Microscopic models for pre-equilibrium emission and (n,xnγ) cross sections

Experimental and theoretical problems around actinides for future reactors
March 17th-19th 2014, ESNT, CEA-Saclay.

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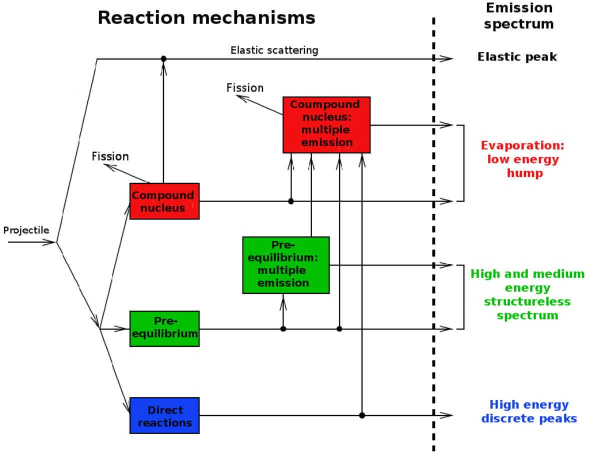
Nuclear reactions modeling



Reaction mechanisms

Emission spectrum

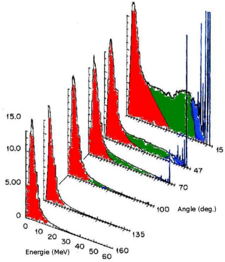
Elastic peak

Evaporation: low energy hump

High and medium energy structureless spectrum

High energy discrete peaks

62 MeV^{56}Fe (p,xp)
Double differential cross sections



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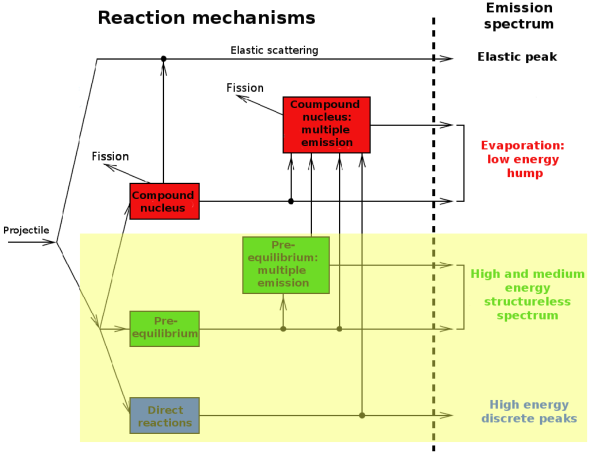


Reaction mechanisms

Emission spectrum

Projectile

Elastic scattering

Elastic peak

Fission

Coumpound nucleus: multiple emission

Fission

Compound nucleus

Evaporation: low energy hump

Pre-equilibrium: multiple emission

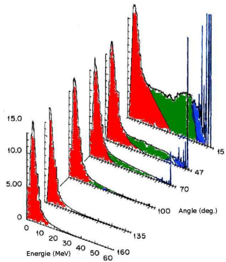
Pre-equilibrium

High and medium energy structureless spectrum

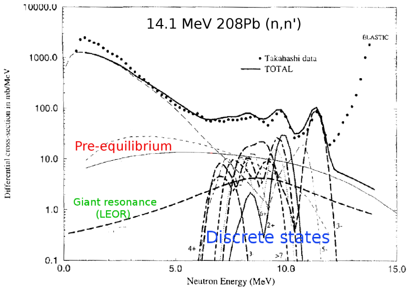
Direct reactions

High energy discrete peaks

62 MeV^{56}Fe (p,xp)
Double differential cross sections



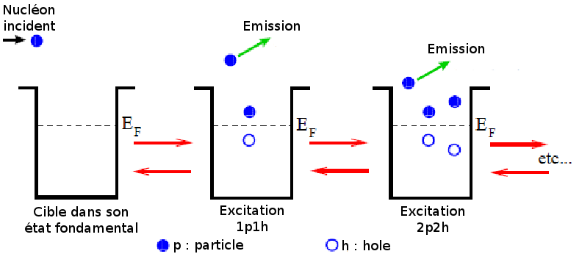
Direct inelastic scattering modeling : phenomenological approach



P. Demetriou et *al.*, Nucl. Phys. A 596, 67 (1996)

- High energy emission :
  - Low energy discrete states excitations : cross sections determined from available measurements (deformation lengths, collective model).
  - Giant resonances : cross sections calculation based on the knowledge of response functions in the continuum which are usually extracted from (e,e'), (h,h'), (h,h'f) measurements or from systematics.
  - Pre-equilibrium emission.
- Depending on the nucleus and the incident energy, the experimental information is not complete and sometimes very scarce: **collective response functions for $L > 3$ and in deformed targets such as actinides.**

Pre-equilibrium reaction mechanism



Doubly differential (n,n') or (p,p') cross sections:

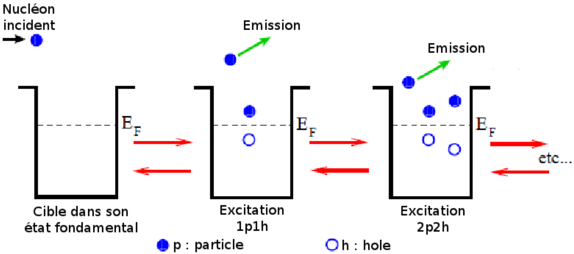
$$\frac{d\sigma(\mathbf{k}_i,\mathbf{k}_f)}{dE_k\,d\Omega_f} \sim \int dE \sum_N f\left(E_{k_i} - E_k - E_N\right) |T_{fi}|^2$$

Transition amplitude (Born Series) :

$$T_{fi} = \langle \chi_f^{(-)}(\mathbf{k}), N | V_{eff} + V_{eff}\frac{1}{E-H_0+i\varepsilon}V_{eff} + V_{eff}\frac{1}{E-H_0+i\varepsilon}V_{eff}\frac{1}{E-H_0+i\varepsilon}V_{eff} + \cdots | \chi_i^{(+)}(\mathbf{k}_i), 0\rangle$$

$f\left(E_{k_i} - E_k - E_N\right)$: spreading functions (damping+escape widths).

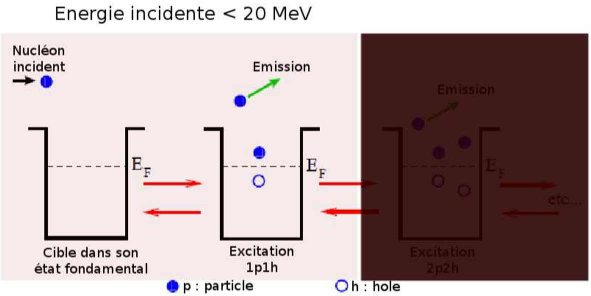
Pre-equilibrium reaction mechanism



- Quantum models (FKK, TUL, NWY), semi-classical (Excitons, intra-nuclear cascade) ...
- Phenomenological ingredients : optical potentials, level densities.
- Adjustable parameters : residual interaction magnitude, coupling matrix elements.

→ Most all the time, all models are able to fit nucleon emission spectra when the right set of ingredients/parameters is selected.

Pre-equilibrium reaction mechanism



Quantum model: doubly differential cross section (n,n')/(p,p') for first order pre-equilibrium emission (E_{in} <20 MeV):

$$\frac{d\sigma(\mathbf{k}_i,\mathbf{k}_f)}{dEd\Omega_f} \sim \int dE \sum_N f\left(E_{k_i} - E_k - E_{ph_N}\right) \left|\langle \chi_f^{(+)}(\mathbf{k}), N | V_{eff} | \chi_i^{(-)}(\mathbf{k}_i), 0\rangle\right|^2$$

- V_{eff} : adjustable parameters
- $\sum_N$: sum over target excitations $|N\rangle = |ph\rangle$

⇒ : FKK model: incoherent particle-hole excitations $|N\rangle = |ph\rangle$.
⇒ : TUL model: allows excitation of collective states (adjusted residual interactions to fit know states properties).

Formal description of direct reactions for elastic and inelastic scattering

- Coupled channels for elastic and few inelastic channels

$$\left(E_{k_i} - T_0 - U_{00}\right)|u_0\rangle = \sum_{n=1}^{k} U_{0n}|u_n\rangle$$

$$\left(E_{k_f} - T_0 - U_{nn}\right)|u_n\rangle = \sum_{n'\neq n} U_{nn'}|u_{n'}\rangle \ ,\ldots$$

- Main ingredient → one-body coupling potentials $U_{nn'} = \langle\psi_n'|V_{eff}|\psi_n\rangle$, calculated from :
  - target states wave functions $\{\psi_n\}$.
  - effective interaction V_{eff} (g-matrix, JLM).
- One-body potential :

$$\langle N'|V_{eff}|N\rangle = \sum_{\alpha\alpha' kk'} \langle\alpha', k'|V_{eff}|\widetilde{\alpha, k}\rangle \rho_{\alpha\alpha'}^{N\rightarrow N'} a_{k'}^{\dagger} a_k$$

- Nuclear structure ingredient → one body density matrix :

$$\rho_{\alpha\alpha'}^{N\rightarrow N'} = \langle N'|a_{\alpha'}^{\dagger} a_{\alpha}|N\rangle$$

Microscopic model for direct inelastic scattering : spherical targets

(n,n') direct inelastic scattering double differential cross section

$$\frac{d\sigma(\mathbf{k}_i,\mathbf{k}_f)}{dE_f\, d\Omega_f} = \int dE_k \sum_N \frac{\mu^2}{(2\pi\hbar^2)^2}\,\frac{k}{k_i}\, f\left(E_{k_i}-E_k-E_N\right)\left|\langle\chi_f^{(-)}(\mathbf{k}),N|V_{eff}|\chi_i^{(+)}(\mathbf{k}_i),\tilde{0}\rangle\right|^2$$

V_{eff} : effective interaction (g matrix).

$$(T+U(E_i))|\chi_i^{(+)}(\mathbf{k_i})\rangle = E_i|\chi_i^{(+)}(\mathbf{k}_i)\rangle$$
$$\left(T+U^{\dagger}(E_f)\right)|\chi_f^{(-)}(\mathbf{k}_f)\rangle = E_f|\chi_f^{(-)}(\mathbf{k}_f)\rangle$$

$U(E_{i/f})$: optical potential (Koning-Delaroche).

