Mark Chadwick, LANL

Overview

- Surrogate Concept
- Statistical theories of compound and preequilibrium reactions
- LANL GNASH code
- Angular momentum distributions, probes
  - GENNIE $(n,x\gamma)$ measurements
  - isomer production
- Some examples, biased towards NNSA needs
- Future challenges

↑

all involve ang. mom. physics

Surrogate Reactions

Can't measure what we want, so:
"You can't always get what you want"

Measure something else that's relevant + Apply physics insights to extrapolate $\Rightarrow$ Predicted values

Some examples

- Fission : Direct reactions can be used to measure fission probabilities P_f.
  These can then be used to infer $\sigma(n,f)$
  (Younes, Britt, Wilhelmy, Gavron, etc)

- Capture : As above. Harder!

- GEANIE : Partial $(n, x\gamma) \Rightarrow$ channel (n,x) cross sections,
  e.g. $^{239}Pu(n,2n)$, $^{193}Ir(n,n')^{193m}$, $^{89}Y(n,2n)^{88g,m1,m2}Y$

- Uranium isotope chain evaluation, ENDF6++
  $n+$ 232, 3, 4, 5, 6, 7, 8, 9, 0, 1U
  expt $n+$ 238U $\rightarrow$ info on 239, 8, 7 barriers
  .... $n+$ 235U $\rightarrow$ .... 236, 5, 4 barriers
  } Allows predictions of $n+$ 237U

- Multi-channel R-matrix, with charge-symmetry / independence
  eg. Hale $n+t$ total x/s from $p+{}^3He$ elastic data
  (LLNL Tom Phillips expt validated Hale predictions)

- Isomer targets, eg. $^{88m2}Y(n,2n)$ from $^{88g}Y(n,2n)$
  $n+$ 235U from $n+$ 235U [illegible]

Physics Insights needed for Surrogate Studies

Interest : $n + (A-1) \Rightarrow A^* \Rightarrow$ Decays Measured e.g. $\frac{\Gamma_i}{\Gamma_{TOT}}$ (channel i)

Surrogate: other reaction ... ← ratio of widths

$$\sigma(n,i) = \sigma_n^{\text{absorption}} \cdot \left(\frac{\Gamma_i}{\Gamma_{TOT}}\right)_{\text{surrogate}}$$

Main concerns:

- The (J,π) spin states populated can be quite different in surrogate method
  - What are the populated spin states?
  - How does (Γ_i/Γ_{TOT}) depend upon J,π?

  } SPIN-DEP. PHYSICS CRUCIAL

- What is the absorption cross section?
  - At higher energies (> few MeV), fairly well known from OM and data [5-10%]
  - At low energies (eg 1-100 keV), OM $\sigma_R = \sigma^{\text{absorp}} + \text{Compound Elastic}$. More complicated.
- Account for Preequilibrium corrections (~ 0 < 5 MeV ; ~15% at 14 MeV ; 90% at 60 MeV)
- Account for width fluctuation corrections in capture.

Compound v. Preequilibrium Reactions

Compound

- Fully equilibrated, "evaporation spectrum"
- Ejectiles symmetric about 90°, ~ isotropic
- Bohr Independence hypothesis
- $t \sim 10^{-16-18}$ sec

Preequilibrium

- Forward-peaked
- High emission energies probable
- Multistep scattering
- $t \sim 10^{-21}$ sec

Statistical Theory

Compound Nucleus :
: long-lived intermediate complex states
: too complex for detailed shell-model understanding (matrix dimension too high)
: statistical model forfeits detailed knowledge, only average prop.
: Describes average behavior of many resonances
: nucleon projectile interacts strongly in interior, & energy exchange with other A nucleons v. fast

Bohr (1936)

- Formation & decay processes independent
- "Memory" of incident channel lost (except J, π)
- Detailed Balance → "Hauser Feshbach"

$$|S_{ab}^{fluct}|^2 = \frac{T_a T_b}{\sum_c T_c}(1+\delta_{ab})$$

↑ elastic enhancement

Regions of validity

keV: n-sep energy, $\Gamma \ll d$ (separated resonances)

10s of MeV: $\Gamma \gg d$

General derivations for all Γ, d { KMT, Verbaarschot

Statistical models focus on average behavior of resonance Γ, d

→ Connects to inputs from <u>phenomenology</u>

eg. Transmission co. (Optical Model)

Level densities (statistical prop. of excited nuclei)

"Phase space dominates!"

<u>Other Statistical Concepts</u> (see other experts here!)

- resonance properties, Porter Thomas distribution of nearest-neighbour spacing — Lynn
- fission — Many people ....
- Statistical Distribution of matrix elements, GOE — Weidenmuller, Yoshida (Kawano talk)
- P, Q Projection operators KMT — Kerman
- Isospin — Grimes

Hauser - Feshbach Compound Nucleus Theory

General formula:

$$\sigma_{a,b} = \pi \lambda^2 \sum_J \omega_a^J \cdot \frac{T_a T_b}{\sum_c T_c} \cdot W_{ab}$$

- ω_a^J: statistical factor
- $\frac{T_a T_b}{\sum_c T_c}$: Transmission coeff.
- W_{ab}: width fluctuation corrections. (elastic enhanced, inelastics reduced) $W \to 1$ at high energy (except for elastic)

Single Derivation CN reactions via well-separated resonances:

$$\sigma_{ab}^J = \pi \lambda^2 \omega_a^J \sum_\lambda \frac{\Gamma_{\lambda a} \Gamma_{\lambda b}}{(E - E_\lambda)^2 + \frac{1}{4}\Gamma_\lambda^2}$$ Breit-Wigner

Total width $\Gamma_\lambda = \sum_c \Gamma_{\lambda c}$

Energy-average cross section (energy interval $\Delta \gg$ res. spacing D)

$$\int_0^\Delta dE \frac{\Gamma_{\lambda a} \Gamma_{\lambda b}}{(E - E_\lambda)^2 + \frac{1}{4}\Gamma_\lambda^2} = 2\pi \frac{\Gamma_{\lambda a} \Gamma_{\lambda b}}{\Gamma_\lambda}$$

so energy average $\langle \sigma_{ab}^J \rangle = \pi \lambda^2 \omega_a^J \cdot \frac{2\pi}{D} \left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle$

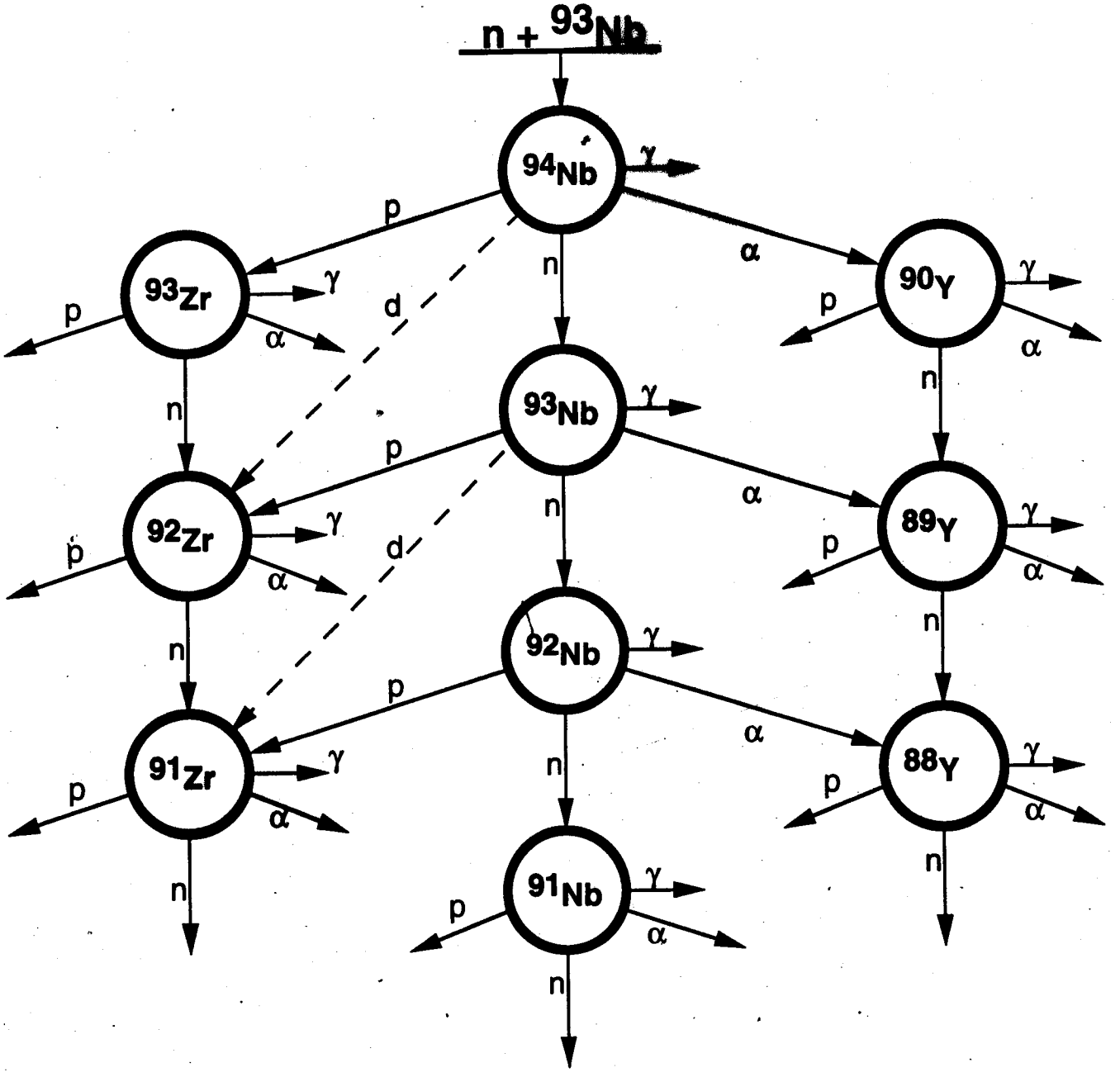
In general, there is a correlation in the widths Γ_a, Γ_b:

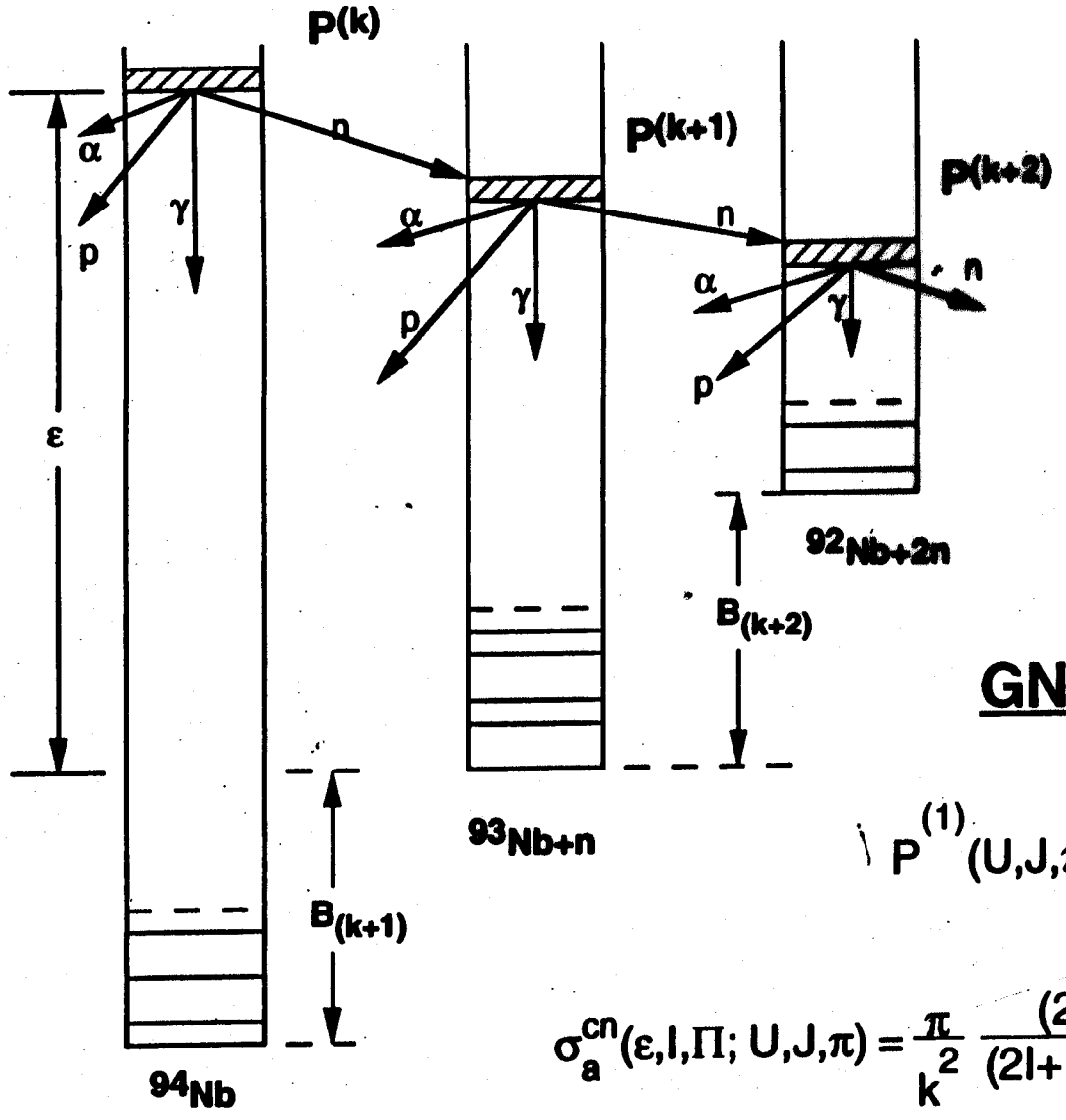
$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = W_{ab} \frac{\langle \Gamma_a \rangle \langle \Gamma_b \rangle}{\langle \Gamma \rangle}$$

Now, with OM trans. co. we can associate $\frac{2\pi\langle\Gamma\rangle}{D} \sim T$ (for $\Gamma \ll D$)

$\Rightarrow$ Hauser-Feshbach result.

SAMPLE REACTION SEQUENCE





GNASH Hauser-Feshbach

$$P^{(1)}(U,J,\pi) = \sigma_a^{cn}(\varepsilon,I,\Pi;\, U,J,\pi)\ \delta(U - \varepsilon - B_a)$$

$$\sigma_a^{cn}(\varepsilon,I,\Pi;\, U,J,\pi) = \frac{\pi}{k^2}\,\frac{(2J+1)}{(2I+1)(2i+1)} \sum_{S=|i-I|}^{i+I} \sum_{\ell=|J-S|}^{J+S} f_\ell(\ell,\pi)\, T_\ell^a(\varepsilon)$$

$$P^{(k+1)}(U',J',\pi') = \rho^{(k+1)}(U',J',\pi') \sum_{J,\pi} \int_{U'+B_{a'}}^{U_{max}} dU\, P^{(k)}(U,J,\pi)\, \frac{\Gamma_{a'}^{(k)}(U,J,\pi;\, U',J',\pi')}{\Gamma(U,J,\pi)}$$

Hauser-Feshbach Theory Use in GNASH

Multistep application of Hauser-Feshbach theory:

$$P^{(k+1)}(U',J',\pi') = \rho^{(k+1)}(U',J',\pi') \sum_{J,\pi} \int_{U'+B_{a'}}^{U_{max}} dU\, P^{(k)}(U,J,\pi) \frac{\Gamma_{a'}^{(k)}(U,J,\pi;\, U',J',\pi')}{\Gamma(U,J,\pi)}$$

Binary reactions populate and then depopulate compound systems of reaction chain.

In GNASH this procedure is also used to calculate gamma cascades.

Initial condition is

$$P^{(1)}(U,J,\pi) = \sigma_a^{cn}(\varepsilon,I,\Pi;\, U,J,\pi)\ \delta(U - \varepsilon - B_a)$$

where

$$\sigma_a^{cn}(\varepsilon,I,\Pi;\, U,J,\pi) = \frac{\pi}{k^2} \frac{(2J+1)}{(2I+1)(2i+1)} \sum_{S=|i-I|}^{i+I} \sum_{l=|J-S|}^{J+S} f_l(I,\pi)\, T_l^a(\varepsilon)$$

Hauser-Feshbach Expressions (Cont'd)

Partial-to-total width ratio:

$$\frac{\Gamma_{a'}(U,J,\pi;\, U',J',\pi')}{\Gamma(U,J,\pi)} = \frac{1}{N(U,J,\pi)} \sum_{S'=|I'-J'|}^{I'+J'} \sum_{l=|J-S'|}^{J+S'} f(l,\pi)\, T_l^{a'}(U - U' - B_{a'})$$

Hauser-Feshbach denominator:

$$N(U,J,\pi) = \sum_{a'} \sum_{I',P'} \sum_{S'=|i'-I'|}^{i'+I'} \sum_{l=|J-S'|}^{J+S'} \int_{E_c'}^{U-B_{a'}} dU'\, f(l,\pi)\, T_l^{a'}(U-U'-B_{a'})\, \rho(U',I',P')) +$$

$$+ \sum_k f(l,\pi)\, T_l^{a'}(U - U_k' - B_{a'})$$

Continuum population increments:

$$\Delta P^{(n+1)}(U',J',\pi') = \rho^{(n+1)}(U',J',\pi') \sum_{J,\pi} \frac{P^{(n)}(U,J,\pi)}{N(U,J,\pi)} \Delta U \sum_{S,l} T_l^{a'}(U-U'-B_{a'})$$

Discrete level population increments:

$$\Delta P_k^{(n+1)}(U',J',\pi') = \sum_{J,\pi} \frac{P^{(n)}(U,J,\pi)}{N(U,J,\pi)} \sum_{S,l} T_l^{a'}(U-U'-B_{a'})$$

Gamma-Ray Strength Functions and Transmission Coefficients

Transmission coefficient definition

$$T^{X\ell}(\varepsilon_\gamma) = 2\pi f_{X\ell}(\varepsilon_\gamma)\, \varepsilon_\gamma^{2\ell+1}$$

Three possibilities in GNASH:

1. Weisskopf strength function

$$f_{X\ell}(\varepsilon_\gamma) = C_{X\ell} = \text{constant}$$

For E1: $C_{E1} = (4.6\text{x}10^{-12})\, A^{1.91}$ [MeV^{-3}]

2. Brink-Axel E1 strength function (standard Lorentzian)

$$f_{E1}(\varepsilon_\gamma) = K_{E1} \frac{\sigma_o \varepsilon_\gamma \Gamma^2}{(\varepsilon_\gamma^2 - E^2)^2 + \varepsilon_\gamma^2 \Gamma^2}$$

where σ_0, Γ, and E are the standard giant dipole resonance parameters, and $K_{E1} = 8.68 \times 10^{-8}$ mb^{-1} MeV^{-2} (nominally).

