



the
abdus salam
international centre for theoretical physics

ICTP 40th Anniversary

SMR.1555 - 23

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

16 February - 12 March 2004

Level Densities

**Mike HERMAN
National Nuclear Data Center
Building 197D
Brookhaven National Laboratory
Upton, NY 11973
U.S.A.**

These are preliminary lecture notes, intended only for distribution to participants

EMPIRE-II level densities

M.Herman

Brookhaven National Laboratory

e-mail: mwherman@bnl.gov

Contents

- general introduction
- Fermi gas model
- Gilbert-Cameron model
- EMPIRE-specific level densities
- parameter systematics
- microscopic Hartree-Fock-BCS approach
- sensitivity of HF calculations to level densities
- fitting discrete levels
- recommendations

Fermi gas model

Density of nuclear levels increases exponentially with increasing energy => Bethe formula derived from the Fermi Gas model

$$\rho(U) = \frac{\sqrt{\pi}}{12a^{1/4}U^{5/4}} \exp(2\sqrt{aU})$$

$$\rho(U, J) = \frac{2J + 1}{2\sqrt{2\pi}\sigma^3} \rho(U) \exp\left[-\frac{(2J + 1/2)^2}{2\sigma^2}\right]$$

where

$a = \pi^2 g/6$ - level density parameter (g single-particle density at Fermi energy)

σ - spin cut-off parameter

Fermi gas model

State equations in the Fermi gas model

$$U = at^2 \quad \text{EXCITATION ENERGY}$$

$$S = 2at \quad \text{ENTROPY}$$

$$\sigma^2 = \langle m^2 \rangle gt = \mathfrak{S}t \quad \text{SPIN-CUT-OFF}$$

$\langle m^2 \rangle$ - mean square of angular momentum projections for single-particle states around Fermi energy

\mathfrak{S} - moment of inertia

Pairing

Odd-even effect observed => accounted for introducing the effective excitation energy U

$$U = E_{exc} - \Delta_Z - \Delta_N \text{ FOR EVEN-EVEN}$$

$$U = E_{exc} - \Delta_Z \text{ FOR EVEN } Z$$

$$U = E_{exc} - \Delta_N \text{ FOR EVEN } N$$

$$U = E_{exc} \text{ FOR ODD-ODD}$$

Δ - phenomenological corrections for even-odd differences in nuclear binding energies

Experimental information

- neutron resonances => level density at neutron binding energy
- discrete levels => level densities at very low energies
- evaporation spectra => broad range of excitation energies but model dependent

Gilbert-Cameron level densities

- Constant temperature formula (up to U_x)

$$\rho_T(E) = \frac{1}{T} \exp[(E - \Delta - E_0)/T],$$

T - nuclear temperature, E - excitation energy ($E = U + \Delta$), E_0 - adjustable energy shift.

- Fermi gas formula (above U_x)

$$\rho_F(U) = \frac{\exp(2\sqrt{aU})}{12\sqrt{2}\sigma(U)a^{1/4}U^{5/4}}.$$

GC level densities (cont.)

- Spin cut-off factor $\sigma^2(U) = 0.146A^{2/3}\sqrt{aU}$.
- T , U_x , and E_0 , such that the level density and its derivative are continuous at the matching point $U_x \Rightarrow$

$$\frac{1}{T} = \sqrt{a/U_x} - \frac{3}{2U_x}.$$

- FITLEV option in EMPIRE \Rightarrow cumulative plots of discrete levels

GC level densities (cont.)

- a parameter
 - constant
 - Ignatyuk type

$$a(U) = \tilde{a} \left[1 + f(U) \frac{\delta W}{U} \right],$$

- δW - shell correction, \tilde{a} - asymptotic value of the a -parameter

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

GC level densities (cont.)

- three systematics for a available in EMPIRE:
 - Ignatyuk et al.
 - Arthur
 - Iljinov et al.
- **No collective effects in Gilbert-Cameron approach!**

EMPIRE-specific level densities

- Features:
 - Collective enhancements due to nuclear vibration and rotation.
 - Super-fluid model below critical excitation energy (GSF)
 - Fermi gas model above critical excitation energy (FG)
 - Rotation induced deformation (spin dependent) => moments of inertia

EMPIRE-specific lev. dens. (FG)

- Prolate nuclei

$$\rho(E, J, \pi) = \frac{1}{16\sqrt{6\pi}} \left(\frac{\hbar^2}{\mathfrak{S}_{\parallel}} \right)^{\frac{1}{2}} a^{1/4} \sum_{K=-J}^J \left(U - \frac{\hbar^2 K^2}{2\mathfrak{S}_{eff}} \right)^{-\frac{5}{4}} \exp \left\{ 2 \left[a \left(U - \frac{\hbar^2 K^2}{2\mathfrak{S}_{eff}} \right) \right]^{\frac{1}{2}} \right\}.$$

EMPIRE-specific lev. dens. (FG)

- Oblate nuclei

$$\rho(E, J, \pi) = \frac{1}{16\sqrt{6\pi}} \left(\frac{\hbar^2}{\mathfrak{S}_{\parallel}} \right)^{\frac{1}{2}} a^{1/4} \sum_{K=-J}^J \left(U - \frac{\hbar^2 [J(J+1) - K^2]}{2|\mathfrak{S}_{eff}|} \right)^{-\frac{5}{4}} \exp \left\{ 2 \left[a \left(U - \frac{\hbar^2 [J(J+1) - K^2]}{2|\mathfrak{S}_{eff}|} \right) \right]^{\frac{1}{2}} \right\}.$$

EMPIRE-specific lev. dens.(FG)

K - spin projection,

\mathfrak{S}_{eff} - effective moment of inertia

defined in terms of perpendicular \mathfrak{S}_{\parallel} and parallel

\mathfrak{S}_{\perp} moments

$$\frac{1}{\mathfrak{S}_{eff}} = \frac{1}{\mathfrak{S}_{\parallel}} - \frac{1}{\mathfrak{S}_{\perp}}.$$

EMPIRE-specific lev. dens. (FG)

- Rotational enhancement automatically taken into account.
- Vibrational enhancement

$$K_{vib} = \exp \left\{ 1.7 \left(\frac{3m_0 A}{4\pi h^2 S_{drop}} \right)^{2/3} T^{4/3} \right\}$$

with $S_{drop} = 17/4\pi r_0^2$ and $r_0 = 1.26$.

- Rotational and vibrational enhancements are damped with increasing energy

Super-fluid (GSF) lev. dens.

- Used below critical energy
- pairing gap $\Delta = 12/\sqrt{A}$
- critical temperature T_{crt} is $T_{crt} = 0.567\Delta$

Super-fluid (BCS) lev. dens.

- The critical value of the level density parameter a is determined by the iteration procedure

$$a_{crt}^{(0)} = \tilde{a} (1 + \gamma \delta_W)$$

$$U^{(n)} = a_{crt}^{(n)} T_{crt}^2$$

$$a_{crt}^{(n+1)} = \tilde{a} \left[1 + \frac{\delta_W}{U^{(n)}} \left(1 - \exp \left(-\gamma U^{(n)} \right) \right) \right]$$

\tilde{a} is the asymptotic value of a

Super-fluid (GSF) lev. dens.

Critical values of relevant quantities

$$E_{cond} = 1.5a_{crt}\Delta^2/\pi^2$$

$$U_{crt} = a_{crt}T_{crt}^2 + E_{cond}$$

$$Det_{crt} = \left(\frac{12}{\sqrt{\pi}}\right)^2 a_{crt}^3 T_{crt}^5$$

$$S_{crt} = 2a_{crt}T_{crt}$$

Super-fluid (GSF) lev. dens.

At excitation energies below U_{crt} we define the parameter $\varphi = \sqrt{1 - U/U_{crt}}$, which allows to express all thermodynamical quantities in terms of their critical values

$$T = 2T_{crt}\varphi \ln^{-1} \left(\frac{\varphi + 1}{1 - \varphi} \right)$$

$$S = S_{crt}T_{crt}(1 - \varphi^2)/T$$

$$Det = Det_{crt}(1 - \varphi^2)(1 + \varphi^2)^2$$

Super-fluid (GSF) lev. dens.

The parallel and orthogonal moments of inertia below the critical temperature T_{crt} are

$$\mathfrak{S}_{\parallel}^{BCS} = \mathfrak{S}_{\parallel} T_{crt} (1 - \varphi^2) / T$$

and

$$\mathfrak{S}_{\perp}^{BCS} = \frac{1}{3} \mathfrak{S}_{\perp} + \frac{2}{3} \mathfrak{S}_{\perp} T_{crt} (1 - \varphi^2) / T$$

Super-fluid (GSF) lev. dens.

Using these results squares of the effective spin cut-off parameters are

$$\sigma_{eff}^2 = \mathfrak{S}_{\parallel}^{BCS} T \quad \text{for } \alpha_2 < 0.005 ,$$
$$\sigma_{eff}^2 = \left(\mathfrak{S}_{\parallel}^{BCS} \right)^{1/3} \left(\mathfrak{S}_{\perp}^{BCS} \right)^{2/3} T \quad \text{for } \alpha_2 > 0.005 ,$$

with α_2 ground state deformation.

Super-fluid (GSF) lev. dens.

$$\rho_{BCS}(U, J) = \frac{2J + 1}{2\sqrt{2\pi}\sigma_{eff}^3\sqrt{Det}} \exp\left(\frac{S - J(J + 1)}{2\sigma_{eff}^2}\right)$$

Correcting for rotational and vibrational effects in the non-adiabatic mode (i.e., including their damping with increasing temperature)

$$\rho(U, J) = \rho_{BCS}(U, J) Q_{rot}^{BCS} K_{rot} Q_{vib} K_{vib} .$$

Super-fluid (GSF) lev. dens.

