Microscopic pre-equilibrium calculations for neutron scattering on deformed nuclei

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- *Microscopic approaches for the multistep direct (MSD) process*
- *Microscopic MSD calculations for neutron scattering on ^{238}U*
- *Conclusions and future work.*

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Microscopic description of the multistep direct (MSD) process : introduction

The **transition amplitude** associated to the “multi-step” direct process reads:

$$T_{f\leftarrow i}=\sum_F \delta(E_{k_i}-E_{k_f}-E_F)\langle\chi^-(\vec{k}_f)\ F\ |V\ +\ VG^+V\ +\ VG^+VG^+V\ +\ \ldots|\ 0\ \ \chi^+(\vec{k}_i)\rangle$$

First step | Second step | Third step

V = Two body interaction (projectile-target's nucleon)

propagator

$$G^+=\frac{1}{E-H_T-H_P+i\epsilon}$$

H_T projectile Hamiltonian (optical potential)

$$H_T|\chi^{+/-}(\vec{k}_{i/f})\rangle=E_{k_{i/f}}|\chi^{+/-}(\vec{k}_i)\rangle$$

H_P target Hamiltonian

Microscopic description of the multistep direct (MSD) process : first step

First order transition amplitude (dominant below 20 MeV)

$$T^{(1)}_{f\leftarrow i}=\sum_F \delta\left(E_{k_i}-E_{k_f}-E_F\right)\langle\chi^-(\vec{k}_f)\;\; F\;\, |V|\;\, 0\;\; \chi^+(\vec{k}_i)\rangle$$

Double differential cross-section can be obtained with different assumption:

-**energy averaging** on projectile energy (experimental energy resolution)
-**ensemble averaging** on the target's excited states (random mixing of ph components)
-decay of the target final states -> **damping widths**

The double differential cross-section reads:

$$\frac{d^2\sigma(\vec{k}_i,\vec{k}_f)}{d\Omega_{k_f}\,dE_{k_f}}\propto\frac{1}{2\Delta}\int_{E_{k_f}-\Delta}^{E_{k_f}+\Delta} dE\,\rho(E-E_F)\left|T^{(1)}_{f\leftarrow i}\right|^2$$

Microscopic description of the multistep direct (MSD) process : second step and spectral decomposition

$$T^{(2)}_{f\leftarrow i}=\sum_F \delta(E_{k_i}-E_{k_f}-E_F)\langle\chi^-(\vec{k}_f)\ \ F\ |VG^+V|\ 0\ \ \chi^+(\vec{k}_i)\rangle$$

$$G^+=\frac{1}{E-H_T-H_P+i\epsilon}\ \xrightarrow{H_T=\sum_n E_n|n\rangle\langle n|}\ G^+=\sum_n\frac{|n\rangle\langle n|}{E-E_n-H_P+i\epsilon}$$

Spectral decomposition of the target Hamiltonian

$$T^{(2)}_{f\leftarrow i}=\sum_{F,n}\delta(E_{k_i}-E_{k_f}-E_F)\langle\chi^-(\vec{k}_f)\ \ F\ |V|n\rangle\underbrace{\frac{1}{E-E_n-H_T+i\epsilon}}\langle n|V|\ 0\ \ \chi^+(\vec{k}_i)\rangle$$

$$|n\rangle=|1\mathrm{p}1\mathrm{h}\rangle$$

$$|F\rangle=|2\mathrm{p}2\mathrm{h}\rangle\ \ \text{or}\ \ |1\mathrm{p}1\mathrm{h}\rangle$$

Explicit calculation of the Green functions

TUL model (Tamura, Udagawa, Lenske)

NWY model(Nishioka, Weidenmuller, Yoshida)

FKK (Feshbach, Kerman, Koonin) model: spectral decomposition of the projectile Hamiltonian

$$G^+=\sum_n\int d\vec{k}\,\frac{|\chi^+(\vec{k})\rangle|n\rangle\langle n|\langle\tilde{\chi}^+(\vec{k})|}{E-E_n-E_k+i\epsilon}$$

On-shell assumption + $|\tilde{\chi}^+(\vec{k})\rangle\simeq|\chi^-(\vec{k})\rangle$

Energy averaging in the intermediate step

Microscopic description of the multistep direct (MSD) process : open questions

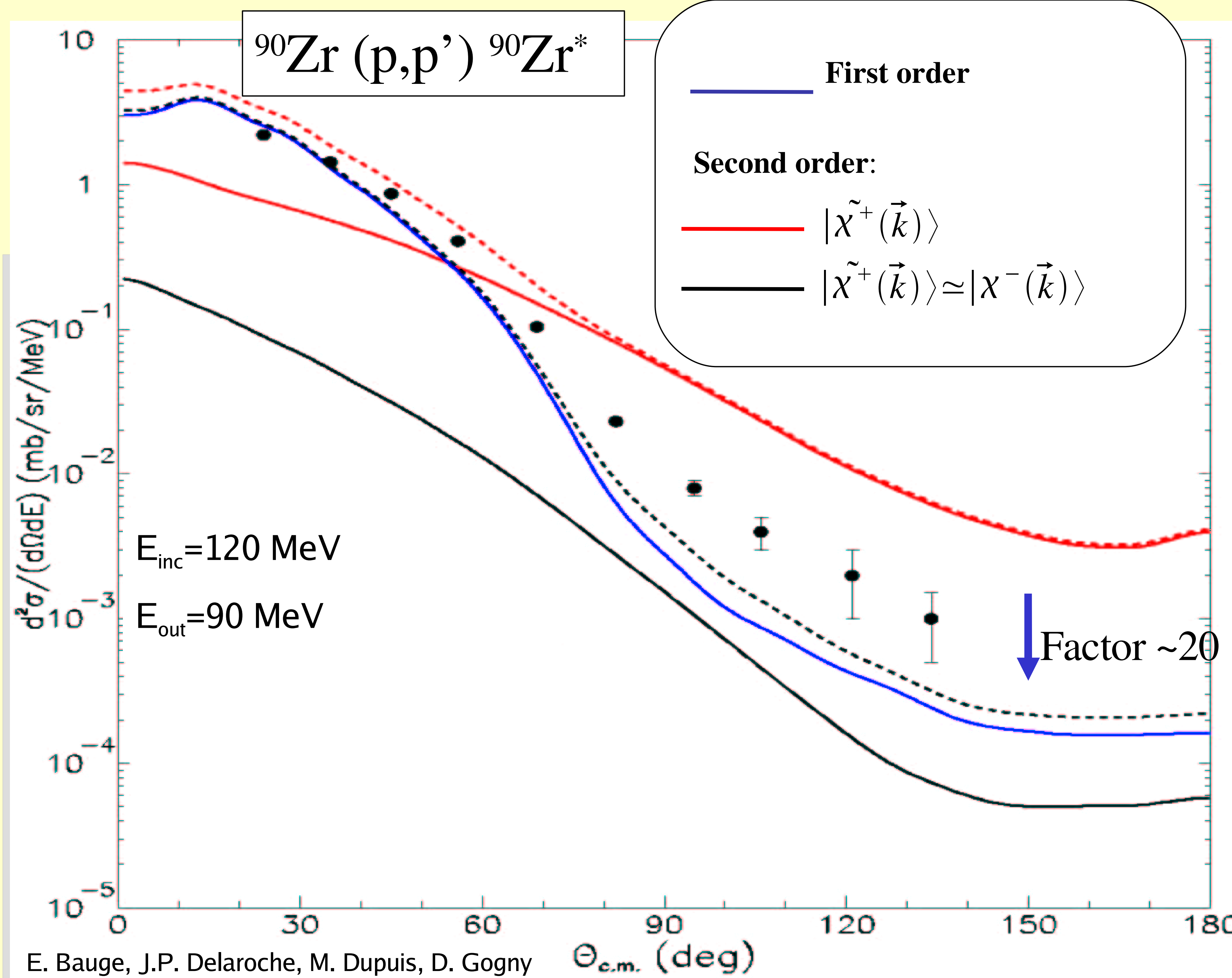
Model	FKK (1980)	TUL (1982)	NWY (1988)
Approximations	Adiabatic+on-shell +distorted wave	Adiabatic	Sudden
Statistical average	Each steps	Each steps	Final step
Target states description	Equidistant	RPA	GOE

Questions which still need answers

- Which two body interaction should be used ?

