Advances in Nuclear Reaction Theory for Deformed Nuclei (Actinides)

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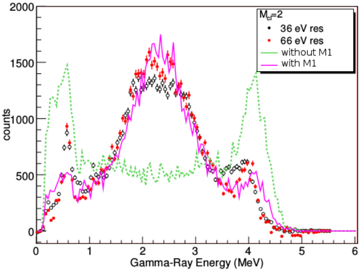
Statistical Model for Strongly Deformed Systems

- Hauser-Feshbach with coupled-channels model essential
  - collective states (rotational band levels) strongly excited
    - neutron inelastic scattering process modified by S-matrix unitarity limit
    - Engelbrecht-Weidenmüller transformation is required
  - M1 giant resonance (scissors mode) at a few MeV
    - neutron radiative capture cross section in the fast energy range enhanced
  - fission is a key process for nuclear data of actinide
    - fission penetration calculation, as well as the barrier parameters, still not accurate enough to predict fission cross sections
- Overview of recent upgrades in nuclear reaction theory for deformed systems, particularly for actinides
  - combining nuclear structure information crucial

γ-Ray Cascade and Capture Cross Section



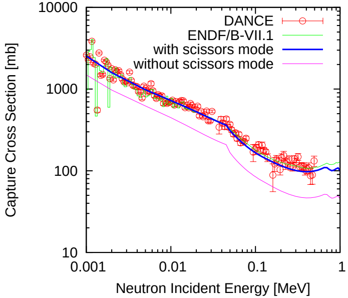
J. Ullmann, et al. PRC **89**, 034603 (2014)

DANCE γ-ray spectrum for multiplicity two

- an additional strength in the low energy region needed
- we assume this is an M1 scissors mode

Including a small M1 component at low energies, the ^{238}U(n,γ) data are well-reproduced without artificial re-normalization of photon strength function

Does correlation exist between M1 and nuclear deformation?

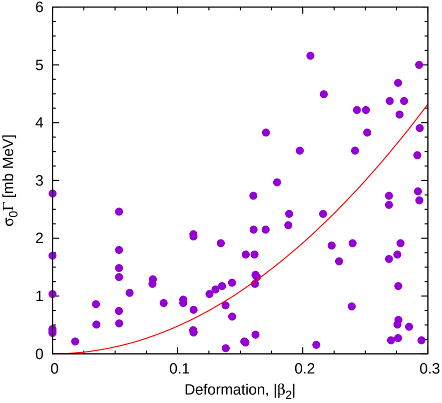


Estimation of M1 Strength from Neutron Capture Data

- compare Hauser-Feshbach calculations with evaluated nuclear data at 100 keV
  - 107 selected, those are based on experimental data
  - eliminate energy variation of cross section
  - avoid both resonance and direct capture dominant regions
- coupled-channels model
  - global optical potential by Kunieda
  - deformation parameters taken from FRDM95
- add M1 strength and adjust the parameter to reproduce the evaluated cross sections at 100 keV

M1 Strength vs. Nuclear Deformation

M1 strength required to reproduce evaluated capture cross section at 100 keV, in addition to the generalized Lorentzian E1



Resonance Energy

- assume oscillation amplitude proportional to the resonance energy
- analysis of ^{238}U DANCE data gave $E \simeq 2$ MeV

$$E_{\mathrm{M1}} = 80|\beta_2|A^{-1/3} \quad \mathrm{MeV}$$

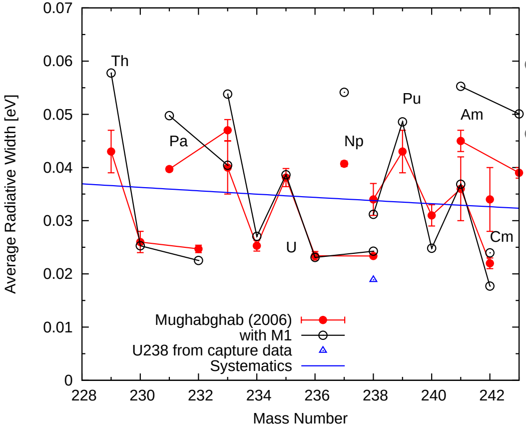
$66\delta A^{-1/3}$ in [D.R. Bes, Phys. Lett. **137B**, 141 (1984)]