The rotational enhancement is

$$K_{rot} = \mathfrak{S}_{\perp} T$$

and is damped with

$$Q_{rot}^{BCS} = 1 - Q_{rot} \left(1 - \frac{1}{\mathfrak{S}_{\perp} T} \right),$$

EMPIRE-specific a-param.

(i) EMPIRE-specific:

- a energy dependent following Ignatyuk et al.

$$a(U) = \tilde{a} \left[1 + f(U) \frac{\delta_W}{U} \right]$$

with

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

δ_W being the shell correction

EMPIRE-specific a -param.

and \tilde{a} the asymptotic value of the a -parameter

$$\tilde{a} = \eta A + \zeta A^{2/3} F_{surf}(R_{max}/R_{min})$$

includes deformation dependent term F_{surf}

EMPIRE-specific systematics

- experimental values extracted from fitting D_{obs}
 - Nix-Moeller shell-corrections:

	$Z < 85$	$Z \geq 85$
$\eta =$	0.094431	$\eta =$ 0.117113
$\xi =$	-0.08014	$\xi =$ -0.09939
$\gamma =$	0.075594	$\gamma =$ 0.094447

EMPIRE-specific systematics

- Myers-Swiatecki shell-corrections:

	$Z < 85$	$Z \geq 85$
$\eta =$	0.052268	$\eta =$ 0.067645
$\xi =$	0.13395	$\xi =$ 0.173358
$\gamma =$	0.093955	$\gamma =$ 0.121465

Use of EMPIRE-specific systematics

- EMPIRE-specific systematics built into the code
- 'local systematics' created during calculations
- spin => deformation => moments of inertia => rotational enhancement and spin distribution of lev. dens.
- automatic adjustment to discrete levels
(needs checking)

Other variants of lev. dens.

(ii) fit to the shell-model s.p.s.:

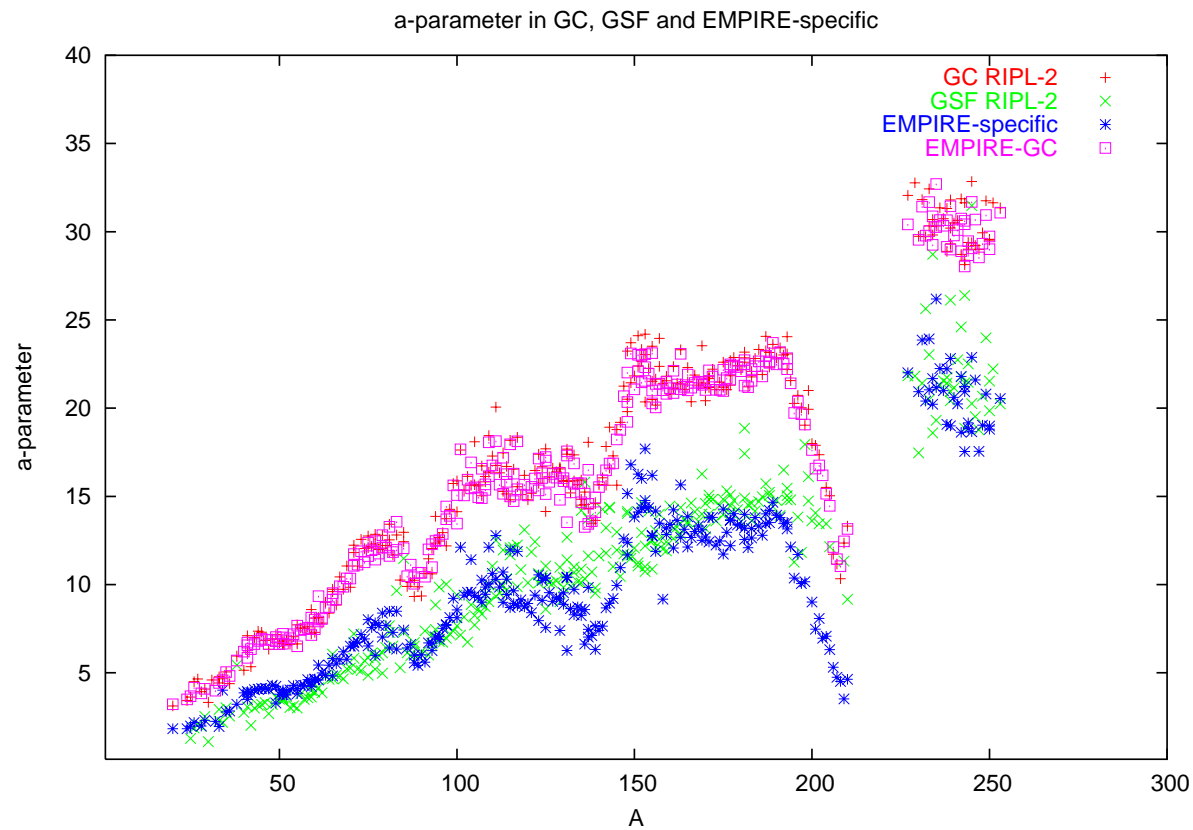
- energy dependent $a(U) = a_1 + a_2 e^{-a_3 U}$ fitted for about 4000 nuclei
- no adjustment to experimental data

(iii) $a = A/\text{constant}$:

- a is constant
- no adjustment to experimental data

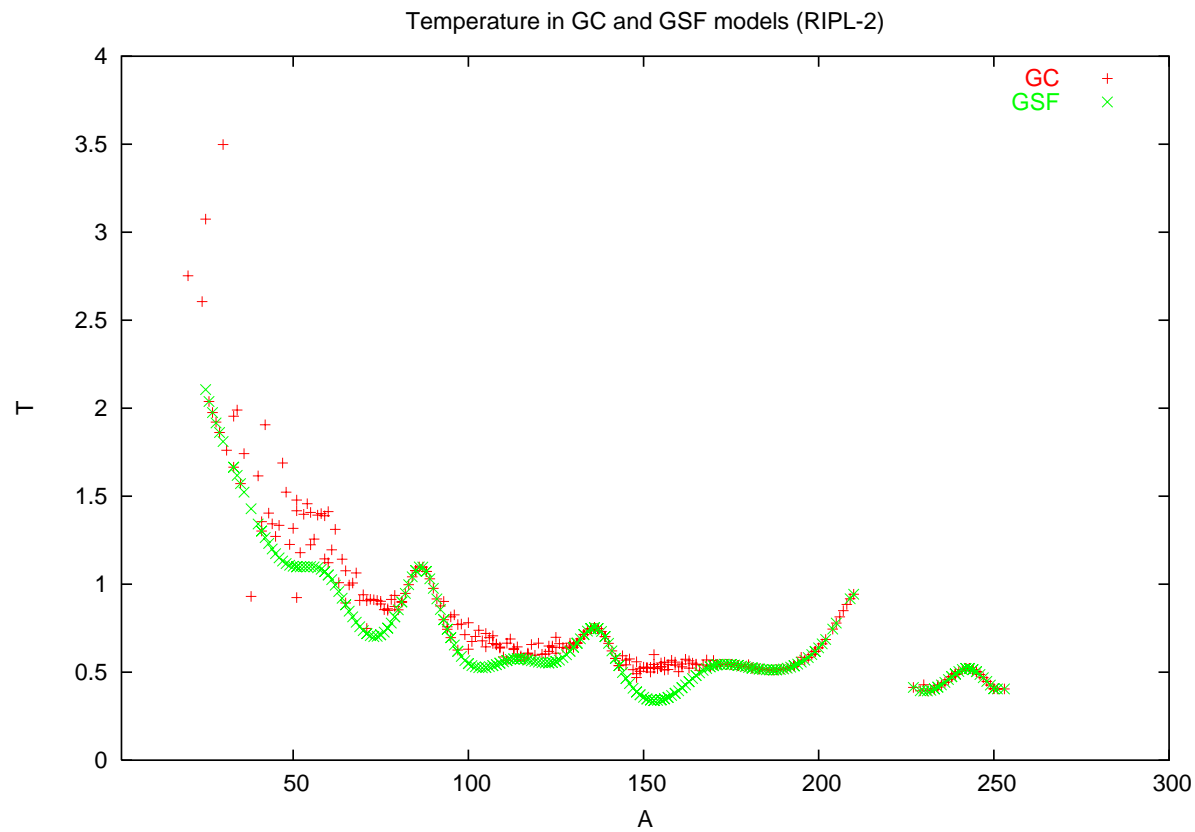
Level density parameters

Comparison of level density parameter a



Level density parameters

Comparison of nuclear temperature T



Hartree-Fock-BCS level densities

- More than 8000 nuclei calculated in the frame of the Hartree-Fock-BCS approach with consistent treatment of
 - shell corrections,
 - pairing correlations,
 - deformation effects and rotational enhancement.
- results re-normalized to the experimental s-wave neutron resonance spacings and adjusted to the cumulative number of discrete levels

Hartree-Fock-BCS level densities

- Using the partition function method, the state density can be obtained as

$$\omega(U) = \frac{e^{S(U)}}{(2\pi)^{3/2} \sqrt{\text{Det}(U)}}$$

- Entropy S and excitation energy U derived from the summation over single particle levels
- Pairing correlations treated within the BCS theory in the constant- G approximation with blocking (single-particle energies replaced by their quasi-particle equivalents)

Hartree-Fock-BCS level densities

Spherical and deformed nuclei treated in a distinct mode

- spherical nuclei:

$$\rho_{sph}(U, J) = \frac{2J + 1}{2\sqrt{2\pi^3}} e^{-J(J+1)/(2\sigma^2)} \omega(U)$$

Hartree-Fock-BCS level densities

- deformed nuclei:

$$\rho_{def}(U, J) = \frac{1}{2} \sum_{K=-J}^J \frac{1}{\sqrt{2\pi\sigma^2}} \omega(U) \times e^{-[J(J+1)/(2\sigma_{\perp}^2) + K^2(1/\sigma^2 - 1/\sigma_{\perp}^2)]/2}$$

Hartree-Fock-BCS level densities

- spin cut-off parameters (σ and σ_{\perp}) are both affected by the pairing correlations, and σ_{\perp} is related to the perpendicular moment of inertia.
- rotational enhancement factor is included and has to be damped with the phenomenological function f_{dam}

$$f_{dam}(U) = \frac{1}{1 + e^{(U - E_{def})/dU}} \left[1 - \frac{1}{1 + e^{(\beta_2 - \beta^*)/d\beta}} \right]$$

Hartree-Fock-BCS level densities

HF-BCS level densities

$$\rho(U, J) = [1 - f_{dam}(U)] \rho_{sph}(U, J) + f_{dam}(U) \rho_{def}(U, J)$$

- single-particle schemes obtained using the Hartree-Fock method with MSk7 Skyrme type force were used in the calculations.
- final results adjusted to resonance spacings at the neutron binding energy and to the cumulative number of discrete levels by applying shift to the excitation energy and a multiplicative factor to the entropy.