-Description of intermediate and final target states ?

-Formulation of the second step process: all the different approximations have not yet been tested.



$^{90}Zr\ (p,p')\ ^{90}Zr^{*}$
First order
Second order:
$|\tilde{\chi}^{+}(\vec{k})\rangle$
$|\tilde{\chi}^{+}(\vec{k})\rangle \simeq |\chi^{-}(\vec{k})\rangle$
E_{inc}=120 MeV
E_{out}=90 MeV
Factor ~20
$d^2\sigma/(d\Omega dE)$ (mb/sr/MeV)
$\Theta_{c.m.}$ (deg)
10
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
0
30
60
90
120
150
180
E. Bauge, J.P. Delaroche, M. Dupuis, D. Gogny

MSD calculations for neutron scattering below 20 MeV

Double differential cross-section :

$$\frac{d^2\sigma(\vec{k}_i,\vec{k}_f)}{d\Omega_{k_f}\,dE_{k_f}} \propto \frac{1}{2\Delta}\int_{E_{k_f}-\Delta}^{E_{k_f}+\Delta} dE \sum_F \frac{1}{(E-E_F)^2+(\frac{\Gamma}{2})^2}|T^{(1)}_{f\leftarrow i}|^2$$

The one-step cross-section is calculated with the DWBA amplitude:

$$T^{(1)}_{f\leftarrow i}=\langle\chi^+\left(\vec{k}_E\right)\ \ F\ \ |V|\ \ 0\ \ \chi^-(\vec{k}_i)\rangle$$

Ingredients : distorted waves $|\chi^-(\vec{k}_i)\rangle$ $|\chi^+(\vec{k}_E)\rangle$

,

two-body interaction V

excited states $|F\rangle$: wave functions, excitation energies, damping widths

Microscopic calculation: motivations

MSD calculations: -done with a **phenomenological interaction** (usually only a central isoscalar interaction with a Yukawa form-factor,strength adjusted to reproduce the experimental data) :

-crude description of excited state: Nilson Model,

-use phenomenological level densities.

→ **Microscopic**, more predictive calculation is **needed**, especially for actinides (experimental data are scarce).

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<u>New calculations with no adjustable parameters:</u>

- **Microscopic** description of **target states**
- **Microscopic two-body interaction for the transition**

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MSD calculation for deformed nuclei

First step of the multistep direct process (MSD): DWBA cross-section

$$\frac{d^2\sigma(\vec{k}_i,\vec{k}_f)}{d\Omega_{k_f}\, dE_{k_f}} \propto \frac{1}{2\Delta}\int_{E_{k_f}-\Delta}^{E_{k_f}+\Delta} dE \sum_F \frac{1}{(E-E_F)^2+\left(\frac{\Gamma}{2}\right)^2} \left|\langle \chi^+\left(\vec{k}_E\right) \; F \; |V| \; 0 \; \chi^-(\vec{k}_i)\rangle\right|^2$$

Axial Hartree-Fock+BCS

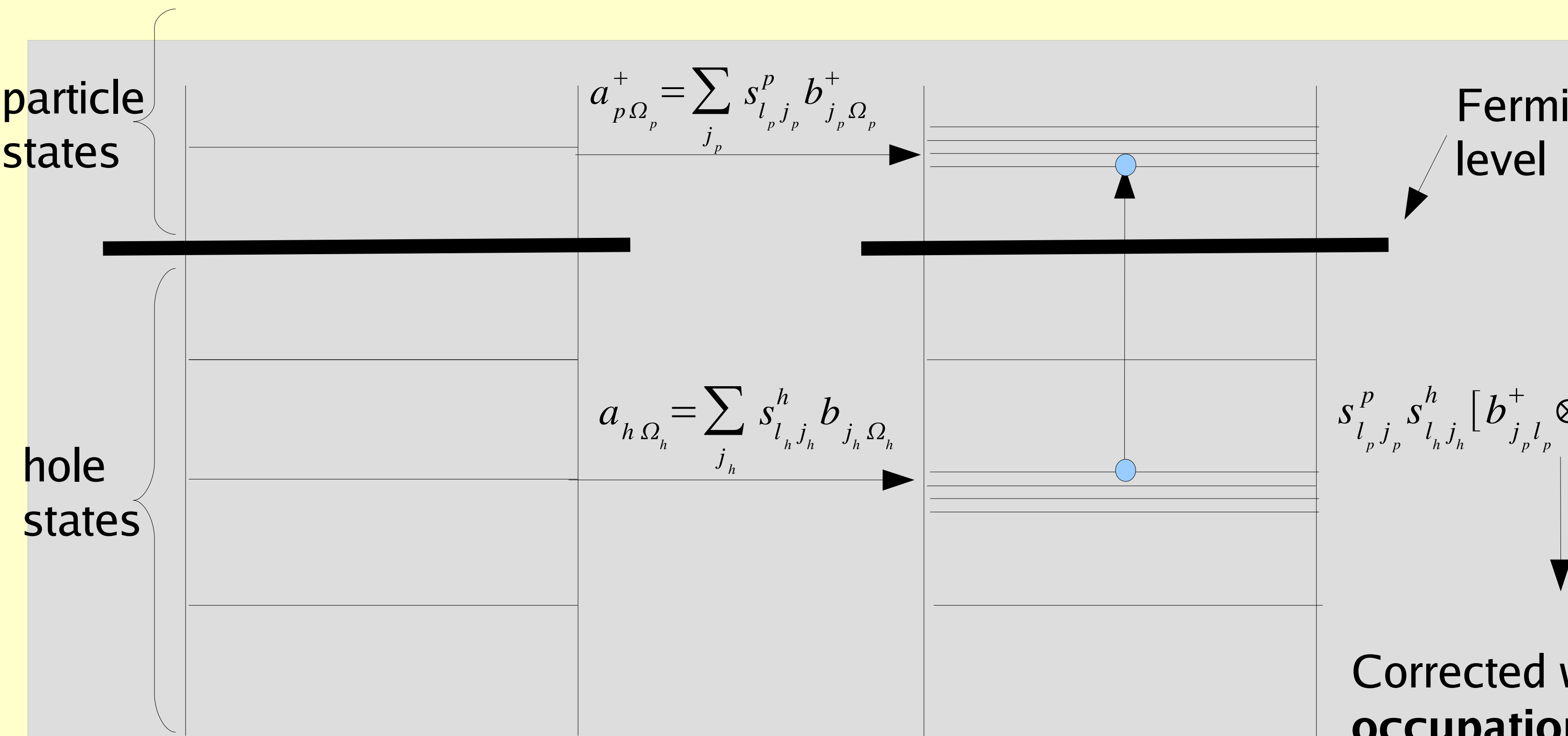
with a Skyrme interaction

Phenomenological distorted waves (Adjusted spherical optical potential to elastic scattering data.)