Gamma-Ray Strength Functions and Transmission Coefficients (Cont'd)

3. Kopecky-Uhl E1 strength function (generalized Lorentzian)

$$f_{E1}(\varepsilon_\gamma, T) = K_{E1}\left[\frac{\varepsilon_\gamma \Gamma(\varepsilon_\gamma)}{(\varepsilon_\gamma^2 - E^2)^2 + \varepsilon_\gamma^2 \Gamma(\varepsilon_\gamma)^2} + \frac{0.7\,\Gamma\, 4\pi^2 T^2}{E^5}\right]\sigma_o\,\Gamma$$

where $\Gamma(\varepsilon_\gamma)$ is an energy-dependent damping width based on Fermi liquid theory

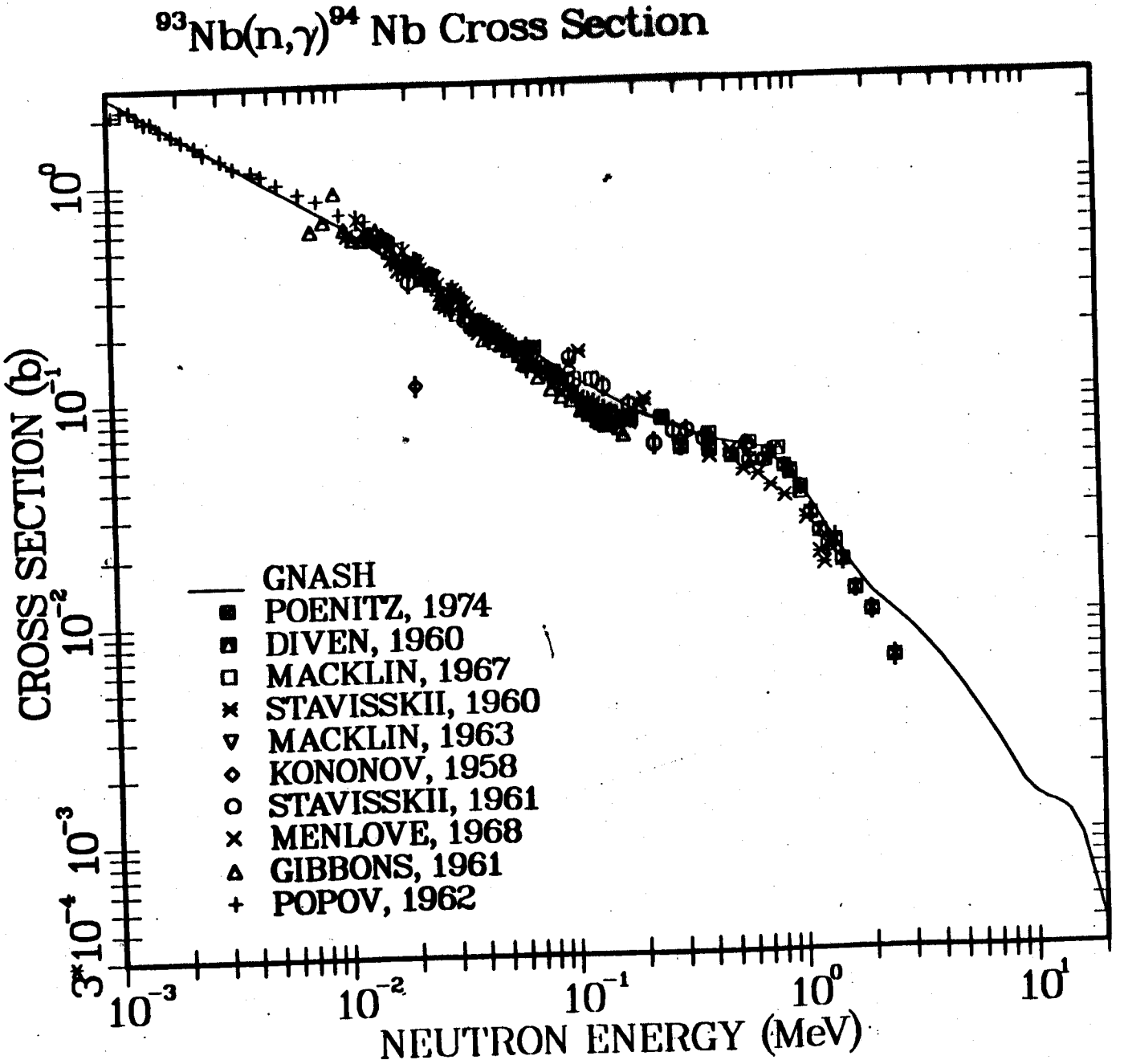
$$\Gamma(\varepsilon_\gamma) = \Gamma\frac{\varepsilon_\gamma^2 + 4\pi^2 T^2}{E^2} \quad \text{with nuclear temperature} \quad T = \sqrt{\frac{B_n - \varepsilon_\gamma}{a}}$$

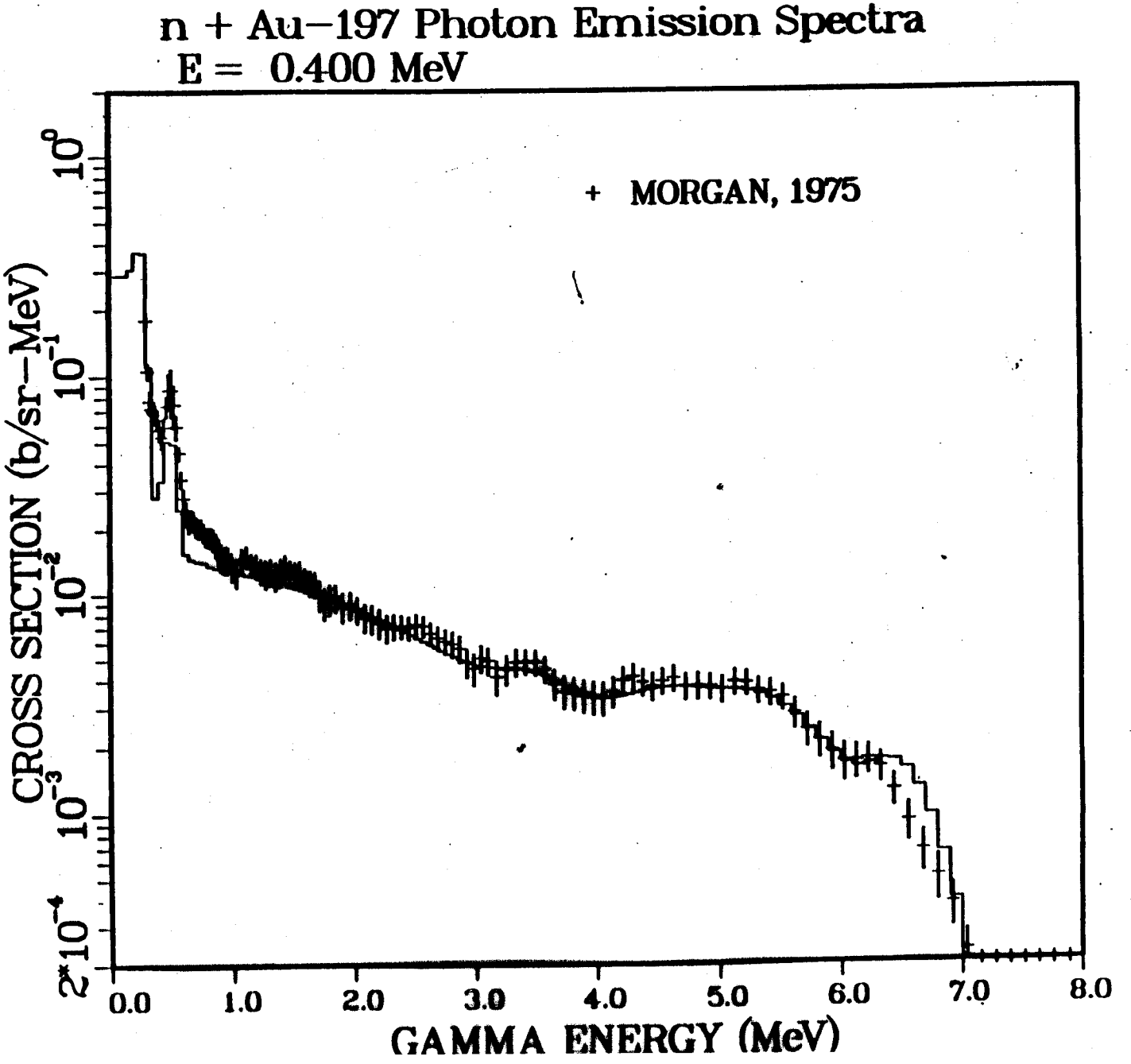
Gamma-Ray Strength Functions and Transmission Coefficients (Cont'd)

Strength Function Normalization

1. Use absolute strength functions built into code
2. Normalize by comparing with low-energy (n,γ) cross section measurements ($E_n \approx$ 1-500 keV)
3. Normalize to experimental information on low energy resonances, that is, the mean gamma-ray width for s-wave neutrons $\langle\Gamma_{\gamma 0}\rangle$, and the mean level spacing for s-wave neutrons, $\langle D_0\rangle$, as follows:

$$\frac{2\pi\langle\Gamma_{\gamma 0}\rangle}{\langle D_0\rangle} = \sum_{J\pi}\sum_{X\ell}\sum_{j'=|J-\ell|}^{J+\ell}\left[\int_0^{S_n-E_c'} d\varepsilon_\gamma\, T^{X\ell}(\varepsilon_\gamma)\, f(\ell,J,j')\, \rho(S_n-\varepsilon_\gamma, j', \pi') + \sum_k T_k^{X\ell}(\varepsilon_\gamma)\, f(\ell,J,j')\right]$$


^{93}Nb(n,γ)^{94} Nb Cross Section
CROSS SECTION (b)
NEUTRON ENERGY (MeV)
GNASH
POENITZ, 1974
DIVEN, 1960
MACKLIN, 1967
STAVISSKII, 1960
MACKLIN, 1963
KONONOV, 1958
STAVISSKII, 1961
MENLOVE, 1968
GIBBONS, 1961
POPOV, 1962


n + Au-197 Photon Emission Spectra
E = 0.400 MeV
+ MORGAN, 1975
CROSS SECTION (b/sr-MeV)
2*10^-4
10^-3
10^-2
10^-1
10^0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
GAMMA ENERGY (MeV)

Nuclear Level Densities

The continuum level density in GNASH is separated into parity, spin, and energy-dependent terms as follows:

$$\rho(U,J,\pi) = F_{\pi}(\pi)\, F_{J}(J,U)\, \rho(U)$$

where U is related to the excitation energy E by $U = E - \Delta$, with Δ being the pairing energy. The spin and parity components are given by

$$F_{J}(J,U) = \frac{(2J+1)}{2\sigma(U)^{2}} \exp\left[-\left(J+\tfrac{1}{2}\right)^{2} / 2\sigma(U)^{2}\right] \quad \text{and} \quad F_{\pi}(\pi) = \frac{1}{2}$$

The spin cutoff function is given by the expression

$$\sigma(U)^{2} = C_{SC}\, A^{2/3} \sqrt{aU}$$

where C_{SC} is a constant equal to either 0.0888 (Gilbert-Cameron) or 0.146 (Facchini), depending upon your input choice.

Nuclear Level Densities (Cont'd)

3. Ignatyuk Model: Both the Gilbert-Cameron and backshifted Fermi gas level densities utilize an energy independent level density parameter, which restricts flexibility at higher energy. This difficulty is compounded by the effects of shell closures on the Fermi gas level density parameter and the need to wash out such effects at higher energies. To address these problems, we implemented the model of Ignatyuk which utilizes an energy dependent level density parameter:

$$a(U) = \alpha\,[1 + f(U)\,\delta W/U] \quad \text{with} \quad \delta W = M_{exp}(Z,A) - M_{ld}(Z,A,\beta)$$

where α is the asymptotic value at higher energies, and shell effects are included in δW [M_{ld} is determined from a standard liquid drop model at deformation β and M_{exp} is an experimental mass. Additional energy dependence occurs in f(U)

$$f(U) = 1 - \exp(-\gamma U)$$

where $\gamma = 0.05$ MeV from Ignatyuk. The asymptotic value of $a(U) \rightarrow \alpha$ is given by

$$\frac{a}{A} = \eta + \beta A$$

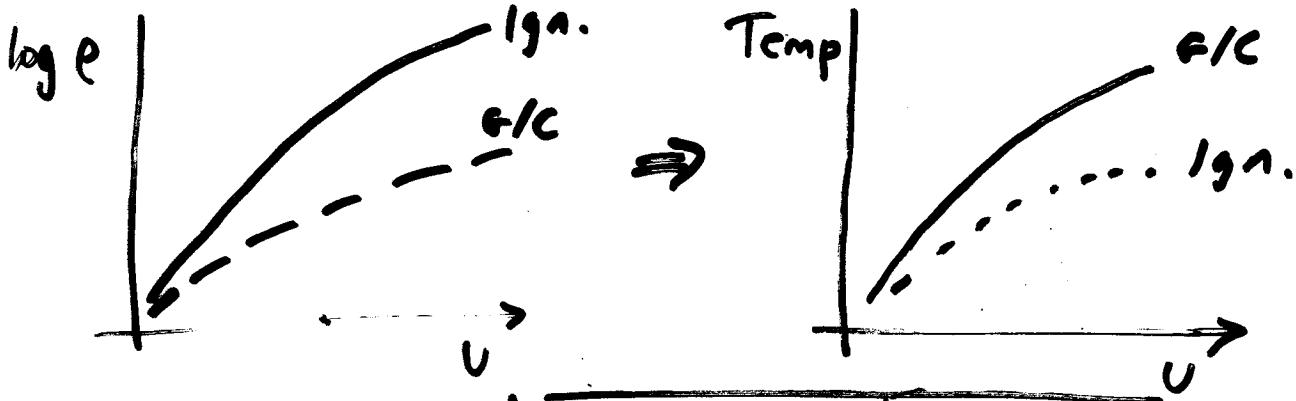
where Ignatyuk gives $\eta = 0.154$, $\beta = 6.3 \times 10^{-5}$. In GNASH we use Arthur's parameterization $\eta = 0.1375$, $\beta = -8.36 \times 10^{-5}$ obtained by fitting Mughabghab's s-wave resonance data. This option utilizes the exact same level density expressions and matchings as does the Gilbert-Cameron model.

LANSCE Pb(n,xγ) data validated Ignatyuk model concepts

→ Washing out of shell effects with incr U (>, few MeV)

e.g. ^{208}Pb a ~ 10 at neutron sep energy (v. low).

Ignatyuk model has a incr. to asymptotic value Gilbert/Cameron has a constant.



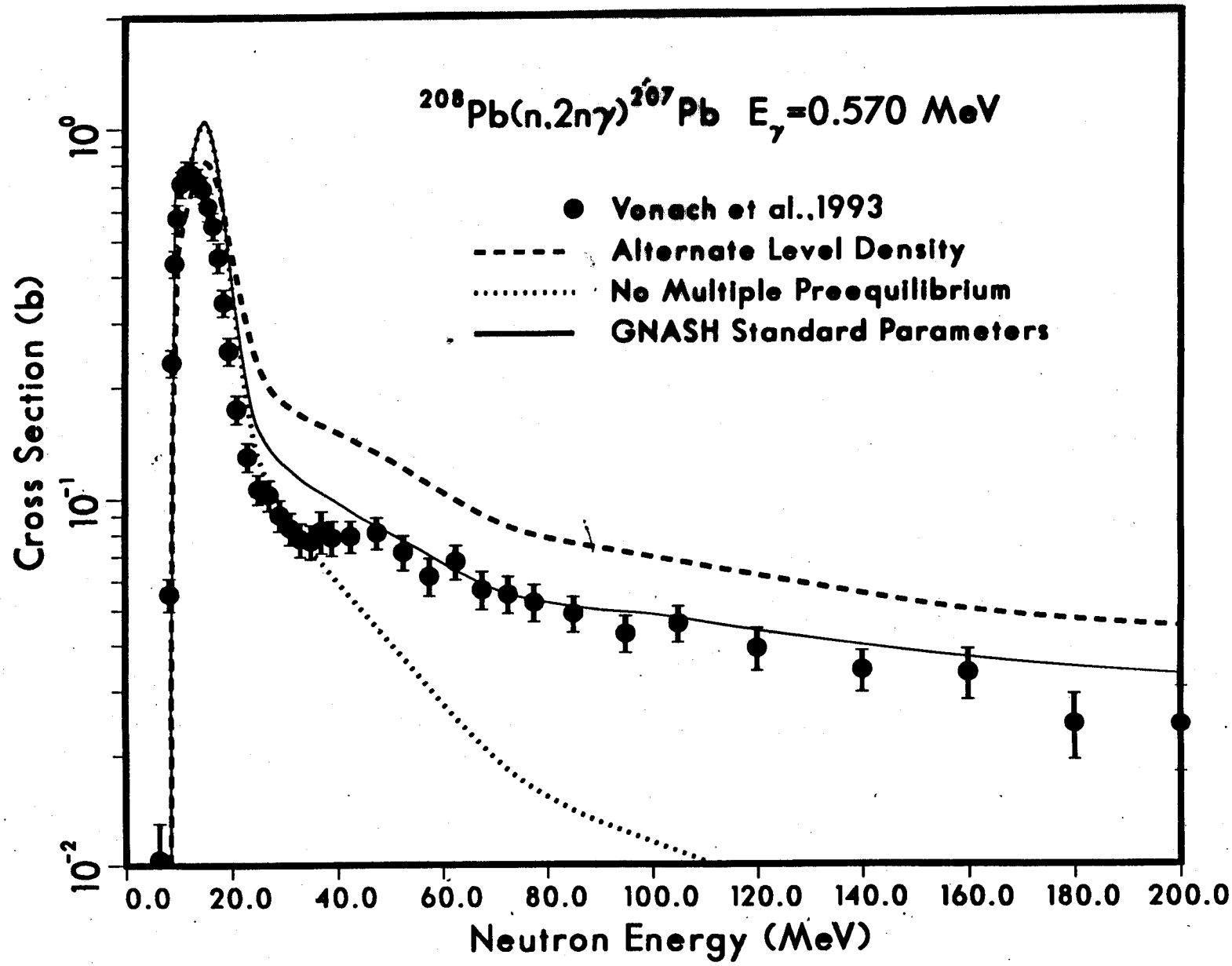
$dU = T\,dS$

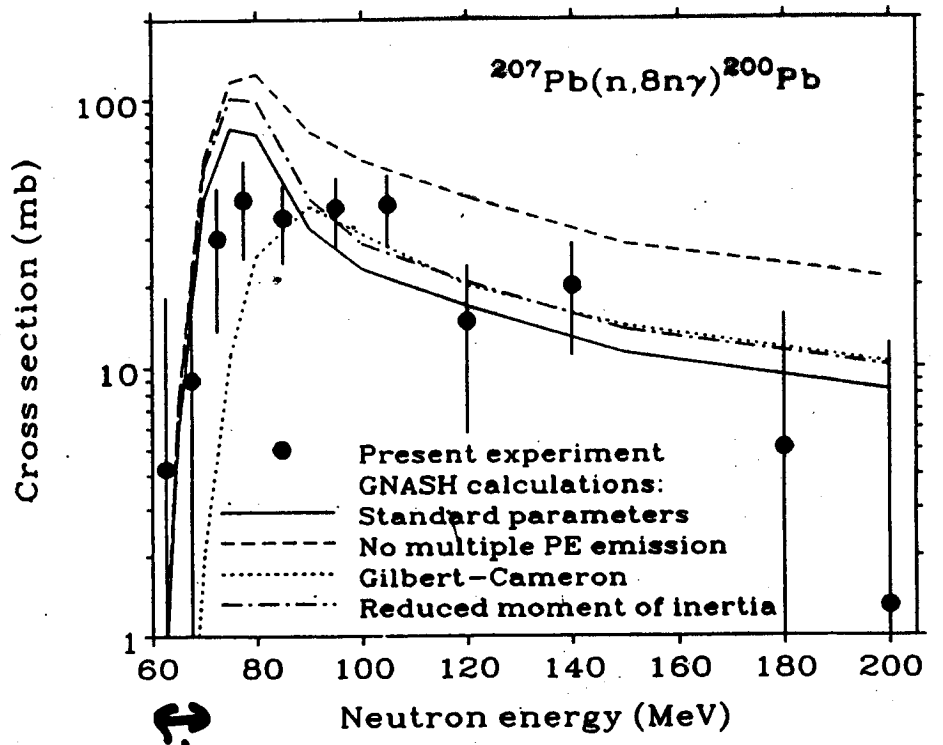
$$T = \frac{dU}{dS} = \frac{1}{\frac{d(\log \rho)}{dU}} \sim \sqrt{\frac{U}{a}}$$

low a ⇒ high T

Evaporated neutrons have a mean k.e. = 2T

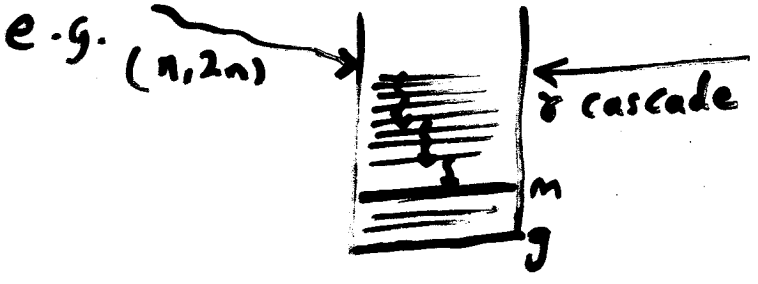
∴ Hauser Feshbach calculation for sequential neutron emission, eg ^{208}Pb(n, 8n) has a higher effective threshold for Gilb./Cameron .... lower .... Ignatyuk


$^{208}Pb(n,2n\gamma)^{207}Pb$ E_γ=0.570 MeV
Vonach et al.,1993
Alternate Level Density
No Multiple Preequilibrium
GNASH Standard Parameters
Cross Section (b)
10^0
10^{-1}
10^{-2}
0.0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0
200.0
Neutron Energy (MeV)



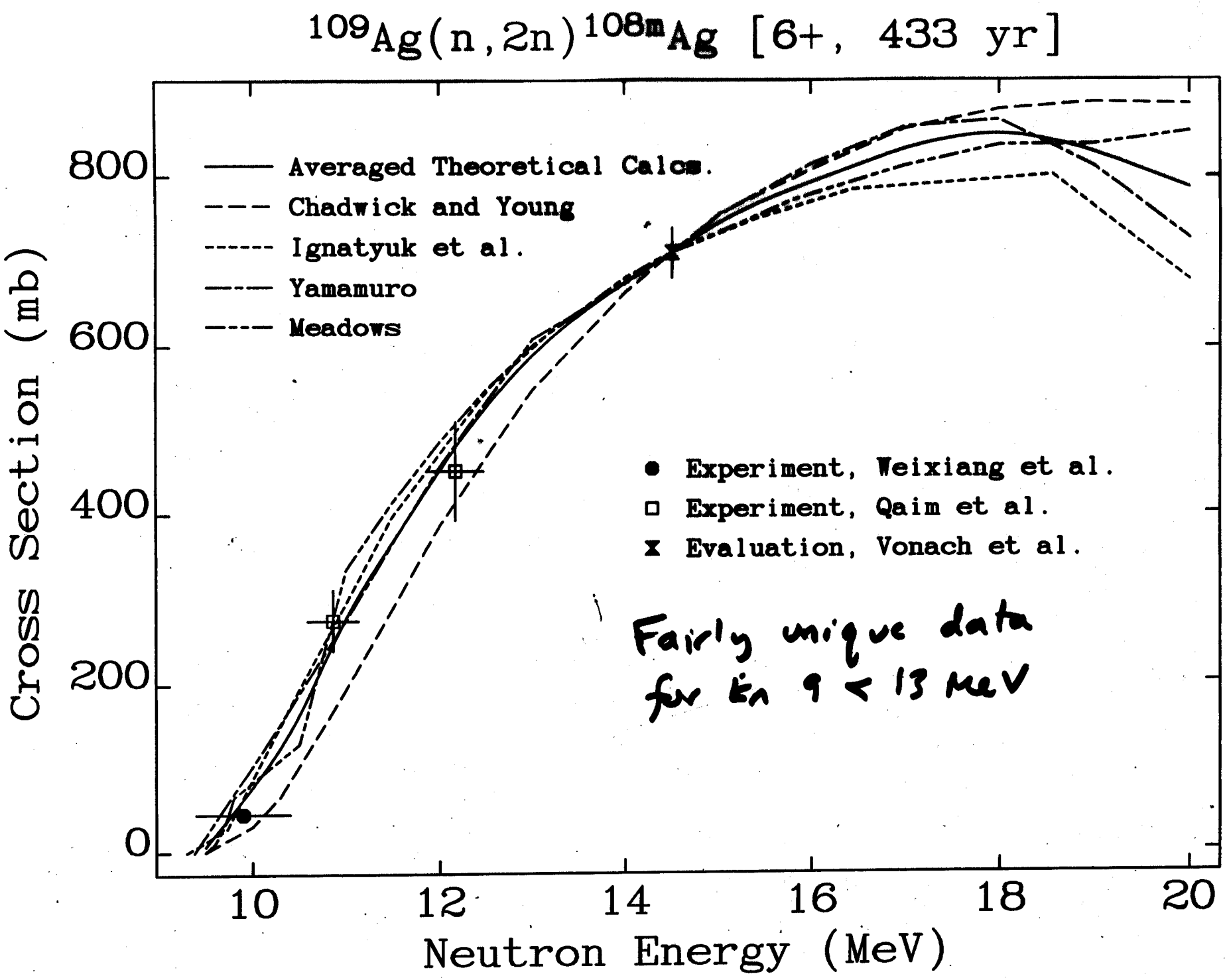
incorrect threshold if washing out of shell effects not included