Hartree-Fock-BCS level densities

- no further phenomenological adjustment needs to be performed by EMPIRE.
- level density tables contain numerical values for 30 spins and extend up to 150 MeV

HF-BCS versus Empire lev. dens.

Common to both approaches:

- use the BCS model at low energies
- rotational enhancement incorporated directly into the level density formula
- phenomenological damping of rotational effects
- deformation effects (in EMPIRE-specific these are also spin dependent)
- adjusted to the available experimental information

HF-BCS versus Empire lev. den.

EMPIRE-specific densities:

- include a vibrational enhancement factor
- use phenomenological a -parameter and closed formula

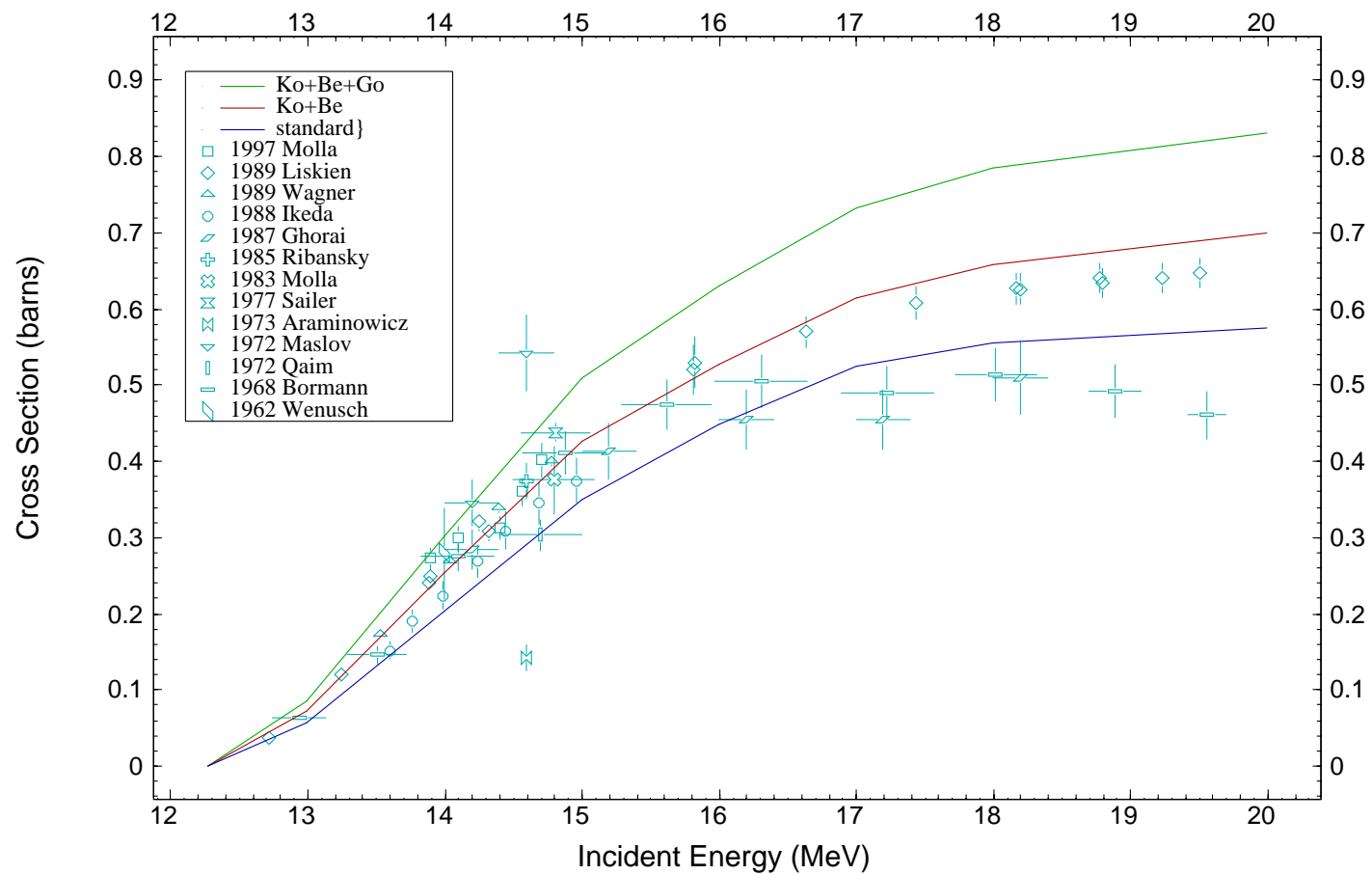
HF-BCS level densities

- derived directly from the microscopic single-particle schemes (expected to be more reliable away from valley of stability)

