Recent analysis of the neutron resonance densities and the neutron strength functions

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- **Neutron resonance parameters and their uncertainties,**
- **Systematics of the level density parameters,**
- **Microscopic statistical and combinatorial calculations of the level densities,**
- **Local systematics of the collective enhancement coefficients,**
- **Test of the level density models through the cross section analysis,**
- **Conclusion.**

Average neutron resonance parameters

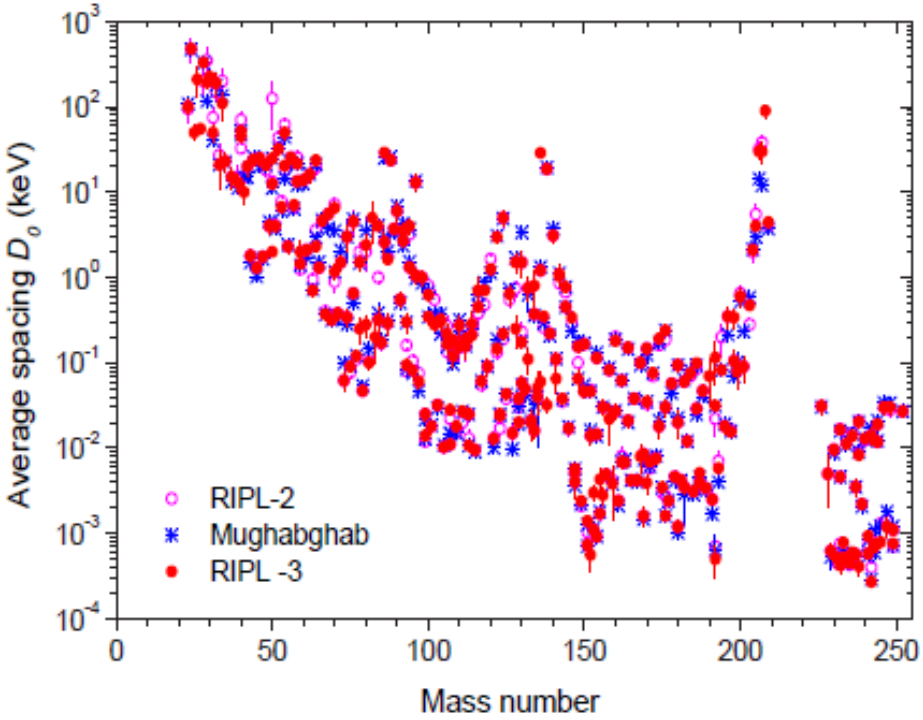
Complete tables of average resonance parameters provided by the Beijing, Bologna and Obninsk groups were collected under the RIPL-1 project (1993-1997). All these parameters are mainly based on the analysis of the resolved resonance parameters presented in the well-known BNL compilation. Despite the common base, many discrepancies were found between the average parameter estimations. These discrepancies were rather large when compared to the parameter uncertainties, especially for cases with less than 20 resonances. In the original BNL compilation the average resonance parameters were obtained for 230 nuclei, the Obninsk group compiled the resonance parameters for 264 nuclei, and the recommended RIPL-1 file included 281 nuclei .