Target excitations

- Nuclear structure model : **Random Phase Approximation** (**RPA**), Gogny D1S interaction.

  Target spectrum : one phonon excitations $|N\rangle = \sum_{ph}\left(X_{ph}^N a_p^{\dagger} a_h - Y_{ph}^N a_h^{\dagger} a_p\right)|\tilde{0}\rangle$.

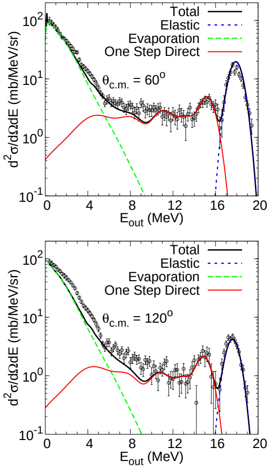
- RPA+D1S model checked for different J^{Π} excitations in magic nuclei (or closed sub-shell nuclei with weak paring) → provides accurate description of **low energy collective states** and **giant resonnances**

- Target excitation widths : $f\left(E_{k_i}-E_k-E_N\right) = \frac{1}{\pi}\frac{\Gamma_N}{(E_{k_i}-E_k-E_N+\Delta_N)^2+\frac{\Gamma_N^2}{4}}$, $\Gamma_N = \Gamma^{\downarrow}+\Gamma^{\uparrow}$, energy shift

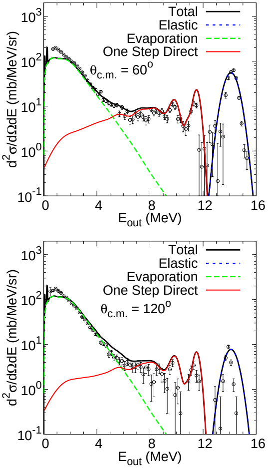
  → phenomenological input.

Direct (n,n') microscopic model : analysis of ^{90}Zr , ^{208}Pb (n,xn) spectra

18 MeV ^{90}Zr(n,xn)



14.1 MeV ^{208}Pb(n,xn)

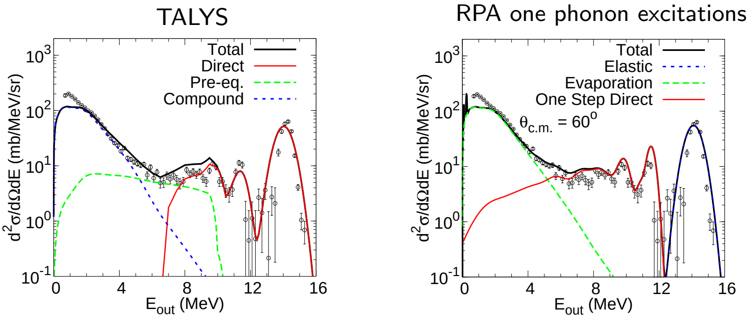


- Calculations performed with one phonon RPA excitations :

→ Reproduce high energy emission : **no adjusted parameters** to get the cross section magnitude.
→ Coherent description of direct inelastic scattering (one-step) : collective and non collective states.

Comparison to TALYS

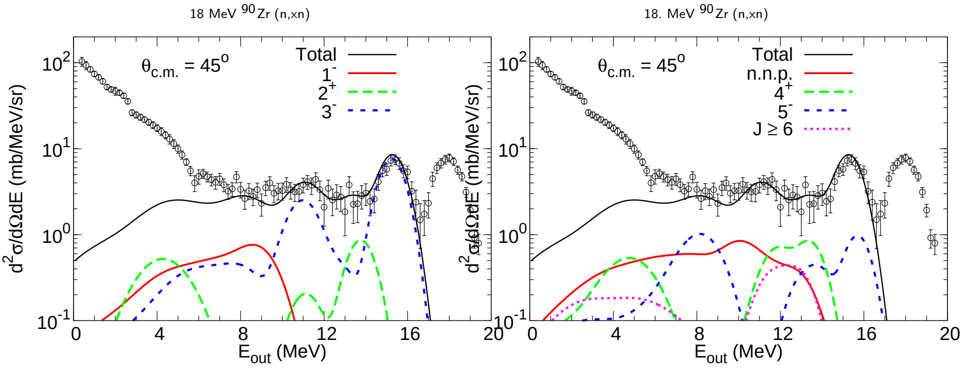
14.1 MeV ^{208}Pb(n,xn) angle=60○



- Discrete states.
- Giant resonances.
- Pre-equilibrium (excitons).

$\Longrightarrow$ (re-)unified description.

Cross sections spin-parity components



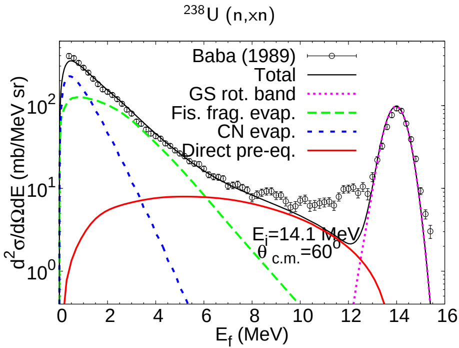
- Major contribution from collective states with total angular momentum from $J = 2$ to 5.