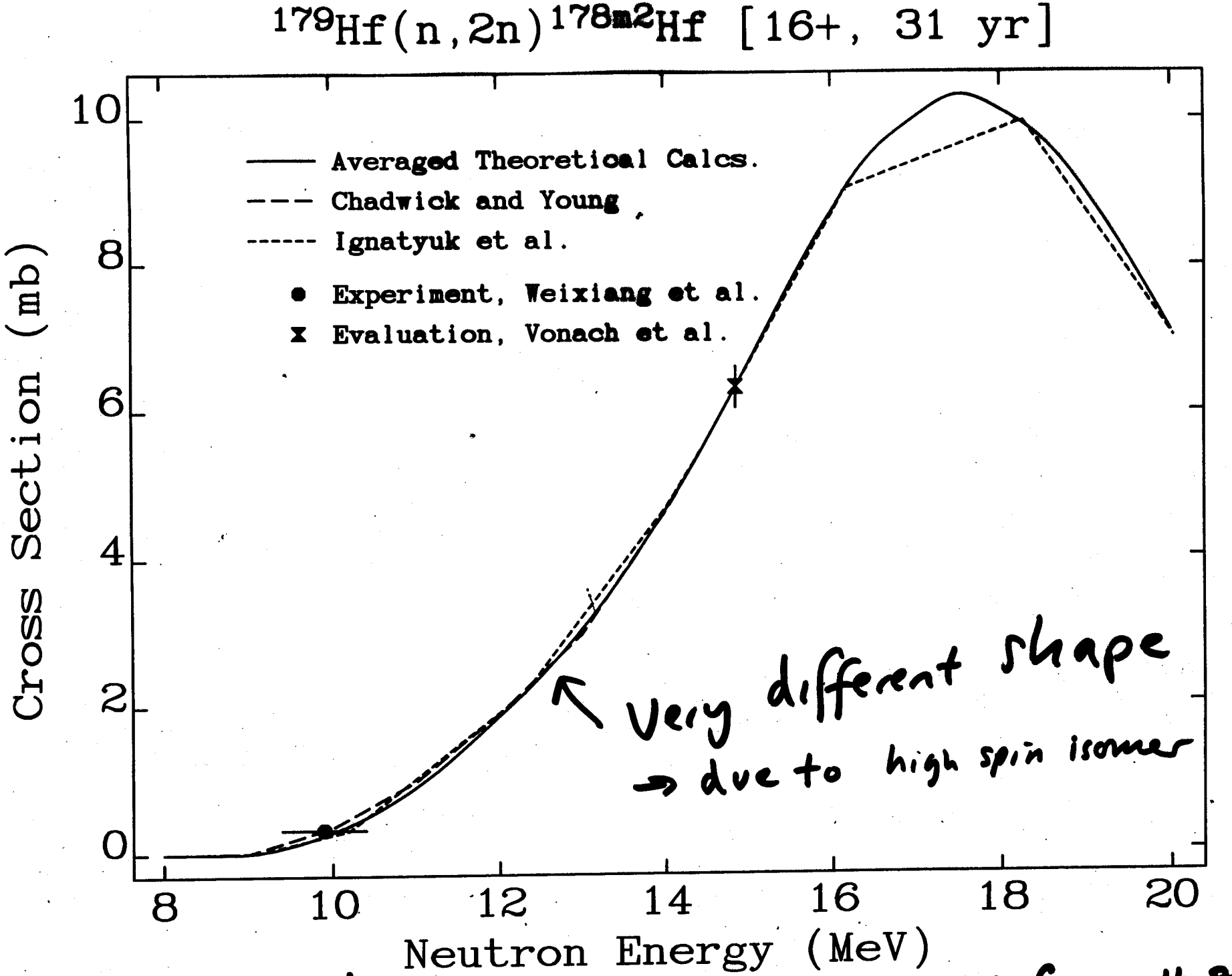
Isomer production provides insights into how well we model spin distributions



2 examples shown: lower spin
v. high spin

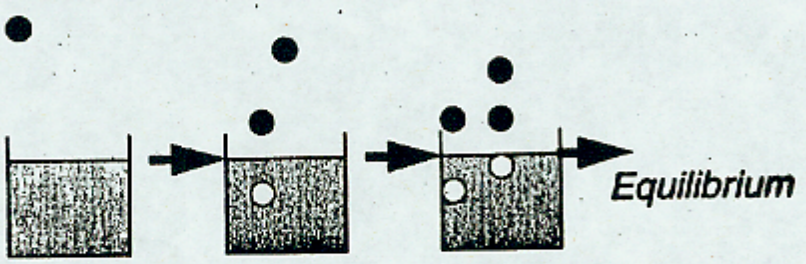
Huizenga - Vandenbosch ansatz:
if J initial in C.N. $\geq \frac{m+g}{2}$, then flux → m
if . . . $< \frac{m+g}{2}$, flux → g


$^{109}Ag(n,2n)^{108m}Ag$ [6+, 433 yr]
Averaged Theoretical Calcs.
Chadwick and Young
Ignatyuk et al.
Yamamuro
Meadows
Experiment, Weixiang et al.
Experiment, Qaim et al.
Evaluation, Vonach et al.
Fairly unique data for En 9 < 13 MeV
Cross Section (mb)
Neutron Energy (MeV)
0
200
400
600
800
10
12
14
16
18
20

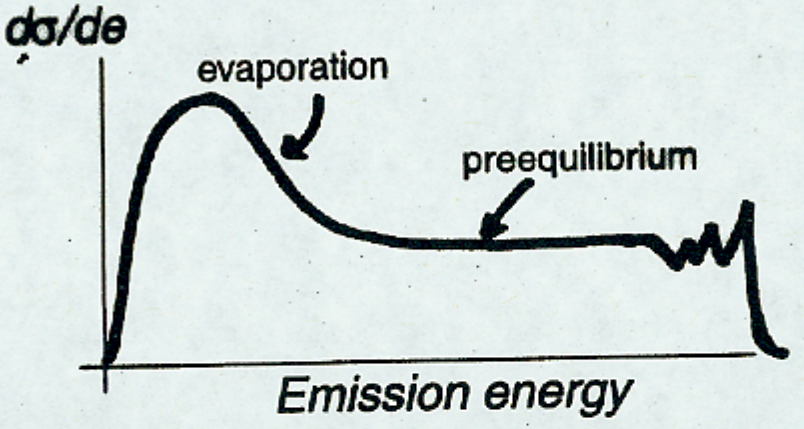


[Physics needed to extend up to 50-100 MeV, eg. spin dist from mult. γ's]

Importance of Preequilibrium Reactions for (p,xn) data



Excitation of particle-hole states
via nucleon-nucleon collisions

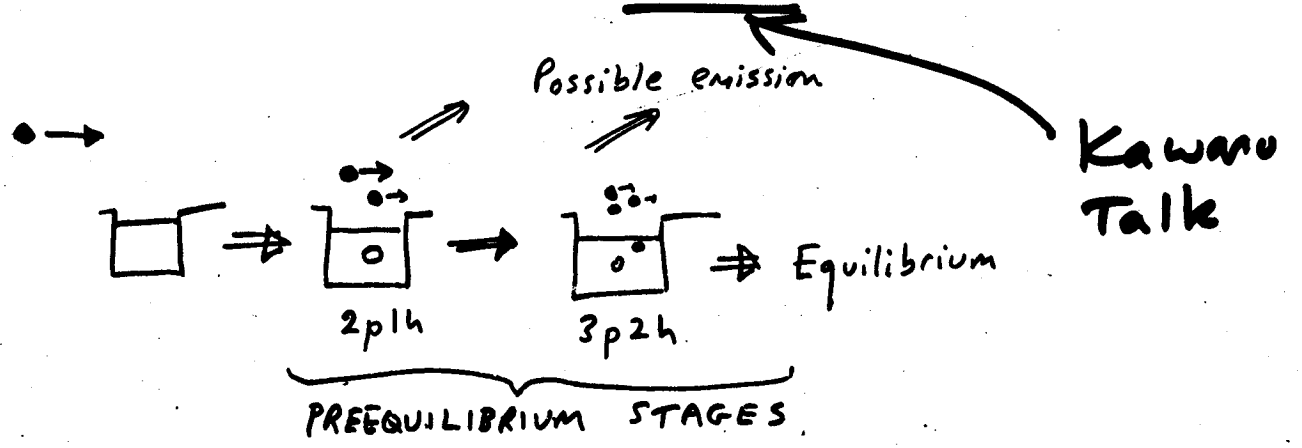


- Preequilibrium reactions are characterized by:
  - — high-energy ejectiles, forward angles
  - — carry a large amount of energy away
  - — one, or a few, scattering creating *p-h* states

- Energy balance applies: Preequilibrium emission:
  - — enhances (p,xn) yields for small x (x=1,2,3. say)
  - — decreases (p,xn) yields for large x (x=8,9,10, say)

History of preequilibrium theories

- 1950 - 1960s — Intra-nuclear Cascade models
- 1960s — semiclassical exciton model (Griffin)
  1970s — semiclassical hybrid model (Blann)
- 1980 — Feshbach-Kerman-Koonin quantum theory
- late 80s — Quantum molecular dynamics
- 1980 — 1990s, FKK, TUL, NYW quantum theories



Statistical Assumptions in Preeq

Quantum approaches

- Chained set of p-h excitations (2-body interaction)
- Coherence & random phase approx for
  - MSD (particle in continuum)
  - MSC (quasi bound)
- Level density of p-h states

Semiclassical (e.g. exciton, HMS)

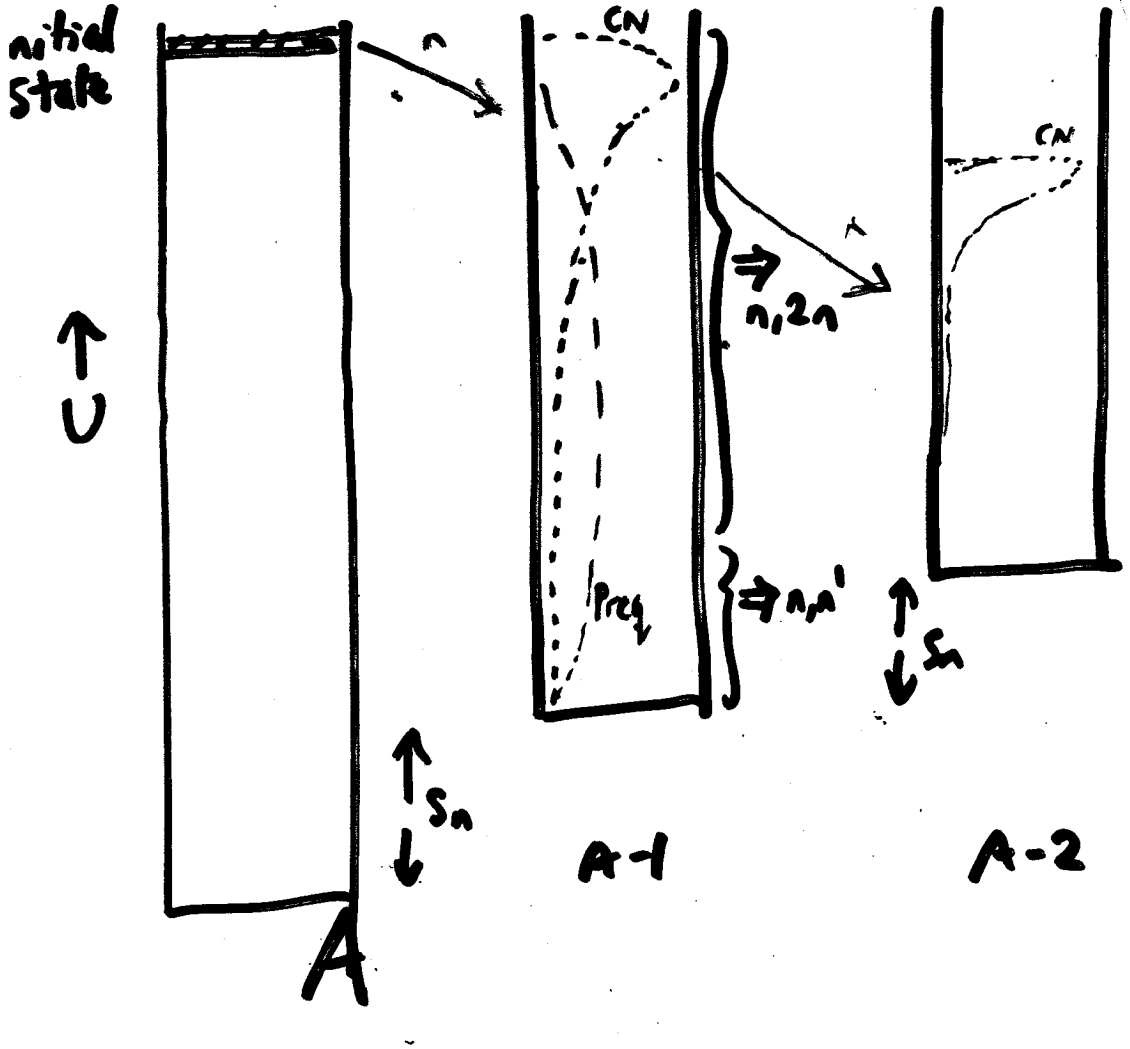
- Equiprobability of p-h configurations
- Detailed balance
- Does not deal in amplitudes, just probabilities
- Different assumption about creation of 1p1h versus 2p2h etc states

How Important is P_{reg} at 14 MeV? (e.g. for spin dist. of residual nuclei)

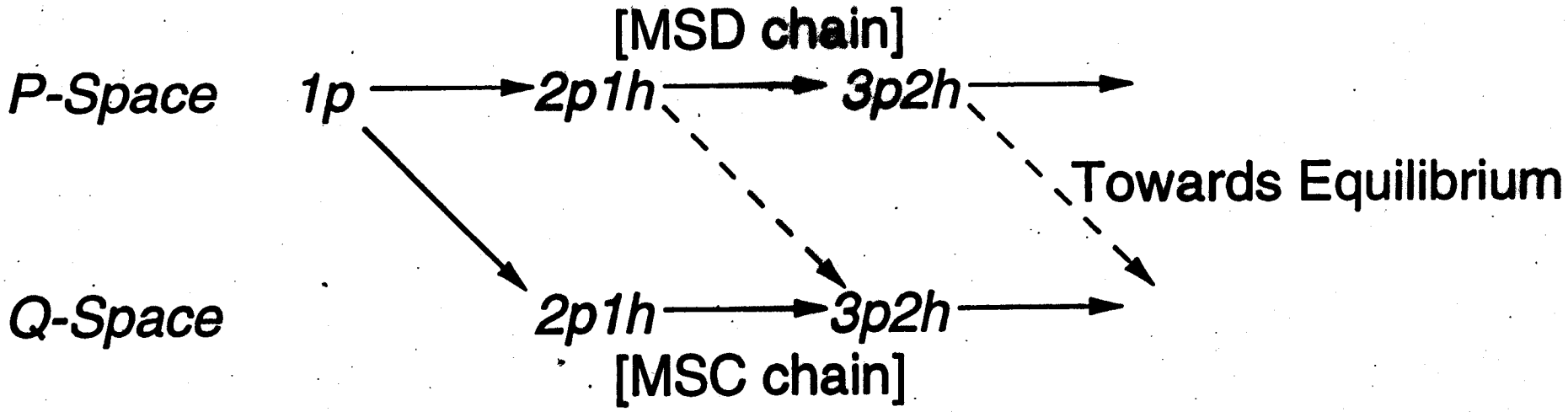
At 14 MeV, $P_{reg} \sim 15\%$ of 1st-Particle emission

But Impact $> 15\%$ for (n, n') channel

$< 15\%$ for $(n, 2n)$ channel



Reaction flux split into two components: Multistep Direct & MultistepCompound



Multistep Direct

At least one particle in continuum
Forward-peaked emission; projectile direction preserved

Multistep Compound

Flux passes through bound configurations
Emission symmetric about 90 degrees
Important for energies below 50 MeV

1-step scattering in the continuum

Previous approach:

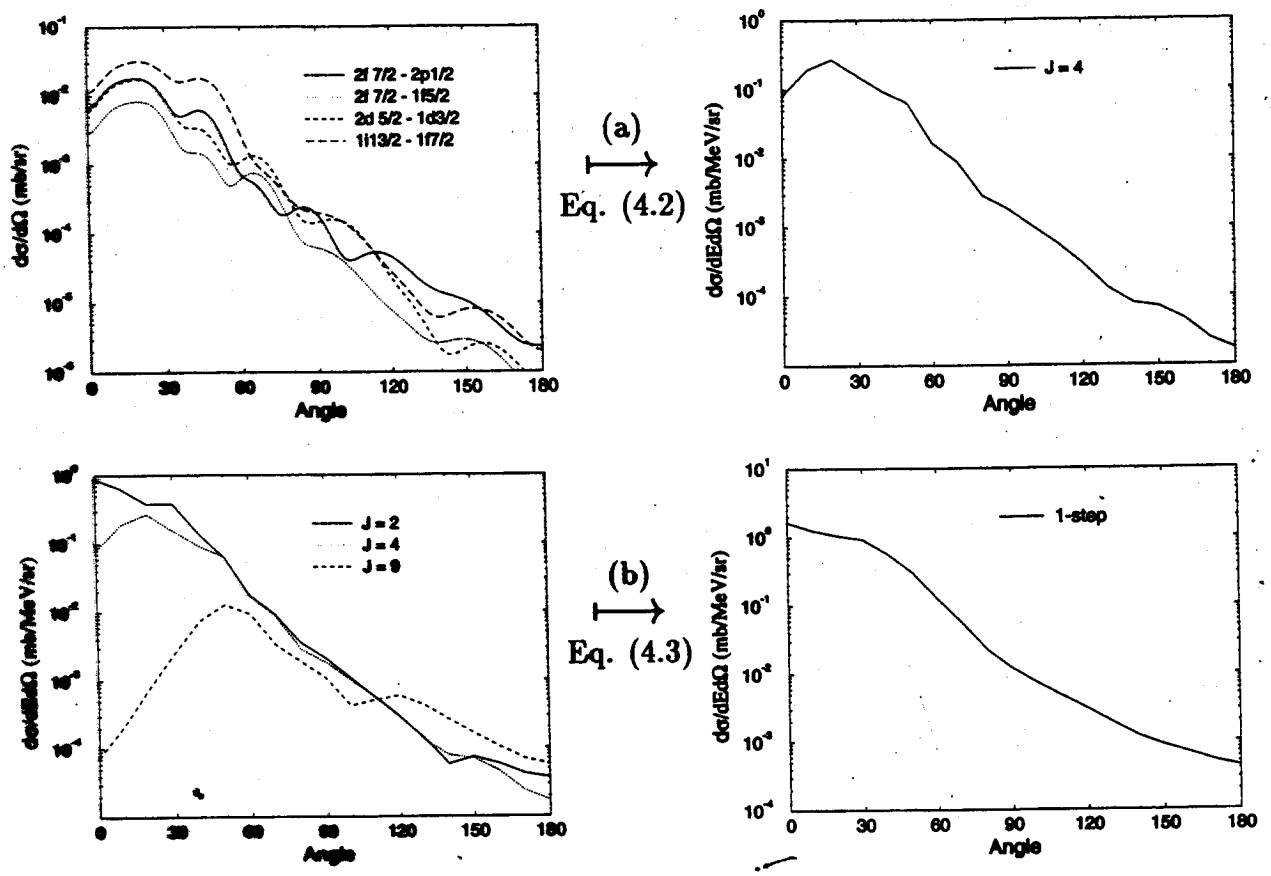
sample DWBA strength, and multiply by level density

$$\frac{d^2\sigma^{(1)}_{j\leftarrow i}}{d\Omega dE} = \sum_J (2J+1)\, R(J)\, \omega(1p,1h,E_x) \left\langle \frac{d\sigma_{j\leftarrow i}(E,\Omega \leftarrow E_0,\Omega_0)}{d\Omega} \right\rangle^{DWBA}_{J}$$

New microscopic approach:

- Calculate all transitions to accessible *1p1h* states
- Use shell model for single-particle states
- No need for level densities

Statistical Averaging, MSD
(1-step)