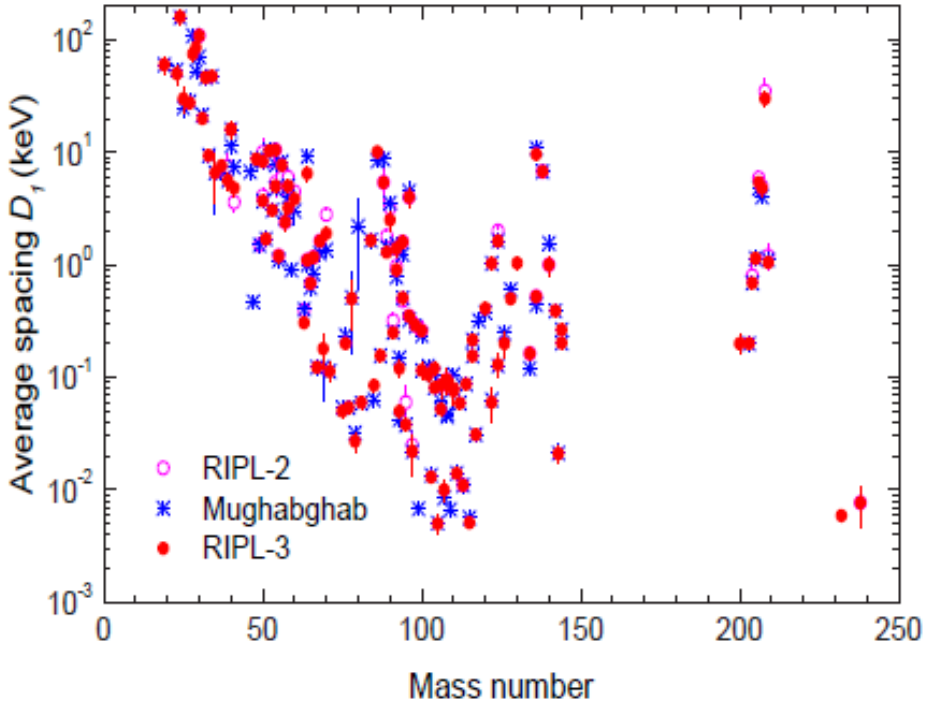
All nuclei available in the alternative files of RIPL-1 but not in the recommended one were re-analyzed during the RIPL-2 stage (1998-2002) on the basis of the updated compilation of the resolved resonance parameters. As a result, 16 nuclei were added to the list of average resonance parameters in the RIPL-2 file. The corresponding average resonance parameters for the p-wave resonances were also added to the updated database .

Some skepticism can arise with respect to the recommended parameters of nuclei for which data are available for a rather small number of resonances, particularly for about 45 nuclei in RIPL-2 in which the number of resonances is equal to or less than five. Any statistical analysis of such data is doubtful. Nevertheless, it was decided to include such cases in the recommended file to provide an estimate that is certainly better than nothing.

Neutron resonance spacing

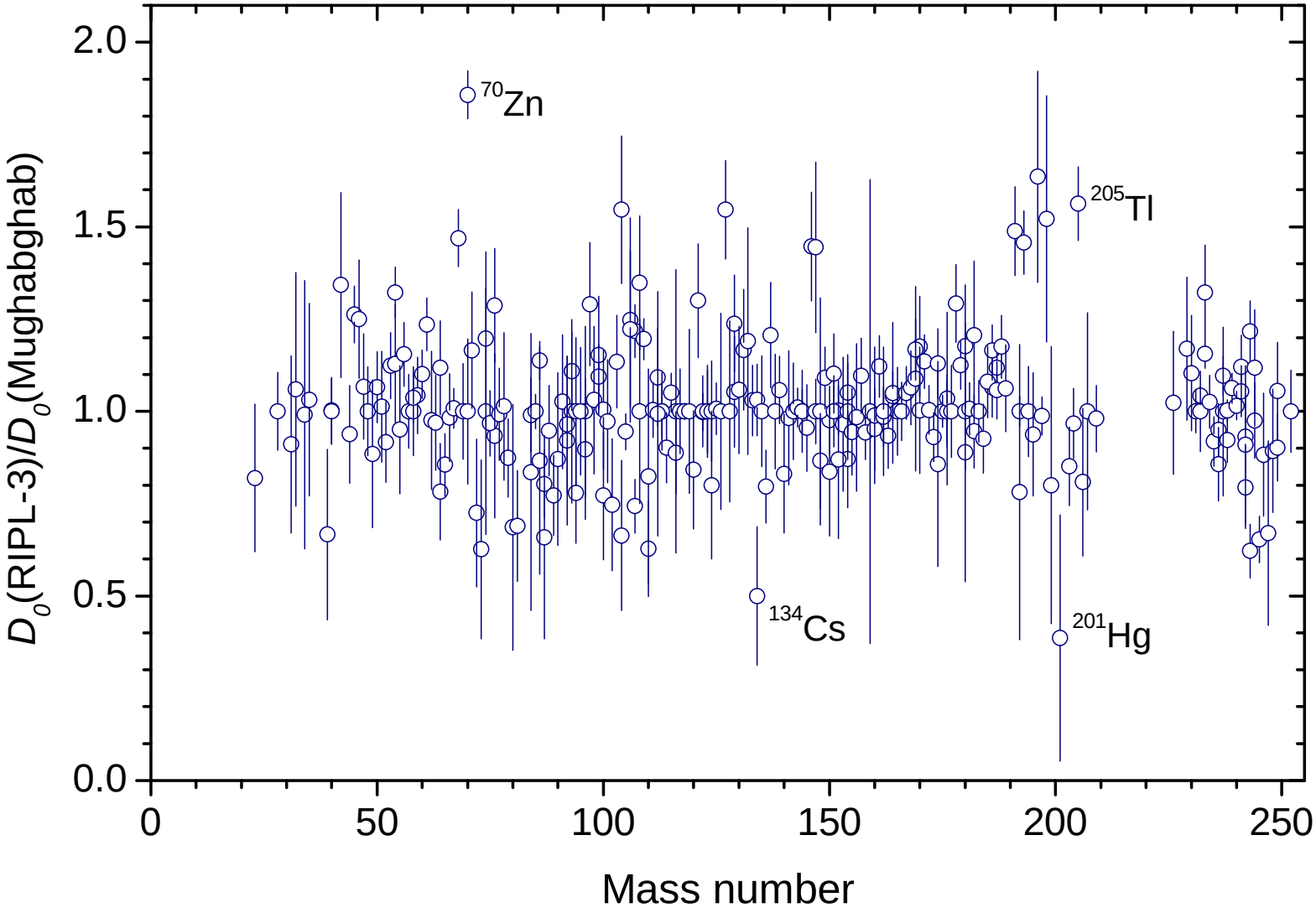
The "Atlas of Neutron Resonances", that was published recently by Mughabghab [2006], includes both an extensive list of individual resonance parameters and the updated average resonance parameters. All differences between the RIPL-2 and Mughabghab data were carefully analyzed during the RIPL-3 project . Main discrepancies between the RIPL-2 average parameters and the Atlas evaluations relate to nuclei for which data are available for less than 20 resonances. All deviations between the RIPL-2 and Mughabghab estimations were re-analyzed on the basis of the individual resonance parameters included in the Atlas. In the case of agreement between the re-evaluated spacings and Atlas data, the last data were included in the RIPL-3 files. However, for contradictory cases the results of the re-evaluated spacings were preferred.