Effect of level densities

28-Nov-2001 15:08

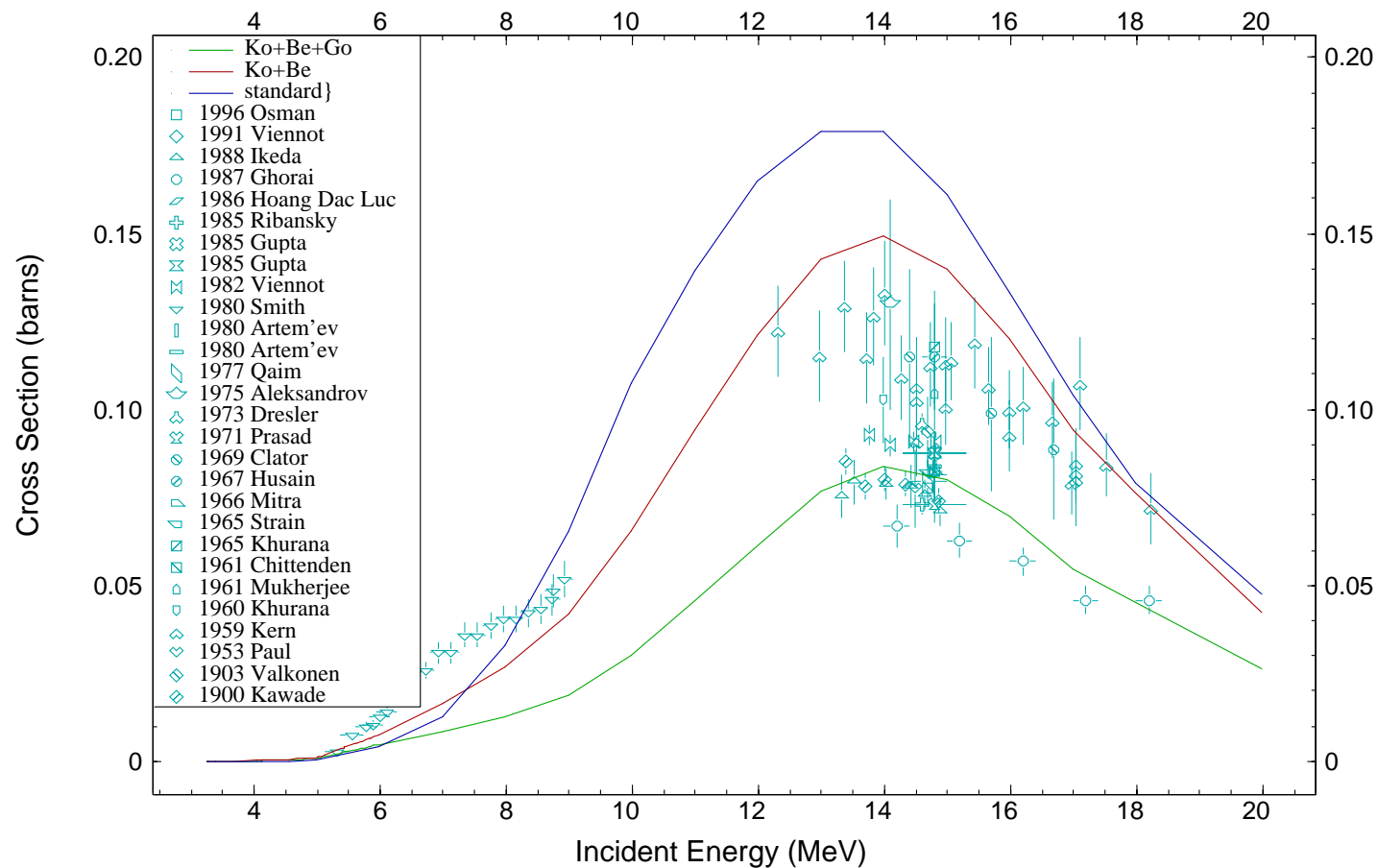
24-CR-52(N,2N),,SIG



Effect of level densities

28-Nov-2001 15:49

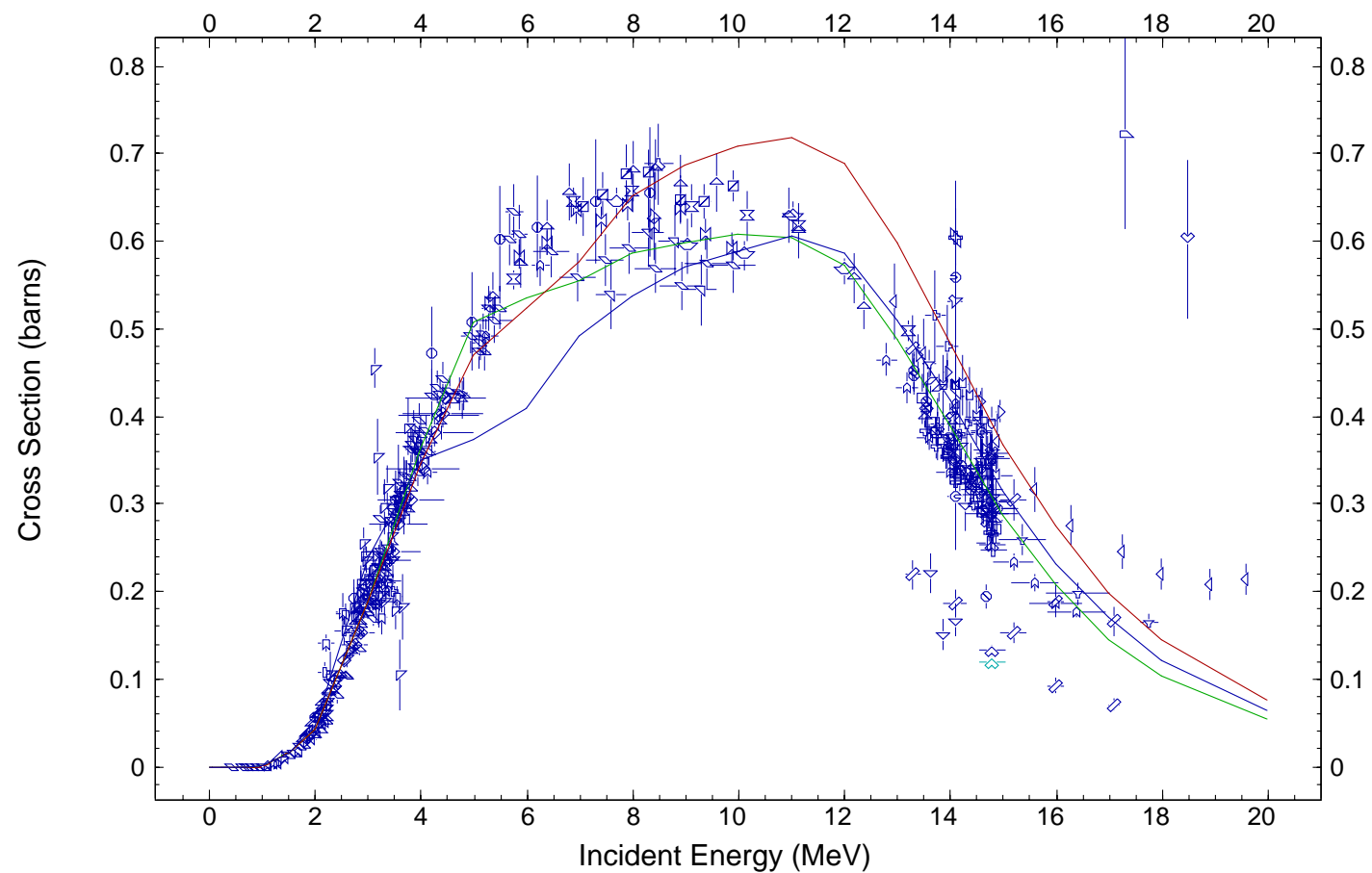
24-CR-52(N,P),,SIG



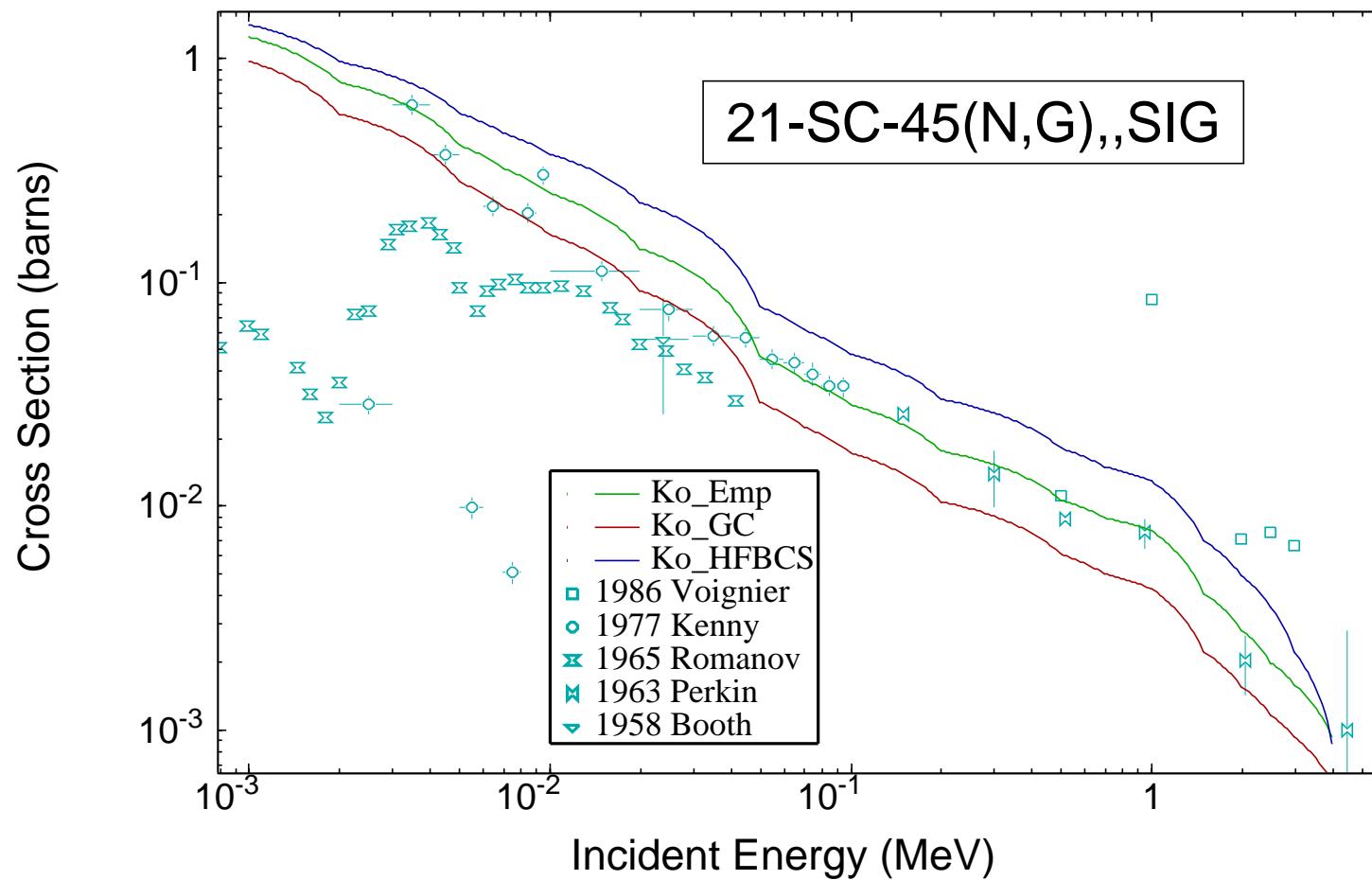
Effect of level densities

28-Nov-2001 15:53

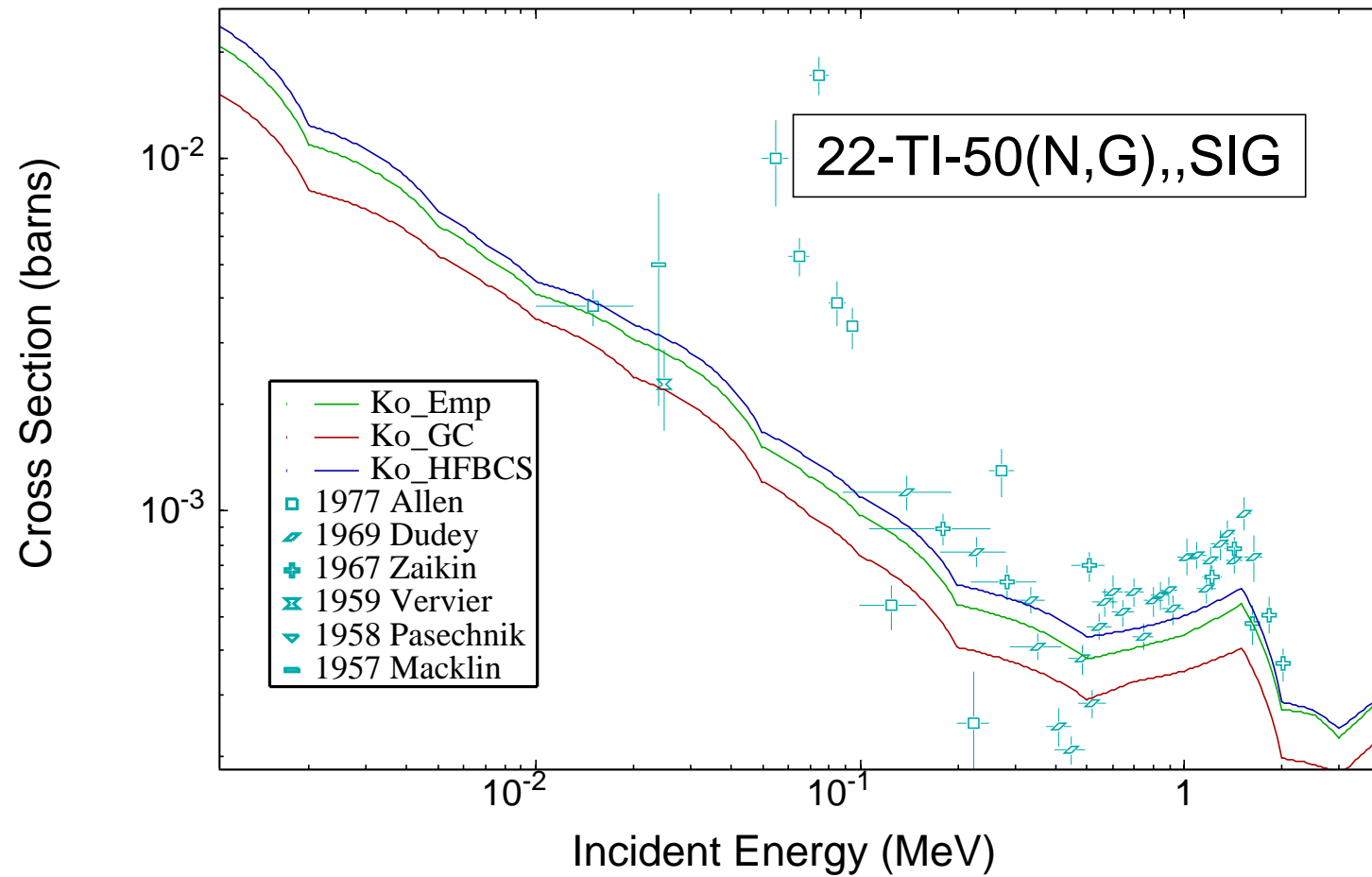