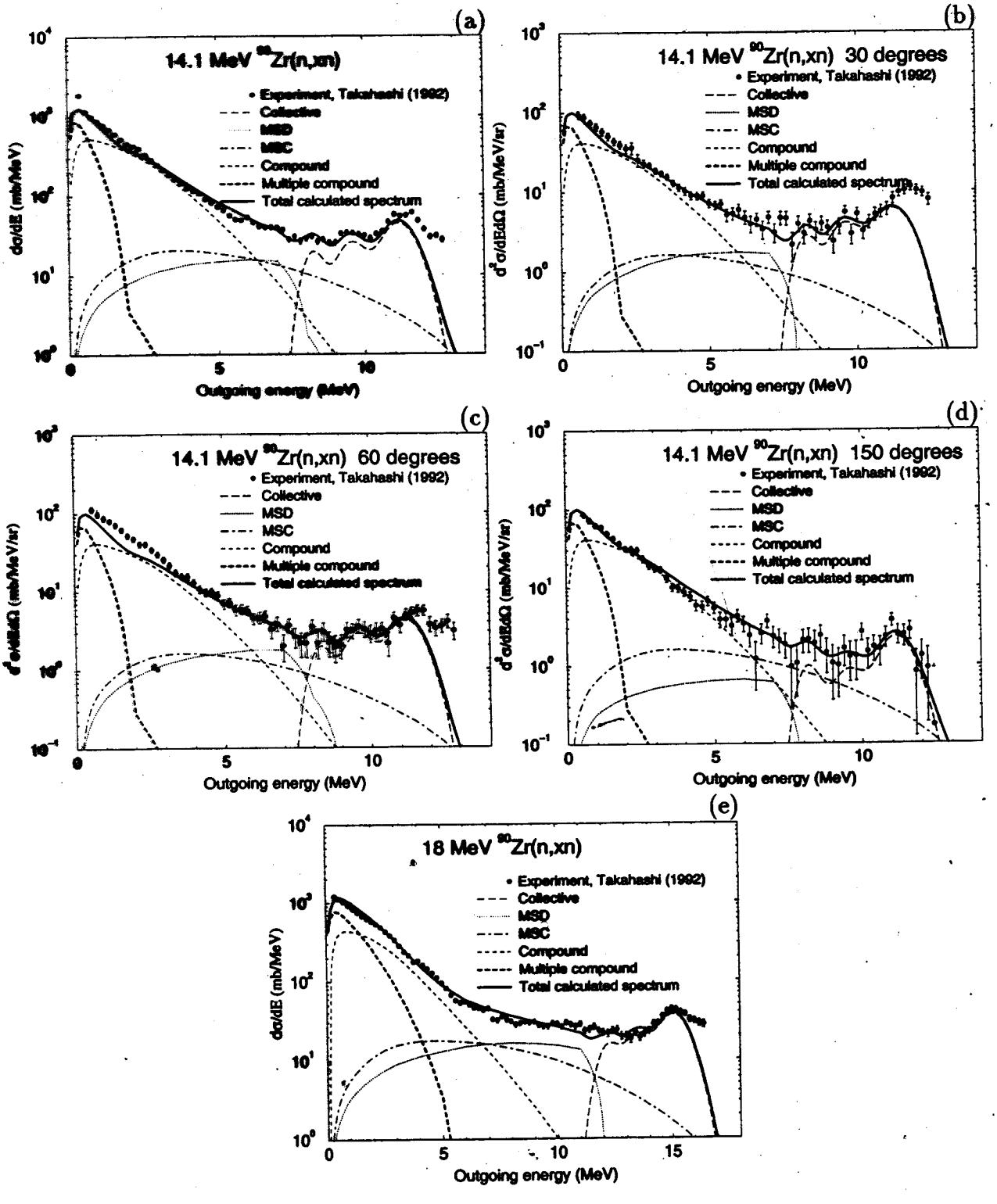
Multistep Direct Scattering (For E > ~20 M

- High density of states leads to **random** phase approximation
- This, along with an on-shell approximation, gives convolution structure
- We explicitly write the summation over intermediate neutron and proton leading particles (2-component model)

$$\frac{d^2\sigma^{(2)}_{j\leftarrow i}(E,\Omega\leftarrow E_0,\Omega_0)}{d\Omega dE} = \frac{m}{4\pi^2\hbar^2}\sum_{k=\pi,\nu}\int \mathrm{d}\Omega_1 \int \mathrm{d}E_1 E_1$$

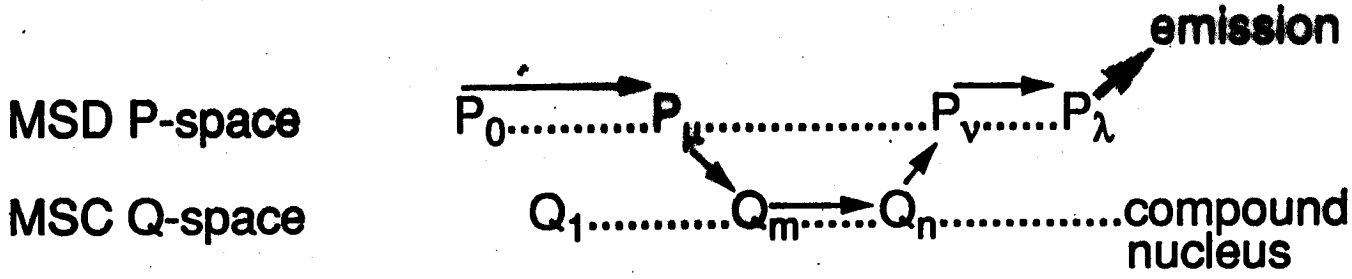
$$\times \quad \frac{d^2\sigma^{(1)}_{j\leftarrow k}(E,\Omega\leftarrow E_1,\Omega_1)}{d\Omega dE}\,\frac{d^2\sigma^{(1)}_{k\leftarrow i}(E_1,\Omega_1\leftarrow E_0,\Omega_0)}{d\Omega_1 dE_1}$$

[Issues here: Non normal DWBA matrix elements]

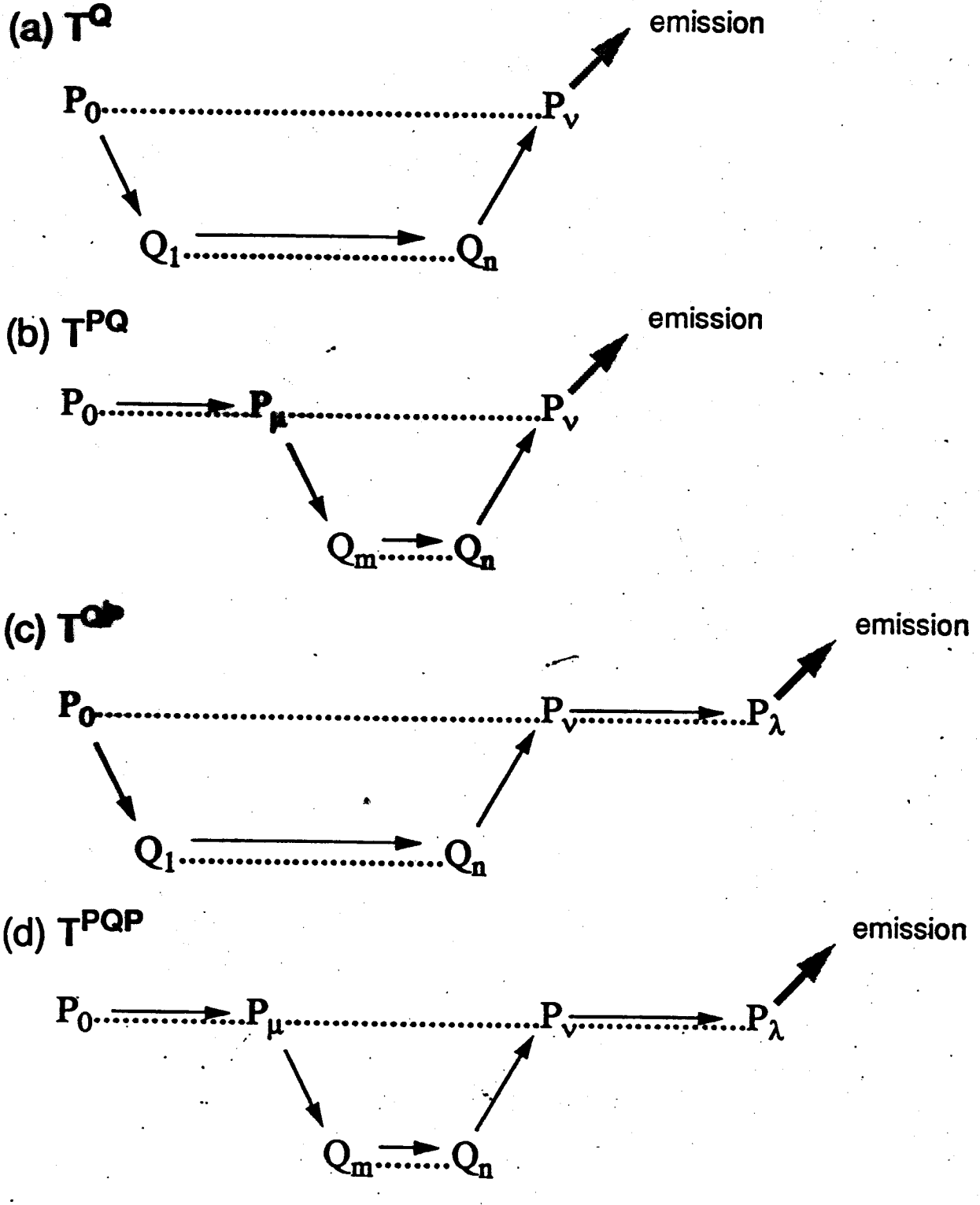

(a)
14.1 MeV ^{90}Zr(n,xn)
• Experiment, Takahashi (1992)
Collective
MSD
MSC
Compound
Multiple compound
Total calculated spectrum
dσ/dE (mb/MeV)
Outgoing energy (MeV)
(b)
14.1 MeV ^{90}Zr(n,xn) 30 degrees
• Experiment, Takahashi (1992)
Collective
MSD
MSC
Compound
Multiple compound
Total calculated spectrum
d²σ/dEdΩ (mb/MeV/sr)
Outgoing energy (MeV)
(c)
14.1 MeV ^{90}Zr(n,xn) 60 degrees
• Experiment, Takahashi (1992)
Collective
MSD
MSC
Compound
Multiple compound
Total calculated spectrum
d²σ/dEdΩ (mb/MeV/sr)
Outgoing energy (MeV)
(d)
14.1 MeV ^{90}Zr(n,xn) 150 degrees
• Experiment, Takahashi (1992)
Collective
MSD
MSC
Compound
Multiple compound
Total calculated spectrum
d²σ/dEdΩ (mb/MeV/sr)
Outgoing energy (MeV)
(e)
18 MeV ^{90}Zr(n,xn)
• Experiment, Takahashi (1992)
Collective
MSD
MSC
Compound
Multiple compound
Total calculated spectrum
dσ/dE (mb/MeV)
Outgoing energy (MeV)

Koning, MSC

Linking of MSD and MSC chains



- *Evidence:-*
  - —"P-Q transitions", Chadwick 1989, Chadwick & Young 1993
  - —"Gradual absorption", Marcinkowski *et al.* 1991,1993
- Phase-space model, e.g. see Marcinkowski *et al.* 1993
- Recent derivation of a linked MSD-MSC theory
  Arbanas, Chadwick, Dietrich, and Kerman, 1994


(a) T^{Q}
emission
P_0
P_ν
Q_1
Q_n
(b) T^{PQ}
emission
P_0
P_μ
P_ν
Q_m
Q_n
(c) T^{Q}
emission
P_0
P_ν
P_λ
Q_1
Q_n
(d) T^{PQP}
emission
P_0
P_μ
P_ν
P_λ
Q_m
Q_n

Results from ACDK Linked MSD-MSC theory

- New MSC formula which includes linking:-

$$\frac{d\sigma}{dE} = \pi\lambda^2 \sum_J (2J+1) \sum_{\mu=0}^{r} \sum_{m=\mu-1}^{\mu+1} \sum_{n=m}^{r} \sum_{\nu=n-1}^{n+1} \sum_{\lambda=\nu}^{r} \sum_{l} \frac{\langle \Gamma_{nJ}^{\uparrow\nu\lambda l}(U) \rangle}{\langle \Gamma_{nJ} \rangle} \left[\prod_{k=m}^{n-1} \frac{\Gamma_{kJ}^{l}}{\Gamma_{kJ}} \right] \frac{2\pi\Gamma_{\mu}}{D_{\mu}^{(i)}}$$

- P-Q transitions given by

$$\frac{2\pi\Gamma_{\mu}}{D_{\mu}^{(i)}} = \int \frac{d\mathbf{k}_1}{(2\pi)^3} \cdots \frac{d\mathbf{k}_{\mu}}{(2\pi)^3} \frac{2\pi\Gamma_0}{D_0^{(\mu)}} \left[\frac{d^2\omega^{(1)}(\mathbf{k}_{\mu} \leftarrow \mathbf{k}_{\mu-1})}{dU_{\mu} d\Omega_{\mu}} \right]$$

$$\times \left[\frac{d^2\omega^{(1)}(\mathbf{k}_{\mu-1} \leftarrow \mathbf{k}_{\mu-2})}{dU_{\mu-1} d\Omega_{\mu-1}} \right] \cdots \left[\frac{d^2\omega^{(1)}(\mathbf{k}_2 \leftarrow \mathbf{k}_1)}{dU_2 d\Omega_2} \right] \left[\frac{d^2\omega^{(1)}(\mathbf{k}_1 \leftarrow \mathbf{k}_i)}{dU_1 d\Omega_1} \right]$$

- Calculated P-Q flux similar to phase-space model, *but only when non-normal DWBA used*

  — further work needed to clarify this issue

Hybrid Monte Carlo Precompound Simulation (HMS)

Blann, Chadwick (ang dist, ...)

- Follows nucleon-nucleon scatterings, creating 1p1h (involves 2,3 quasiparticle distributions, partial state densities) [equiprob. statist. assumption]
  Consistent with nucleon-nucleon nuclear matter scattering kinematics, Kikuchi-Kawai

- No limit on number of particles emitted (Multiple Preq)

- Angular scattering $G(\theta) \sim \exp(a \cos\theta)$

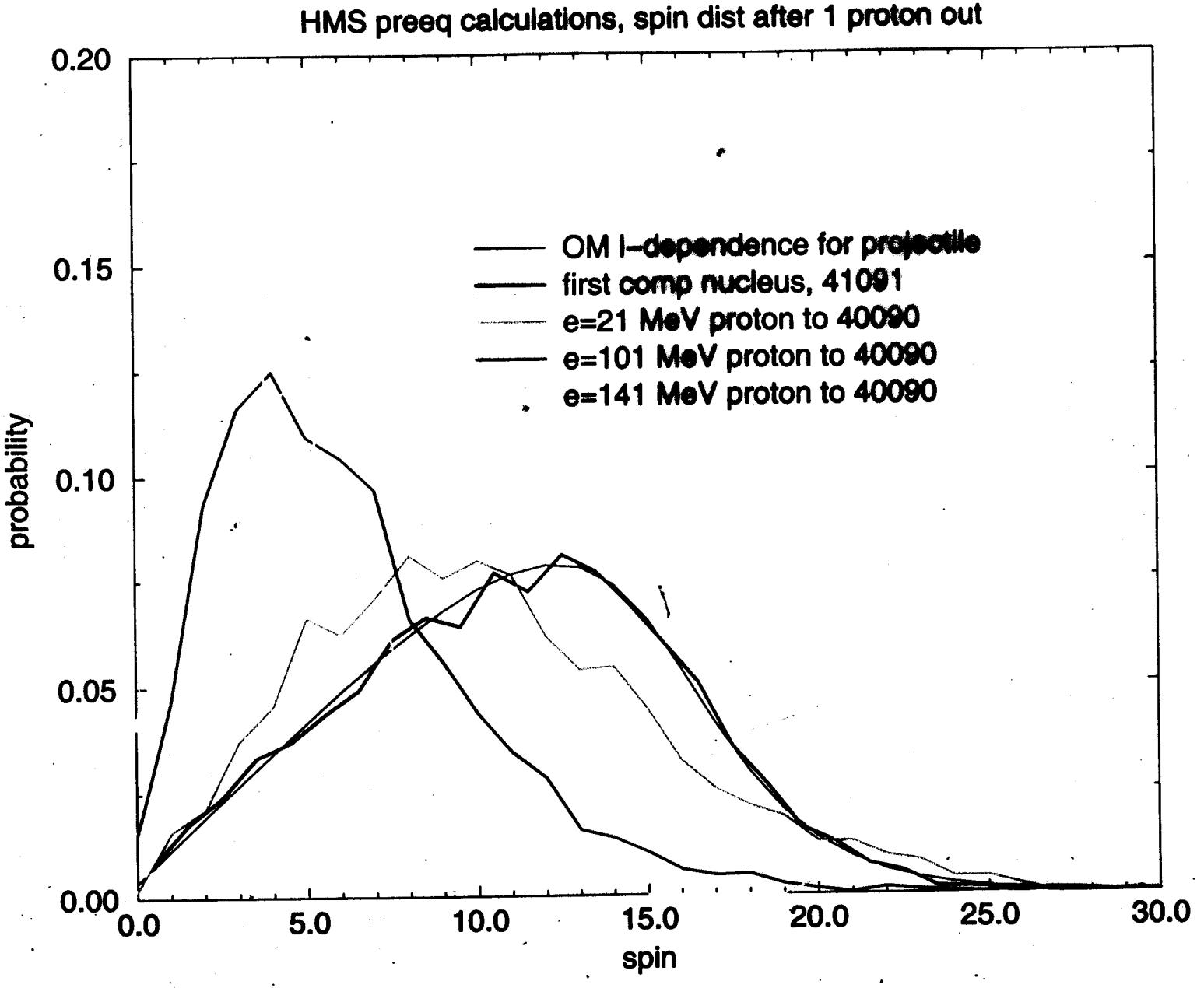
Forward peaking : $a = \dfrac{3 K \cdot k}{2 n m e_{av}}$ K: tot mom, k: scatt. mom, n = # excitons

(Basis for Kalbach Phenomenology)

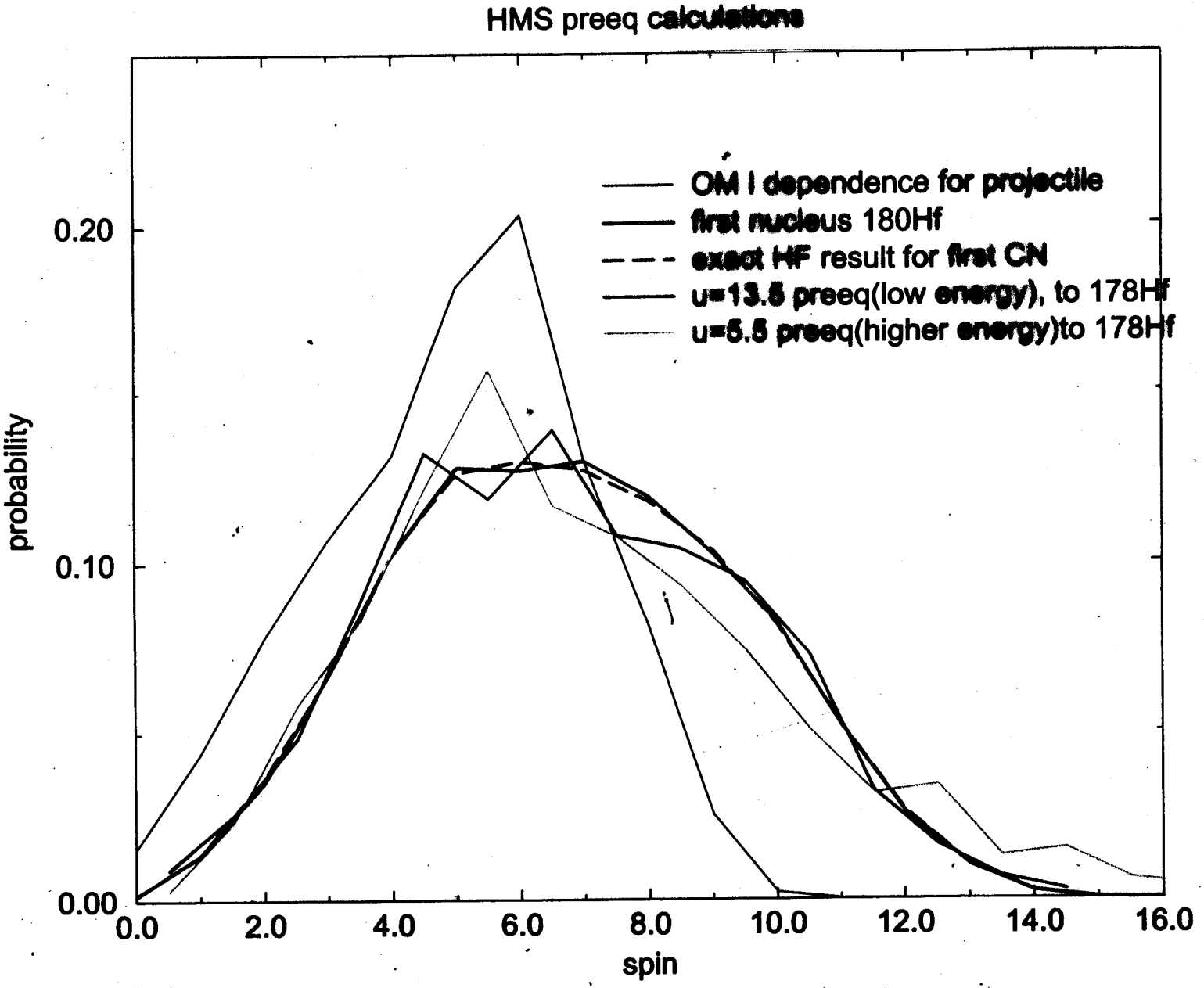
(Central limit theorem, momentum distributions)