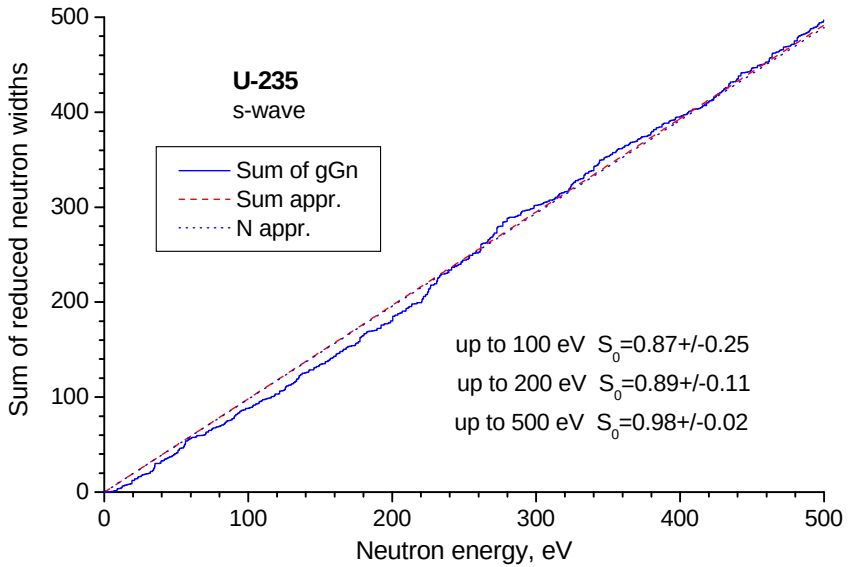
Nuclear data week at BNL (November 3-7, 2008)

