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Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety

16 February - 12 March 2004

Pre-Equilibrum Models of Nuclear Reactions

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PREEQUILIBRIUM NUCLEAR REACTIONS

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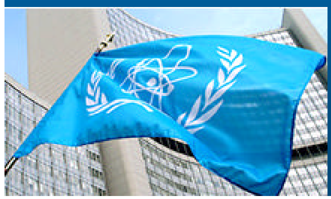
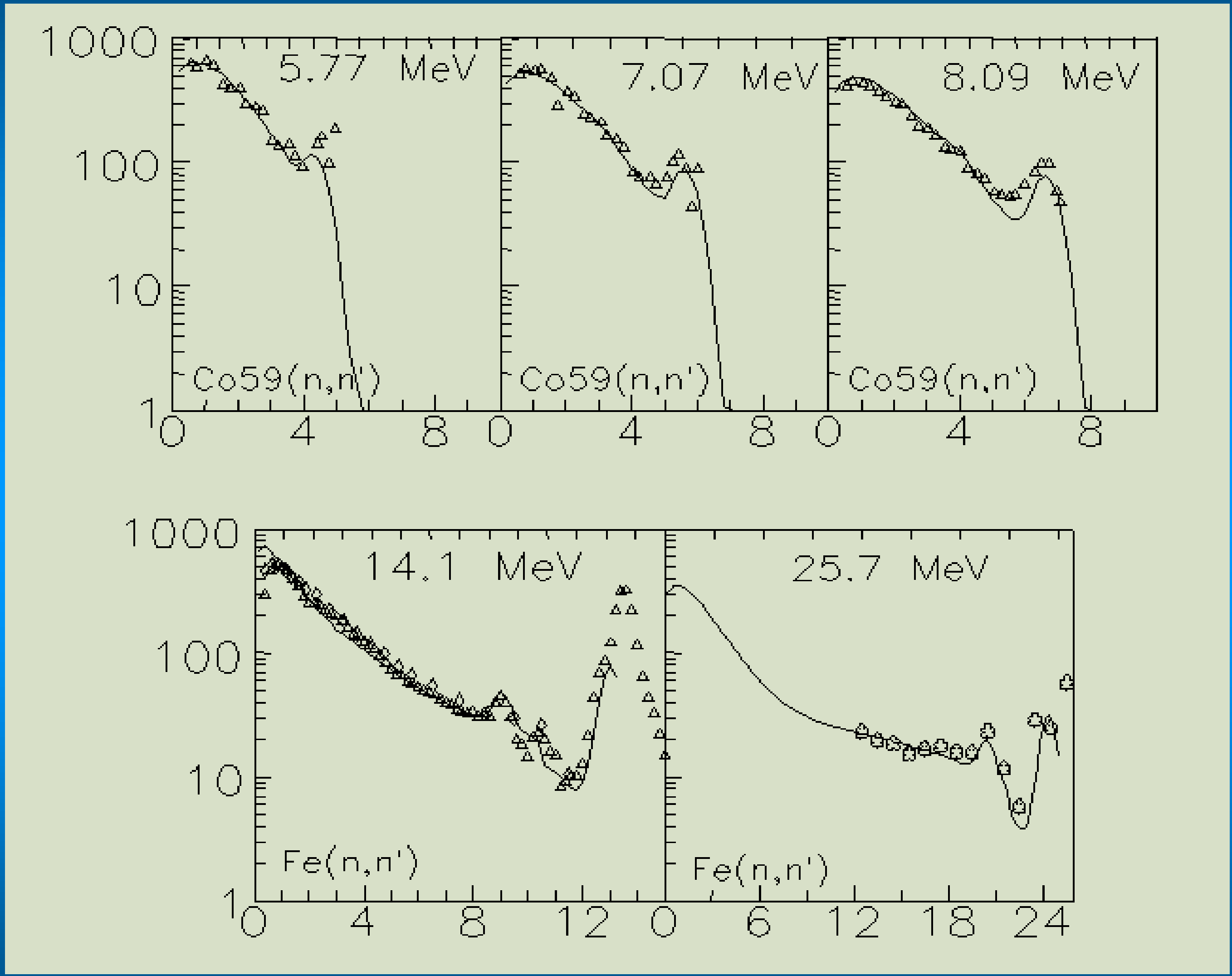