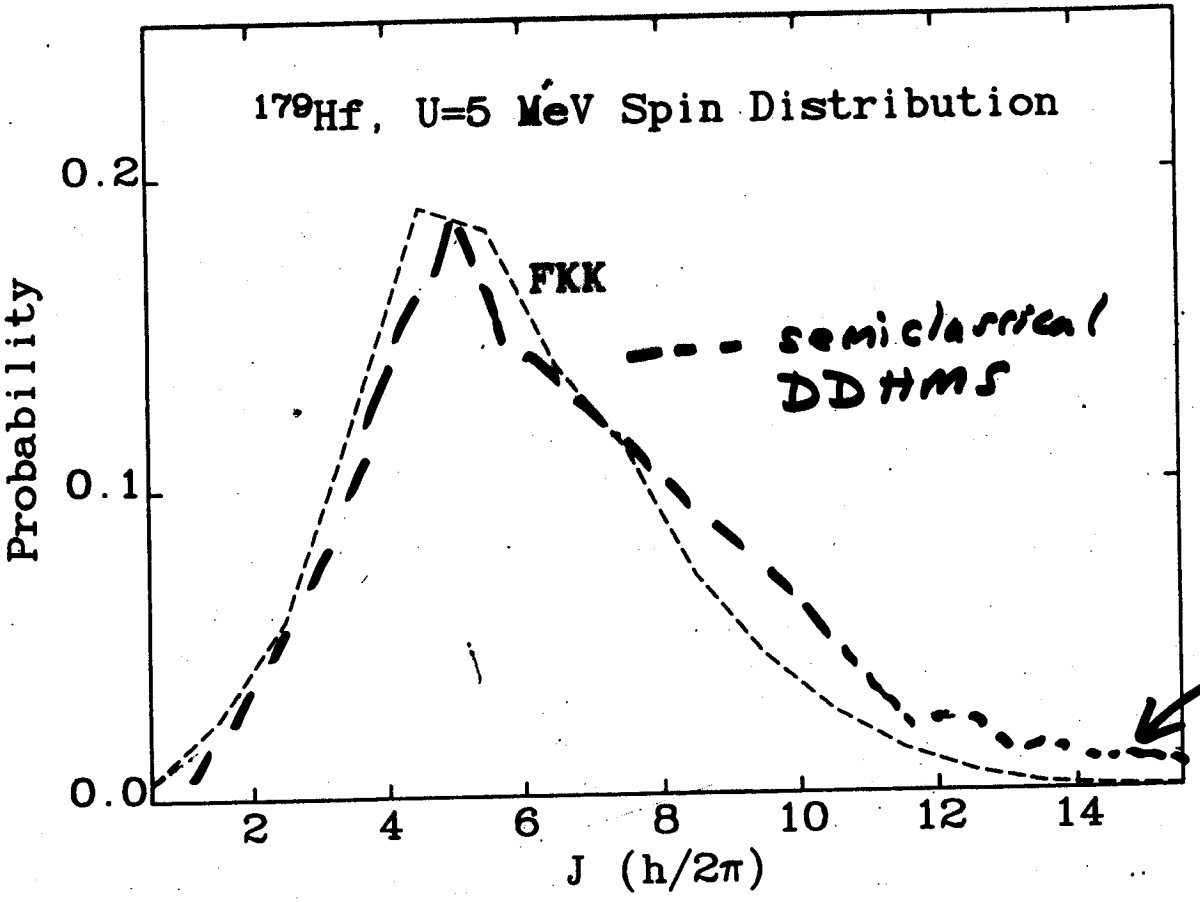
- Angular momentum transfer from semiclassical calc.
  - $\underline{r} \times \underline{p}$
  - r sampled from impact param
  - $\boxed{\text{high energies} \Rightarrow \text{more forward peaking} \Rightarrow \text{smaller a.m. transfer}}$

160 MeV p+90Zr



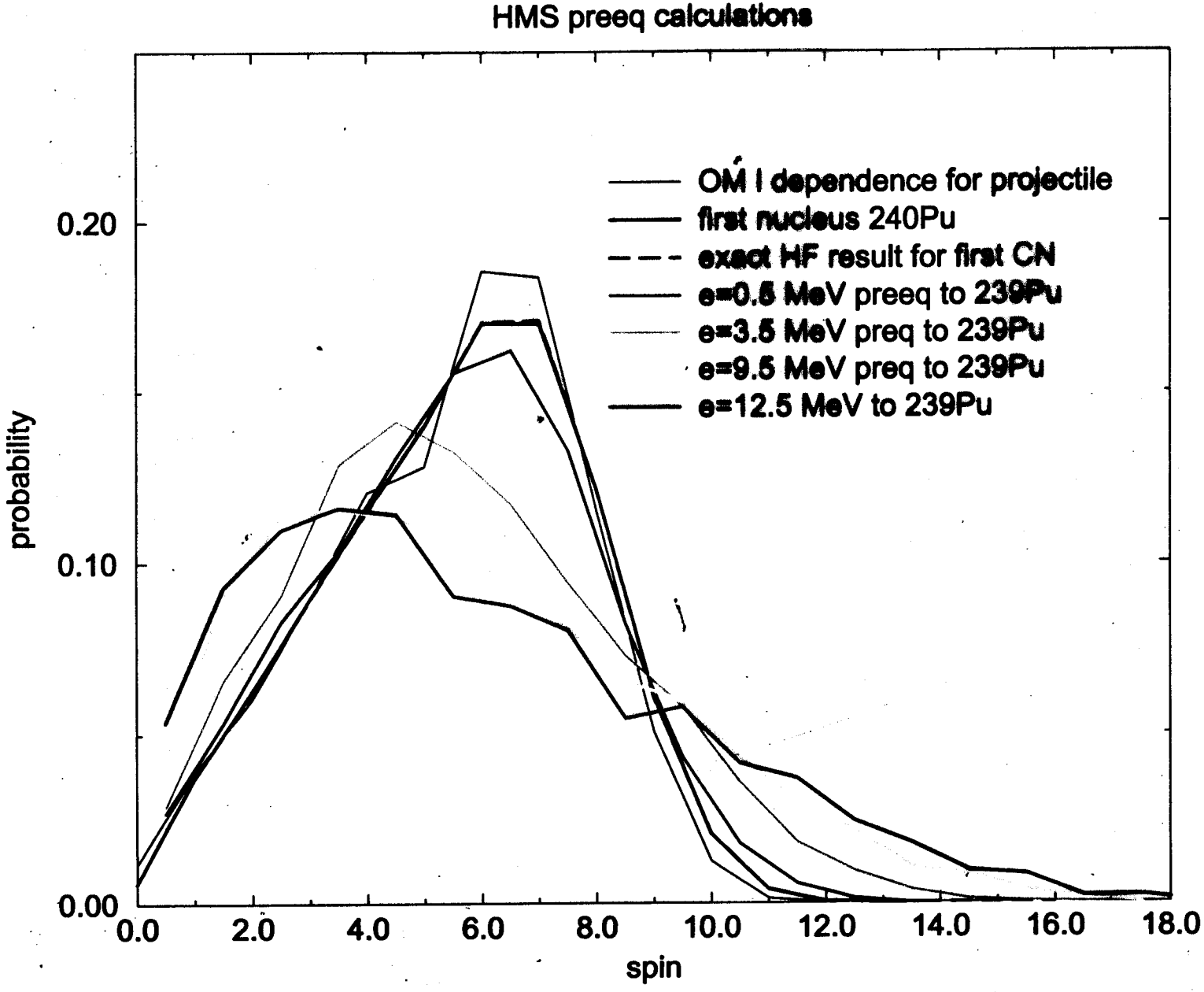
14 MeV n+179Hf (4.5 spin target)



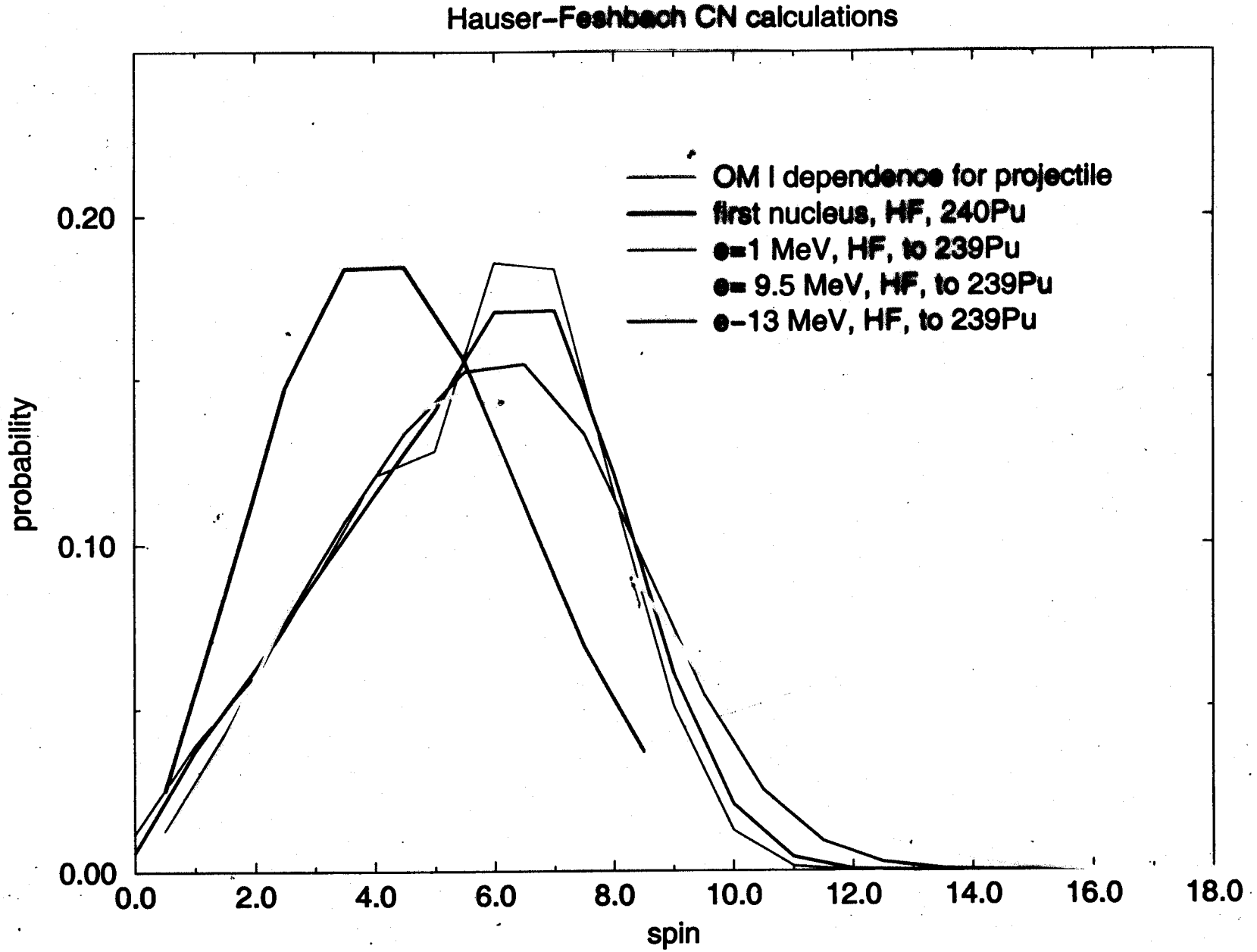


finite value out here unphysical, since available high-spin level dens → 0

14 MeV n+239Pu (0.5 spin target)



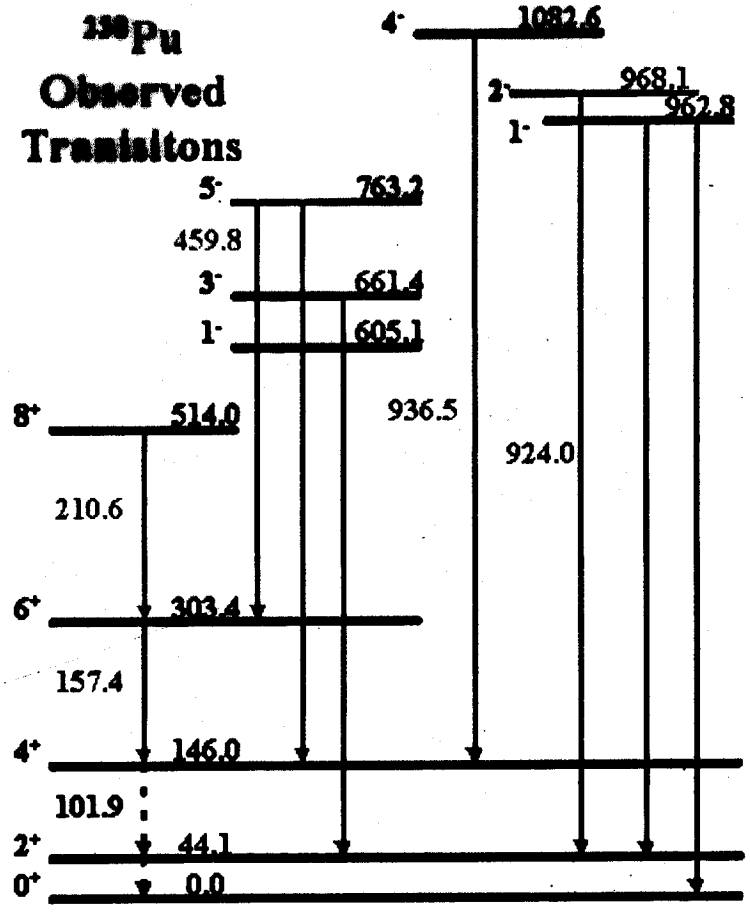
14 MeV n+239Pu (0.5 spin target)



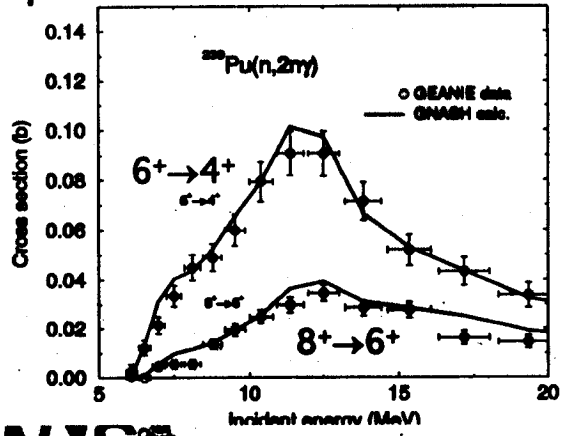
^{239}Pu(n,2n):

New technique was developed to determine this cross section

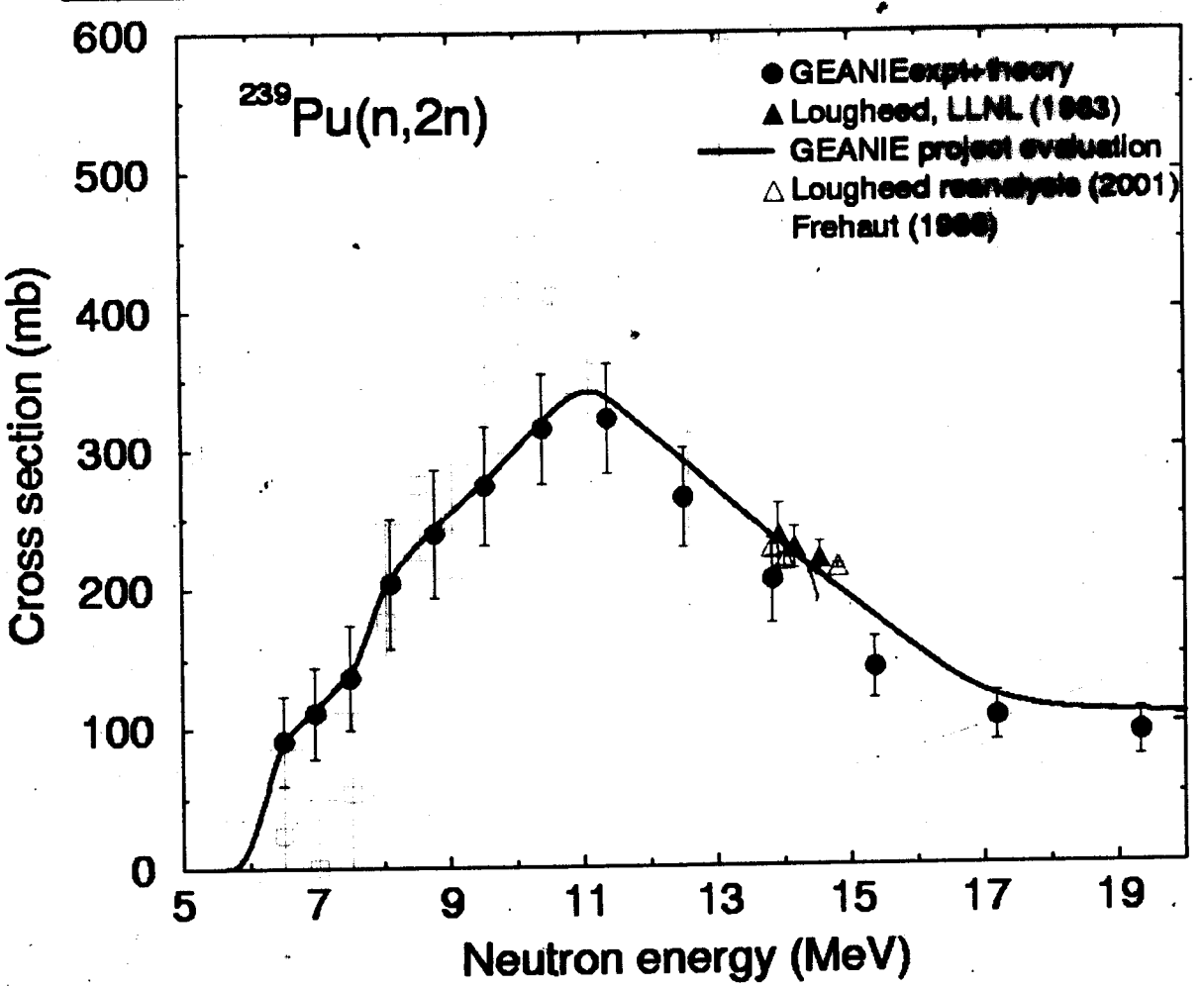
Measure partial gamma-ray cross sections and combine with theory (GNASH) predictions of unmeasured transitions, to obtain total (n,2n) cross section



Exp. & calc. excitation functions:



Final evaluated data from GEANIE project: Experiment + theory



These evaluated data, with 1-sigma error bands, are available for use by designers using legacy and new ASCI codes

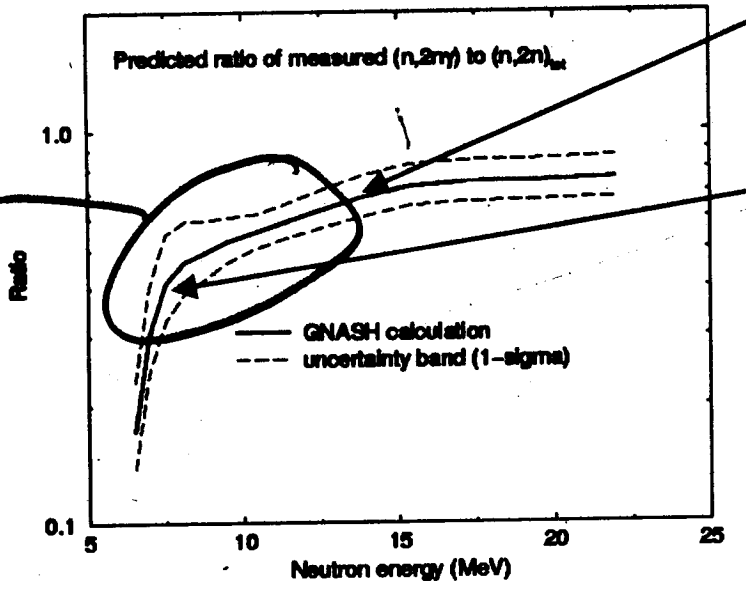
Procedure for inferring (n,2n) cross section

Theory contribution to (n, 2n)

The GEANIE experiment measured 6 independent γ-rays. To infer the total (n, 2n) cross section, we use :

$$\sigma(n,2n) = \sum_i \sigma_i^{expt}(n,2n\gamma)\left[\frac{\sigma^{theory}(n,2n)}{\Sigma_i\,\sigma_i^{theory}(n,2n\gamma)}\right]$$

By summing 6 γ-rays, we use as much of the experimental information as possible, and mitigate against weaknesses in the predictions of individual gamma-rays



Recent validation of this shape (Talk to MBC)