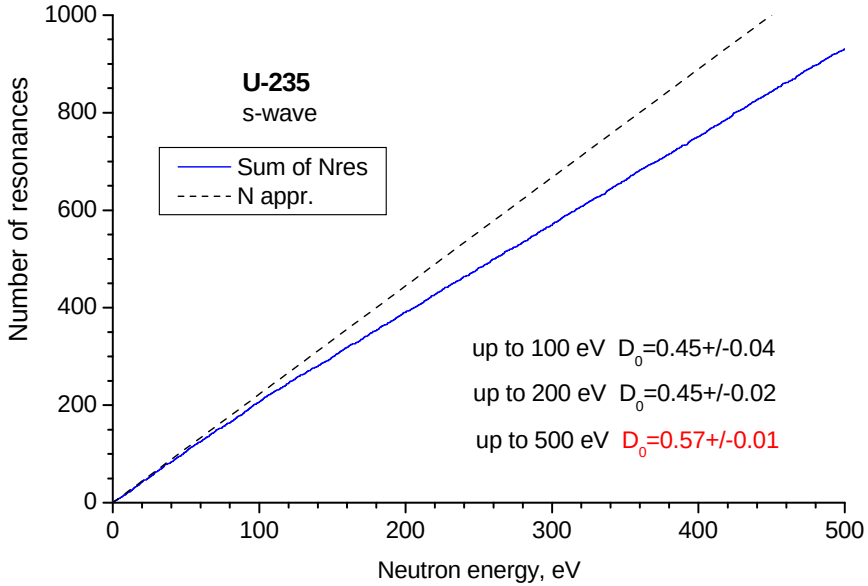
Ratios of the RIPL-3 spacings for the s-wave resonances to the spacings recommended by Mughabghab [2006]

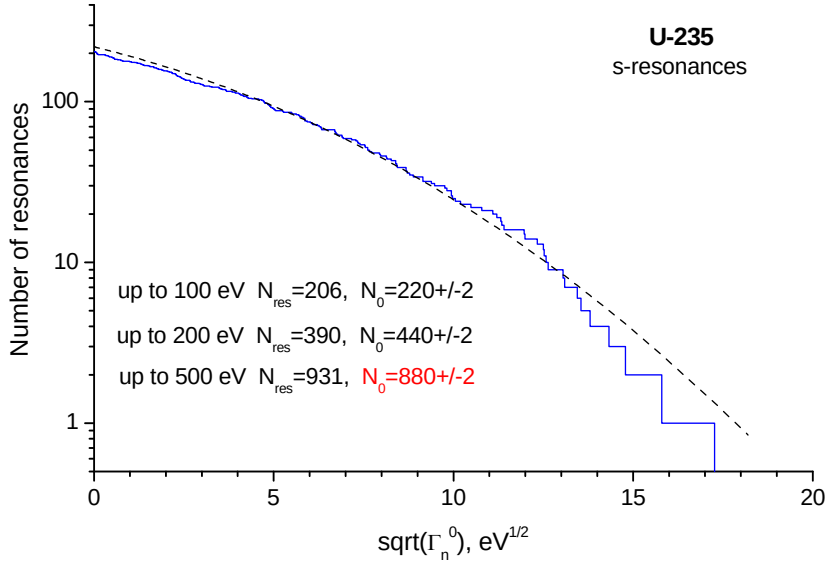


Analysis of the resonance parameters for ^{235}U

The set of resonances at the energy region up to 2.25 keV contains 849 s-wave resonances with J=3 and 1565 s-wave resonances with J=4 [L.Leal et al., Report ORNL/TM-13516, 1997]. It was recognized that the energy range below 100 eV should be used to analyze the statistical properties of resonances.







Average resonance parameters for ^{238}U:

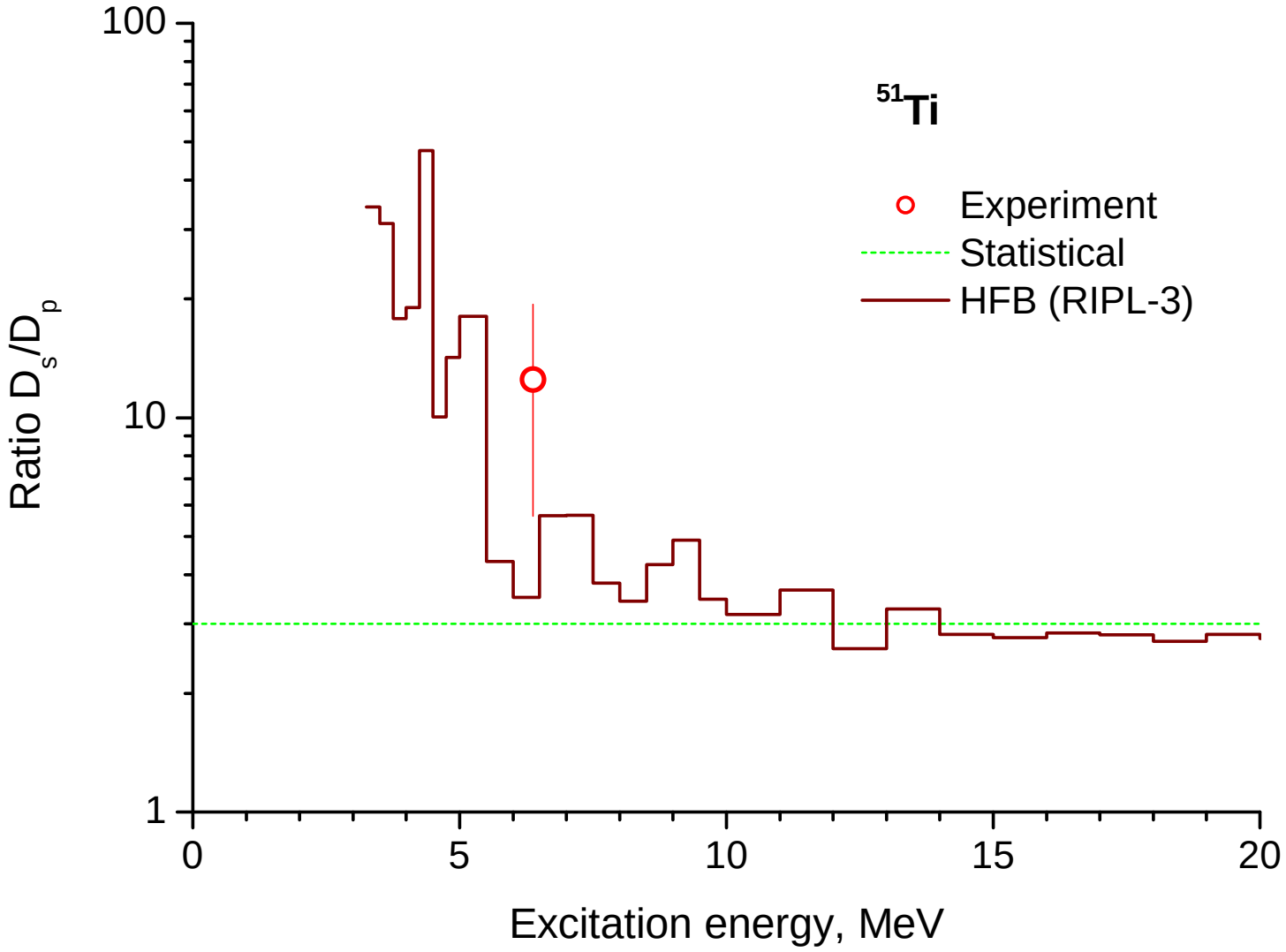
	D0, eV	D1, eV	S0, 10-4	S1, 10-4
1965, Gil.-Cam.	17.7±0.7	--	--	--
1979, Rohr et al.	21.5±2.2	--	1.02 ±0.16	--
1984, Mughabghab	20.9±1.1	7.2±0.4	1.2±0.1	1.7±0.3
1986, Ignatyuk et al.	21.7 ±0.9	7.3±0.5	1.15±0.12	1.7±0.5
1996, Beijing, RIPL-1	21.0 ±0.05	--	0.93±0.06	--
2002, RIPL-2 (10 keV)	20.8±0.3	7.7±1.0	1.03±0.08	1.6±0.4
2004, Leal et al., (20 keV)	--	--	1.07±0.07	1.71±0.07
2006, Mughabghab	20.26±0.72	7.42±0.23	1.29±0.13	2.17±0.19
2007, RIPL-3 (20 keV)	20.3±0.6	7.7±0.3	1.03±0.08	1.6±0.2

Analysis of the resonance spacing for ^{50}Ti:

The set of resonances for ^{50}Ti contains three s-wave resonances with the energies 56.5, 185.6 and 307.0 keV and about 20 p-wave resonances. The following estimations for the resonance spacing were made on this basis:

	D0, keV	D1, keV	S1, 10-4
1970, M.Baba	18±6 (≈3D1)	--	--
1979, G.Rohr et al.	71±40	--	--
1981, S.Mughabghab	125±70	10±3	0.40±0.17
1986, A.Ignatyuk et al.	Mug. 1981 was adopted for all		
1996, Bologna, RIPL-1	103±42	--	--
1996, Beijing, RIPL-1	84.8±24.4	--	--
2002, RIPL-2	125±70	10±3	0.40±0.17
2006, S.Mughabghab	24.9±1.5 (≈3D1)	8.30±0.53	0.54±0.10
2008, RIPL-3	Mug. 2006 was adopted for all. Is it OK???		

