Connecting structure and direct reaction modeling

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Perspective on Nuclear Data for the Next Decade 2 - 14-17/10/2014, CEA-TGCC.

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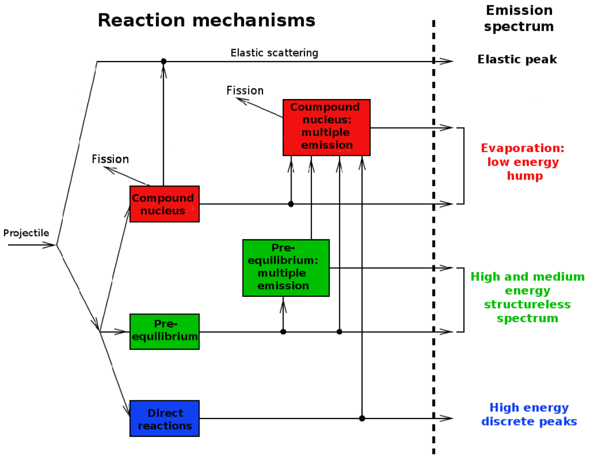
Nuclear reactions modeling



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

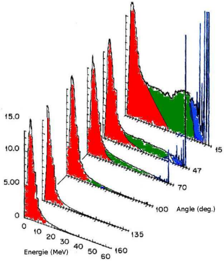
Pre-equilibrium

High and medium energy structureless spectrum

Direct reactions

High energy discrete peaks

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



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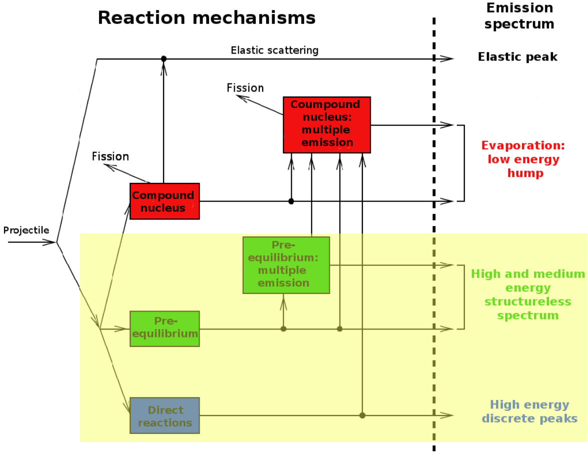

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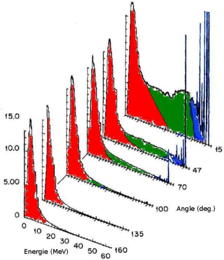
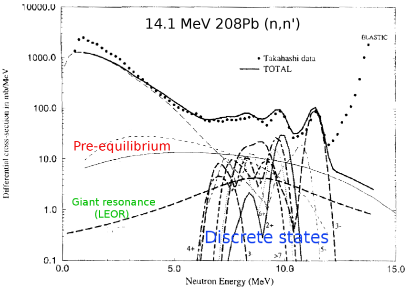


Direct inelastic scattering modeling : phenomenological approach



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.**

Microscopic model for direct inelastic scattering : spherical targets

Nuclear structure model : **Random Phase Approximation ((Q)RPA)**, D1S interaction

Target excitations $|N\rangle = \sum_{ph} \left(X^N_{ph} a^\dagger_p a_h - Y^N_{ph} a^\dagger_h a_p \right) |\tilde{0}\rangle$.

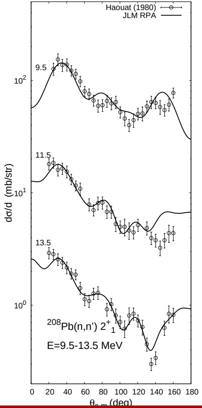
DWBA calculations :

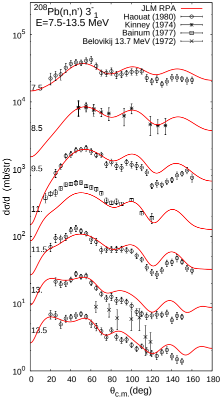
$$\frac{d\sigma}{d\Omega} \sim \left| \langle \chi^{(-)}, N | V_{eff} | 0, \chi^{+} \rangle \right|^2$$