28-NI-58(N,P),,SIG



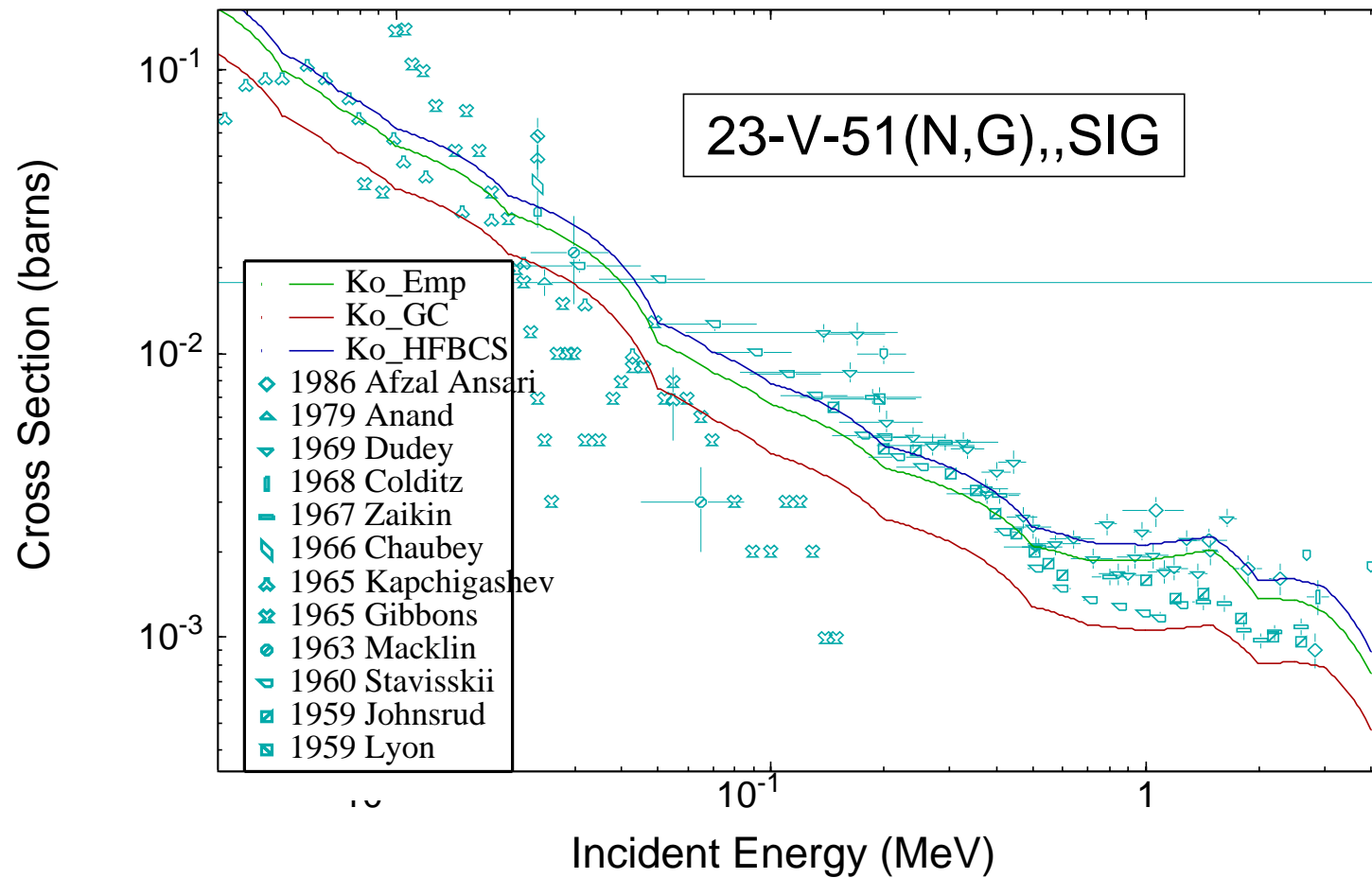
Effect of level densities



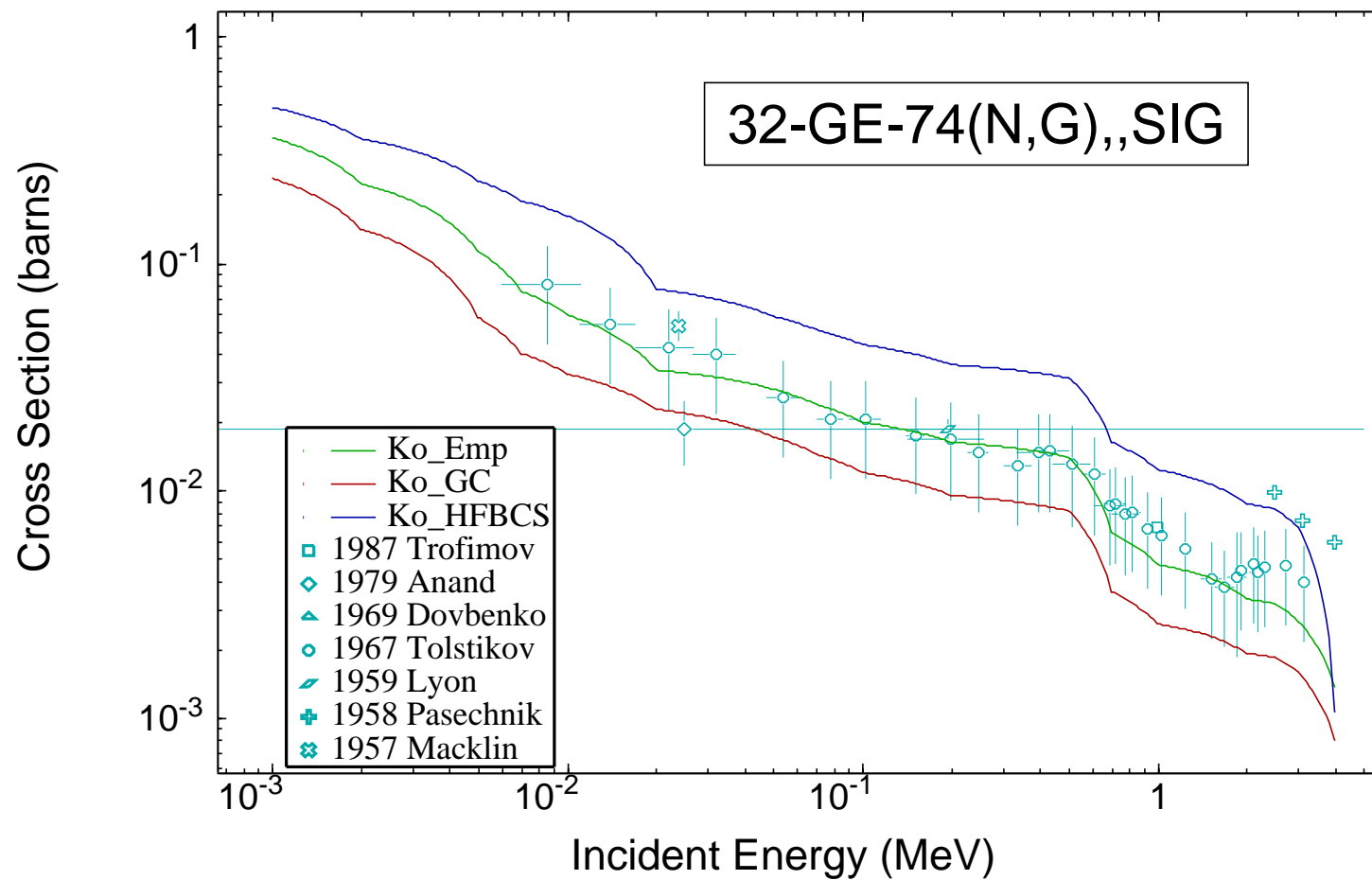
Effect of level densities



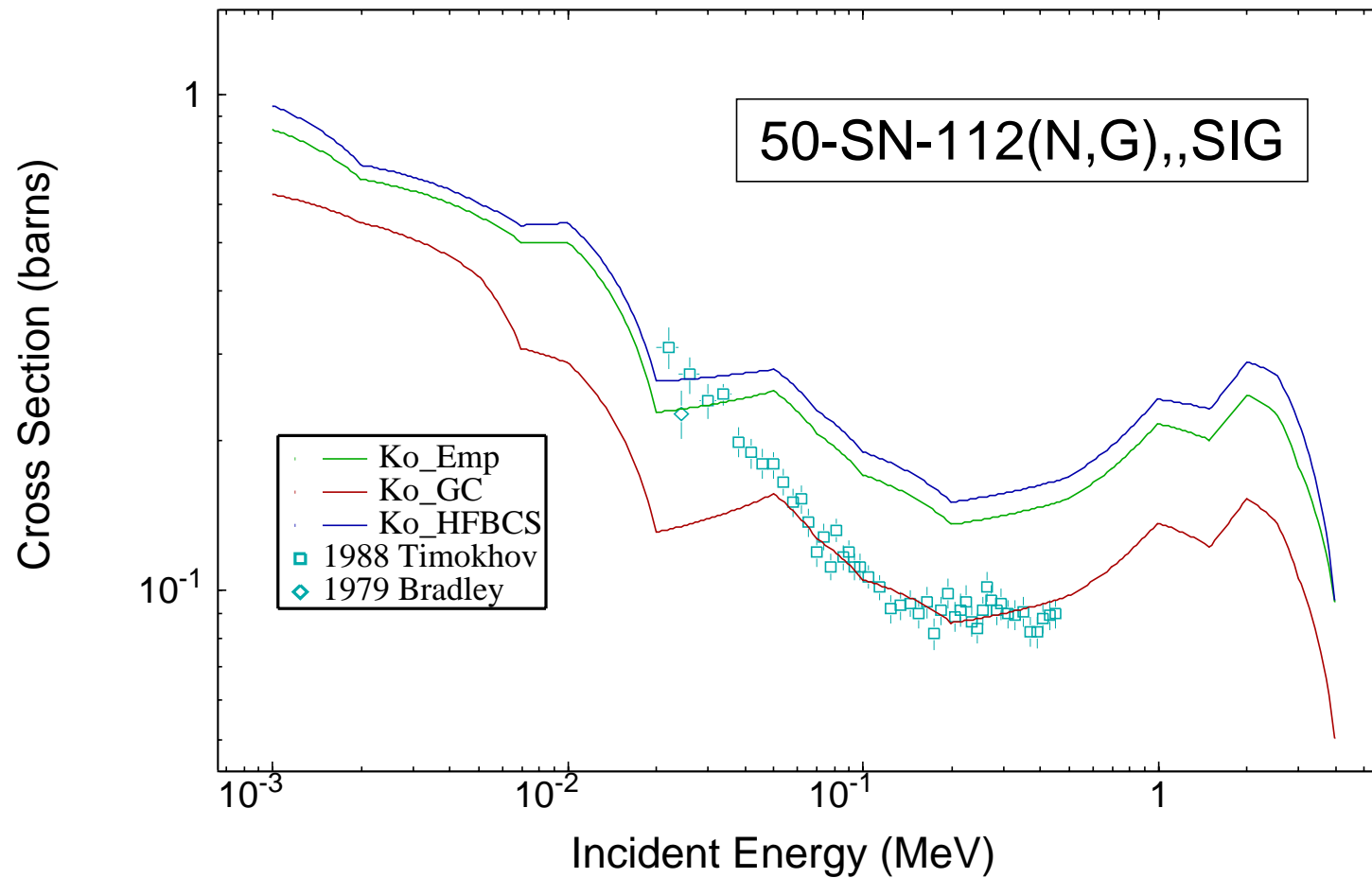
Effect of level densities



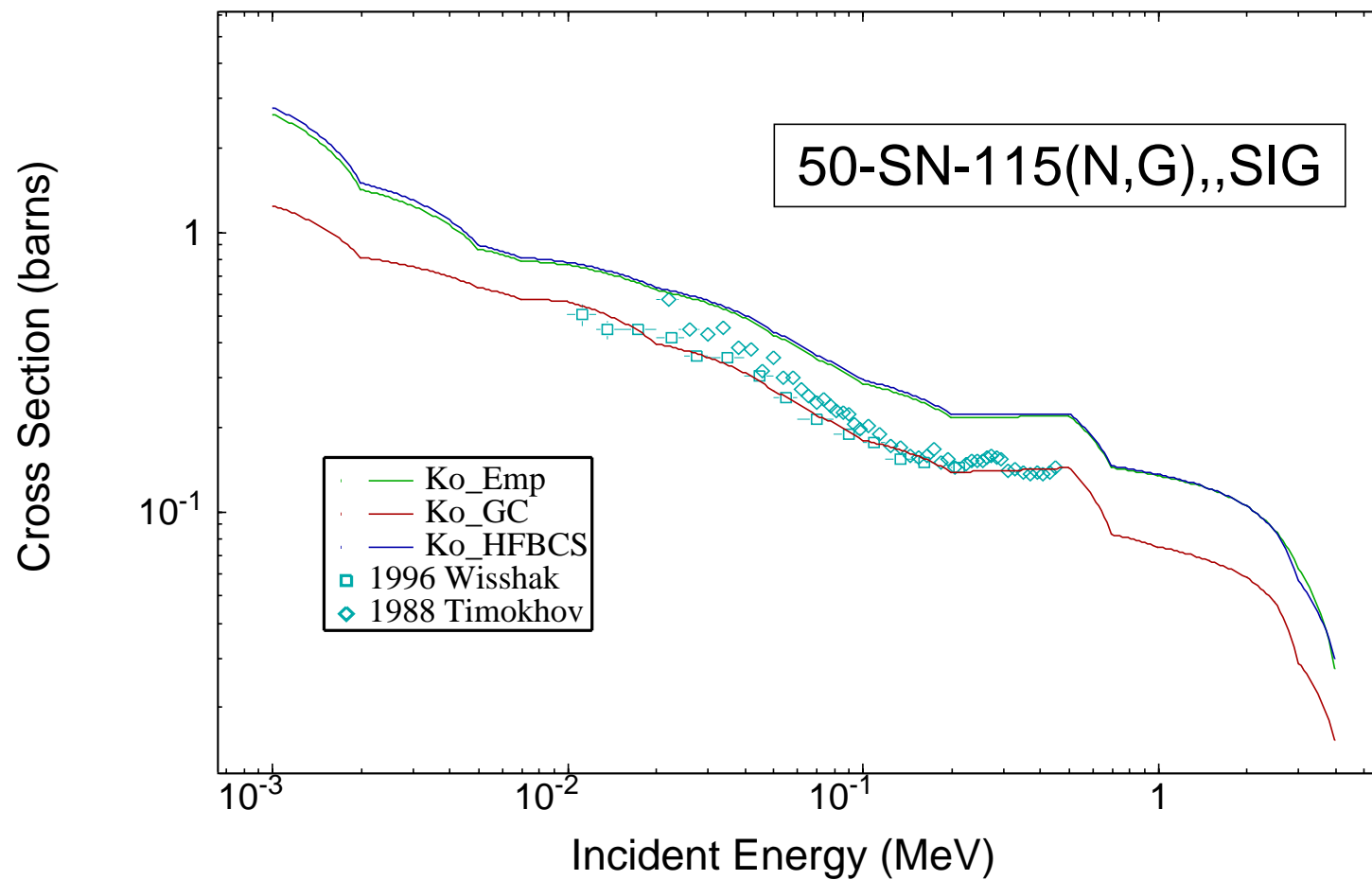
Effect of level densities



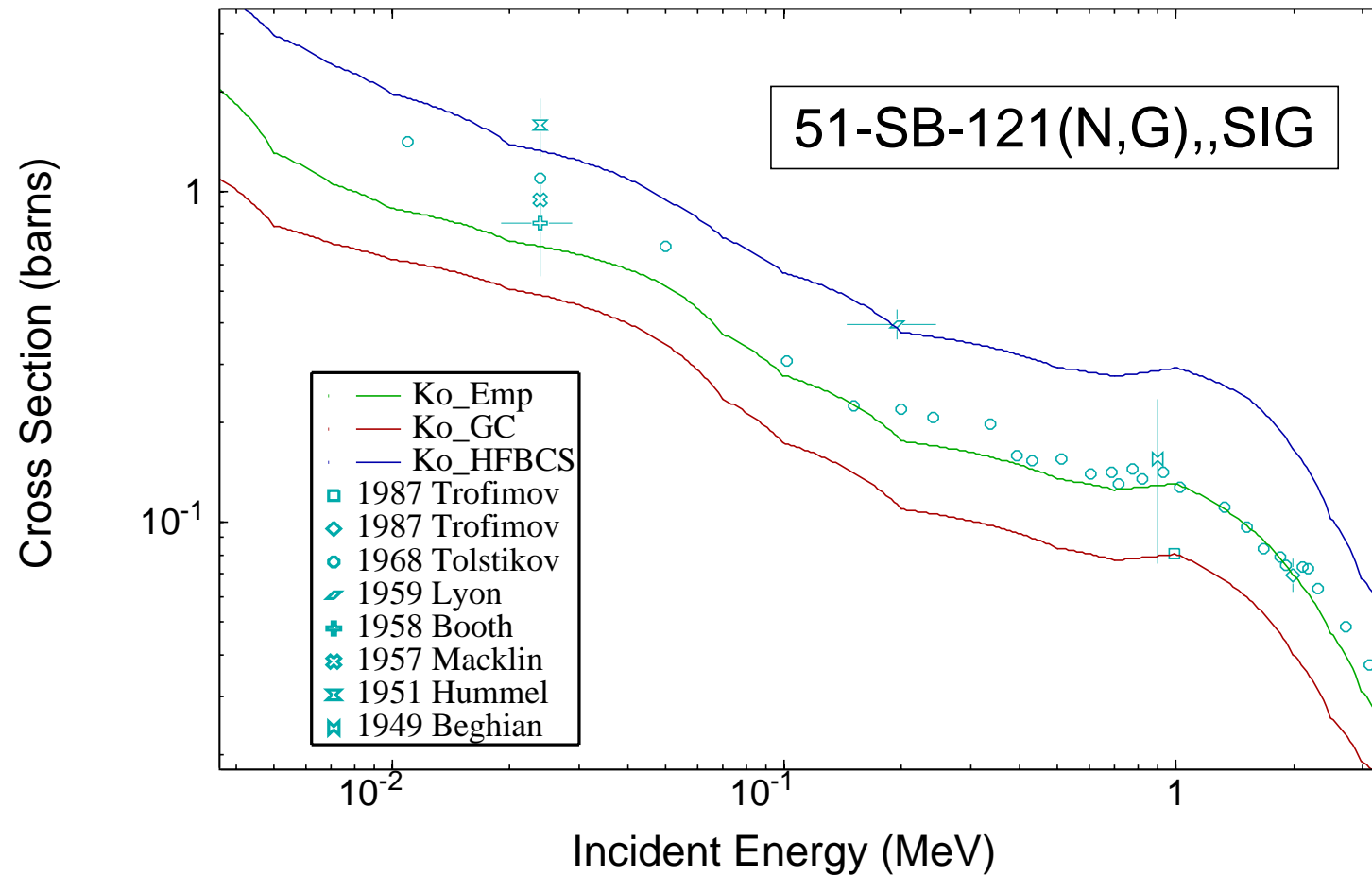
Effect of level densities