Transition: M3Y interaction

N. Anantaraman et al, Nucl. Phys. A398, 269 (1983).

Particle-hole excitations in a deformed nucleus



$$s^{p}_{l_p j_p} s^{h}_{l_h j_h} [b^{+}_{j_p l_p} \otimes b_{j_h l_h}]^{J}_{M=\Omega_p-\Omega_h} |\phi_0>$$

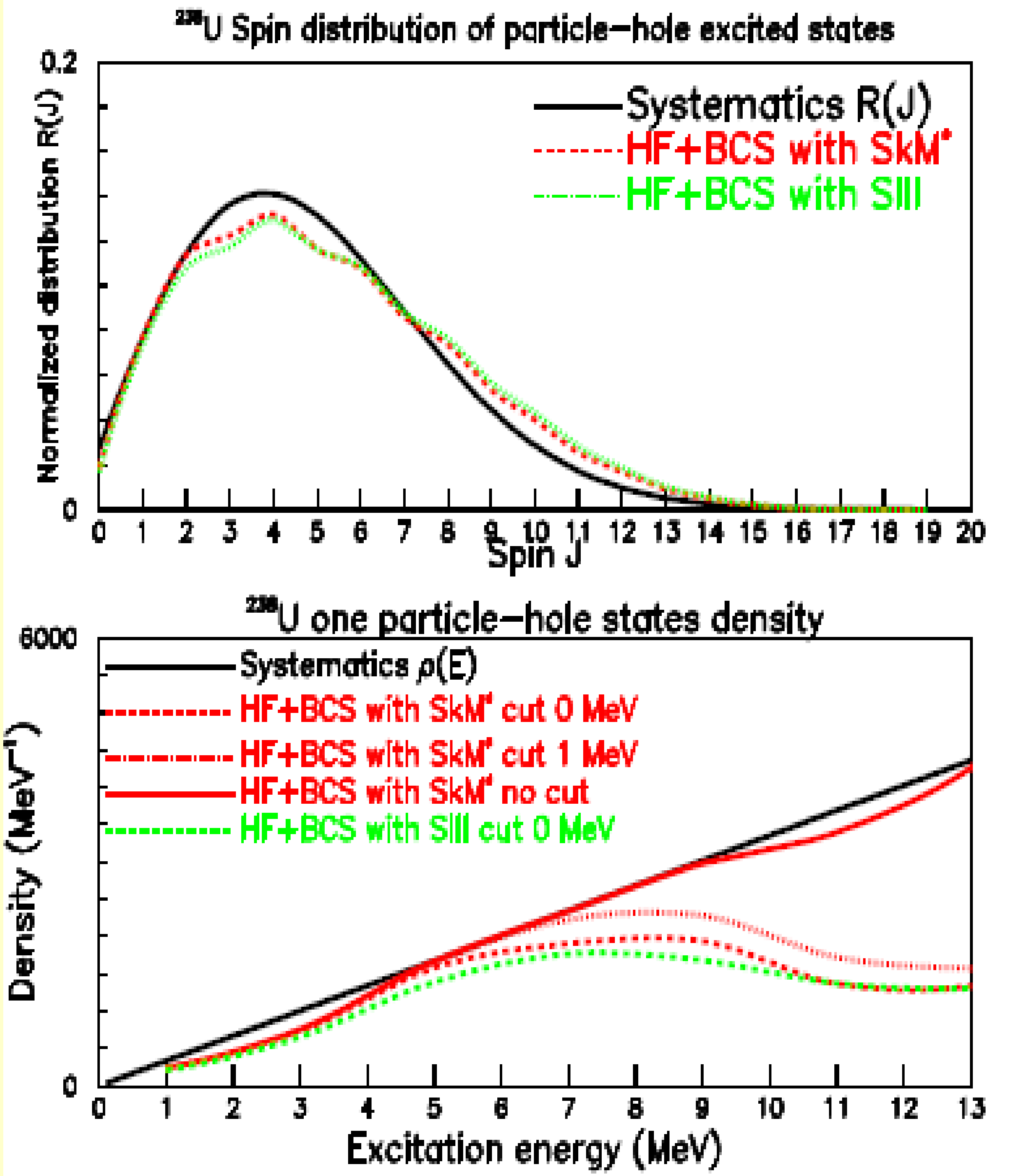
Corrected with **BCS occupation probabilities**

The deformed single particle states are projected on spherical states

Approximation: each spherical component of a deformed single particle state is considered as single particle state of a spherical nuclei with a fractional occupation number.

Particle-hole excitations:

$$u^2_p v^2_h s^{p}_{l_p j_p} s^{h}_{l_h j_h} [b^{+}_{j_p l_p} \otimes b_{j_h l_h}]^{J}_{M=\Omega_p-\Omega_h} |\phi_0>$$



State densities and spin distribution

Comparison to phenomenological expressions:

-one particle-hole spin-distribution (Gruppelaar, Brookhaven Nat. Lab. Rep. 251, (1983)):

$$R(J) = \frac{(J+\frac{1}{2})}{\sqrt{2\pi\sigma^2}} \times e^{-\frac{(J+\frac{1}{2})^2}{2\sigma^2}}$$

$$\sigma^2 = 0.24 \times 2 \times A^{\frac{2}{3}}$$

-level density for one particle-hole states (Beták and Dobes, Z. Phys A 279, 319 (1976))