→ A description of collective states for all angular momentum is mandatory to account for direct nucleon emission well.

M. Dupuis, T. Kawano, J.-P. Delaroche, E. Bauge, **PRC83, 014602 (2011)**.

Microscopic model for direct inelastic scattering off axially deformed targets

- Calculation with p-h excitations : Interaction fit to match (n,xn) data. ⇒ underestimates high energy emission [T. Kawano et *al.*, Phys.Rev. C63, 034601 (2001)].
- Collective (vibrations) states in actinides (low energy and giant resonances) : not well characterized in experiments, usually not included in reactions modeling.
- Temporary solution used in evaluations : pseudo states = collective states with properties (energy and deformation length) adjusted to fit the observed high energy neutron emission (used in ENDF-BVII, BRC).



QRPA model that describes collective excitations in axially deformed nuclei has been recently develloped in Bruyres and used to describe the excitations spectra in actinides :
S.Peru, G.Gosselin, M.Martini, M.Dupuis, S.Hilaire, J.-C.Devaux, **Phys.Rev.C 83**, *014314 (2011)*.

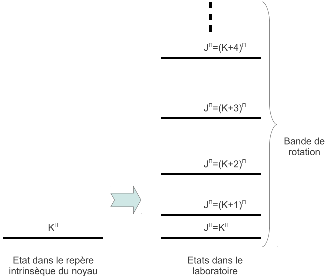
Excitation spectrum of a nucleus with a static axial deformation

- QRPA method : axial deformation, projection K of the total angular momentum on the symmetry axis is a good quantum number, parity is conserved.
- Target excitations in the **intrinsic frame : one phonon excitations.**

$$|\alpha K\Pi\rangle = \Theta^{+}_{\alpha K\Pi}|\tilde{0}_I\rangle = \frac{1}{2}\sum_{ij\in(K\Pi)}\left(X^{\alpha K\Pi}_{ij}\eta^{+}_{ip_i\Omega_i}\eta^{+}_{jp_j\Omega_j} - (-)^{K}\,Y^{\alpha K\Pi}_{ij}\eta_{ip_i-\Omega_i}\eta_{jp_j-\Omega_j}\right)|\tilde{0}_I\rangle$$

- Target states in the **laboratory frame : projection on total angular momentum → rotational band for each intrinsic excitation, with angular momenta $J \geq K$**

$$|\alpha JMK\Pi\rangle = \sqrt{\frac{2J+1}{16\pi^2}}\int d\Omega\,\mathscr{D}^{J}_{MK}{}^{*}(\Omega)R(\Omega)|\alpha K\Pi\rangle + (-)^{J+K}\mathscr{D}^{J}_{M-K}{}^{*}(\Omega)R(\Omega)|\alpha\bar{K}\Pi\rangle$$



Direct inelastic scattering cross section for axially deformed targets

Doubly differential cross section :

$$\frac{d\sigma(\mathbf{k}_i,\mathbf{k}_f)}{dEd\Omega_f} \sim \int dE \sum_N f\left(E_{k_i} - E_k - E_N\right) \frac{d\sigma_N(\mathbf{k}_i,\mathbf{k})}{d\Omega}$$

- Sum over target excitations : $\sum_N = \sum_{K^\Pi} \sum_{J \geq K}$

  → K^Π intrinsic excitations, $J \geq K$ rotational band states,
  → ~4000-10000 intrinsic excitations $E = 11 - 18$ MeV, 20,000 and 50,000 states in total.

- For one excitation : $\frac{d\sigma_N(\mathbf{k}_i,\mathbf{k})}{d\Omega}$

  → need coupling potential $U_L(r) = \int V_L(r,r')\rho_L^{QRPA}(r')r'^2 dr'$

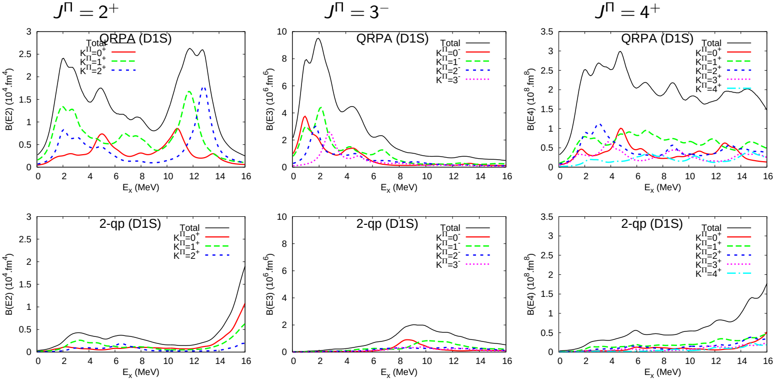
- V **JLM Bruyères interaction** (*E. Bauge, J. P. Delaroche, and M. Girod, Phys. Rev. C63, 024607 (2001), Phys. Rev. C58, 1118 (1998)*)
- $\rho_L(r)$: multipole of order L of the **QRPA radial transition density** between the GS and an intrinsic excitation.