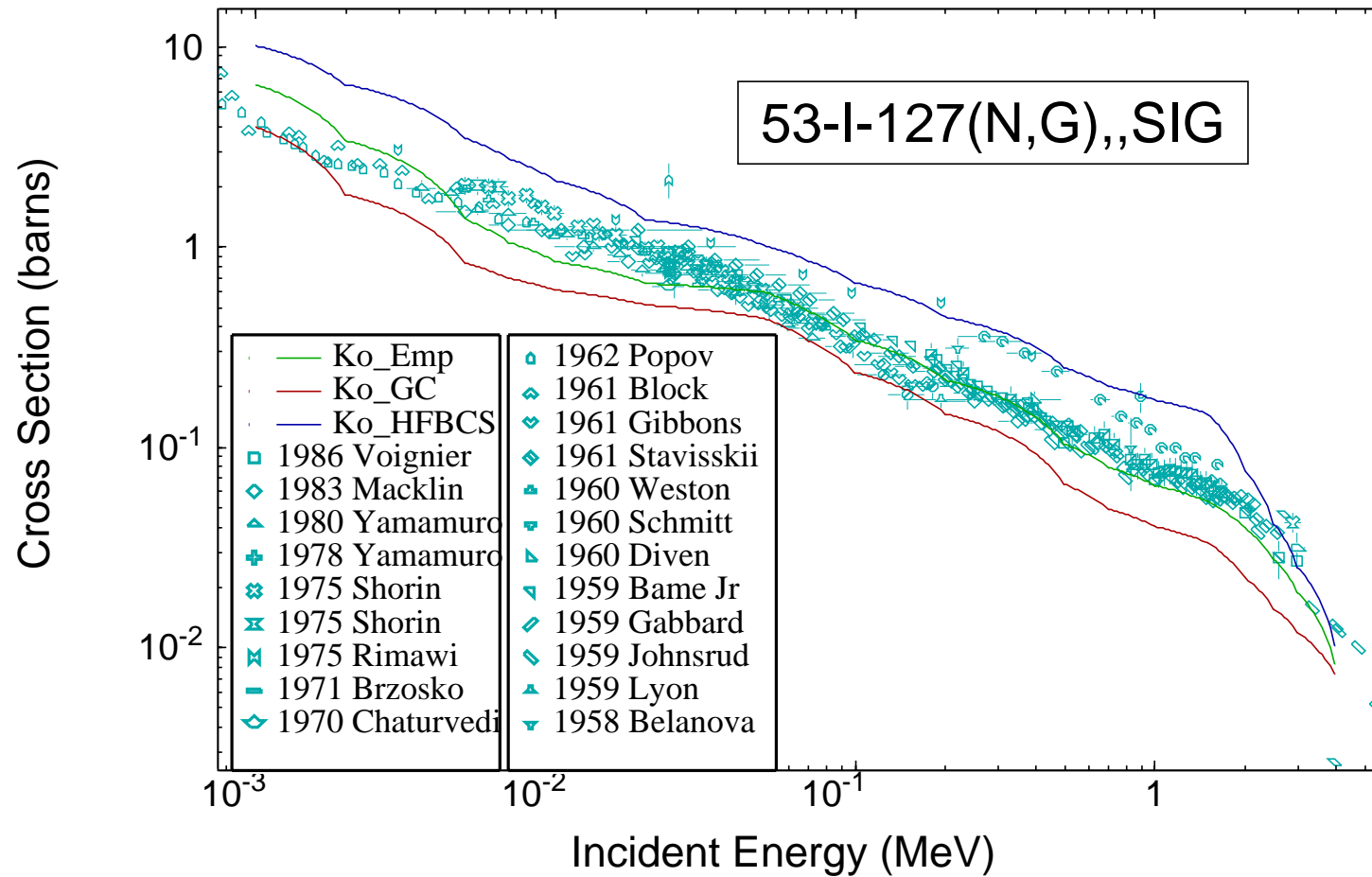
Effect of level densities



Effect of level densities

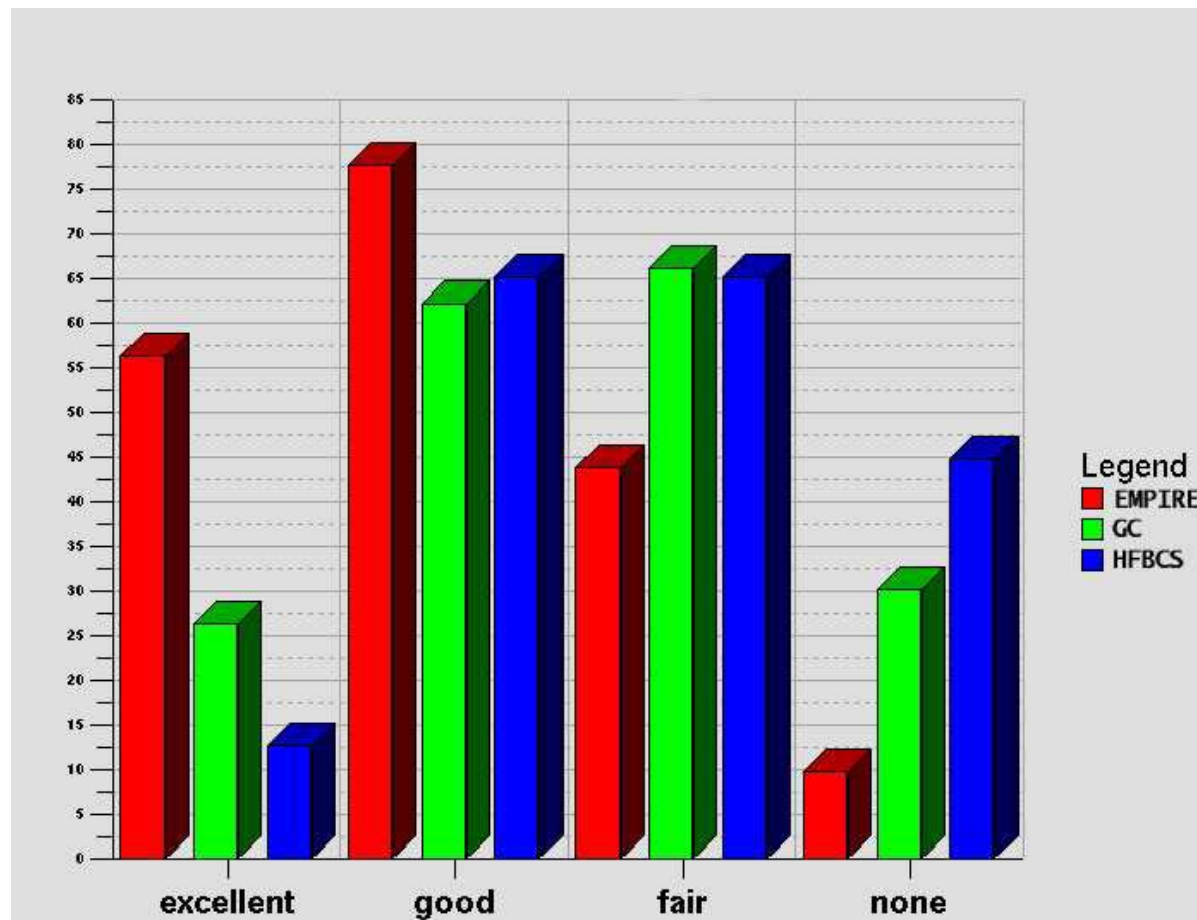


Effect of level densities



Effect of level densities

Agreement of capture calculations with exp. data



Fitting discrete levels

EMPIRE fits level densities to the cumulative number of discrete levels for