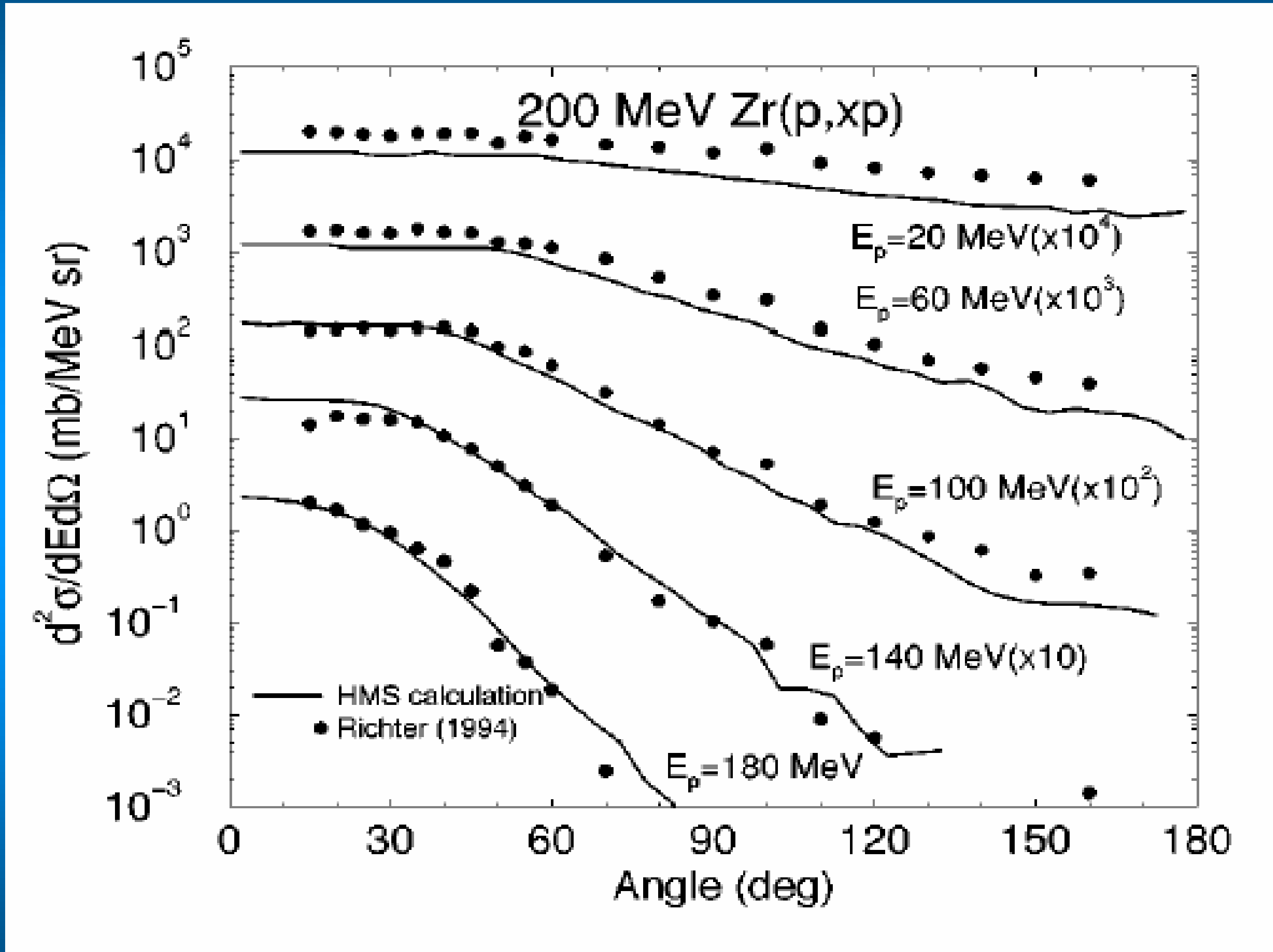
OVERVIEW

- Introduction
- Semiclassical theory of PE emission : Exciton and HMS models
- Quantum-Mechanical (microscopic theories) : SMD/SMC
- EMPIRE implementation

EQUILIBRIUM, DIRECT and ???



ISOTROPIC DISTRIBUTION ???



EXCITON MODEL

- Griffin J.J., *Phys.Rev.Lett.* ***17****(1966) 478; Phys.Lett.* ***B24****(1967) 5*

- Cline C.K., Blann M., “The preequilibrium sttistical model: Description of the nuclear equilibration process and parameterization of the model”, *Nucl. Phys.* ***A172****(1971) 225*
- Cline C.K., *Nucl. Phys.* ***A193****(1972) 417*
- Ribansky I., Oblozhinsky P., Betak E., *Nucl. Phys.* ***A205****(1973) 545*

MASTER EQUATION: KINETIC EQUATION DESCRIBING THE TIME EVOLUTION OF THE PROBABILITY DISTRIBUTION *P(n,t)*

$$\frac{dP}{dt}(n,t) = l^{+}(n-2)P(n-2,t) + l^{-}(n+2)P(n+2,t) - \left[l^{+}(n) + l^{-}(n) + W(n) \right] P(n,t)$$

P(n,t) – Probability that system will be in the state with *n* excitons during time *t*

W(n) – Total emission rate

$l^{+}(n)$, $l^{-}(n)$ - internal transition rates to states with $n \pm 2$

EXCITON MODEL

•Williams F.C., *Phys.Lett.* ***31B****(1970) 184*

•Oblozhinsky P., Ribansky I., Betak E., *Nucl.Phys.* ***A226****(1974) 347*

•Kalbach-Cline C., *Nucl.Phys.*, ***A210****(1973) 590* $<M^2> = KA^{-3}E^{-1}$

$$l^{+}(n) = \frac{2p}{\hbar}\left\langle M^{2}\right\rangle \frac{g^{3}\left[U - A^{W}(p,h)\right]^{2}}{2(n+1)} \quad ; \quad l^{-}(n) = \frac{2p}{\hbar}\left\langle M^{2}\right\rangle \frac{1}{2}\, gph(n-2)$$

NEVER COME-BACK ASSUMPTION: $l^{+}(n) >> l^{-}(n)$

EXCITON MODEL

- Gadioli E., Gadioli Erba E., Sona P.G., *Nucl.Phys.* ***A217****(1973) 589*
- Machner H., *Z.fur Phys.* ***A302****(1981) 125*

$$l^{+}(n) = \frac{a}{k_{mfp}} U' \quad ; \quad l^{-}(n) = \frac{a}{k_{mfp}} \frac{1}{g^{2}} \frac{ph(n-2)(n-1)}{U'}$$

Gupta S.K., *Z.fur Phys.*, ***A303****(1981) 329* → Additional 3/8 factor

NEVER COME-BACK ASSUMPTION: $l^{+}(n) >> l^{-}(n)$

EXCITON MODEL

$$W(n) = \sum_{b} \int_{0}^{e_{MAX}} de_{b} \, W_{b}(U, n, e_{b})$$

Using detailed balance :