QRPA response functions in ^{238}U

Reduce transition probabilities (proton+neutron) $B(EJ) \sim |\int \rho_J^{\tilde{0}_I,\alpha K\Pi}(r) r^{J+2} dr|^2$ (L> 2) : provide a measure of excitations collectivity (cross sections magnitude approximately proportional to $B(EJ)$)

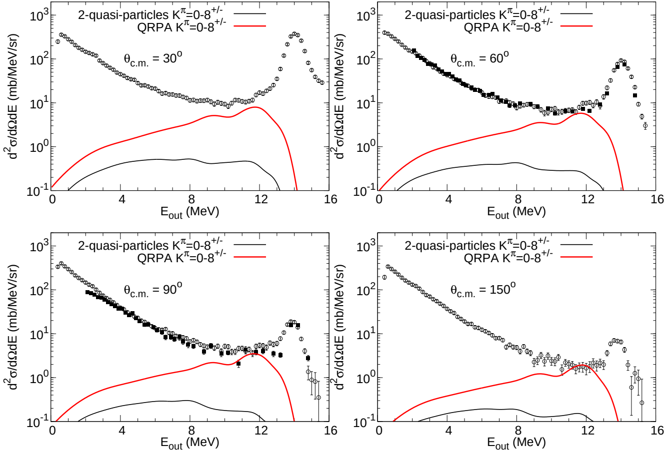
QRPA
$\Theta^\dagger|\tilde{0}\rangle$

2 quasi-particles :
$\eta^\dagger\eta^\dagger|HFB\rangle$

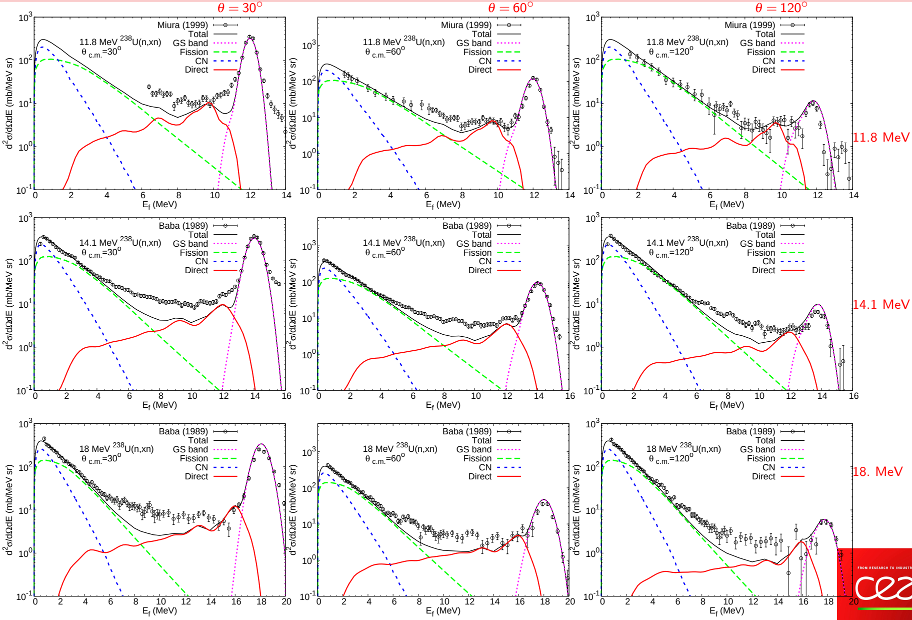


- Large number of collective excitations at low energy

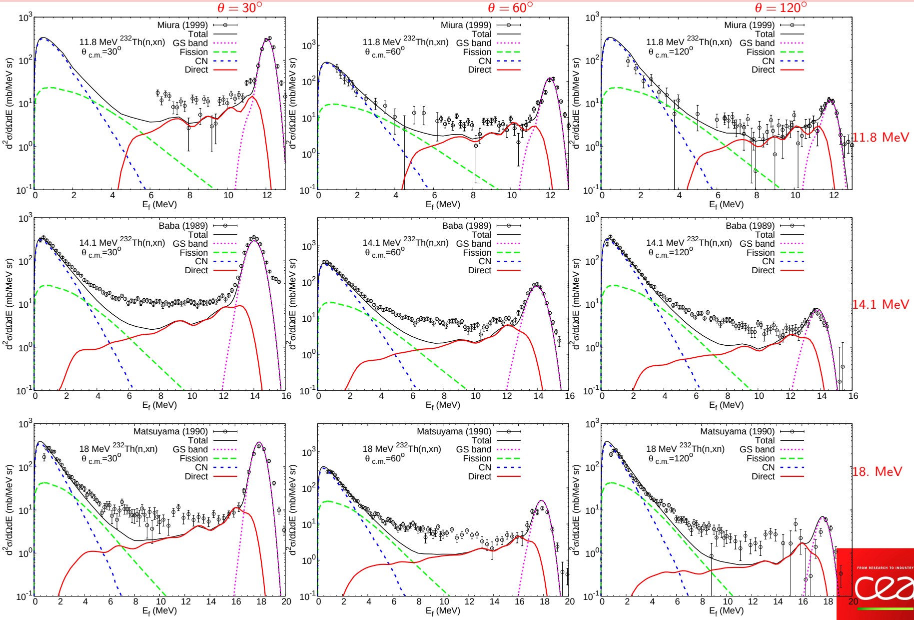
Impact of collective excitations on cross sections : 14.1 MeV (n,n') ^{238}U