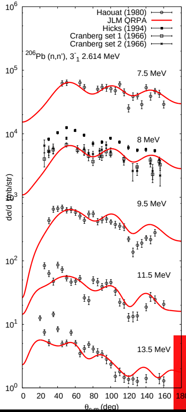
Optical potentials : $U = \langle \tilde{0} | V_{eff} | \tilde{0} \rangle$

Transition potentials : $U_{tr} = \langle N | V_{eff} | \tilde{0} \rangle$

Folding model with $V_{eff} \equiv$ JLM interaction from E. Bauge, J. P. Delaroche, and M. Girod, Phys. Rev. C63, 024607 (2001).







JLM model validation : Rearrangement

Transition potential

Optical potential: $U = V.\rho,\ \rho = \rho_{IS} = \rho_p + \rho_n$.

Transition potential: $U_{tr} = \beta_L \frac{dU}{dR} = \frac{dU}{d\rho}\beta_L \frac{d\rho}{dR}$.

Transition density identified to: $\rho_L^{tr}(r) = \beta_L \frac{d\rho}{dR}$.

Rearrangement (Cheon):

If $V \equiv V(\rho) \Rightarrow \frac{dV(\rho)\rho}{d\rho} = V(\rho) + \rho \frac{dV(\rho)}{d\rho}$.

Regular term: $U_{tr} = V(\rho)\rho_L^{tr}(r)$

Rearrangment term: $U_{tr}^R = \rho \frac{dV(\rho)}{d\rho}\rho_L^{tr}(r)$

See T. Cheon ***etal*****., Nucl. Phys. A437, 301 (1985) : done in (p,p') ^{16}O (N=Z).**

New rearrangement:

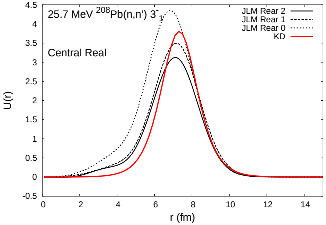
If $V \equiv V(\rho_p, \rho_n) \equiv V(\rho_{IS}, \rho_{IV})$, $\rho_{IV} = \rho_n - \rho_p$.

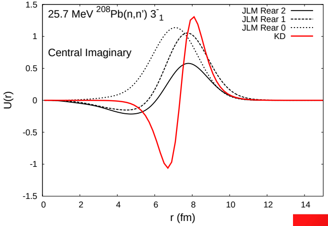
Regular term: $U_{tr} = V(\rho)\rho_L^{tr,,IS}(r)$.

Rearrangment term 1 (IS): $U_{tr}^{R1} = \rho_{IS}\frac{dV}{d\rho_{IS}}\rho_L^{tr,IS}(r)$.

Rearrangment term 2 (IV): $U_{tr}^{R2} = \rho_{IS}\frac{dV}{d\rho_{IV}}\rho_L^{tr,IV}(r)$.

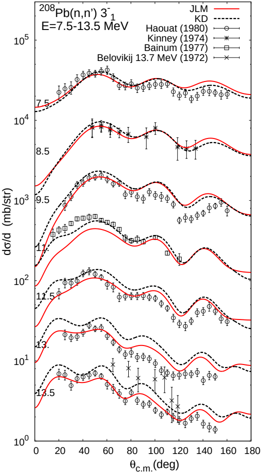
KD : collective model with Koning Delaroche potential ($\beta_3 = 0.120$).