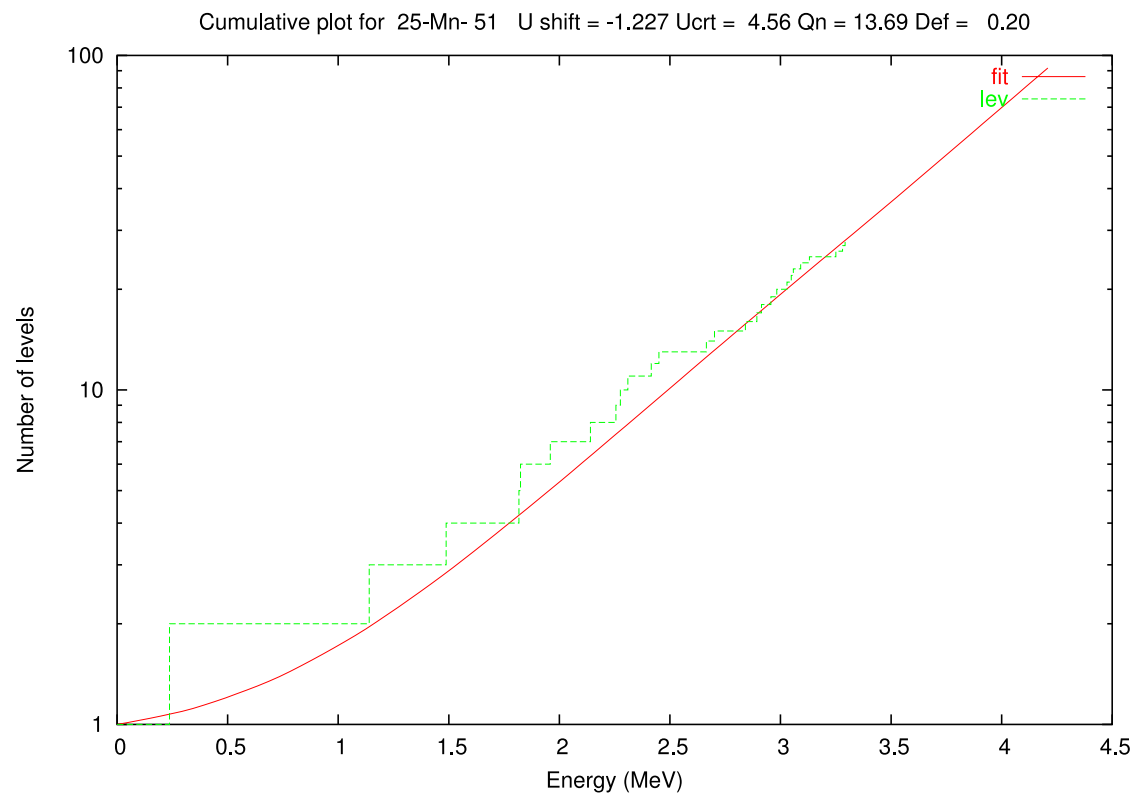
- EMPIRE-specific level densities (LEV DEN=0)
- Gilbert-Cameron level densities (LEV DEN=2)

Fit is automatic but **MUST NOT** be trusted blindly

- check with the FITLEV input option
- adjust number of discrete levels

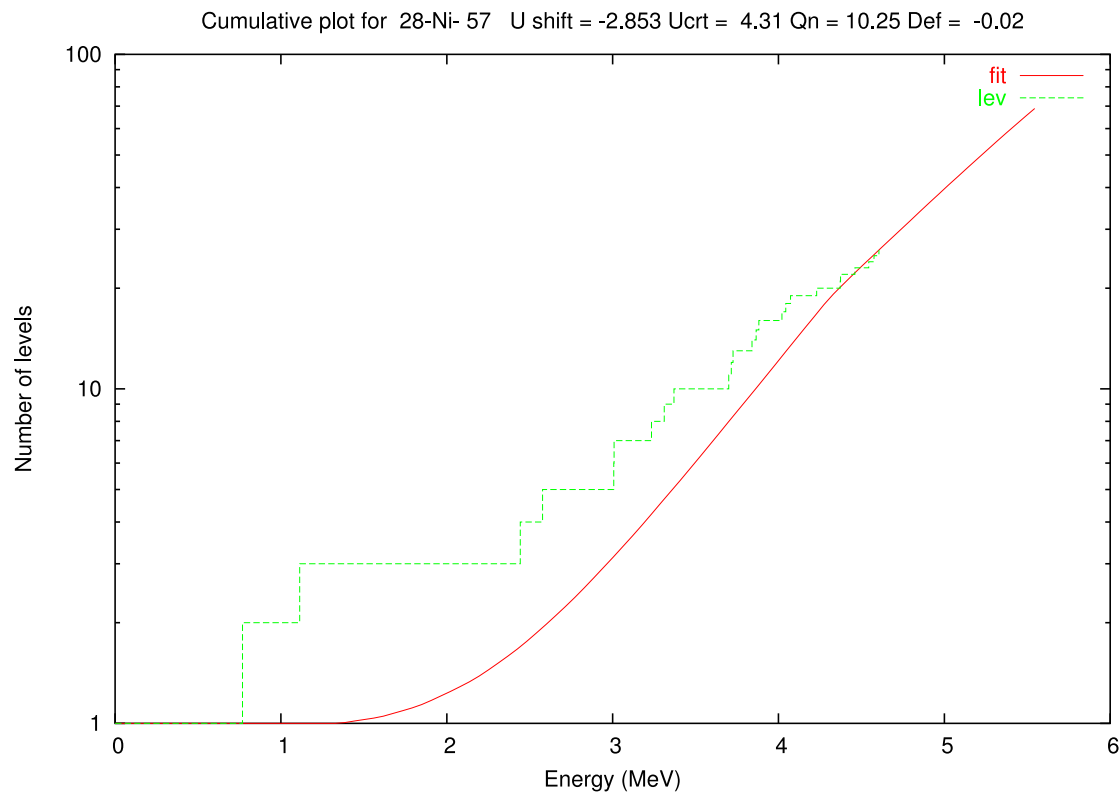
Fitting discrete levels

Example of a good fit