At 14 MeV:
measured ~ 70%
theory ~ 30%

Near threshold:
theory comprises a higher %

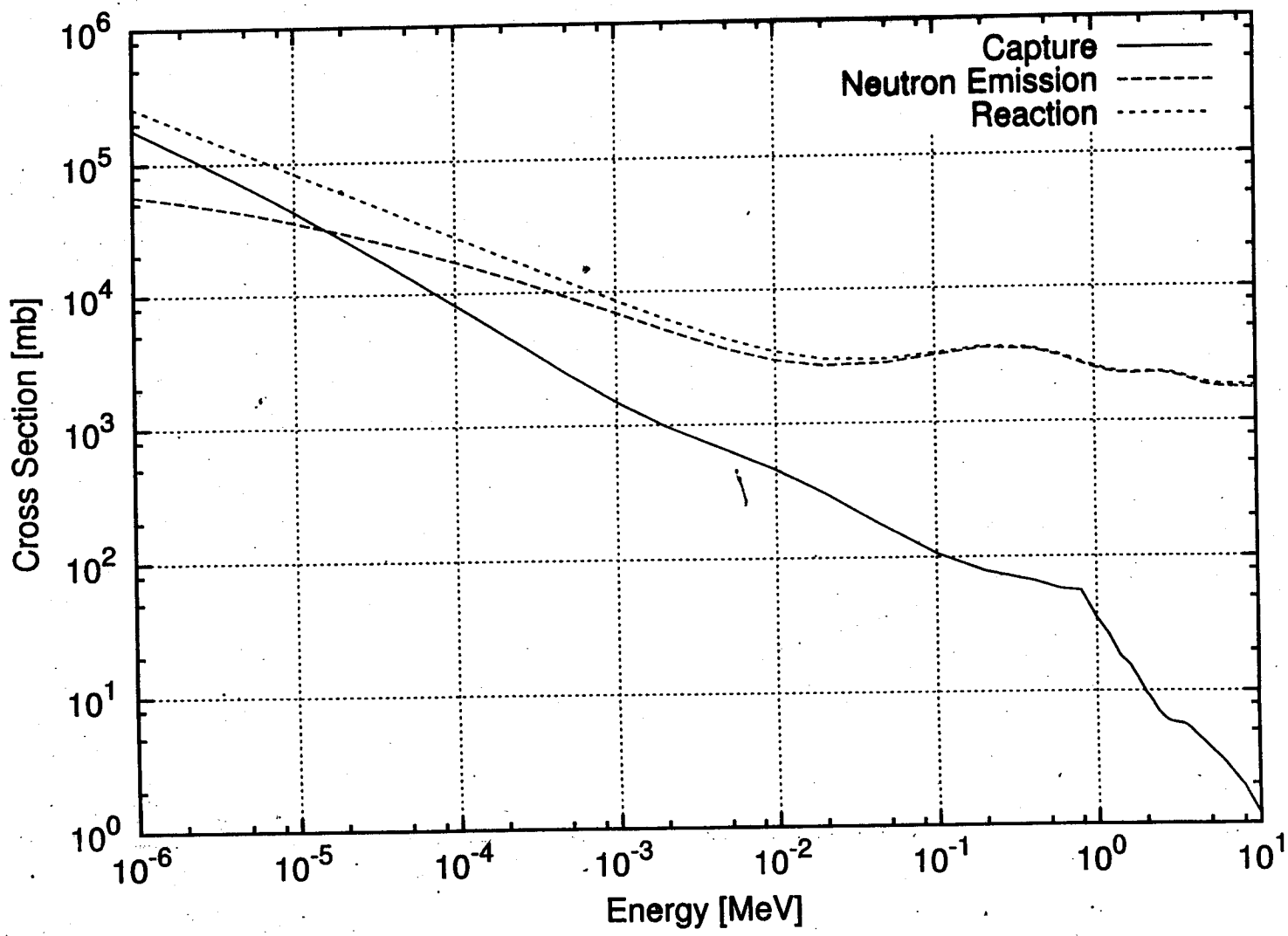
n + 87Y

→ capture

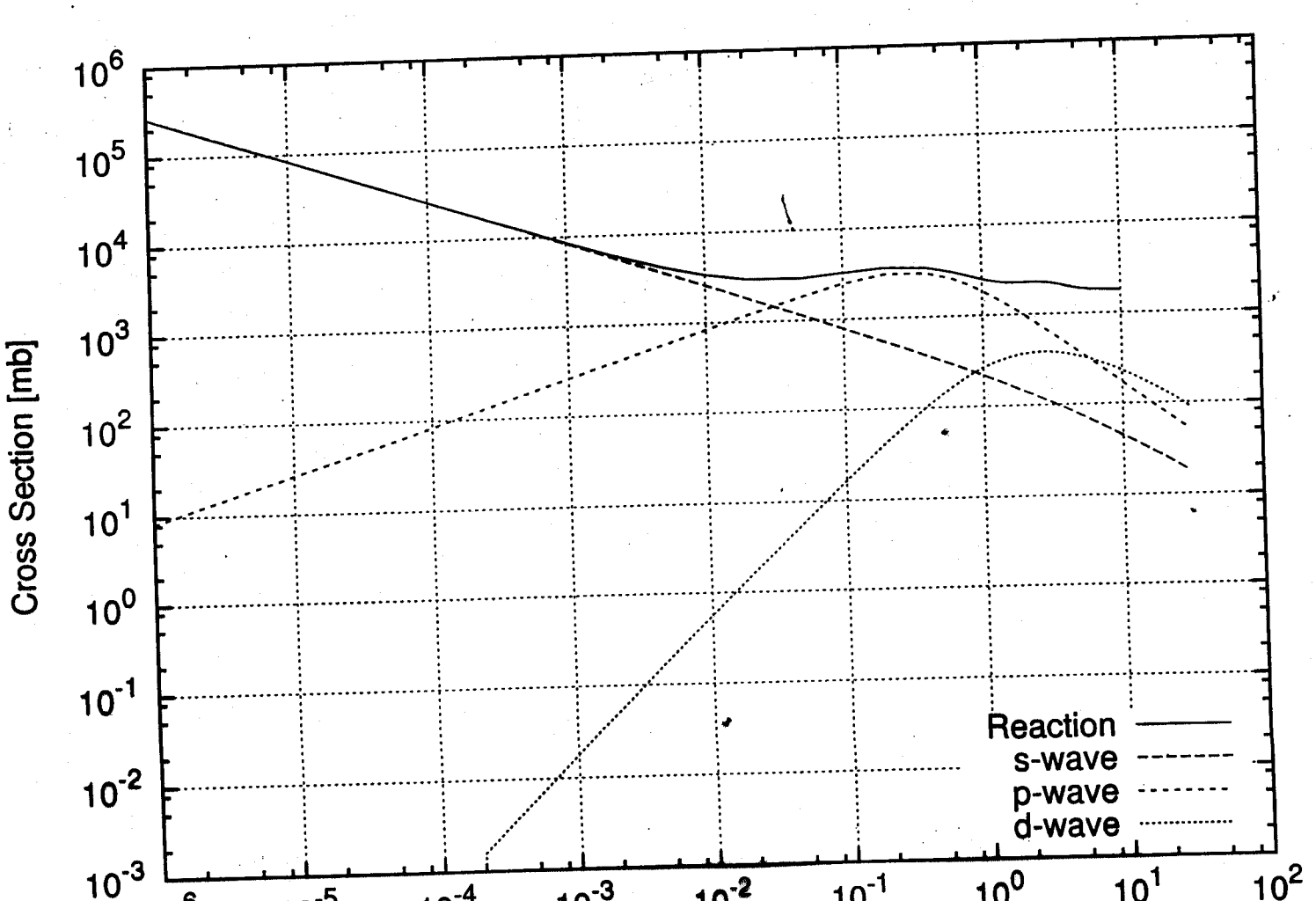
(Kawano)

87Y + n reactions

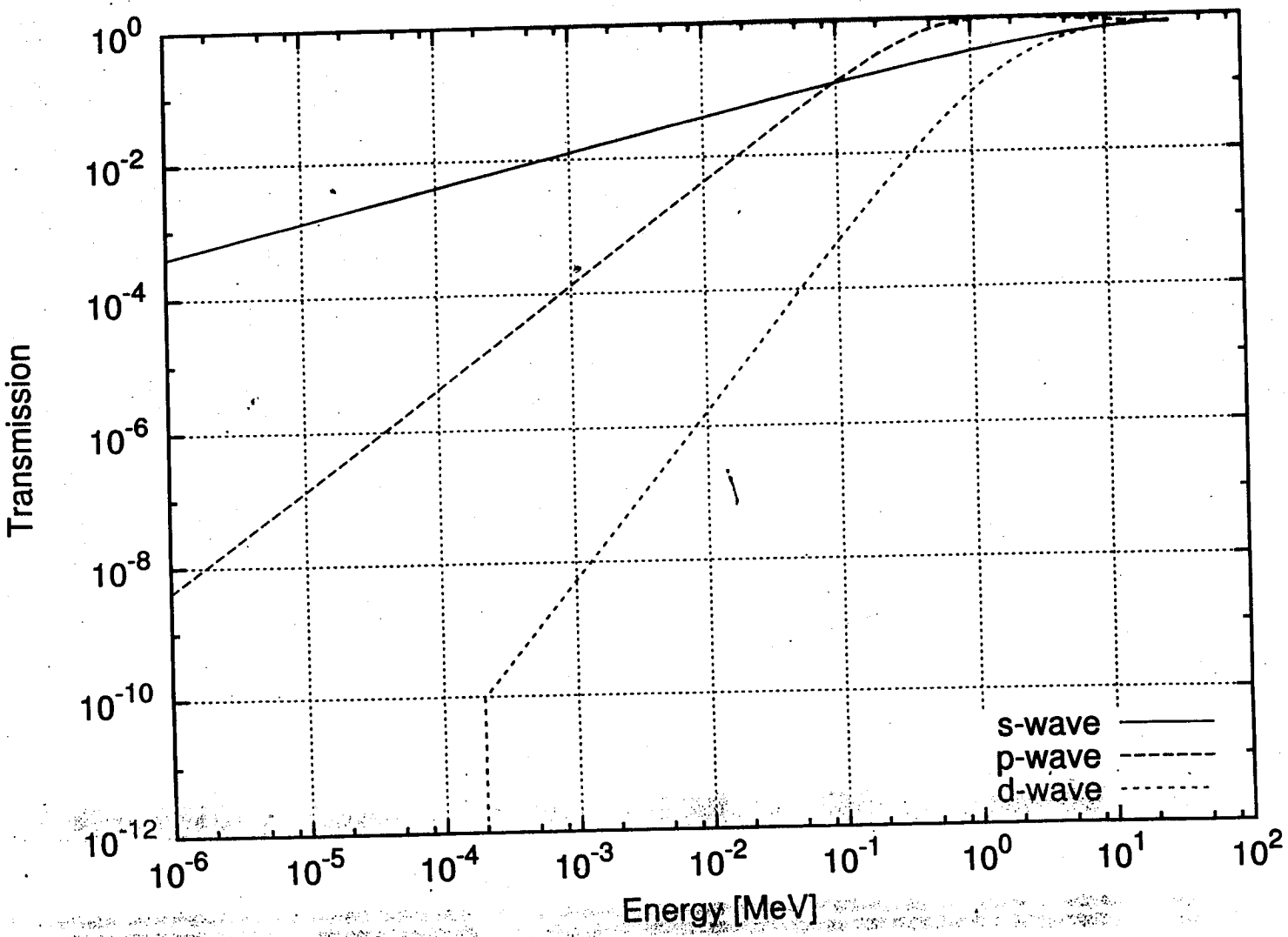
HFM calc.



$$\sigma^J = \frac{\pi}{k^2}(2J+1)\,T_J$$



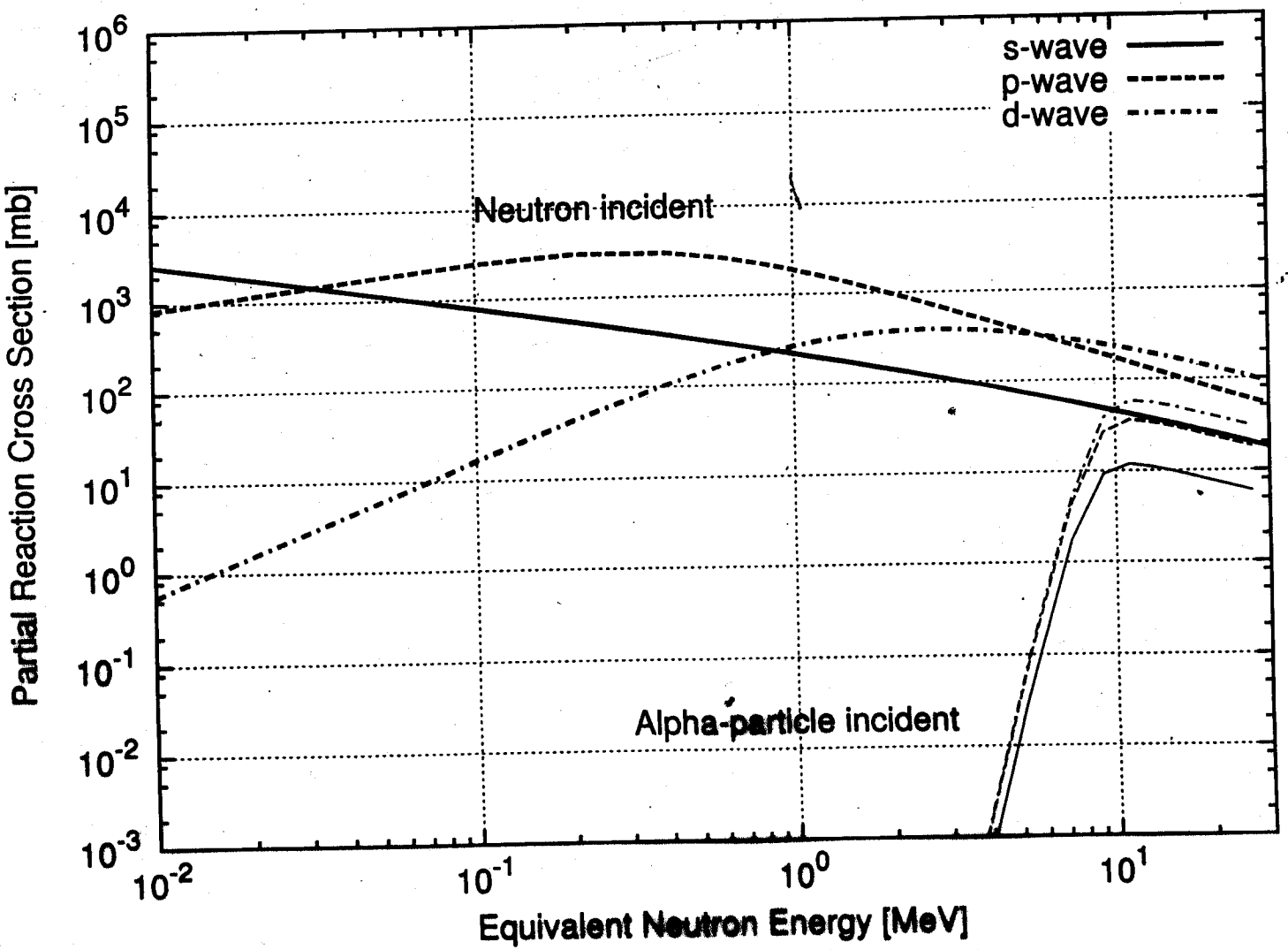
neutron transmission (spin averaged)