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

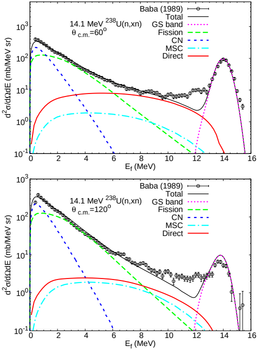


Analysis of 11-18 MeV (n,xn) ^{232}Th spectra

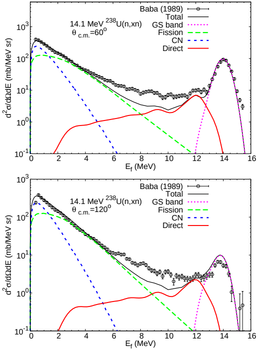


Comparison to previous more phenomenological calculations

Kawano one-step direct :

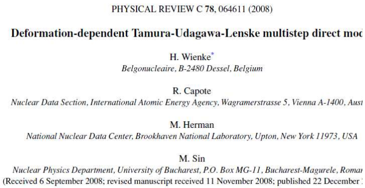


Microscopic model with QRPA :



- High energy cross section ($E_f > 10$ MeV): rather good.
- Clearly underestimated at $E_f \simeq 6$-10 MeV

Comparison to pre-equilibrium TUL model implemented in EMPIRE



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Deformation-dependent Tamura-Udagawa-Lenske multistep direct mo

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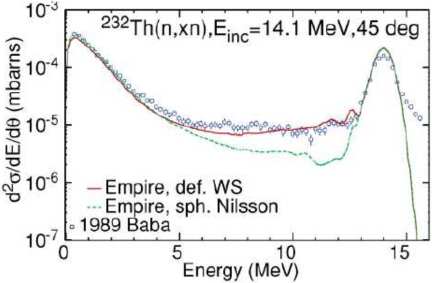
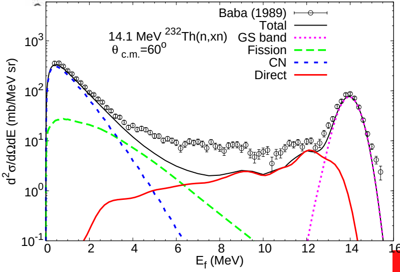
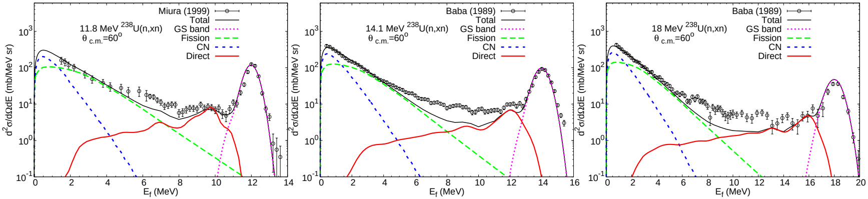


QRPA one phonon excitations



Direct pre-equilibrium emission for: 11-18 MeV (n,n') ^{238}U



Improve the present direct pre-equilibrium emission model for axially deformed targets

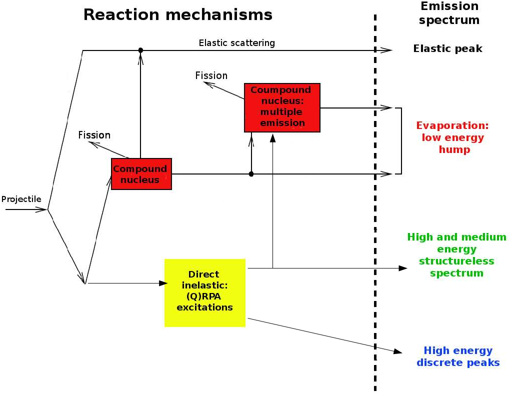
- Non-natural parity transitions: tensor interactions.
- Model approximations (local density approximation, coupling scheme), ingredients are of course not perfect (effective interaction, damping widths, QRPA response functions): need to estimate error on overal normalization.

Microscopic model with realistic ingredients and no adjustable parameter: discrepancies with data allow to identify model deficiencies, important reaction mechanisms that were neglected.

- High one-phonon state density: excitation of two-phonons states → multi-step could be important even at these low incident energies.
- Multi-step compound contributions ?
- Close comparison with TUL model.

(n,xnγ) cross sections

How new direc inelastic xs impact on (n,n'γ) xs.