Nucleon emission :

$$W_{b}(U, n, e_{b}) = \frac{2s_{b} + 1}{p^{2} \hbar^{3}} m_{b} \, e_{b} \, s_{b}^{inv}(e_{b}) \frac{w_{res}(p - b, h, U)}{w_{comp}(p, h, E)} Q_{b}(p, h)$$

EXCITON MODEL

For cluster emission :

- Iwamoto A., Harada K., *Phys.Rev.* ***C26****(1982) 1821*
- Sato K., Iwamoto A., Harada K., *Phys.Rev.* ***C28****(1983) 1527*

$$W_a(U,n,e_a) = \frac{1}{p^2\hbar^3} m_a e_a s_a^{inv}(e_a) \frac{\sum_{l+m=4} F_{lm}(e_a)\, Q_{lm}^{a}(p,h)\, w_{res}(p-l,h,U)}{w_{comp}(p,h,E)}$$

EXCITON MODEL

Gamma emission :

- Pluyko V.A., Prokopets G.A., *Phys.Lett.*, ***76B****(1978) 253*
- *Betak E., Dobes J., Phys.Lett.,* ***84B****(1979) 368*
- Akkermans J.M., Gruppelaar H., *Phys.Lett.*, ***157B****(1985) 95*

$$W_g(U,n,e_g) = \frac{1}{p^2 \hbar^3 c^2} e_g^2 \, s_g^{inv}(e_g) \frac{\sum_{k=n-2}^{n} b(k \rightarrow n, e_g)\, w_{res}(p,h,U)\Big|_{p+h=k}}{w_{comp}(p,h,E)}$$

EXCITON MODEL

Initial condition: $P(n,t=0)=d_{n,n0}$

$$-P(n,t=0)= l^{+}(n-2)t(n-2,t)+l^{-}(n+2)t(n+2,t)-\left[l^{+}(n)+l^{-}(n)+W(n)\right]t(n,t)$$

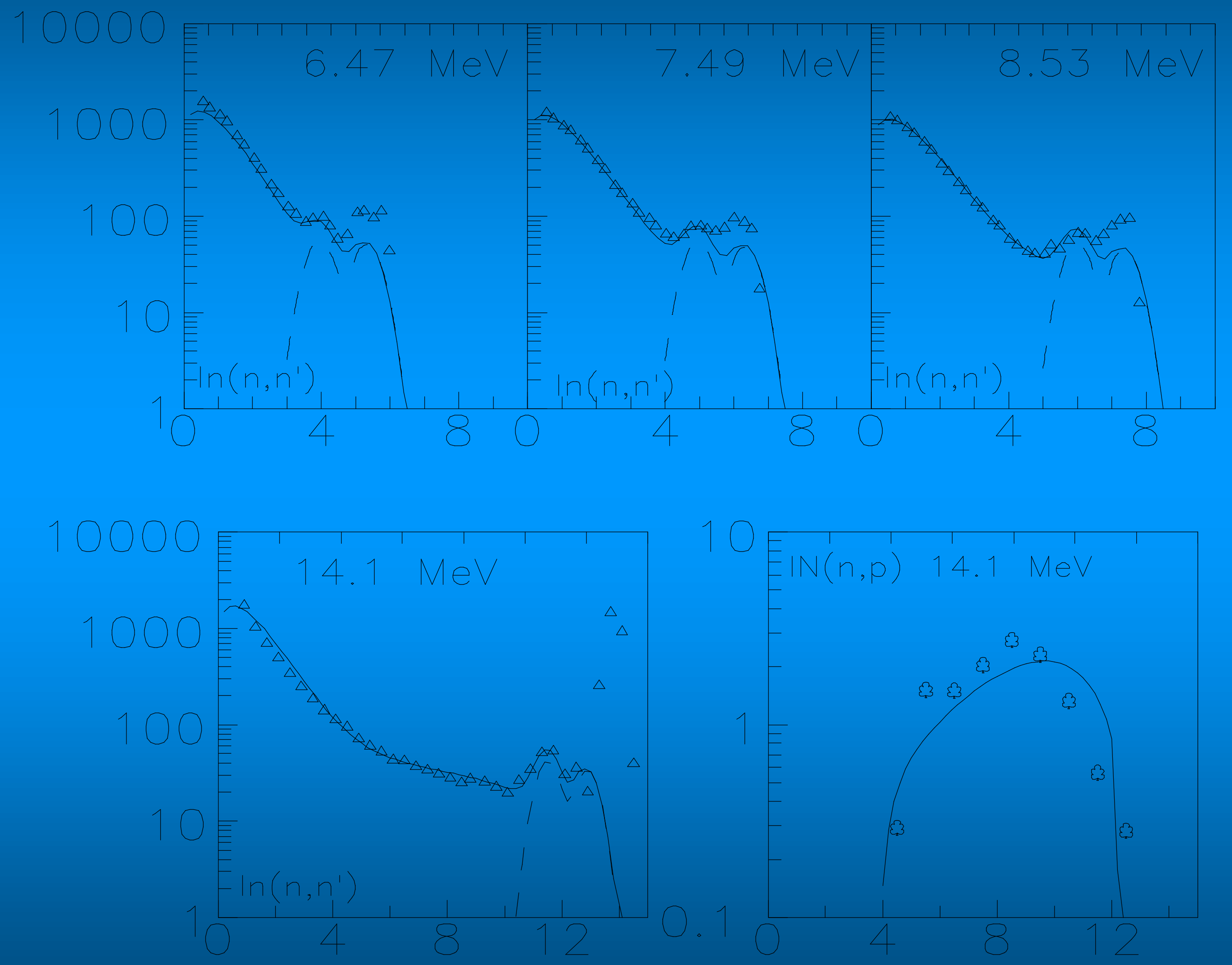
Emission spectra :

$$\frac{ds_{ab}}{de_{b}}(e_{b})=s_{ab}^{reacc}(E_{inc})D_{ab}(E_{inc})\sum_{n=1}^{n_{equil}}W_{b}(U,n,e_{b})t(n)$$