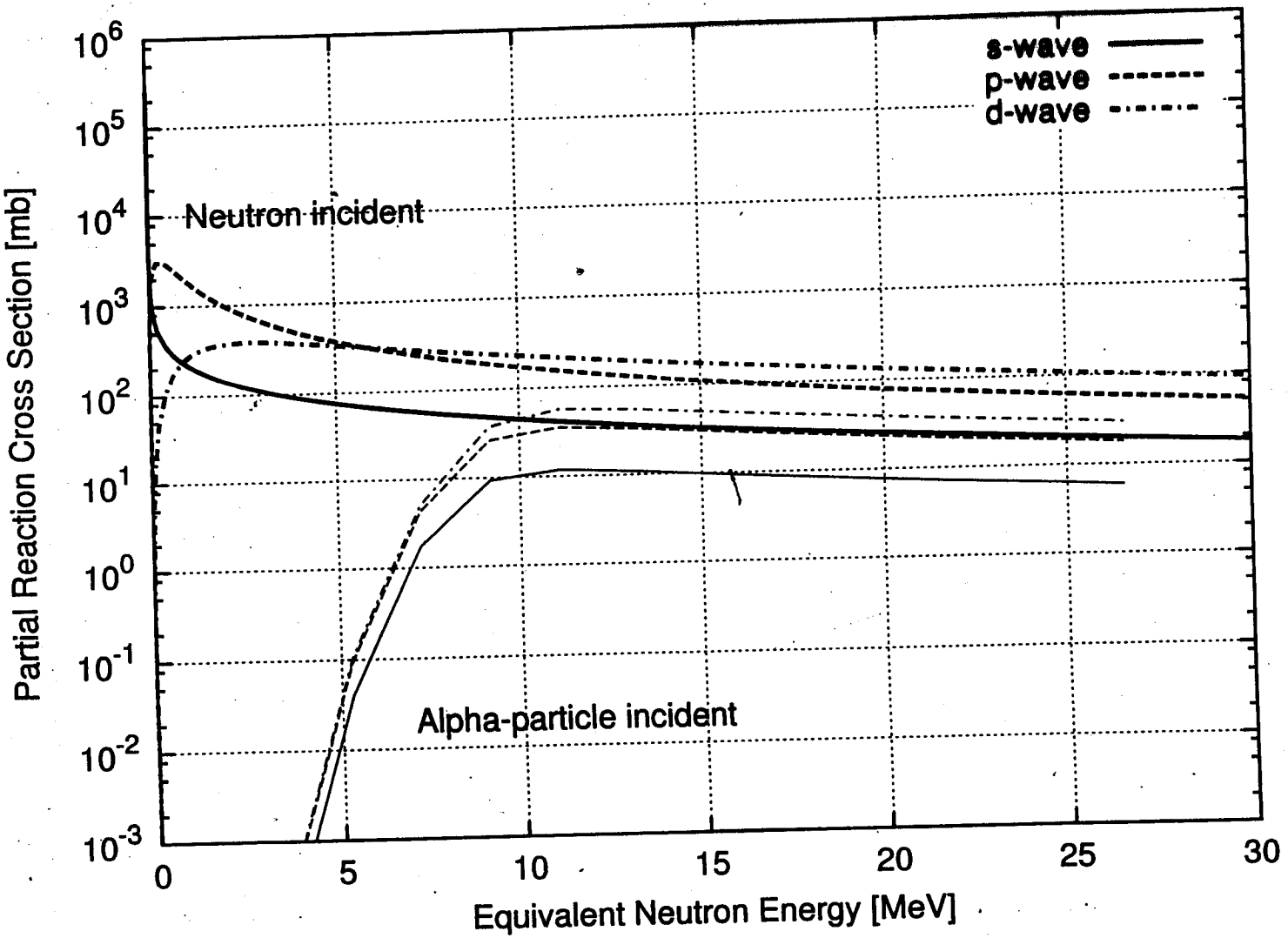


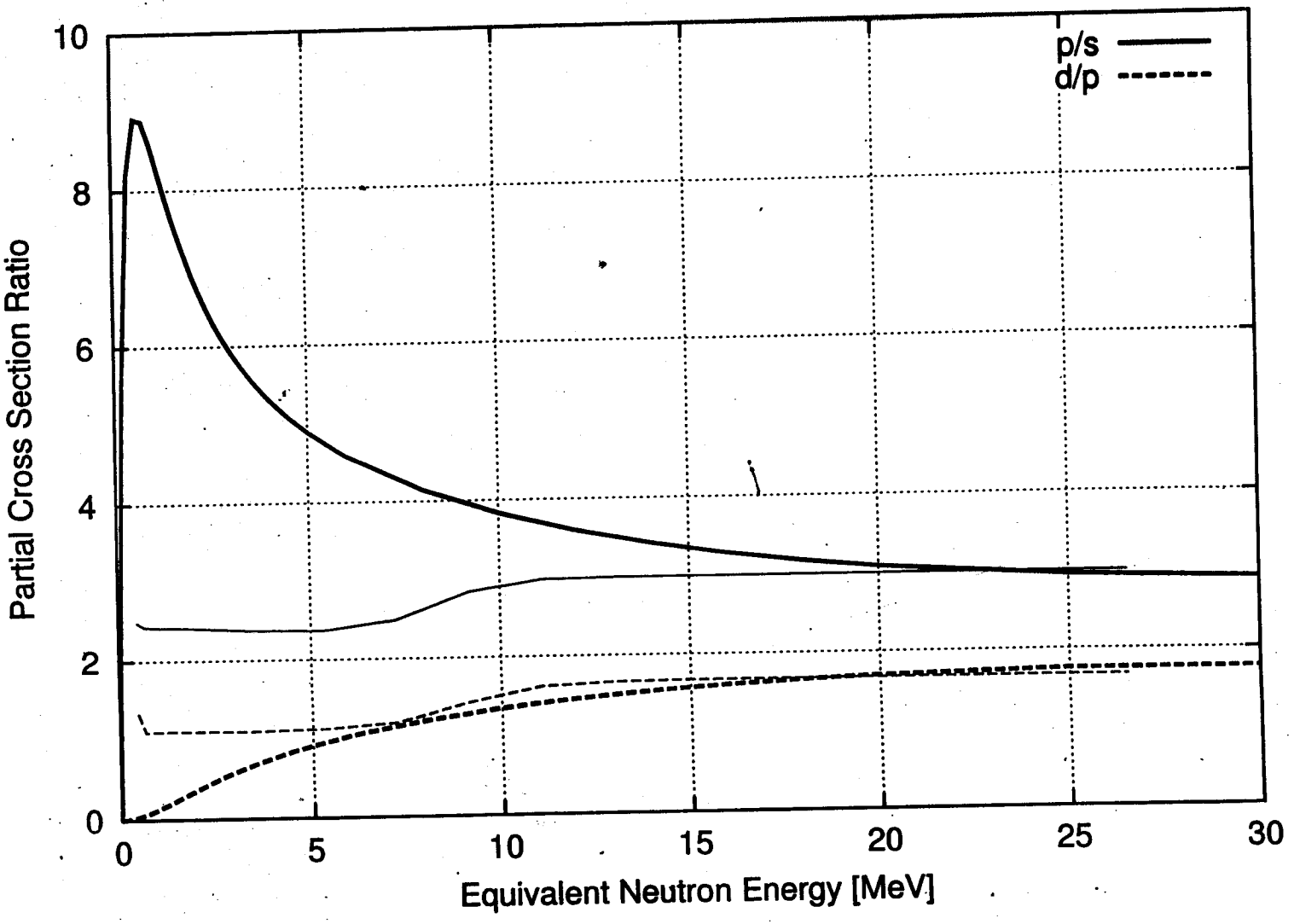
$^{87}Y + n \rightarrow {}^{88}Y^*$

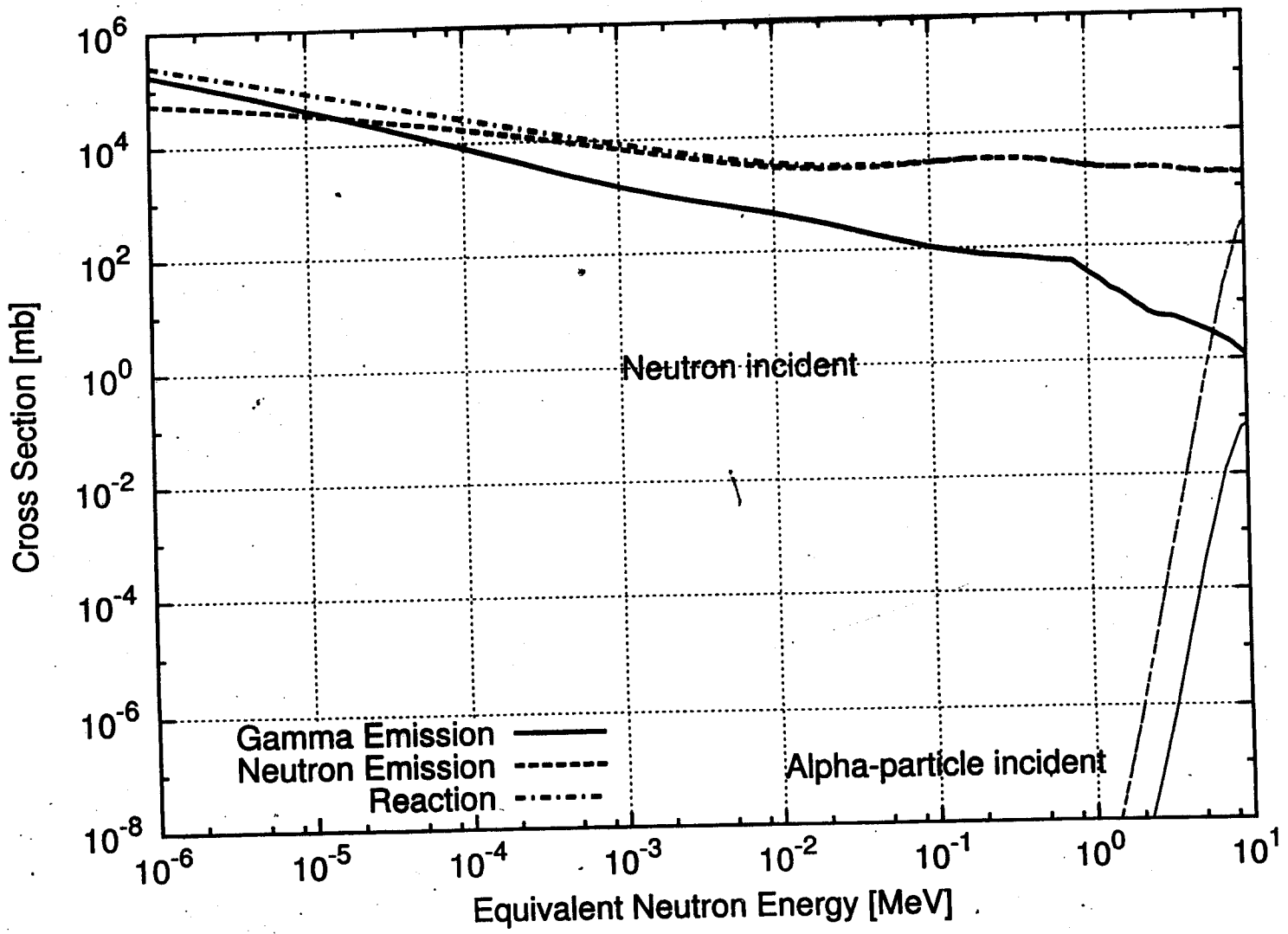
$^{84}Rb + \alpha$

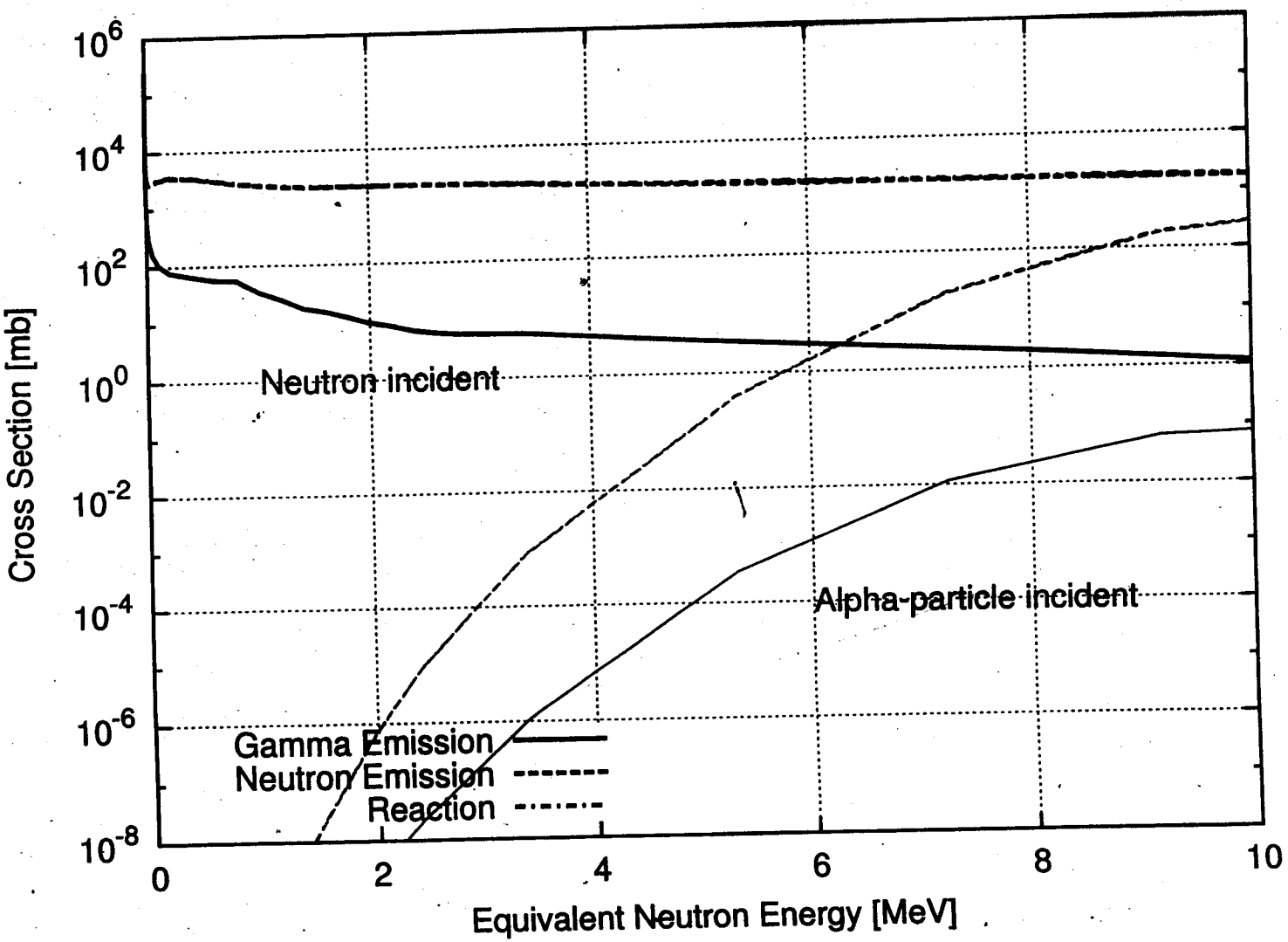
$E_\alpha = 1.09 E_n + 2.5$

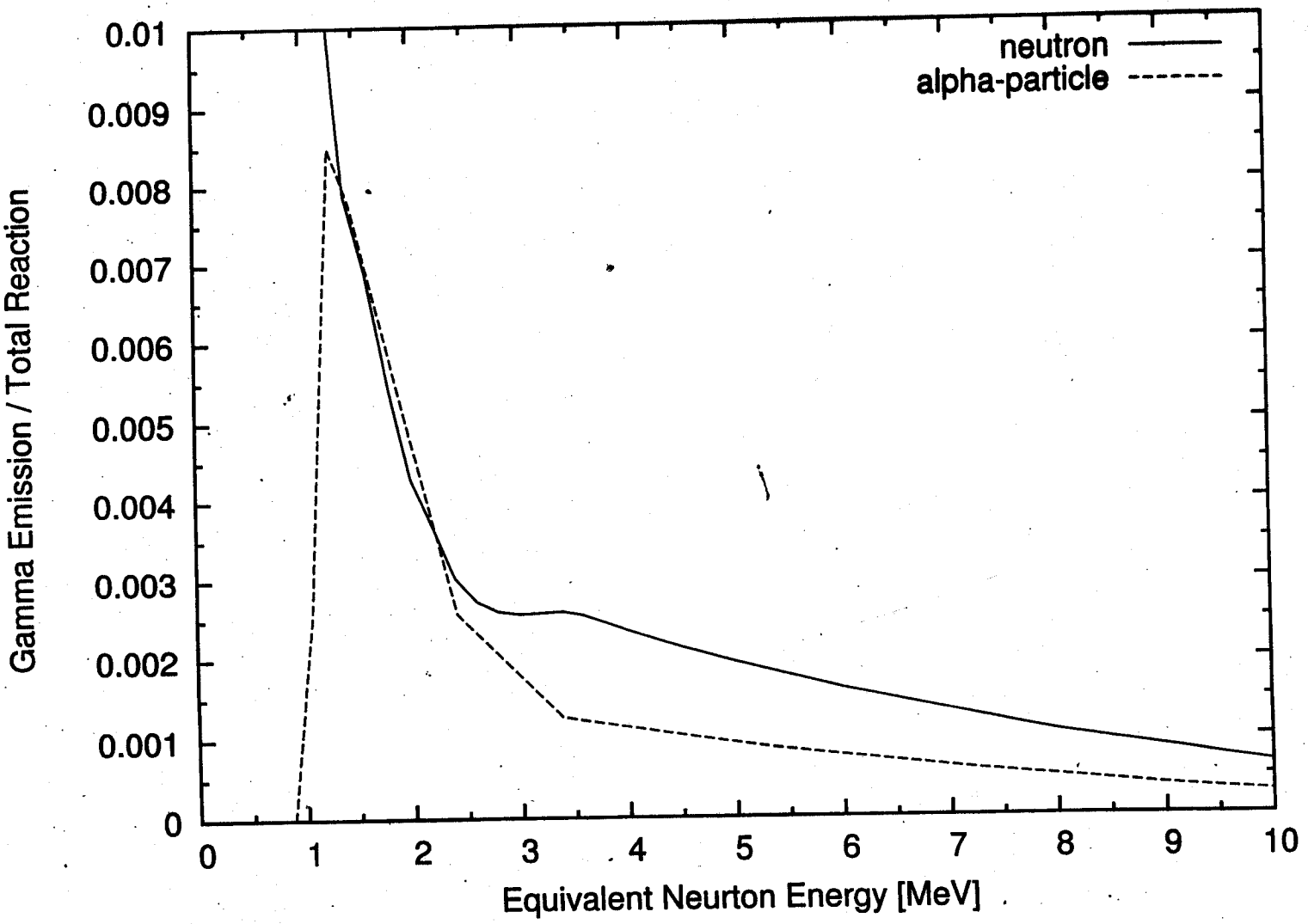


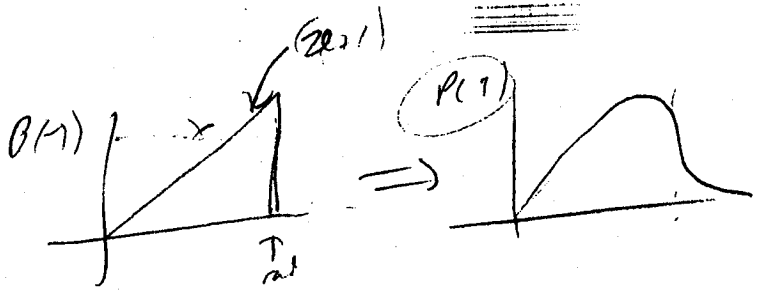

s-wave
p-wave
d-wave
Neutron incident
Alpha-particle incident
Partial Reaction Cross Section [mb]
Equivalent Neutron Energy [MeV]
10^6
10^5
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
0
5
10
15
20
25
30

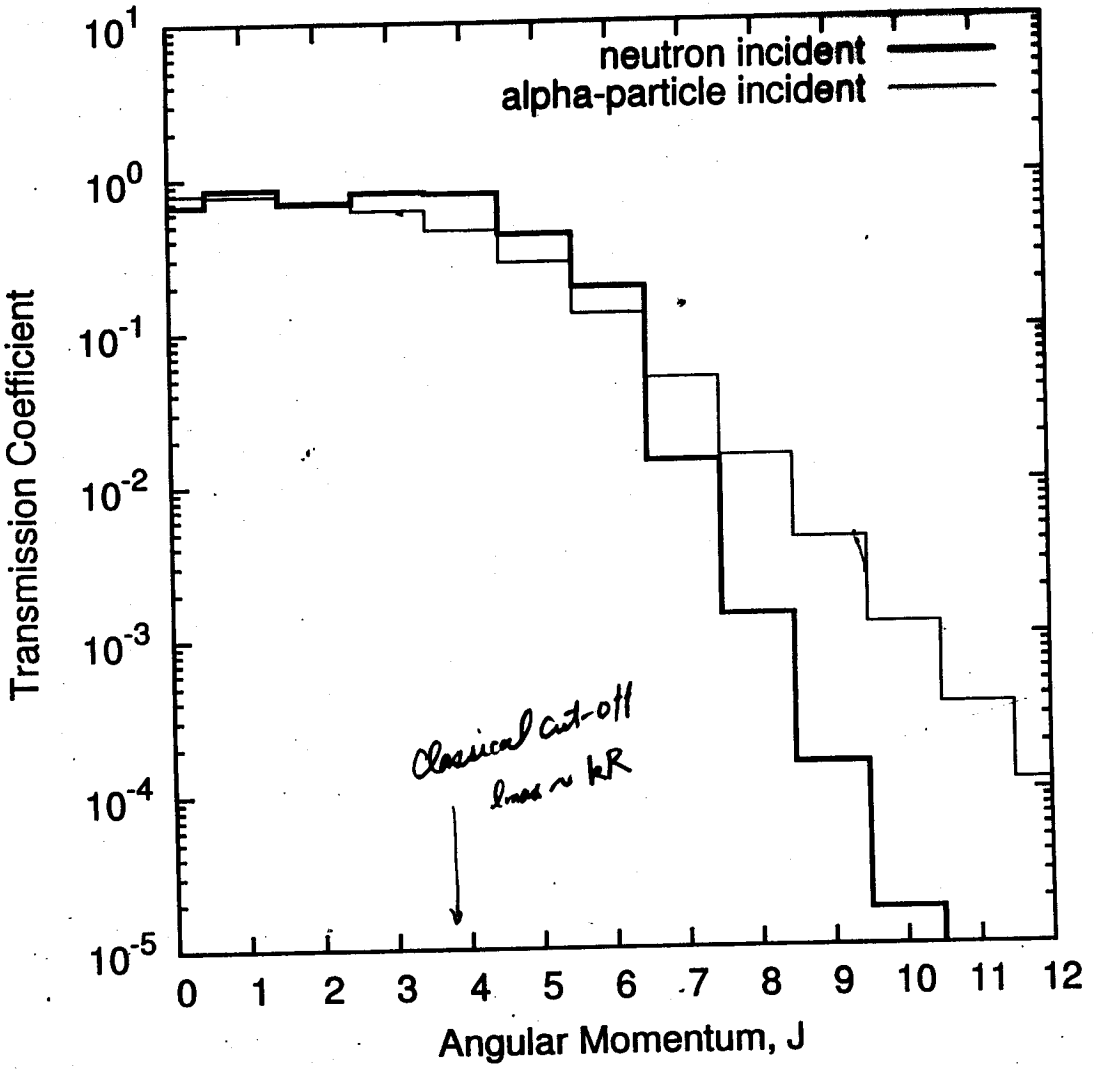

p/s
d/p
Partial Cross Section Ratio
Equivalent Neutron Energy [MeV]
0
2
4
6
8
10
0
5
10
15
20
25
30


Cross Section [mb]
Equivalent Neutron Energy [MeV]
Neutron incident
Alpha-particle incident
Gamma Emission
Neutron Emission
Reaction


Cross Section [mb]
10^6
10^4
10^2
10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
Neutron incident
Alpha-particle incident
Gamma Emission
Neutron Emission
Reaction
0
2
4
6
8
10
Equivalent Neutron Energy [MeV]


neutron
alpha-particle
Gamma Emission / Total Reaction
Equivalent Neurton Energy [MeV]
0.01
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
0
1
2
3
4
5
6
7
8
9
10



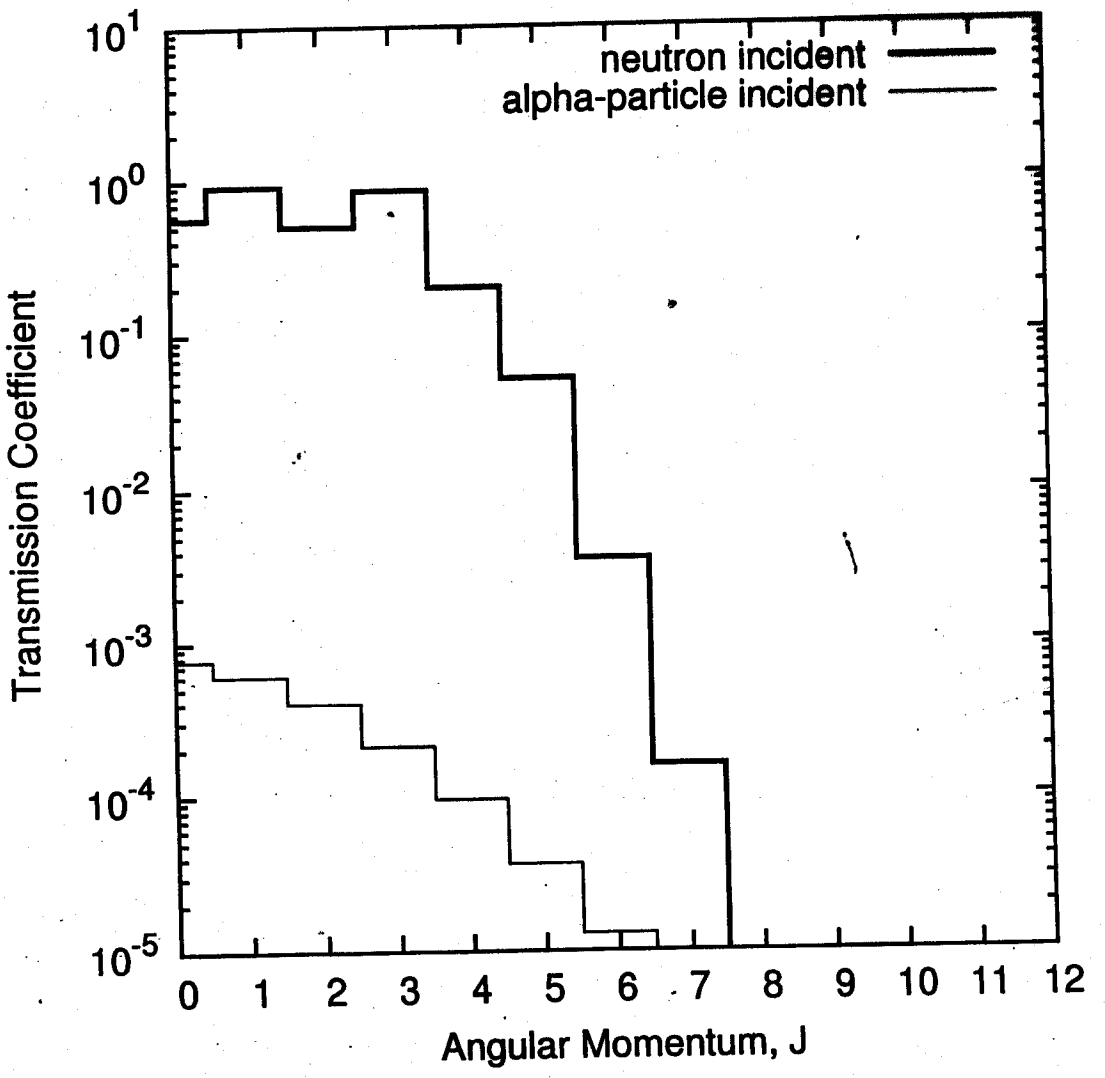


$^{87}Y + n$

$^{89}Rb + \alpha$

$E_n = 10$

$E_x = 12.8$



$^{87}Y + n$

$^{84}Rb + \alpha$

$E_n = 5\ MeV$

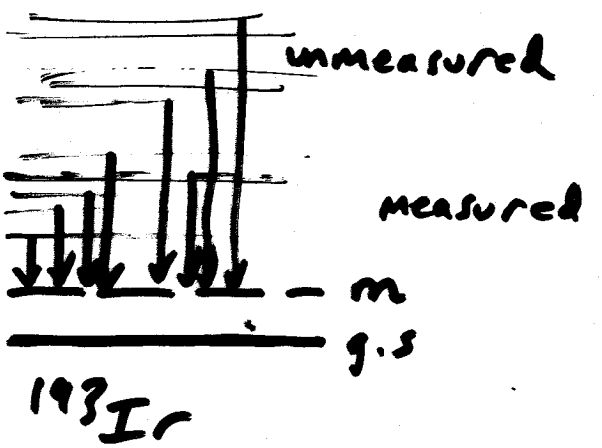
$E_\alpha = 2.67\ MeV$

(Talon talk)

$^{193}Ir(n,n')^{193m}Ir$ isomer for radchem

- unique detector for mid-range (fission) neutrons
- GEANIE measured this; theory needed