Peak Cross Section and Width

$$\sigma_{\mathrm{M1}}\Gamma_{\mathrm{M1}} = 50\beta_2^2 \quad \mathrm{mb\ MeV}$$

Average Gamma Width, Actinide Region

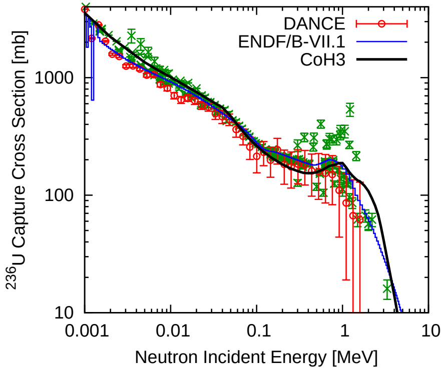
$$\langle\Gamma_\gamma\rangle = \frac{D_0}{2\pi}\sum_{XLJ'}\int_0^{S_n+E_n} T_{XL}(E_\gamma)\rho(S_n+E_n-E_\gamma, J')dE_\gamma \qquad (1)$$



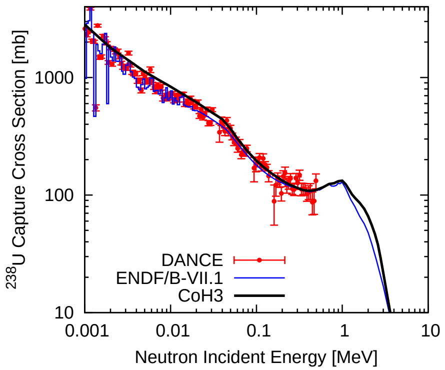
- actinide data not included in the search
- ^{238}U value
  - 23.36±0.31 meV (ATLAS)
  - 23.6 meV (RIPL)
  - 24.3 meV (this work)
  - 18.9 meV from σ_{capt}

^{236}U and ^{238}U Capture Cross Sections

^{236}U(n,γ)



^{238}U(n,γ)



Inclusion of Direct Channel in Hauser-Feshbach

Cross section calculations for strongly deformed systems

- Approximated Method
  - calculate transmissions from Coupled-Channels S-matrix

$$T_a = 1 - \sum_c |\langle S_{ac}\rangle\langle S^*_{ac}\rangle|^2 \tag{2}$$

  - $\sum_a T_a$ gives correct compound formation cross section
  - HF performed in the direct-eliminated cross-section space
- Engelbrecht-Weidenmüller (EW) transformation
  - diagonalize S-matrix to eliminate the direct channels
  - HF performed in the diagonal channel space
  - transform back to the cross section space
- Theory of Kawai-Kerman-McVoy (KKM)
  - correct at the limit of channel degree of freedom $\nu = 2.0$

Moldauer and Engelbrecht-Weidenmüller

- In the actual cross section calculation, there are a lot of uncoupled channels (e.g. fission and capture)
- Solving GOE triple-integral for all channels is impractical
- Apply Moldauer's estimate to the transformed cross sections

$$P_{ab} = \delta_{ab} - \sum_c \langle S_{ac} \rangle \left\langle S^*_{bc} \right\rangle, \qquad (UPU^\dagger)_{\alpha\beta} = \delta_{\alpha\beta} p_\alpha \tag{3}$$