Depletion factor :

$$\mathrm{D}_{\mathrm{ab}}(E_{inc})=1-\frac{s_{ab}^{dir}(E_{inc})}{s_{ab}^{reacc}(E_{inc})}$$

EXCITON MODEL



EXCITON MODEL + spin

$$\begin{aligned}\frac{dP(E,J,n,t)}{dt} &= P(E,J,n-2,t)\lambda^{+}(E,J,n-2)\\ &+ P(E,J,n+2,t)\lambda^{-}(E,J,n+2)\\ &+ P(E,J,n,t)\left[\lambda^{+}(E,J,n)+\lambda^{-}(E,J,n)+L(E,J,n)\right]\\ &+ \sum_{J',n',x}\int P(E',J',n',t)\lambda_{x}\left(\left[E',J',n'\right]\rightarrow[E,J,n]\right)d\varepsilon\end{aligned}$$

$$\lambda^{+}(n)=\frac{2\pi}{\eta}\left\langle M^{2}\right\rangle\frac{g^{3}\left[U-A^{W}(p,h)\right]^{2}}{2(n+1)}$$

$$\lambda^{\pm}(E,J,n)=\frac{2\pi}{\hbar}|M|^{2}Y_{n}^{\downarrow}X_{nJ}^{\downarrow}$$

$$\frac{dP}{dt}(n,t)=l^{+}(n-2)P(n-2,t)+l^{-}(n+2)P(n+2,t)-\left[l^{+}(n)+l^{-}(n)+W(n)\right]P(n,t)$$

EXCITON MODEL + spin

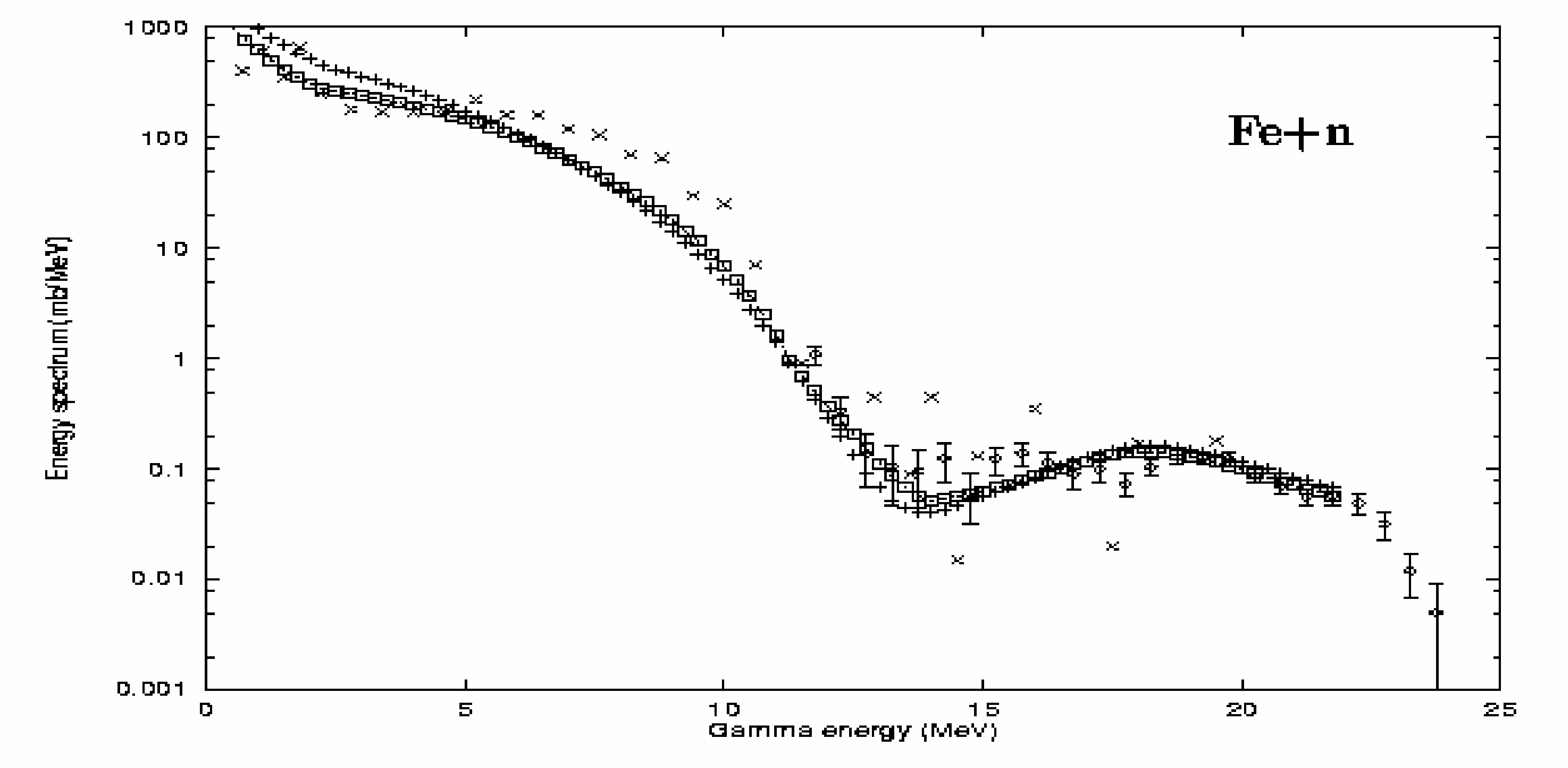
Emission rates :

$$\lambda_{\pi,\nu}([E,J,n] \rightarrow [U,S,n-1]) = \frac{1}{h}\frac{\omega(n-1,U,S)}{\omega(n,E,J)}\Re_{\pi,\nu}(n)\sum_{j=|S-1/2|}^{S+1/2}\sum_{l=|J-j|}^{J-j} T_l(\varepsilon),$$