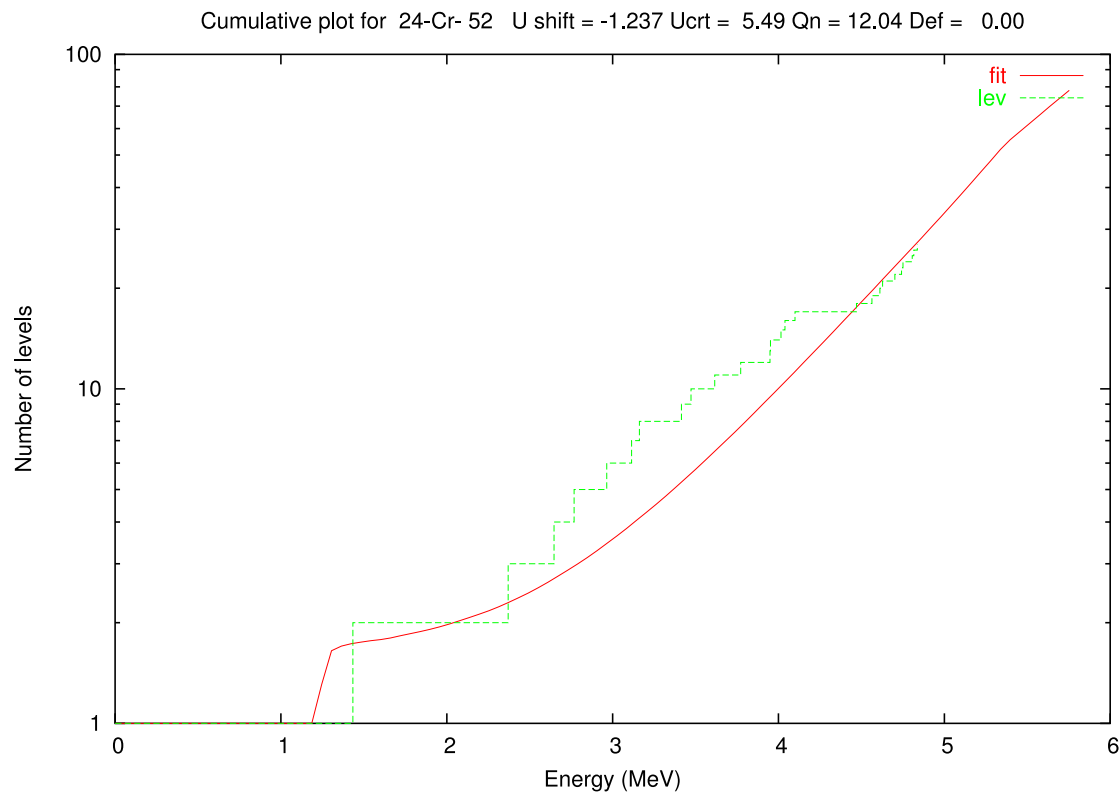
Fitting discrete levels

Example of a bad fit



Fitting discrete levels

Example of an ambiguous fit



Recommendations

- Generally, EMPIRE-specific level densities should be preferred along the stability line
- Gilbert-Cameron works better for Sn isotopes
- HF-BCS might be more reliable far from the stability line