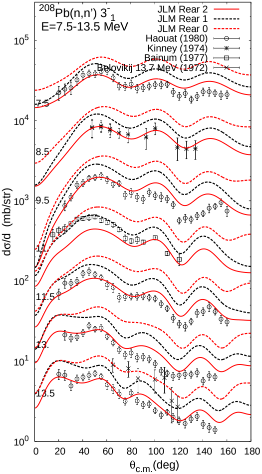


JLM model validation : Rearrangement

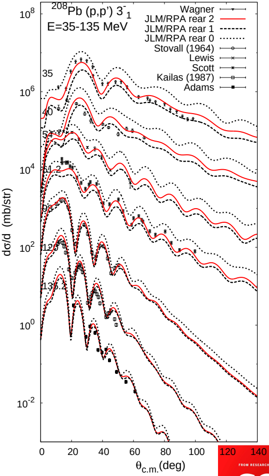
Comparison JLM - Collective model



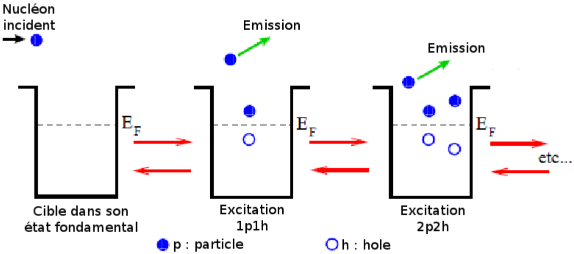
Impact of rearrangement : **(n,n')**



Impact of rearrangement : **(p,p')**



Pre-equilibrium reaction mechanism



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

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

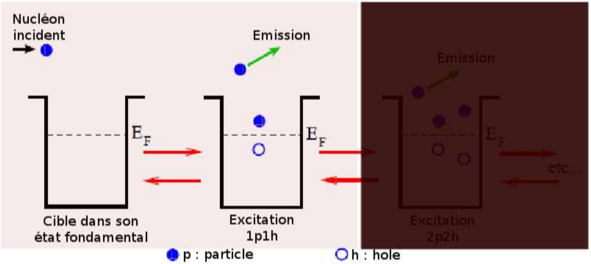
Transition amplitude (Born Series) :

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

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

Pre-equilibrium reaction mechanism

Energie incidente < 20 MeV



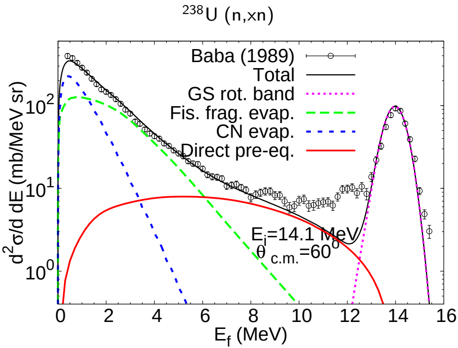
Doubly differential cross section (n,n')/(p,p')

Usually at E<20 MeV : reduced to one-step direct process ≡ sum of DWBA cross sections.

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

Microscopic model for direct inelastic scattering off axially deformed targets

- Calculation with p-h excitations : Interaction fit to match (n,*x*n) 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)*.

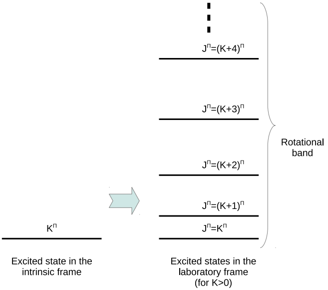
Excitation spectrum of a nucleus with a static axial deformation

- 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 :

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

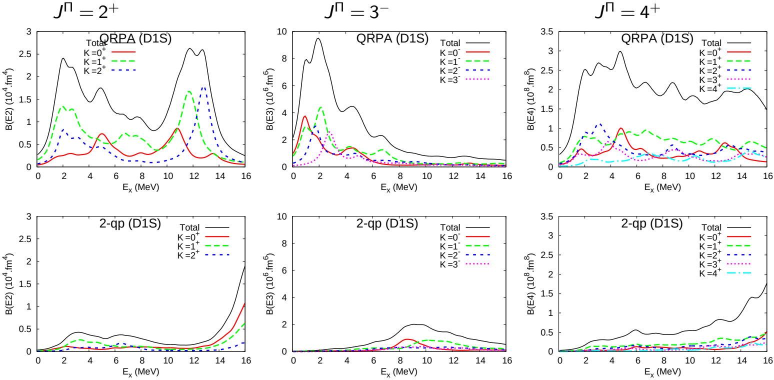
- Sum over target excitations : $\sum\limits_N = \sum\limits_{K^\Pi} \sum\limits_{J \geq K}$