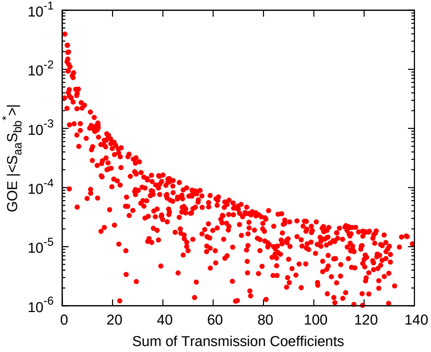
$$\begin{aligned} \langle \sigma^{\mathrm{fl}}_{ab} \rangle &= \sum_{\alpha\beta} U^*_{\alpha a} U^*_{\beta b} \left\{ U_{\alpha a} U_{\beta b} + U_{\alpha a} U_{\beta b} (1 - \delta_{\alpha\beta}) \right\} \left\langle |\tilde{S}_{\alpha\beta}|^2 \right\rangle \\ &\quad + U^*_{\alpha a} U^*_{\beta b} U_{\alpha a} U_{\beta b} \left\langle \tilde{S}_{\alpha\alpha} \tilde{S}^*_{\beta\beta} \right\rangle \end{aligned} \tag{4}$$

$$\left\langle \tilde{S}_{\alpha\alpha} \tilde{S}^*_{\beta\beta} \right\rangle \simeq e^{i(\phi_\alpha - \phi_\beta)} \left(\frac{2}{\nu_\alpha} - 1 \right)^{1/2} \left(\frac{2}{\nu_\beta} - 1 \right)^{1/2} \sigma_{\alpha\beta} \tag{5}$$

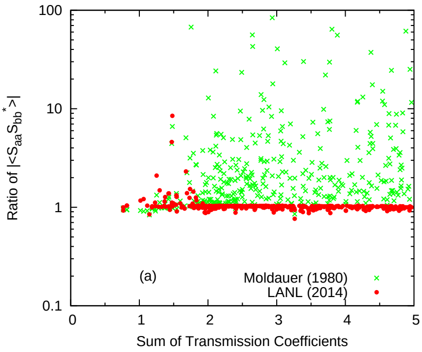
Moldauer's $\langle S_{\alpha\alpha} S^*_{\beta\beta} \rangle$ Term

Applying systematics of $\nu_a = f(T_a, \sum T_a)$ to randomly generated S-matrix

exact $\langle S_{\alpha\alpha} S^*_{\beta\beta} \rangle$ by GOE



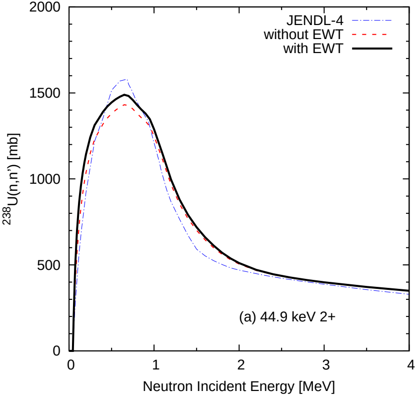
Moldauer/GOE

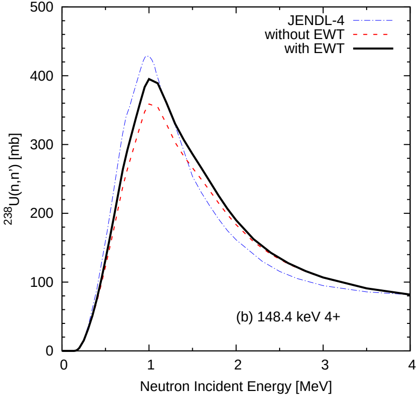


GOE simulations imply that Moldauer's ansatz seems to be correct.

U-238 Inelastic Scattering Cross Section

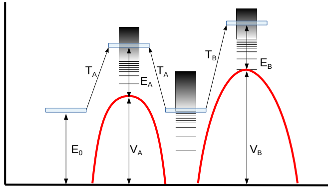
Full EW transformation implementation into the CoH_3 code

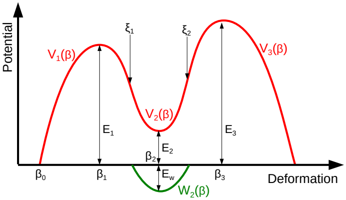




Probably we have been underestimating the inelastic scattering cross sections of actinides by 10 – 15%.