$$\rho(E) = g^2 E \quad (MeV^{-1})$$

$$g = A/13 \quad MeV^{-1}$$

Other contributions to the neutron spectrum

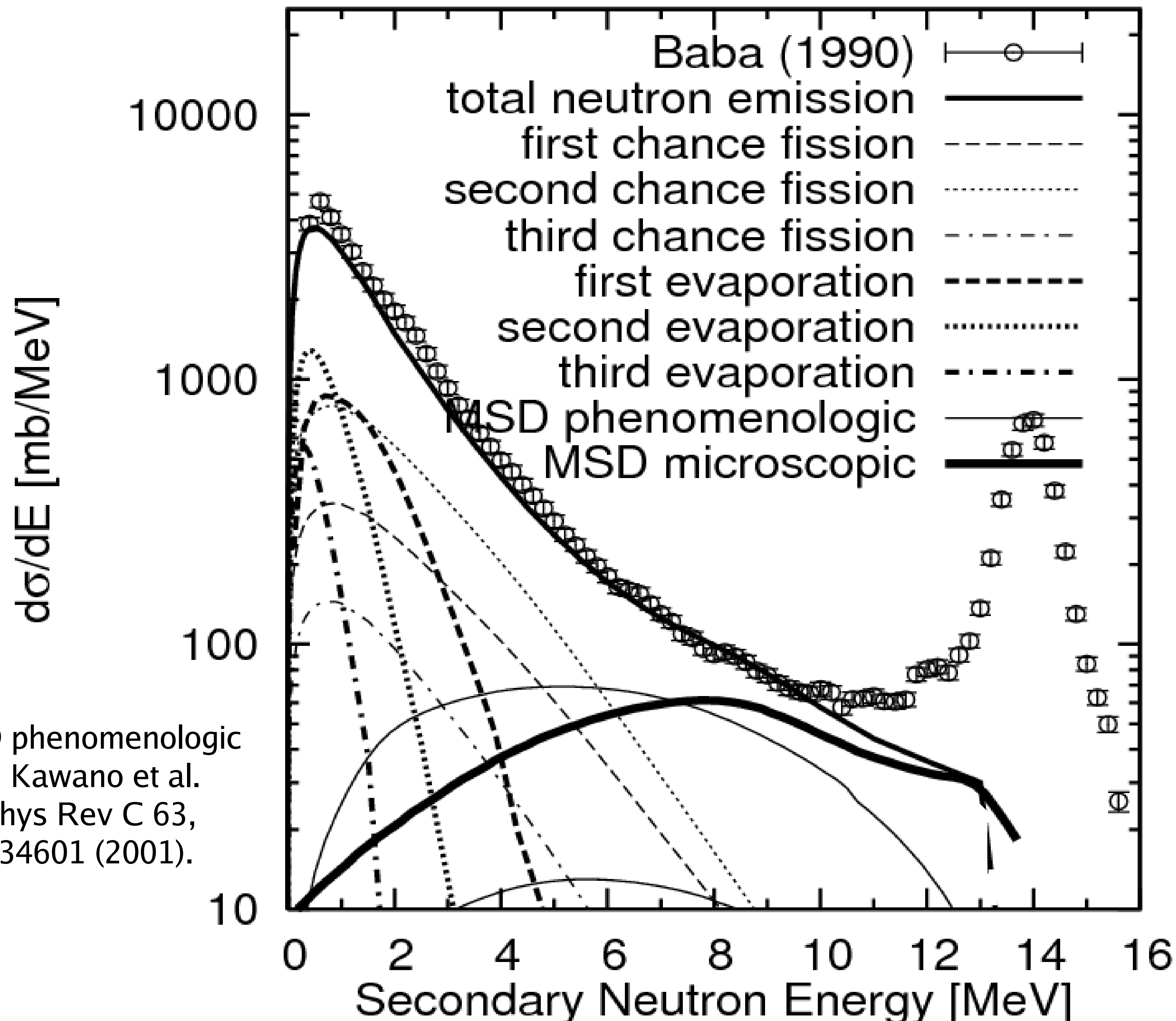
<u>For 10~20 MeV incident neutrons on ^{238}U, processes involved in (n,xn) reactions :</u>

Multistep compound: microscopic or statistic model (small contribution).

Evaporation : Hauser-Feshbach model (n,n') , (n,2n) , (n,3n).

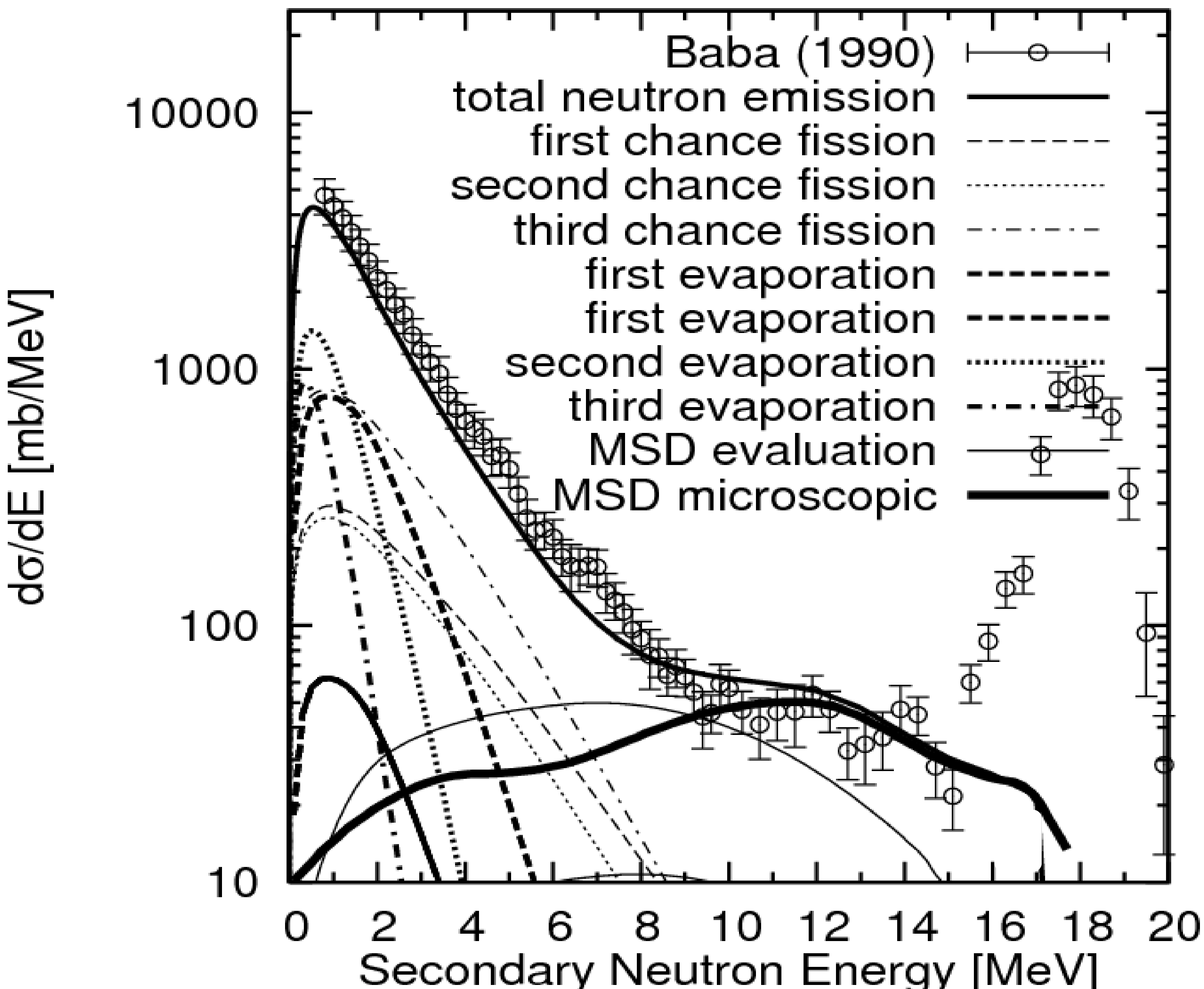
Multiple chance fission: Madland and Nix model (up to 3 chances).