  → K^Π intrinsic excitations, $J \geq K$ rotational band states,
- For one excitation : $\dfrac{d\sigma_N(\mathbf{k}_i,\mathbf{k})}{d\Omega}$

  → need coupling potential $U_L(r) = \int V_L(r,r')\rho_L^{QRPA}(r')r'^2dr'$ (JLM folding model).
- $\rho_L(r)$: 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 $B(EJ)$)



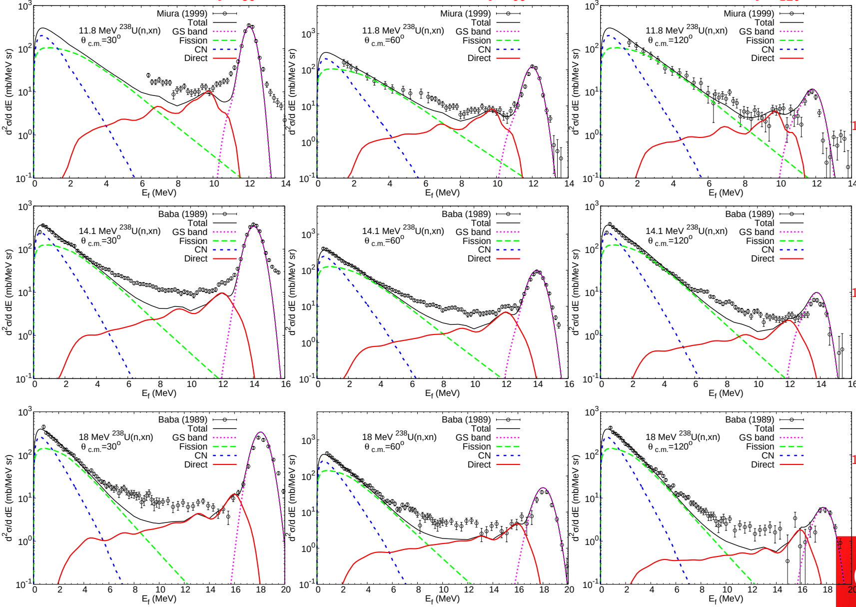
QRPA
$\Theta^\dagger|\tilde{0}\rangle$

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

- Large number of collective excitations at low energy

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

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



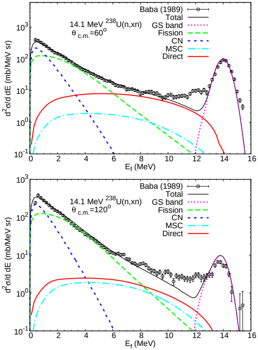
11.8 MeV

14.1 MeV

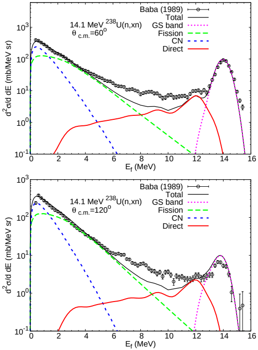
18. MeV

Comparison to previous more phenomenological calculations

Kawano one-step direct :



Microscopic model with QRPA :

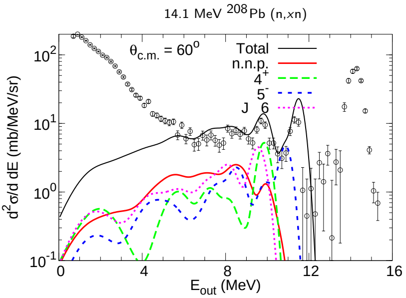


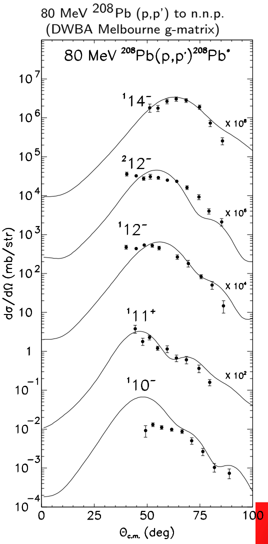
- High energy cross section (E_f >10 MeV): rather good.
- Clearly underestimated at $E_f \simeq$6-10 MeV