Fission Transmission for Arbitrary Potential Shape





Solving One-dimensional Schrödinger equation

J.D. Cramer, J.R. Nix, Phys. Rev. C **2**, 1048 (1970)

$$\frac{d^2}{d\beta^2}\phi(\beta) + \frac{2\mu}{\hbar^2}\left\{E - (V(\beta) + iW(\beta))\right\}\phi(\beta) = 0 \quad (6)$$

with the boundary conditions of

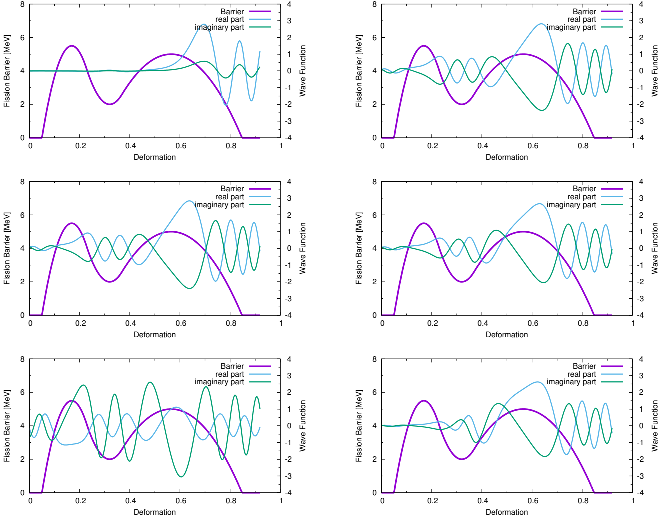
$$\phi(\beta) \simeq \begin{cases} u^{(-)}(k\beta) - S\,u^{(+)}(k\beta) & \beta > \beta_{\max} \\ Au^{(-)}(k\beta) & \beta < \beta_0 \end{cases} \quad (7)$$

where

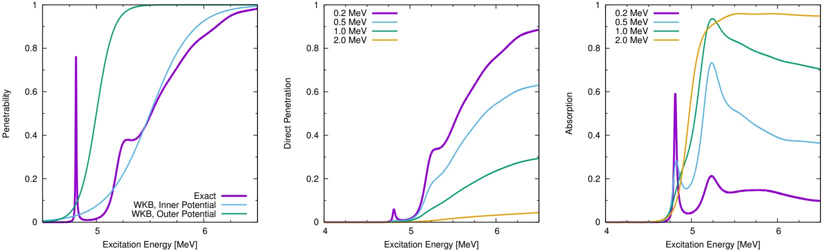
$$u^{(\pm)}(k\beta) = \cos(k\beta) \pm i\sin(k\beta) \quad (8)$$

Wave Functions for Double-Humped Fission Barrier

real potential | complex potential



Fission Transmission Coefficients



- Empire has a similar capability, but WKB approximation
- T_f solver already implemented in CoH_3
- We still need to model indirect fission for the complex potential case
    - absorbed flux goes into the fission channel,
    - or come back to the initial compound nucleus (capture or inelastic)

Post-Scission Phenomena

- Fission produces a lot of observable quantities
- Post-scission modeling should reproduce these data consistently
  - prompt fission neutron and γ-ray spectra
  - fission product yields, $\overline{\nu}$, total kinetic energy, etc.
- Monte Carlo technique to simulate de-excitation of fission fragments
  - CGMF (LANL) and FREYA (LLNL)

Conclusion

- Hauser-Feshbach calculations for actinide significantly improved in the last decade
- However, model parameters still need to be refined for better prediction
  - photon strength functions — generalized E1, enhanced E1, M1 scissors
  - level density with realistic spin and parity distributions
  - realistic fission path
    - coupled-channels calculation for rotational-vibrational nuclei, and potential parameters
- Mean-field theories may help better understanding
- Exchange expertise among similar code projects important
  - Empire at BNL and IAEA, TALYS at CEA/DAM, CCONE at JAEA, CoH_3 at LANL, and LLNL code