MSD angle integrated cross section for 14.2 MeV neutron scattering on ^{238}U

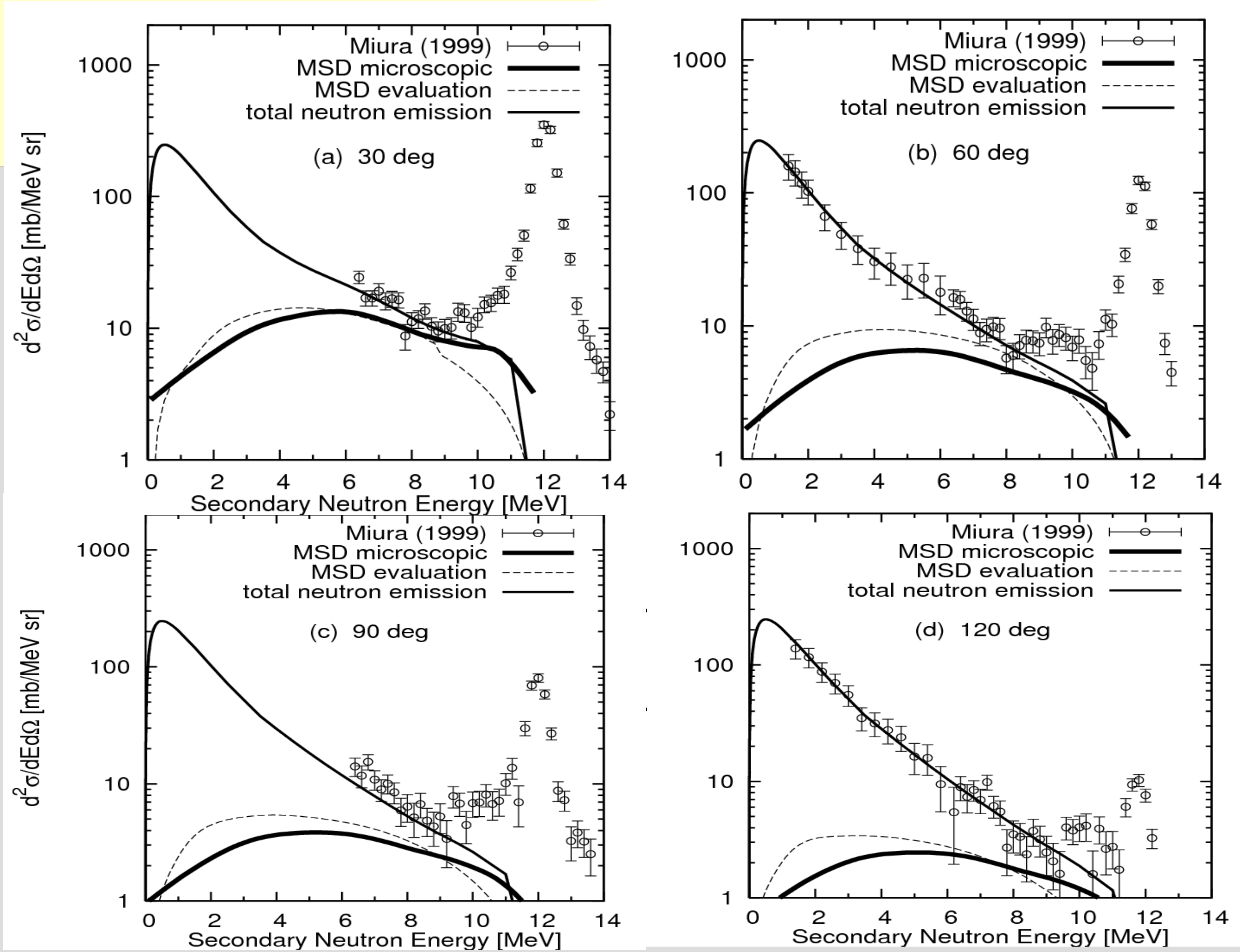


MSD phenomenologic
T. Kawano et al.
Phys Rev C 63,
034601 (2001).

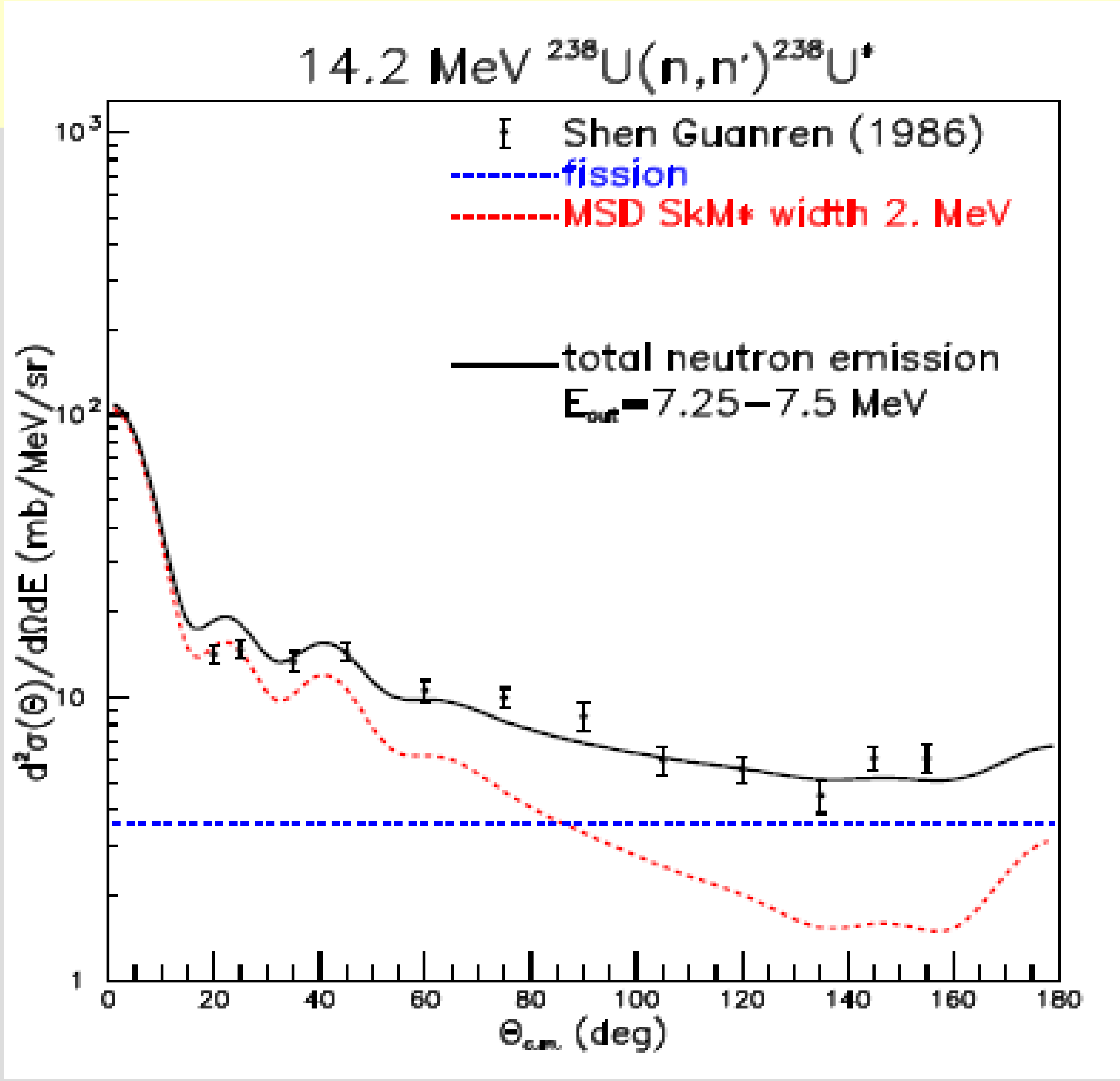
MSD angle integrated cross section for 18. MeV neutron scattering on ^{238}U