Emission spectra :

$$\frac{d\sigma_x}{d\varepsilon_x} = \sum_{J_c,J_r,n}\int \sigma(E_c,J_c)\tau(E_c,J_c,n)\lambda_x([E_c,J_c,n] \rightarrow [E_r,J_r,n-1])\,dE_r\,.$$

ROLE OF SPIN IN PE calculations



- Betak E., Acta Physica Slovaca 45 (1995) 625

HYBRID MC SIMULATION (*HMS*)

Blann M., *Phys.Rev.C.* ***54****(1996) 1341, "New precompound decay model"*

This work addresses a new formulation for precompound decay processes in nuclear reactions, made to reduce inconsistencies and limitations of earlier models. To date, precompound formulations have relied upon a summation over assumed populations based on a sequence of few quasiparticle (''exciton'') partial state densities [1–3]. It was shown that the first exciton density of the summation used for nucleon induced reactions (three exciton) followed consistently from a consideration of nucleon-nucleon scattering kinematics in nuclear matter [4]. But Bisplinghoff [5] clearly demonstrated for all existing precompound decay formulations that the use of higher order partial state densities was inconsistent with the results expected by consistent folding over the assumed two body scattering processes.

DDHMS: Blann M., Chadwick M., *Phys.Rev.C.* ***57****(1998) 233*

[5] Bisplinghoff J., *Phys.Rev.C.* ***33****(1986) 1569*

HYBRID MC SIMULATION (*HMS)*

Advantages :

- It avoids multi-exciton level densities *(as critiziced by Bisplinghoff)*
- No physical limit on the number of preequilibrium emissions
- Provides complete set of observables, including DDCS, cross sections for productions of the residuals and spectra of recoils.
- Spin and excitation-energy dependent population of residual nuclei could be obtained, allowing for an easy coupling to the CN model

BASED on HYBRID MODEL: Blann M., *Phys.Rev.Lett.* ***27****(1971) 337; Phys.Rev.Lett.* ***28****(1972) 757*

HYBRID MC SIMULATION (*HMS*)

The calculation flow in the DDHMS model can be summarized in terms of the following steps:

1. draw collision partner for the incoming nucleon (2p-1h state created)
2. draw energy (ε) of the scattered nucleon (if bound go to step 5)
3. draw scattering angles for both particles
4. decide whether the scattered nucleon will be emitted, re-scattered or trapped
   (a) if emitted appropriate cross section is augmented
   (b) if re-scatters additional particle-hole is created and we return to step 2
   (c) if trapped leave it and go to step 5
5. draw excitation energy of a particle in the remaining 1p-1h configuration (between $0 \div (U - \varepsilon)$), if unbound go to step 3, if bound choose another existing 1p-1h pair and repeat step 5.

HYBRID MC SIMULATION (*HMS*)

For choosing a collision partner it is assumed that the unlike interaction is 3 times more probable than the like one ($\sigma_{np} = 3\sigma_{nn}$). Thus, for the incident neutron we have P_{nn} and P_{np} for the probability of exciting neutron and proton respectively

$$P_{nn} = \frac{(A-Z)}{(A-Z)+3Z},$$

$$P_{np} = 1 - P_{nn}$$

and similarly for the incident proton

$$P_{pp} = \frac{Z}{Z+3(A-Z)},$$

$$P_{pn} = 1 - P_{pp}.$$

HYBRID MC SIMULATION (*HMS*)

Energy distribution ⇒

$$P(\varepsilon)d\varepsilon = \frac{\rho_{n-1}(E-\varepsilon)g}{\rho_n(E)}d\varepsilon$$

$$\rho_2(E) = \frac{g(gV)}{2} \quad if \quad E > V,$$

$$\rho_2(E) = \frac{g(gE)}{2} \quad if \quad E \leq V,$$

$$\rho_3(E) = \frac{g^3[V(2E-V)]}{4} \quad if \quad E \geq V.$$

$$T_3(\varepsilon',E) = \int_{\varepsilon=0}^{\varepsilon'} \frac{\rho_2(E-\varepsilon)g\, d\varepsilon}{\rho_3(E)}$$

$$T_2(\varepsilon',U) = \int_{\varepsilon=0}^{\varepsilon'} \frac{g^2 d\varepsilon}{\rho_2(U)}$$

V is the potential well depth

HYBRID MC SIMULATION (*HMS*)