$\Longrightarrow$**TUL calculations in EMPIRE: fit the (n,*x*n) data well.**

$\Longrightarrow$**What is missing ?**

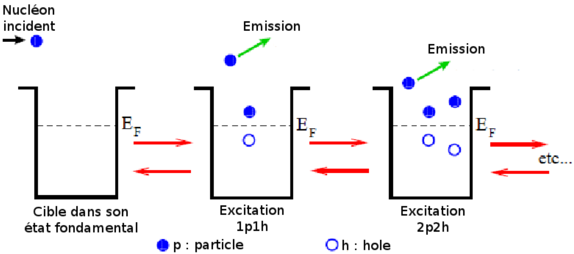
Non-natural parity excitations





- Contribution of **non-natural partity (n.n.p.)** excitations ($\pi = (-)^{L+1}$): up to 20% of the emission cross section.
- Transition not-possible within the JLM convolution model ($\Delta S = 1$).
- Adjust a new interaction for folding models with missing terms (start from gmatrix or effective interaction from Nuclear Structure approach).
- Low cost-short term solution : level densities folded with averaged cross-sections.

Two-step process to two-phonons states



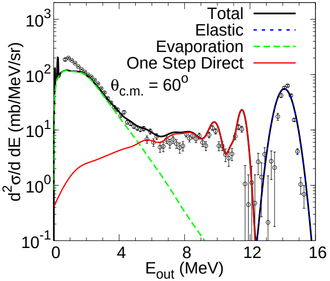
Two-steps process

Second order transition amplitude to two-bosons states:

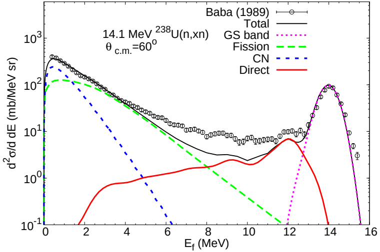
$$T_{fi} = T_{fi}^{(1)} + \langle \chi_f^{(-)}(\mathbf{k}), N_1, N_2 | V_{eff} \frac{1}{E - H_0 + i\varepsilon} V_{eff} | \chi_i^{(+)}(\mathbf{k}_i), 0 \rangle$$

$|N_1, N_2\rangle = \Theta^+_{N_1} \Theta^+_{N_2} |\tilde{0}\rangle$: two bosons state. Two-step: already included in TUL-EMPIRE model $\Longrightarrow$ need to carefully compare the components of the two models

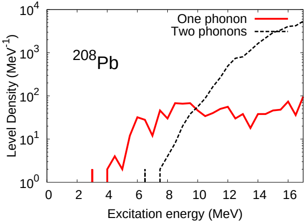
Perspective : two-step process

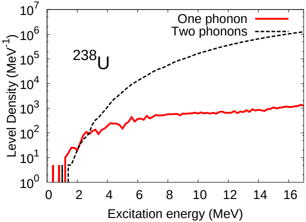


14.1 MeV ^{208}Pb (n,xn)



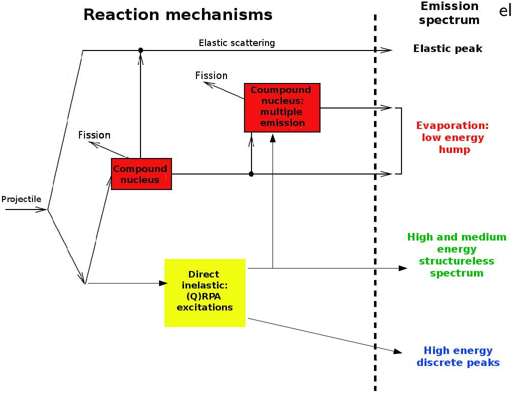
14.1 MeV ^{238}U (n,xn)

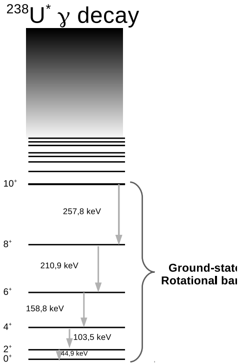




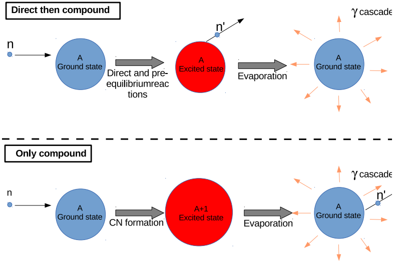
$(n,xn\gamma)$ cross sections

Impact new direc inelastic xs on $(n,n'\gamma)$ xs.