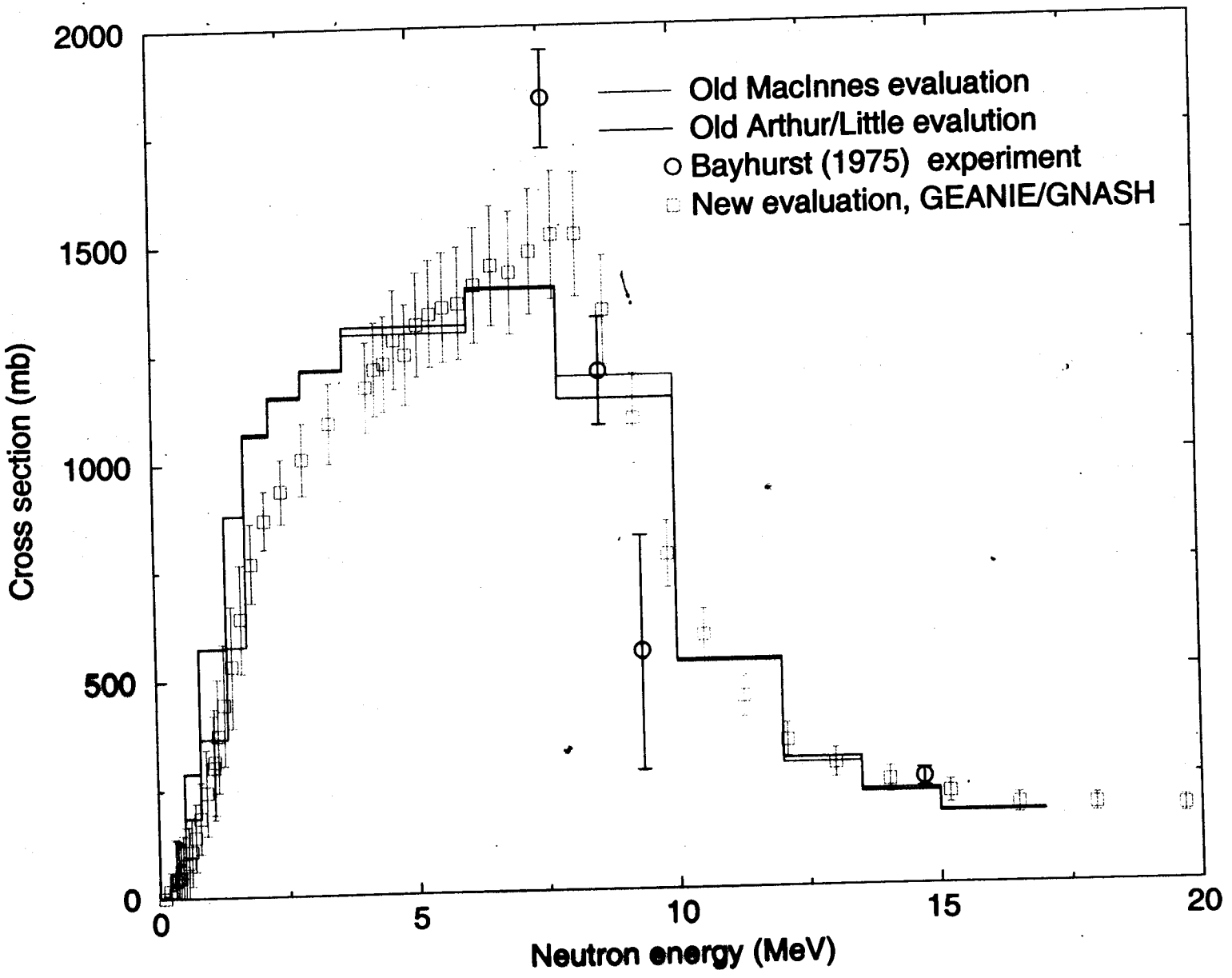
$\sum_{4\gamma s}(n,n'\gamma)$ = surrogate, for (n,n') isomer prod.

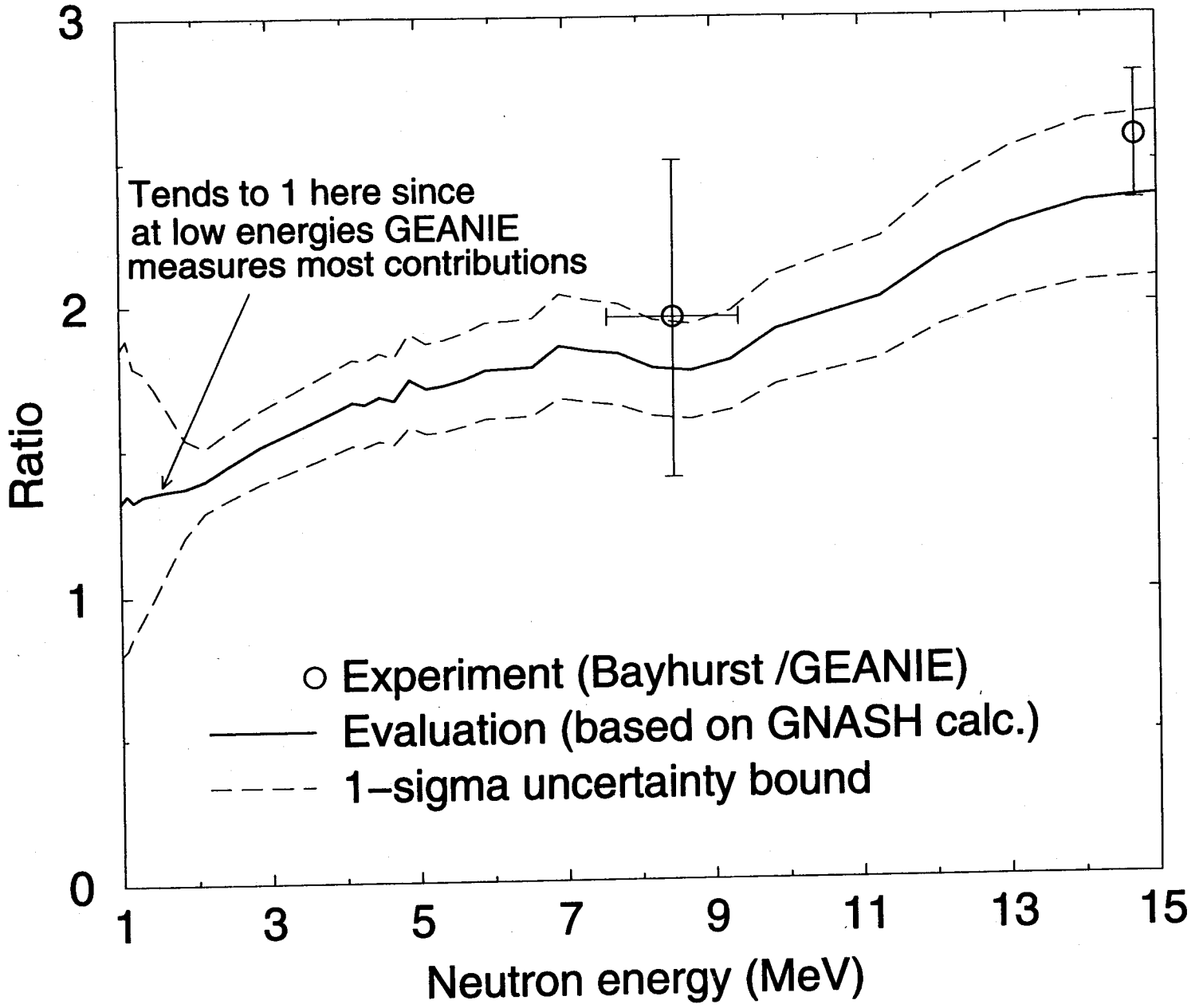


GNASH can be used to predict the ratio

$$\left\{ \frac{(n,n')^{193m}Ir}{\sum_{4\gamma s}(n,n'\gamma)^{193m}Ir} \right\}$$

Ir193 (n,n') isomer



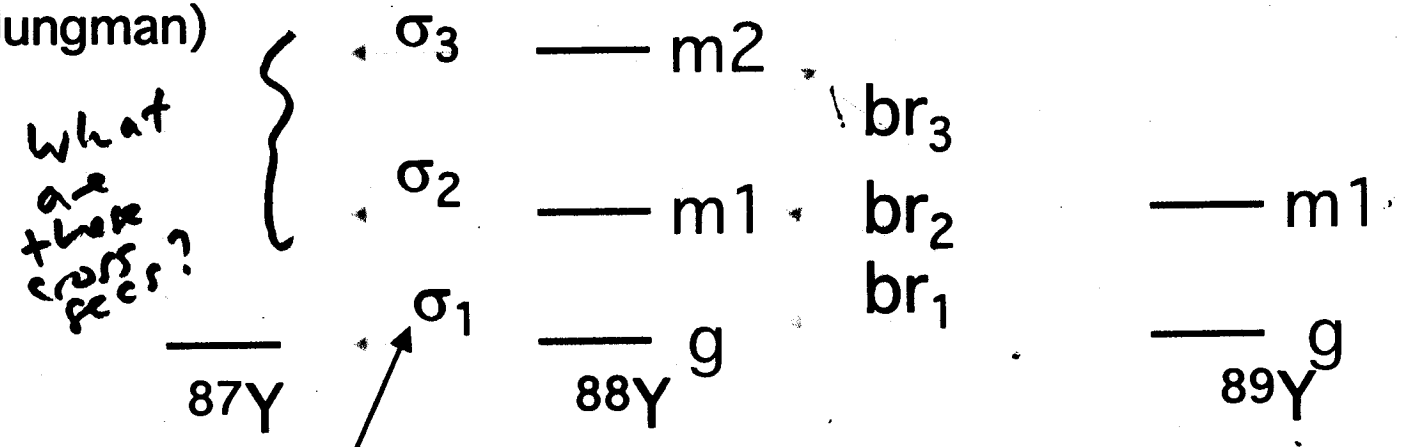

Ratio [^{193}Ir(n,n')^{193m}Ir / GEANIE Σ_4 γ rays]
Tends to 1 here since
at low energies GEANIE
measures most contributions
Experiment (Bayhurst /GEANIE)
Evaluation (based on GNASH calc.)
1–sigma uncertainty bound
Ratio
Neutron energy (MeV)
0
1
2
3
1
3
5
7
9
11
13
15

Yttrium cross sections off stability

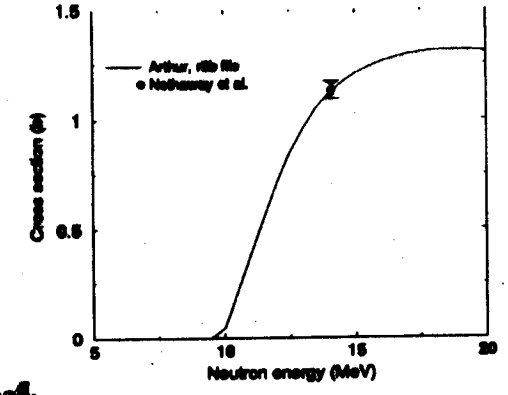
GEANIE exp + theory to determine cross sections
Transitions to, and from, isomers must be understood

Average ^{88}Y(n,2n)= $\sigma_{88\to87}$= br_1*σ_1 + br_2*σ_2 + br_3*σ_3 ; 87/88 =1/2$\sigma_{88\to87}$ Φ

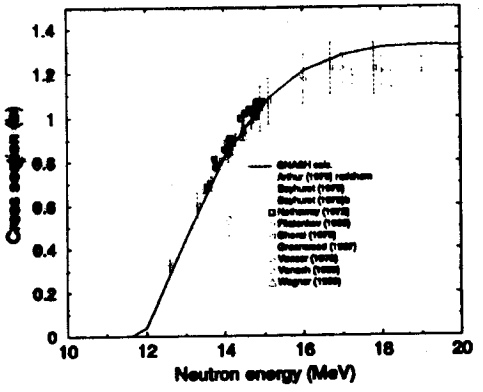
(Jungman)



Total ^{88g}Y(n,2n)



Total ^{89g}Y(n,2n)

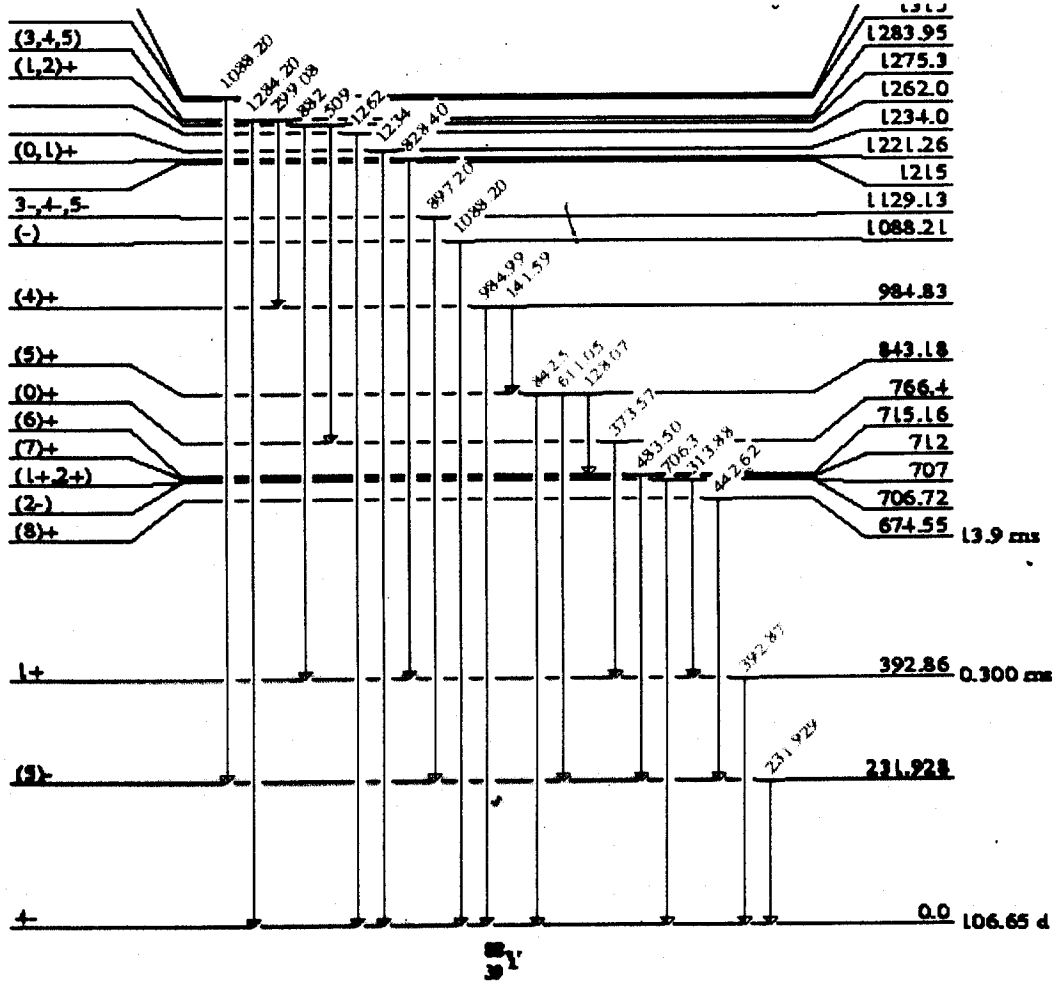


This work determines branching ratios and assesses impact on $\sigma_{88\to87}$ uncertainties

LANSCE GEANIE experiment by Garrett, Becker (LLNL) and Nelson, Fotiados, Devlin (LANL)

^{88}Y spectroscopy: gamma-decay scheme

m2 isomer is part of a $(g_{9/2})_p(g_{9/2})_n^{-1}$ multiplet ($8^+,7^+,6^+,5^+\ldots$)

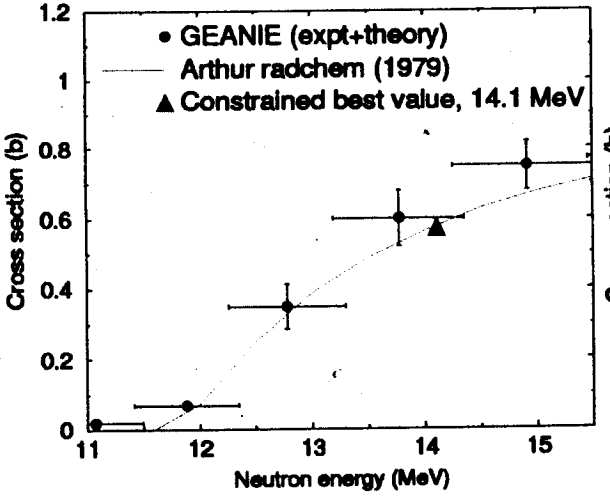


NNSA

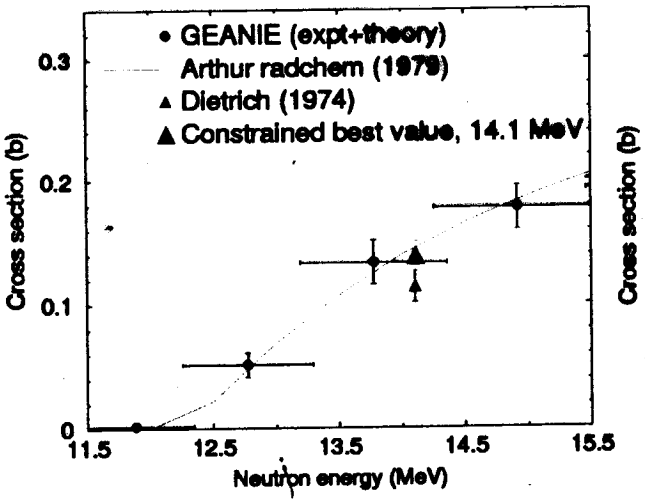
• Los Alamos

Best estimate of ^{89}Y(n,2n) to g, m1, m2 at 14.1 MeV. *(Kawano)*
Use GEANIE/GNASH project + Dietrich measurements

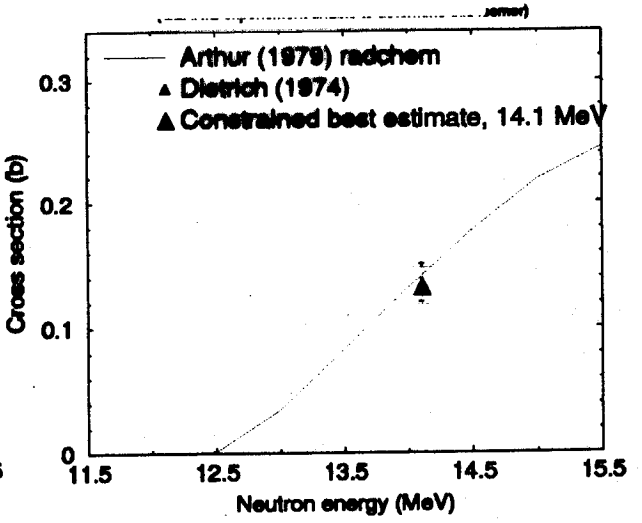
ground



m1 isomer



m2 isomer



Constrained best estimates of the 14.1 MeV cross Sections. Constraint is that (n,2n) total =845 mb (±2%):

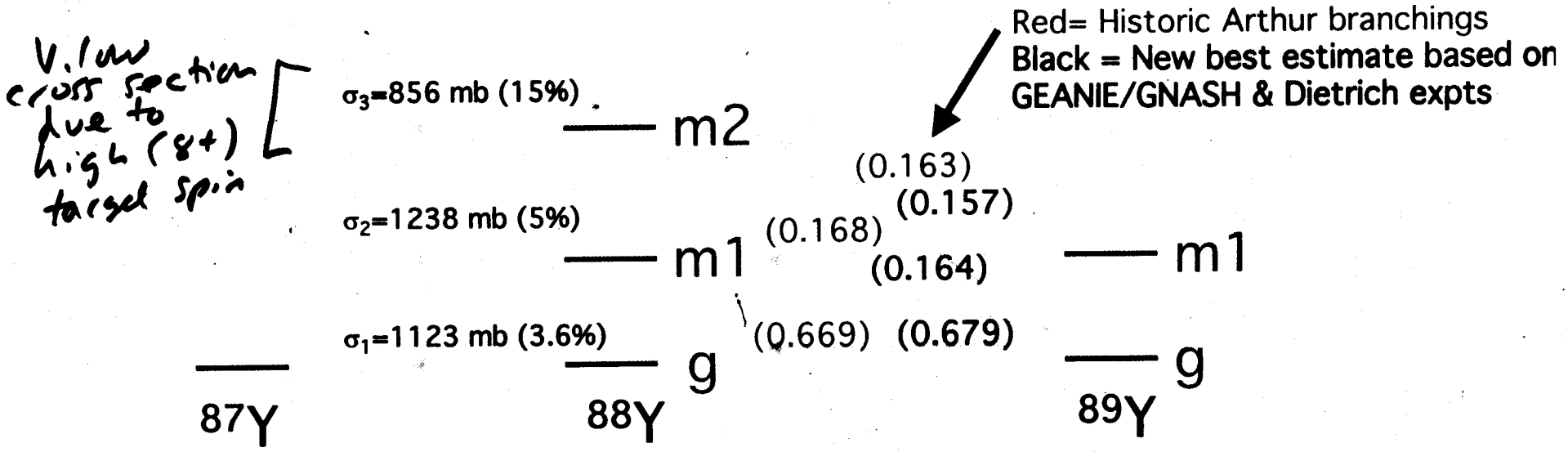
g = 576 mb (3.2%)
m1 = 139 mb (8.3%),with correlations:
m2 = 133 mb (11.0%)

	g	m1	m2
g	100%		
m1	61%	100%	
m2	77%	3%	100%

GEANIE/GNASH Validation of Historic NNSA Radchem Data & Uncertainty Quantification in Yield

Average $^{88}Y(n,2n) = br_1*\sigma_1 + br_2*\sigma_2 + br_3*\sigma_3$
Best estimate from a covariance error analysis, including uncertainties & correlations in 89->88 and 88->87 transitions

V. low cross section due to high (8+) target spin



Red= Historic Arthur branchings
Black = New best estimate based on GEANIE/GNASH & Dietrich expts

Average $^{88}Y(n,2n)$ cross sec at 14.1 MeV:
Historic value in NNSA databases: 1099 mb
This work: 1104 mb (±4.0%)
(good agreement!)

Contibution to total uncertainty due to 89->88 branching uncertainties Is small (~0.5%) because of correlations