruyères-le-Châtel**)

Thank you