Reaction mechanisms for (n,n'γ)



Direct then compound

n

A Ground state

Direct and pre-equilibriumreactions

n'

A Excited state

Evaporation

A Ground state

γ cascade

Only compound

n

A Ground state

CN formation

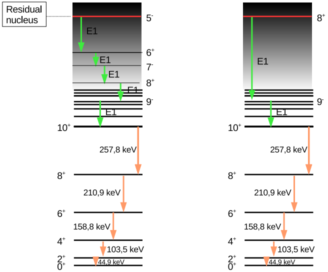
A+1 Excited state

Evaporation

n'

A Ground state

γ cascade

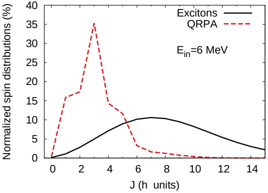


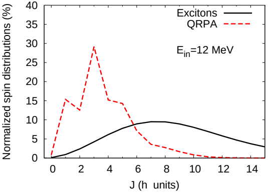
Residual nucleus spin distribution in ^{238}U

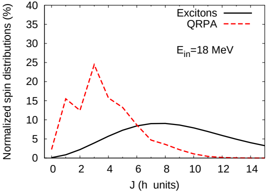
- Direct inelastic scattering ^{238}U (n,n') :
  $\rightarrow$ hypothesis : equilibration to a compound nucleus with excitation energy E, spin-parity J,Π.
- Spin distribution :

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

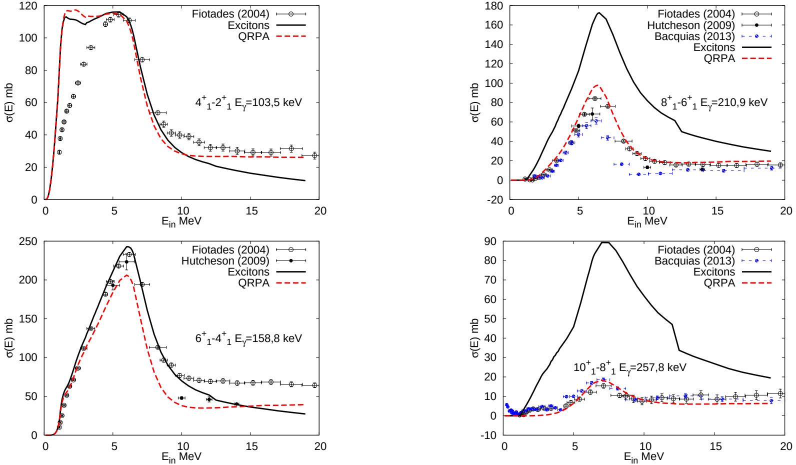
  Results form QRPA inelastic scattering model : $R(J,E_{\text{in}})=\dfrac{\sigma_J(E_{\text{in}})}{\sum_J \sigma_J(E_{\text{in}})}$, $\sigma_J(E_{\text{in}})$: cross section summed over all states of spin J.





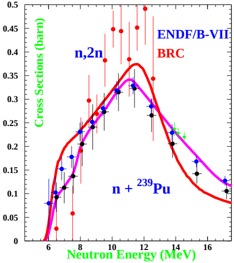


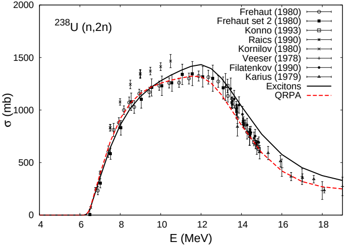
^{238}U (n,n'γ) cross sections for transitions in the GS rotational band

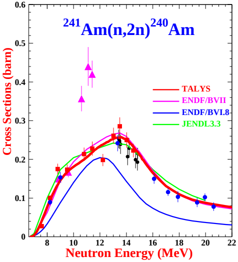


Collaborations IPHC (Strasbourg)-CEA/DAM-IFIN : (n,n'γ)^{238}U et ^{232}Th.