Emission probability

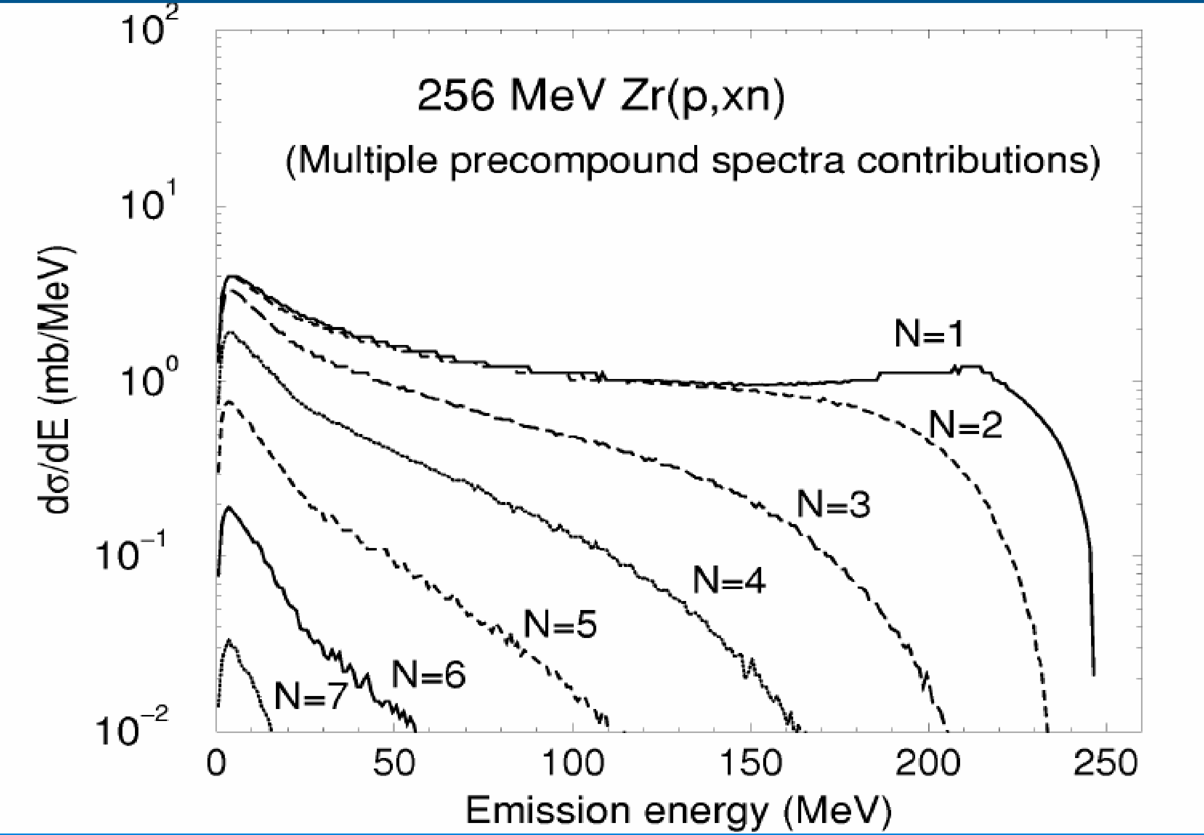
$$P_v(\varepsilon - Q) = \frac{\lambda_c(\varepsilon - Q)}{\lambda_c(\varepsilon - Q) + \lambda_+(\varepsilon)},$$

Particle emission rate

$$\lambda_c(\varepsilon - Q) \sim \frac{\sigma_v(\varepsilon - Q)(\varepsilon - Q)(2S+1)\mu_v}{g}.$$

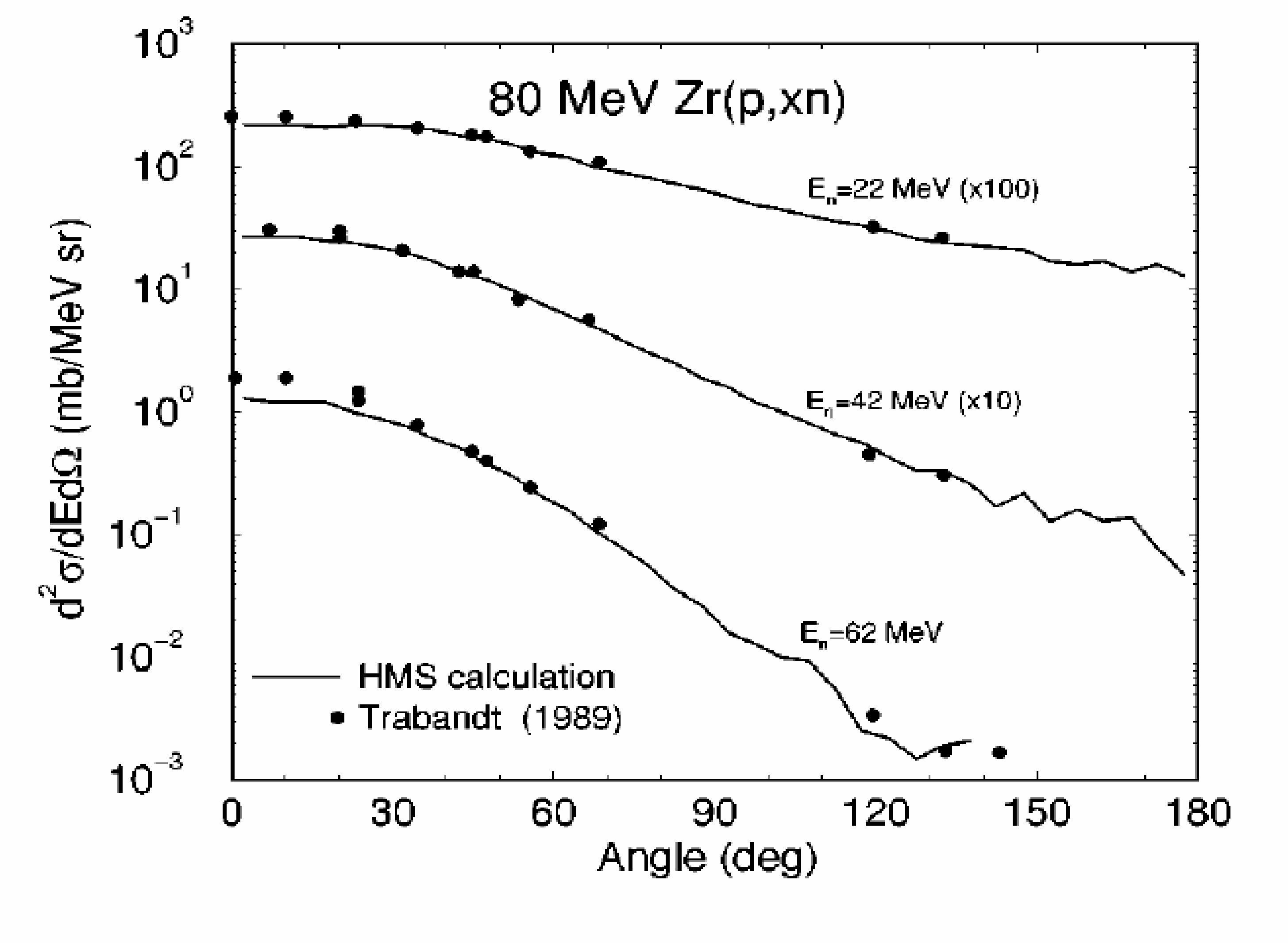
being Q – the binding energy, S – spin, g - sp density