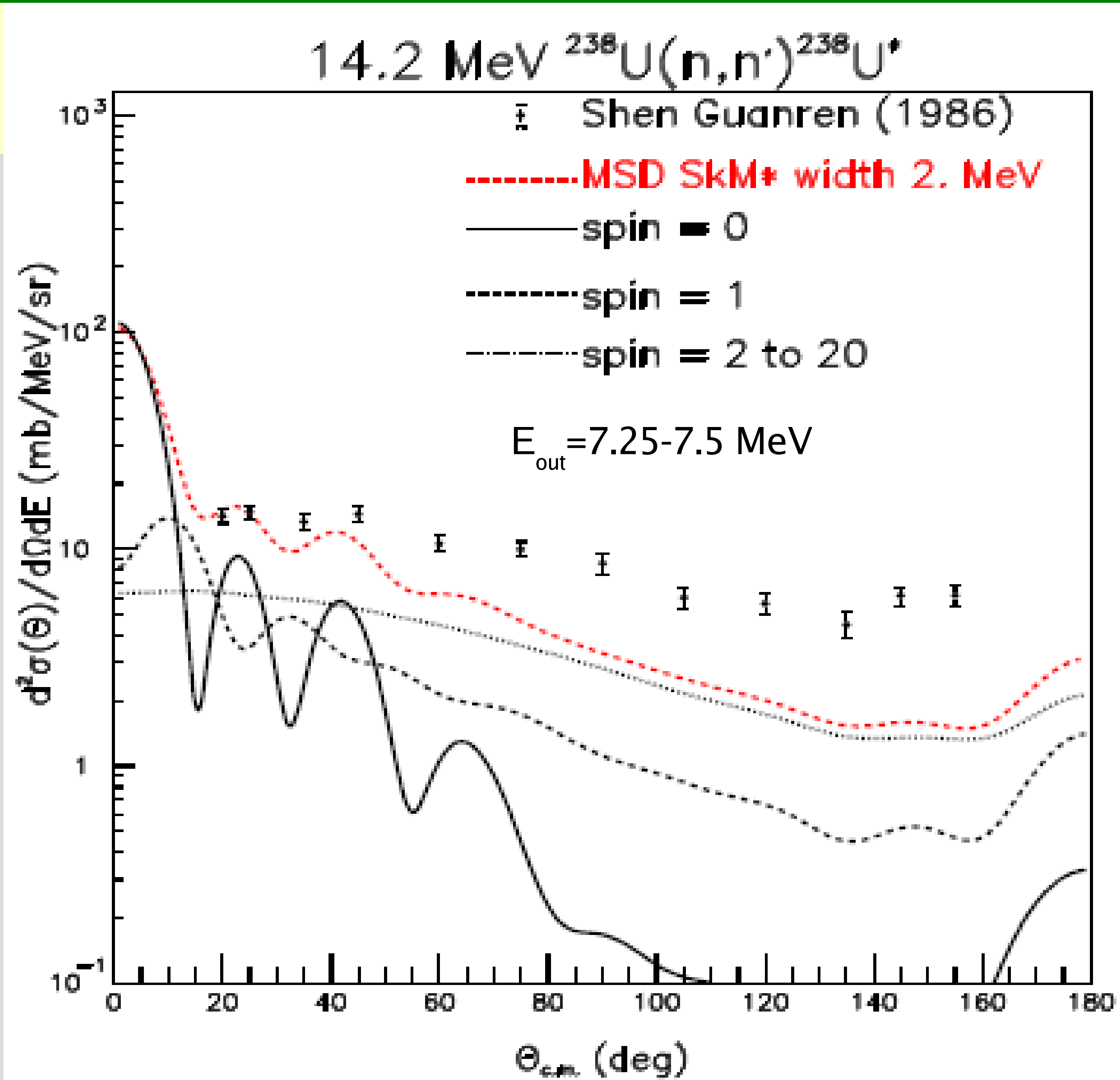
MSD double differential cross section for 11.8 MeV neutron scattering on ^{238}U



MSD angular distribution for 14.2 MeV neutron scattering on ^{238}U



MSD angular distribution : cross section spin distributions



Some details on the present calculations: neutron inelastic scattering on ^{238}U

$$\frac{d^2\sigma(\vec{k}_i,\vec{k}_f)}{d\Omega_{k_f}\,dE_{k_f}} \propto \frac{1}{2\Delta}\int_{E_{k_f}-\Delta}^{E_{k_f}+\Delta} dE \sum_F \frac{1}{(E-E_F)^2+(\frac{\Gamma}{2})^2}\left|\langle \chi^+\left(\vec{k}_E\right)\ F\ |V|\ 0\ \chi^-(\vec{k}_i)\rangle\right|^2$$

<u>**Code**</u> DWBA 98 J. Raynal, parallelized.

<u>**Required computations time for a calculation on 42 2GHz opteron processors:**</u>

Incident energy (MeV)	Number of ph configurations	Computation time
11.8	260 000	18 min
14.1	310 000	21 min
18.	380 000	26 min

Sensitivity to the model parameters

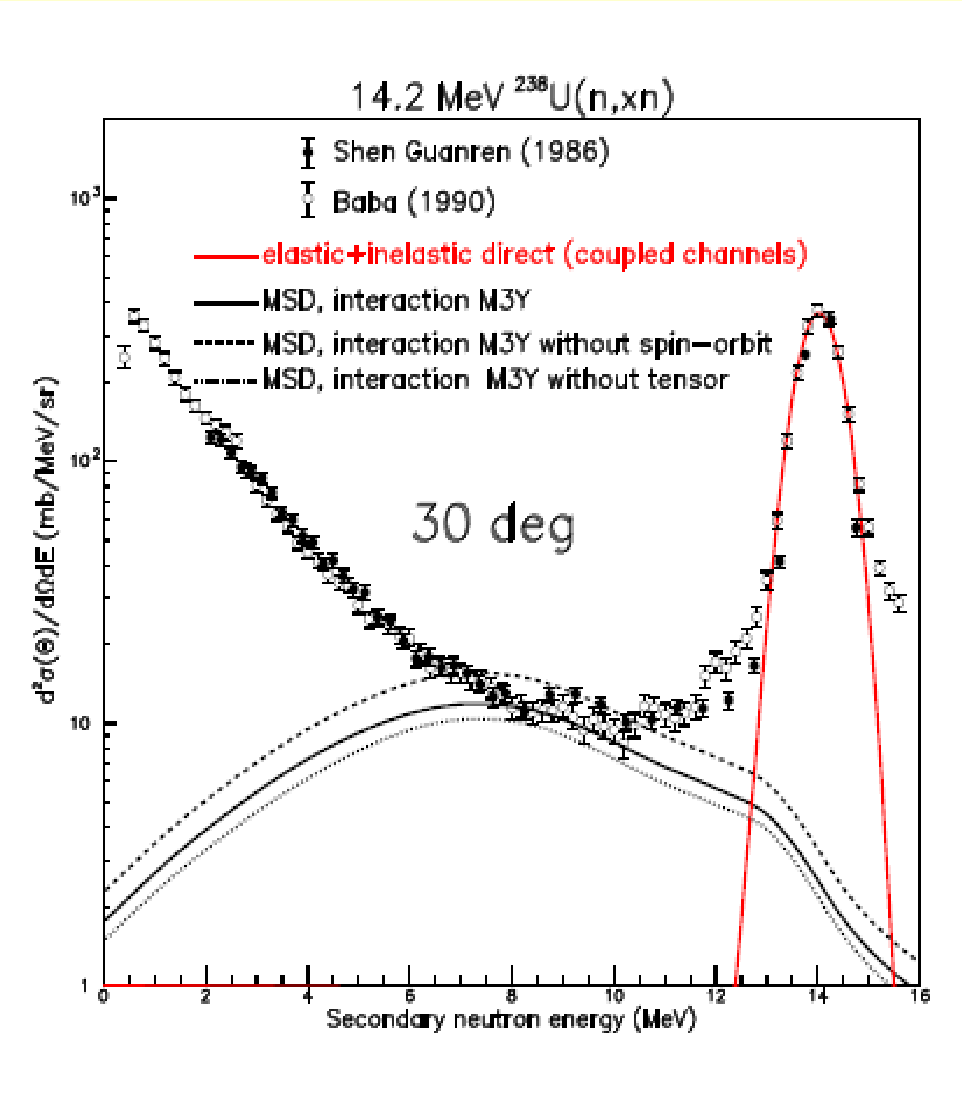
These MSD calculations depend on different parameters:

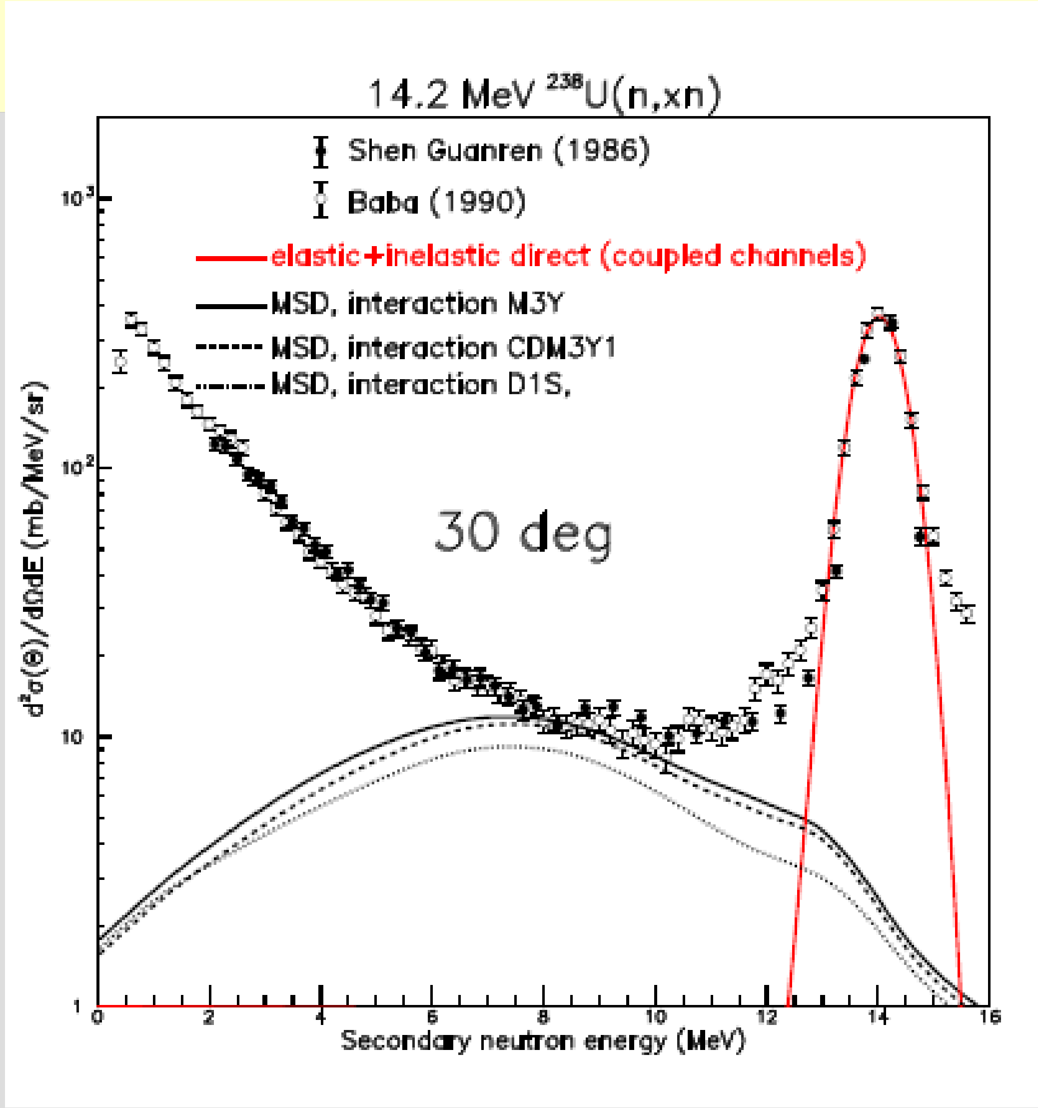
- **two-body interaction between the projectile and the target's nucleons:**
  the effective interaction is not well known, especially at low energy. Different calculations with the M3Y, density dependent M3Y, D1S interactions.

- **structure description of the single particle states:**
  with the projected HF+BCS approach, comparison between two Skyrme interactions.