Discussion (n,2n)





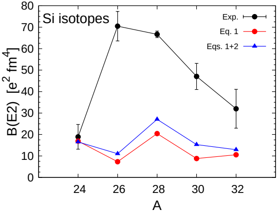


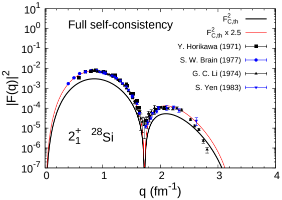
- Exp. data: similar (n,2n) slope for ^{238}U and ^{241}Am.
- Microscopic calculation of direct inelastic scattering: does not change ^{238}U (n,2n) slope.
- Perspectives :

→ 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 ?

Light targets : multiparticle-multihole (mpmh) configurations method

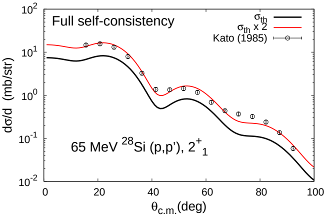
Nuclear excitations : sum of 0p0h,1p1h, 2p2h ... mpmh type excitations on a correlated GS.
Nuclear structure observables : first results in limited configurations space (sd-shell)





Nucleon induced reactions : DWBA calculations with mpmh wave-functions $\Longrightarrow$ complementary test of nuclear sturcture.

DWBA with Melbourne g-matrix



- (p,p') cross-section display the same behavior as for (e,e').
- Calculation in **larger space** (not limited to sd-shell) and a **new effective interaction** (extended Gogny force : tensor, finite range everywhere)

$\Longrightarrow$ expected **reliable nuclear struture input** for direct **reaction models** for nucleon scattering on **light nuclei** (ex : ^{16}O).

Mpmh worker : N. Pillet, C. Robin, D. Peña, J. Lebloas
Refs.: J. LeBloas et *al*. Phys.Rev.C 89, 11306 (2014), N. Pillet et *al*. Phys.Rev.C 85, 44315 (2012), C. Robin : PhD manuscript (2014).

Conclusions and future work

Microscopic models for nucleon inelastic scattering off spherical or axially deformed nuclei

- One phonon excitations predicted form (Q)RPA calculation (D1S interaction).
- Observed high energy neutron emission is well reproduced (pour $E_{in} < 20$ MeV).
  → QRPA low energy collective states explain the pseudo states origin.
- No arbitrary distinction between direct inelastic scattering and pre-equilibrium emission.
- Improve the description of ^{238}U (n,n'γ) reactions for ^{238}U .
- Discrepancy between predictions and data at lower emission energy in ^{238}U and ^{232}Th : highlight the needs to introduce other reaction mechanisms such as two-step process.

In progress

- Analysis of (n,xn) and (n,xnγ) to ^{232}Th, ^{239}Pu et ^{241}Am (weak coupling approximation for odd nuclei).
- ^{239}Pu (n,2n) cross section extracted from (n,2nγ) data : new analysis with microscopic direct reaction modeling.
- Comparison of QRPA response functions used in the TUL model and the present model (R. Capote).

Future work

Non natural parity excitations for axially deformed targets: enlight the need of a better effective interaction at low energy.

- Fit new effective interaction to low energy from g-matrix, problem of non-locality.

Calculation of second order with two phonons excitations.

- Millions of transition to consider : approximations needed.
- Use D1S-QRPA response functions in TUL-like model.
- Fit deformation parameters from collective model analysis, use them in the secon order calculation.

Whithin ten years ...

- Coupled channel calculations with QRPA transition densities including interband coupling.
- Extension of RPA-OMP (G. Blanchon) to direct inelastic scattering.
- Coupled channel with non-local potentials : mandatory if we want to use fully microscopic potentials.
- Use of mpmh wave functions for reactions on light nuclei.
- Introduce progresses in microscopic nuclear reaction models in global nuclear reaction codes (TALYS, EMPIRE ...) to improve (step by step) nuclear data evaluation.

THANK YOU

FOR YOUR ATTENTION

Collaborators

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