HYBRID MC SIMULATION (*HMS*)

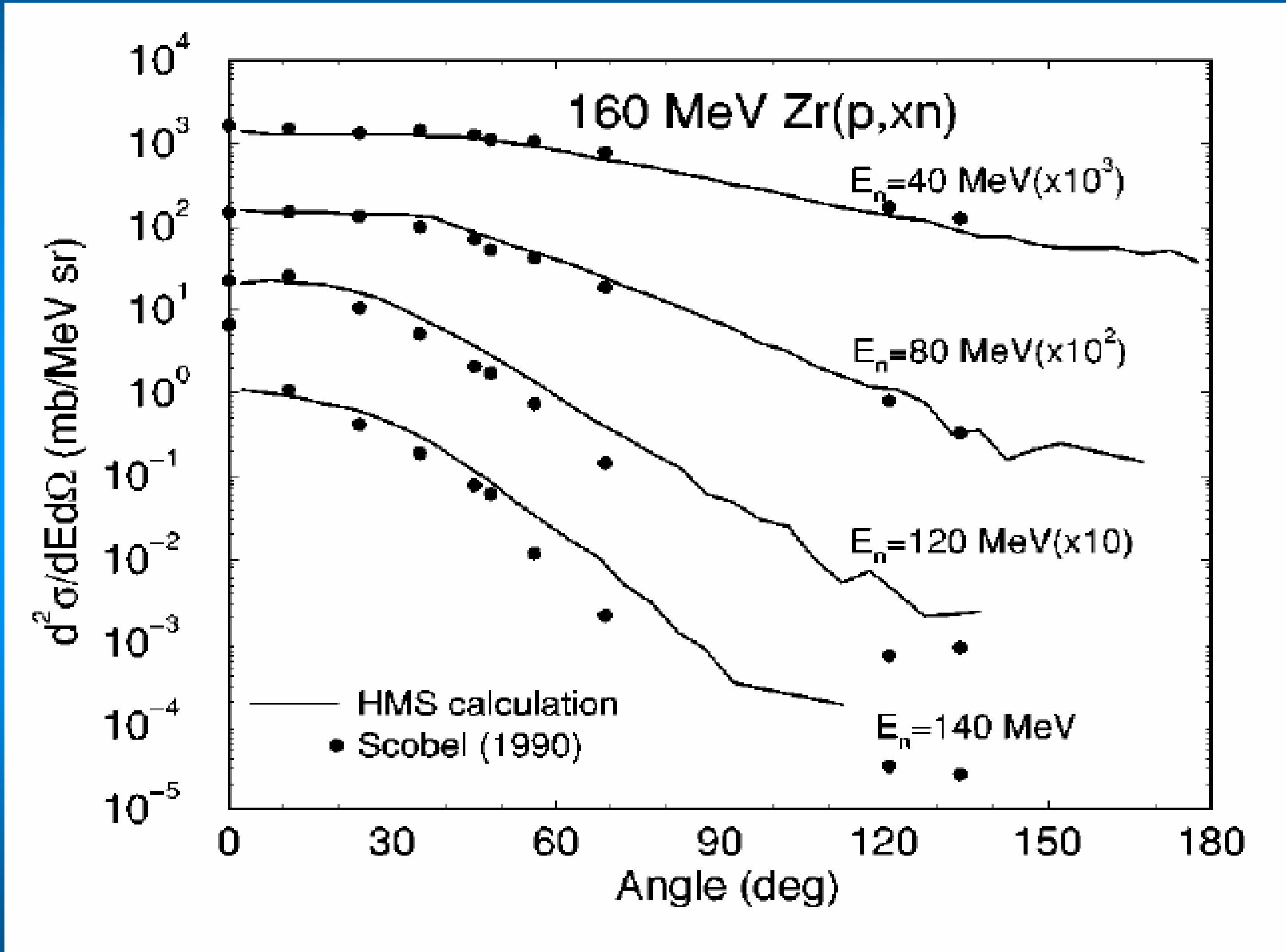


We would emphasize that the "$N=$" numbers in Fig. 1 do not represent exciton numbers in terms of older exciton models; all emissions in the HMS model are treated with respect to $2p1h$ or $1p1h$ configurations. The "$N=$" numbers represent only the fact that there have been $N-1$ precompound nucleons emitted prior to the one for which the spectrum is being shown.