Reaction mechanisms

Emission spectrum

Projectile

Elastic scattering

Elastic peak

Fission

Compound nucleus

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Coumpound nucleus: multiple emission

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Direct inelastic: (Q)RPA excitations

High and medium energy structureless spectrum

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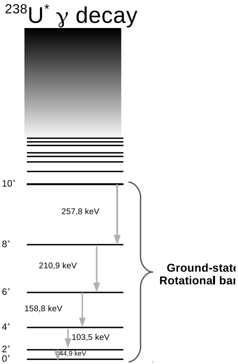
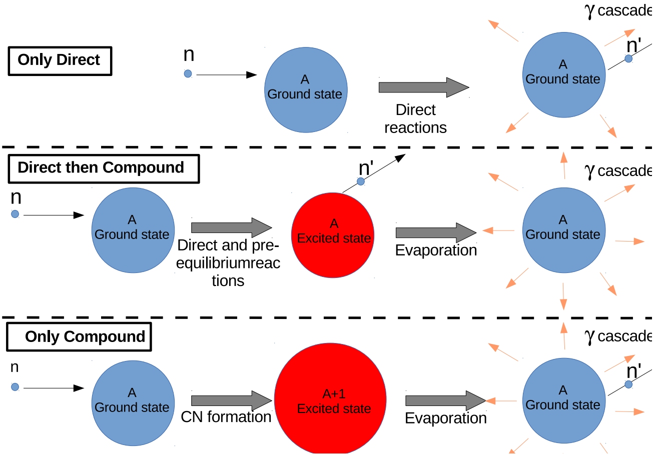
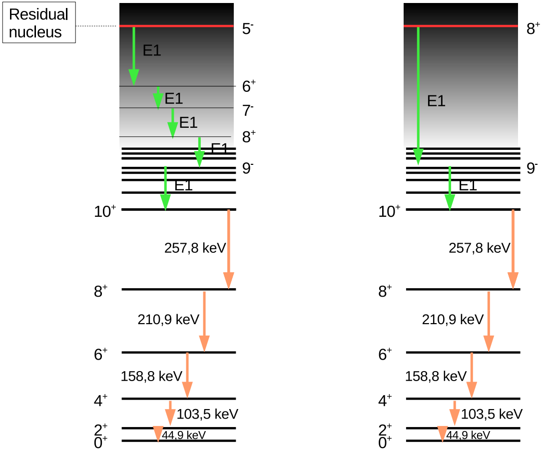


Reaction mechanisms for (n,n'γ)



Reaction mechanisms for (n,n'γ)



Residual nucleus spin distribution in ^{238}U

Direct inelastic scattering ^{238}U (n,n')

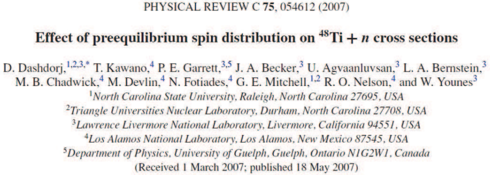
Equilibration to a compound nucleus with:

- excitation energy E
- spin-parity J, Π.

Spin distribution

Default in TALYS (for E <20 MeV): $R(J) = \frac{(2J+1)^2}{2\sqrt{2\pi}\sigma^{\frac{3}{2}}} e^{\frac{-(J+\frac{1}{2})^2}{2\sigma}}$ $\sigma = 0.72A^{\frac{2}{3}}$

- CN level density while **direct reactions** (i.e. one-step pre-equilibrium process) **populate particle-hole or one phonon states**.
- Does not take into account the **propability of excitation via the direct process: low angular momentum transfer favored**.



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Effect of preequilibrium spin distribution on ^{48}Ti + n cross sections

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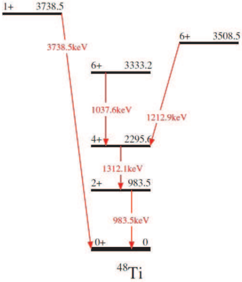
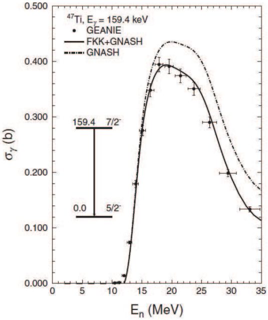


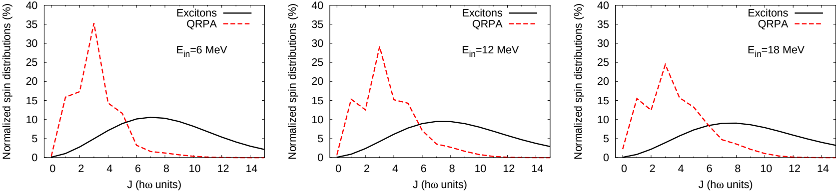


Residual nucleus spin distribution in ^{238}U

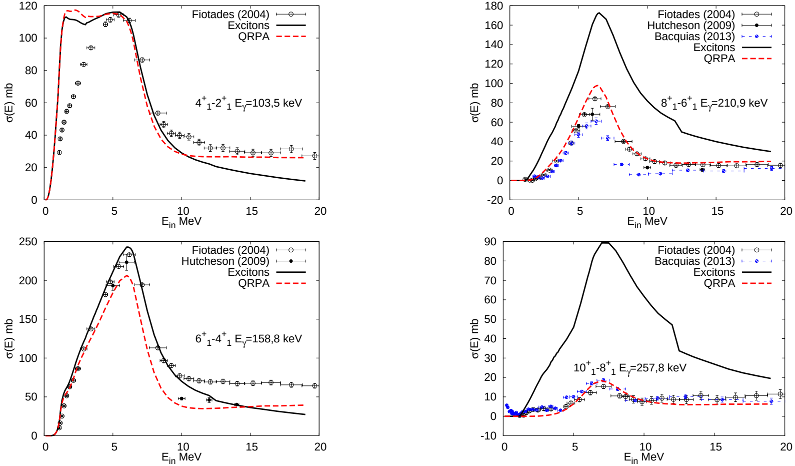
Spin distribution from direct reaction calculation

Results form QRPA inelastic scattering model : $R(J, E_{\text{in}}) = \dfrac{\sigma_J(E_{\text{in}})}{\sum_J \sigma_J(E_{\text{in}})}$,

$\sigma_J(E_{\text{in}})$: cross section summed over all states of spin J.