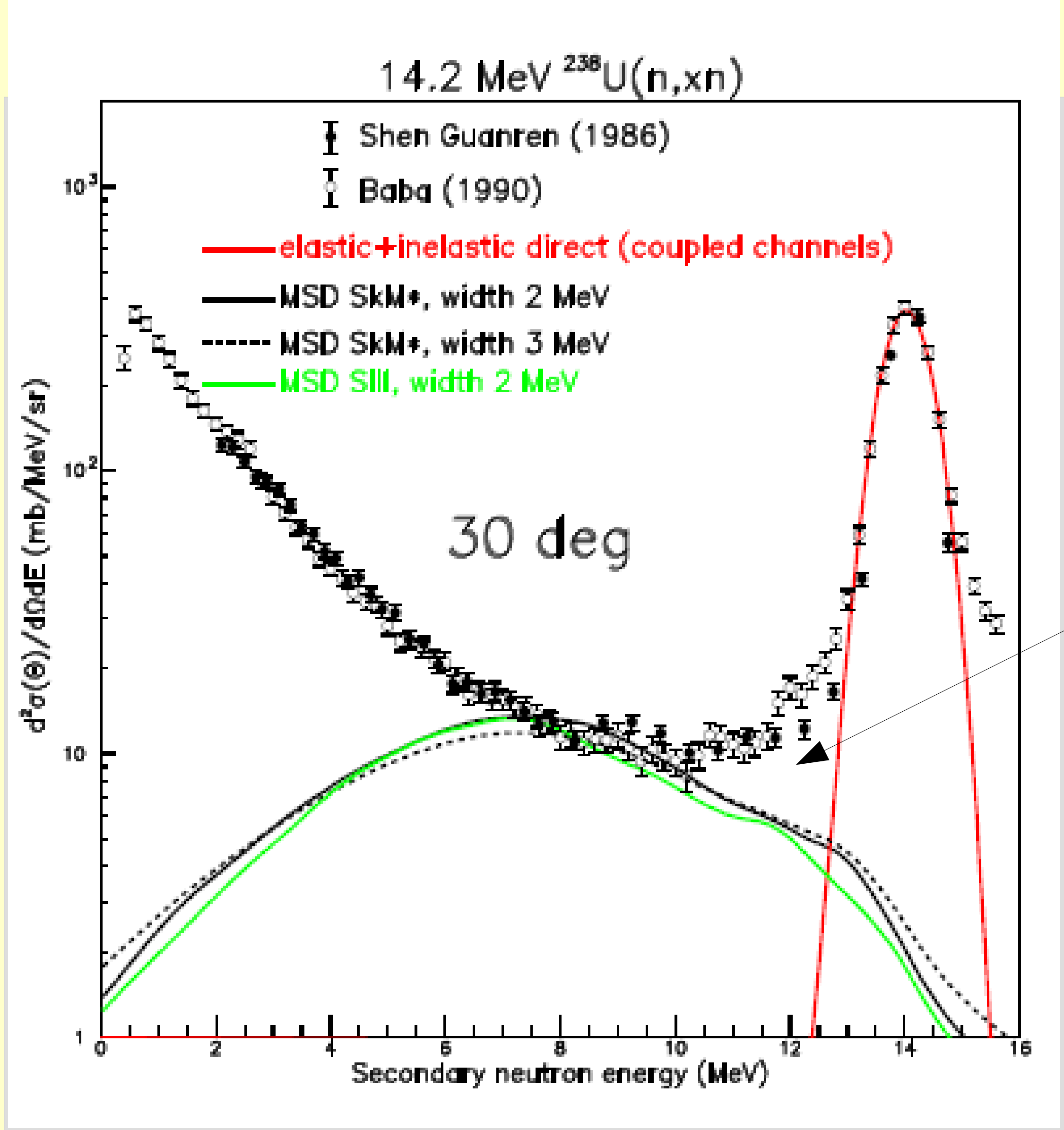
- **widths of particle-hole excited states**
  the widths are not yet predicted by microscopic calculations, but we can test different phenomenological prescriptions.

Sensitivity to the two-body interaction





Sensitivity to the nuclear structure calculation and the damping widths



Data not reproduced:

-better form factor for the elastic direct contribution ? (experimental resolution)

-collective states ? No predictions but a full QRPA calculation is needed

-residual interaction: energy shift of the particle-hole energies

-not so evident in the 11.8 and 18 MeV analyses: experimental data needs to be corrected ?

Conclusions

- **MSD cross sections** calculations have been achieved **without adjustment**: results are in fair agreement with experimental data for ^{238}U.

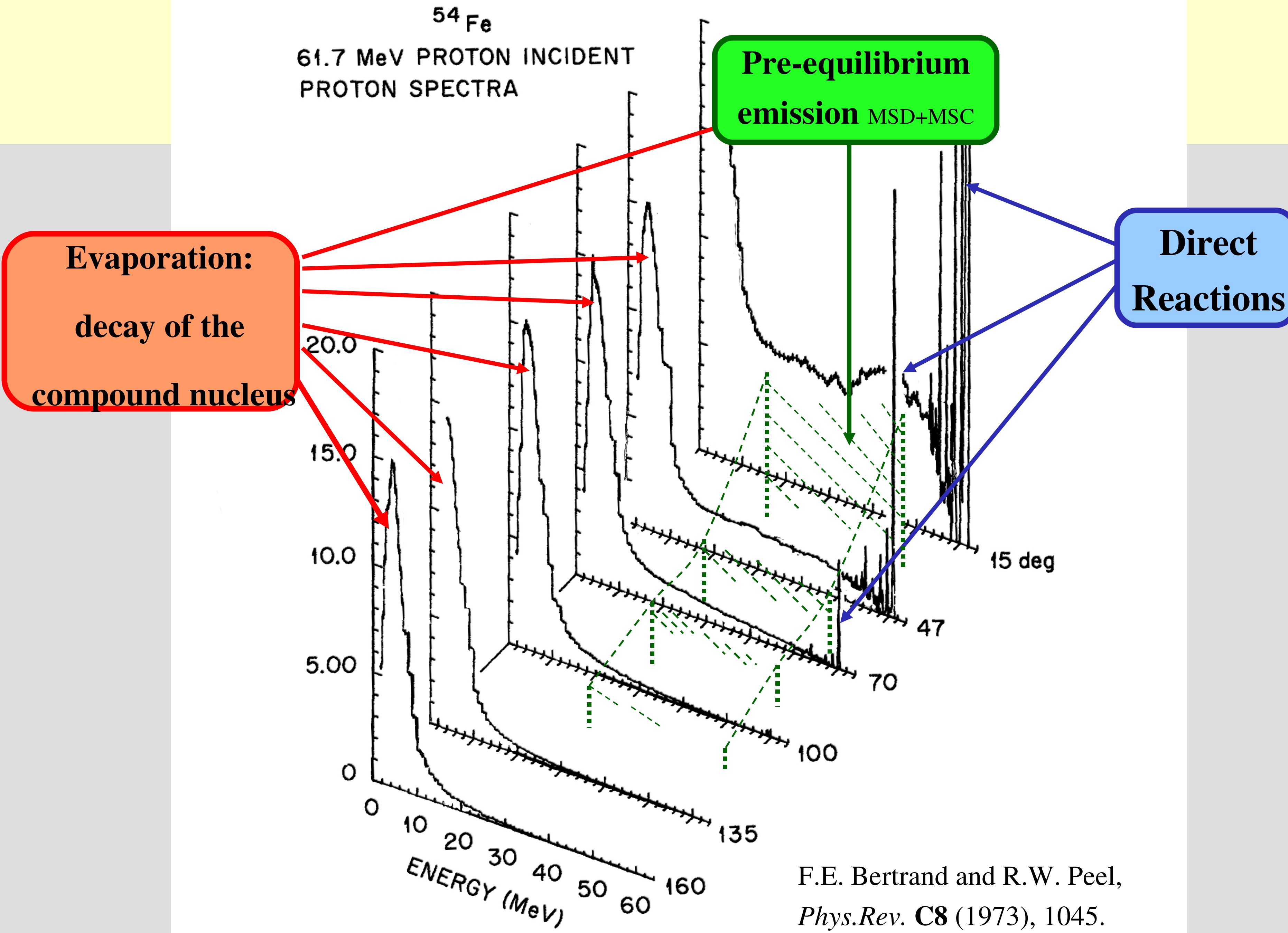
- **Microscopic calculations** are now **required**:
  - more **predictive,**
  - computation time is no longer a problem.

Future work

- <u>Consistent calculation of pre-compound process and compound nucleus formation</u>
- Treatment of continuum states in particle-hole excitations.
- Microscopic calculation of the compound nucleus formation (replace the projectile continuum state with a bound state).

- Correction of s.p. energies + damping widths due to the residual interaction**S** :**coupling between 1p1h excitations and to 2p2h excitations.**
- More realistic description of the target excited states: excitations built with **HFB and QRPA calculations** (with the gogny force) : answer for collective states .

Different reaction models



F.E. Bertrand and R.W. Peel, *Phys.Rev.* **C8** (1973), 1045.