HYBRID MC SIMULATION (*HMS*)



HYBRID MC SIMULATION (*HMS*)



Quantum-Mechanical theories : SMD/SMC

Dr. Mike Herman, BNL, USA

EMPIRE NON-EQUILIBRIUM MODELS

To avoid double-counting when combining different models EMPIRE applies the following priorities:

ECIS provides inelastic scattering to collective levels independently of settings for the remaining models.

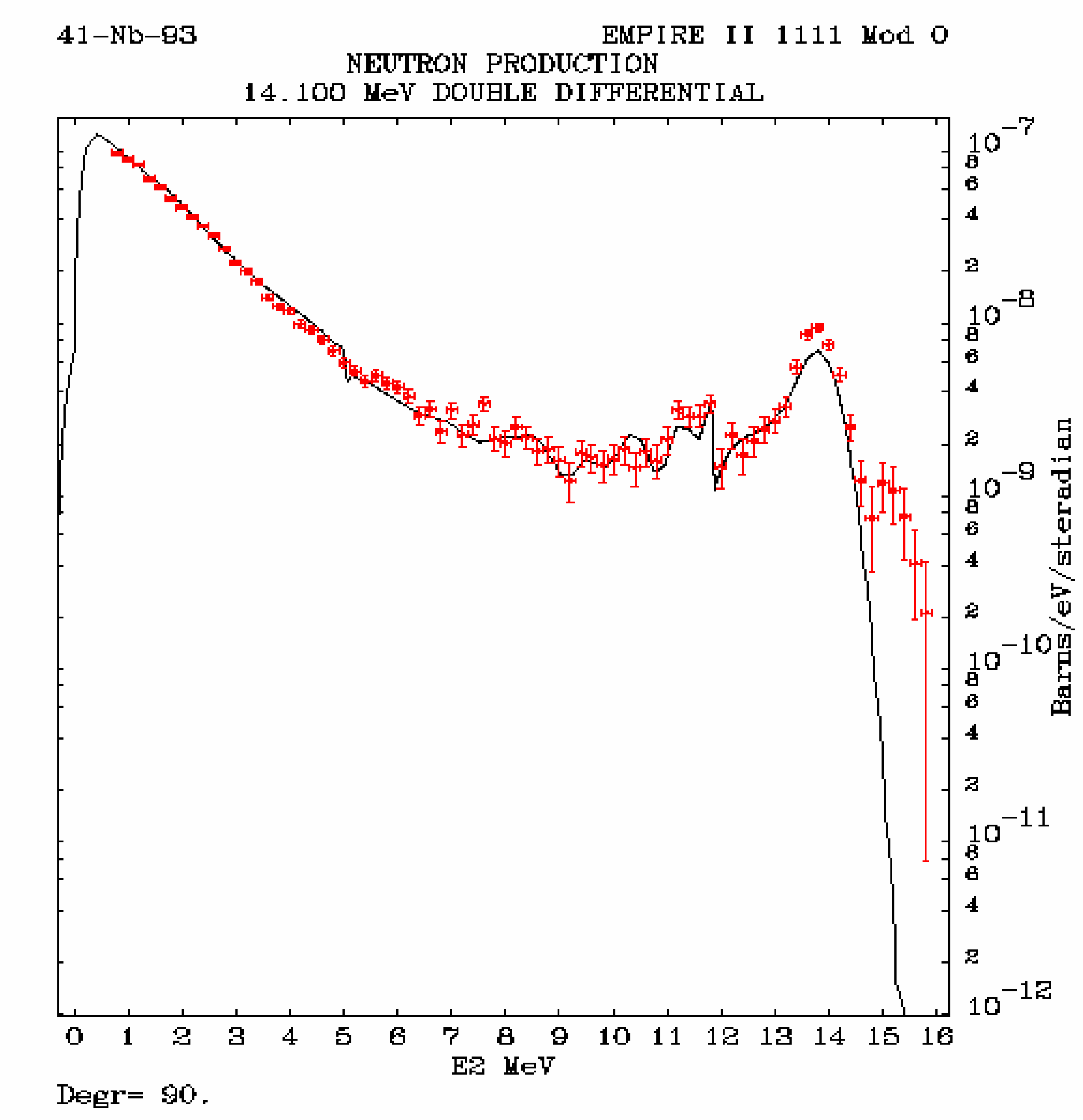
MSD provides inelastic continuum independently of other settings. Inelastic to the discrete levels is suppressed if ECIS is active. Note the provision for the second-chance preequilibrium emission after MSD.

MSC results are taken for the inelastic and charge-exchange to the continuum if not suppressed by use of DEGAS or HMS.

DEGAS provides inelastic and charge-exchange to the continuum and to discrete levels if MSD and MSC are not active. Otherwise, only the charge-exchange contribution is used. Gamma emission is used if not provided by the MSC.

HMS provides inelastic and charge-exchange to the continuum and to discrete levels if MSD and MSC are not active. Otherwise only the charge-exchange contribution is used. Suppresses DEGAS results for particle emission if DEGAS is active. Does not provide γ-rays, thus DEGAS or MSC results are taken.

PCROSS provides inelastic and charge-exchange to the continuum if MSD and MSC are not active. Provides **alpha and light ion emission** to the continuum and PE **gamma emission** (if not MSC)


41-Nb-93
EMPIRE II 1111 Mod 0
NEUTRON PRODUCTION
14.100 MeV DOUBLE DIFFERENTIAL
E2 MeV
Barns/eV/steradian
Degr= 90.

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Trieste, Febr.2004

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