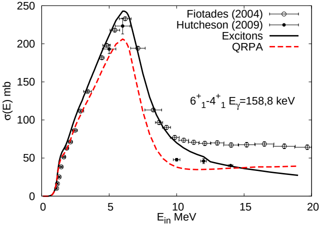


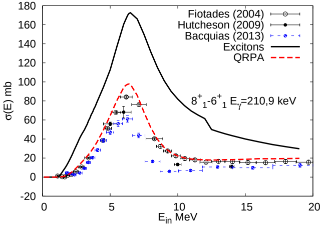
^{238}U (n,n'γ) cross sections for transitions in the GS rotational band

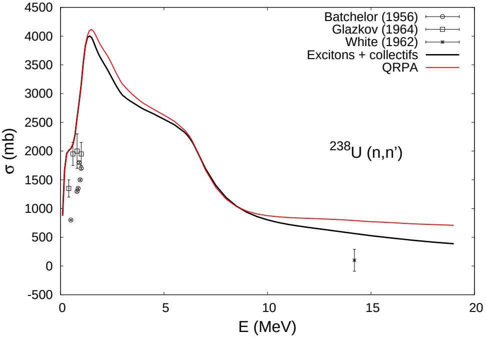


A. Bacquias, M. Kerveno - IPHC (preliminary)

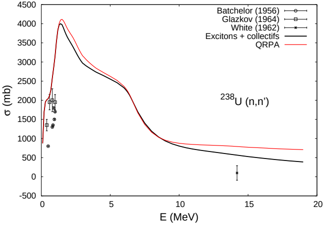
Link with (n,n') cross section

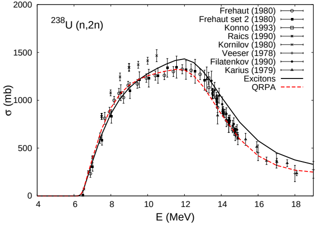


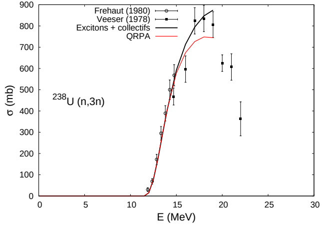




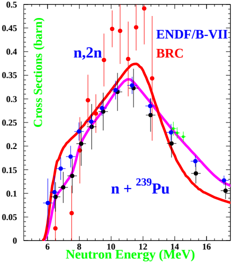
^{238}U (n,n'), (n,2n), (n,3n) cross sections

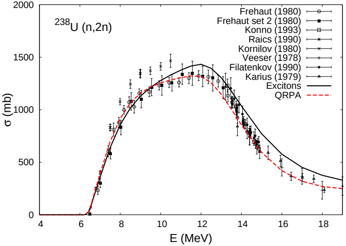


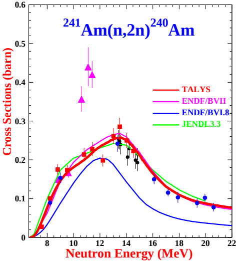




^{239}Pu (n,2n) problem







- Exp. data: similar (n,2n) slope for ^{238}U and ^{241}Am.
- Microscopic calculation of direct inelastic scattering: does not change ^{238}U (n,2n) slope.
- Perspectives :

→ Same calculation in progress for ^{239}Pu , but ...
→ ... we expect similar results that in ^{238}U :
⟹ could other reaction mecanisms explain the (n,2n) slope in ^{239}Pu ?
⟹ New (n,2n) data interpretation in ^{239}Pu ?

Conclusions

Microscopic models for direct nucleon inelastic scattering off spherical nuclei: RPA one-phonon excitations

- Observed high energy neutron emission is well reproduced (pour E_{in} <20 MeV).
- No arbitrary distinction between direct inelastic scattering and pre-equilibrium emission.

Microscopic models for direct nucleon inelastic scattering off axially deformed nuclei: QRPA one-phonon excitations

- QRPA low energy collective states explain the pseudo states origin.
- Impact on ^{238}U (n,n'γ) cross sections: global improvement transition in GS band.
- Discrepancy between predictions and data at lower emission energy in ^{238}U and ^{232}Th : other reaction mechanisms such as two-step process, non-natural parity excitations ?

Future work

- Non natural parity excitations for axially deformed targets.
- Estimate of second order with two phonons excitations, multistep-compound ?
- Impact on spin distribution, new (n,n'γ) analysis ?
- Interband (n,n'γ) in ^{238}U .
- Same study in ^{232}Th .
- Use present results to help interpret (n,2nγ) measures ?