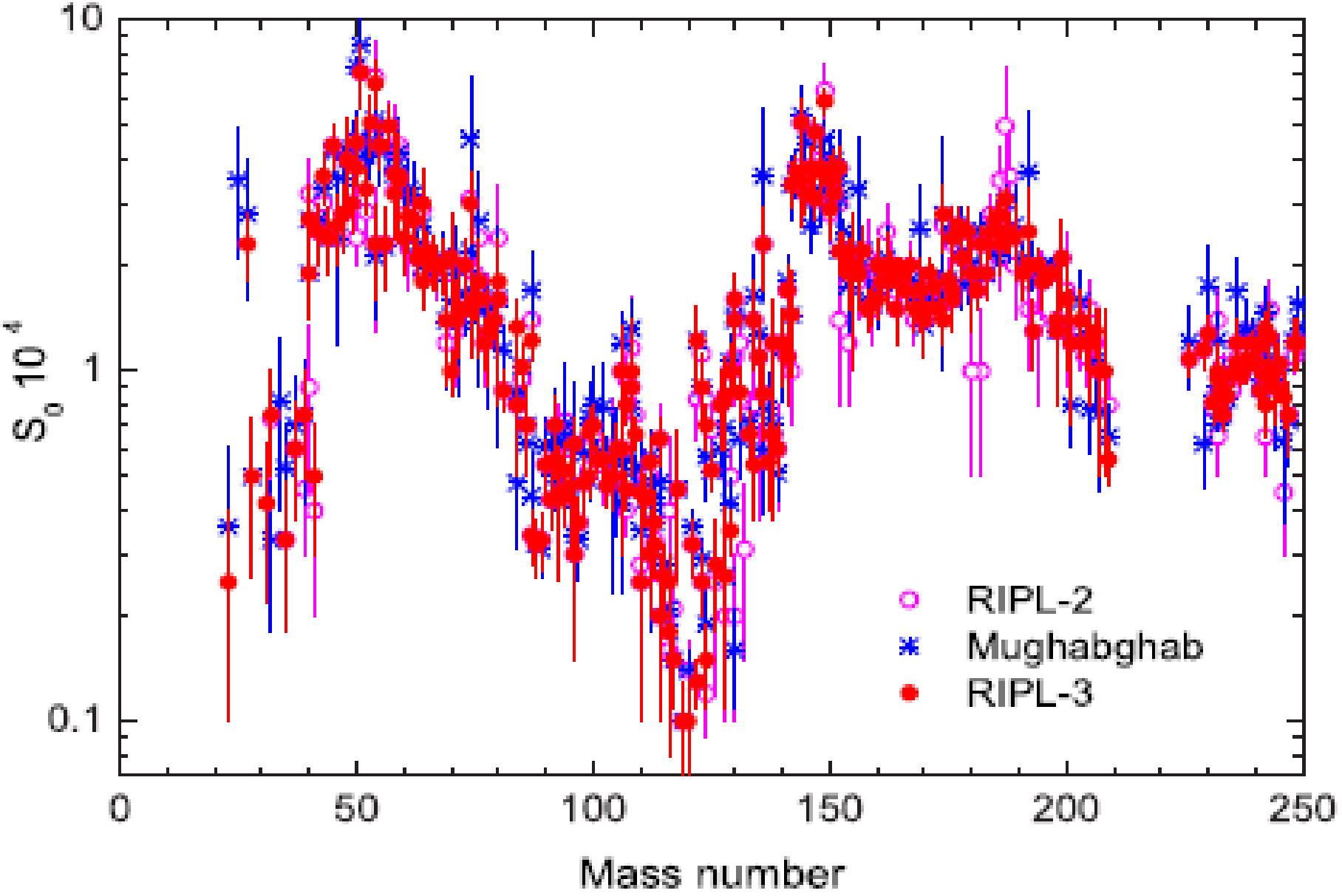
Parity dependence of the level densities: the ratio of the resonance spacings for s- and p-wave neutrons



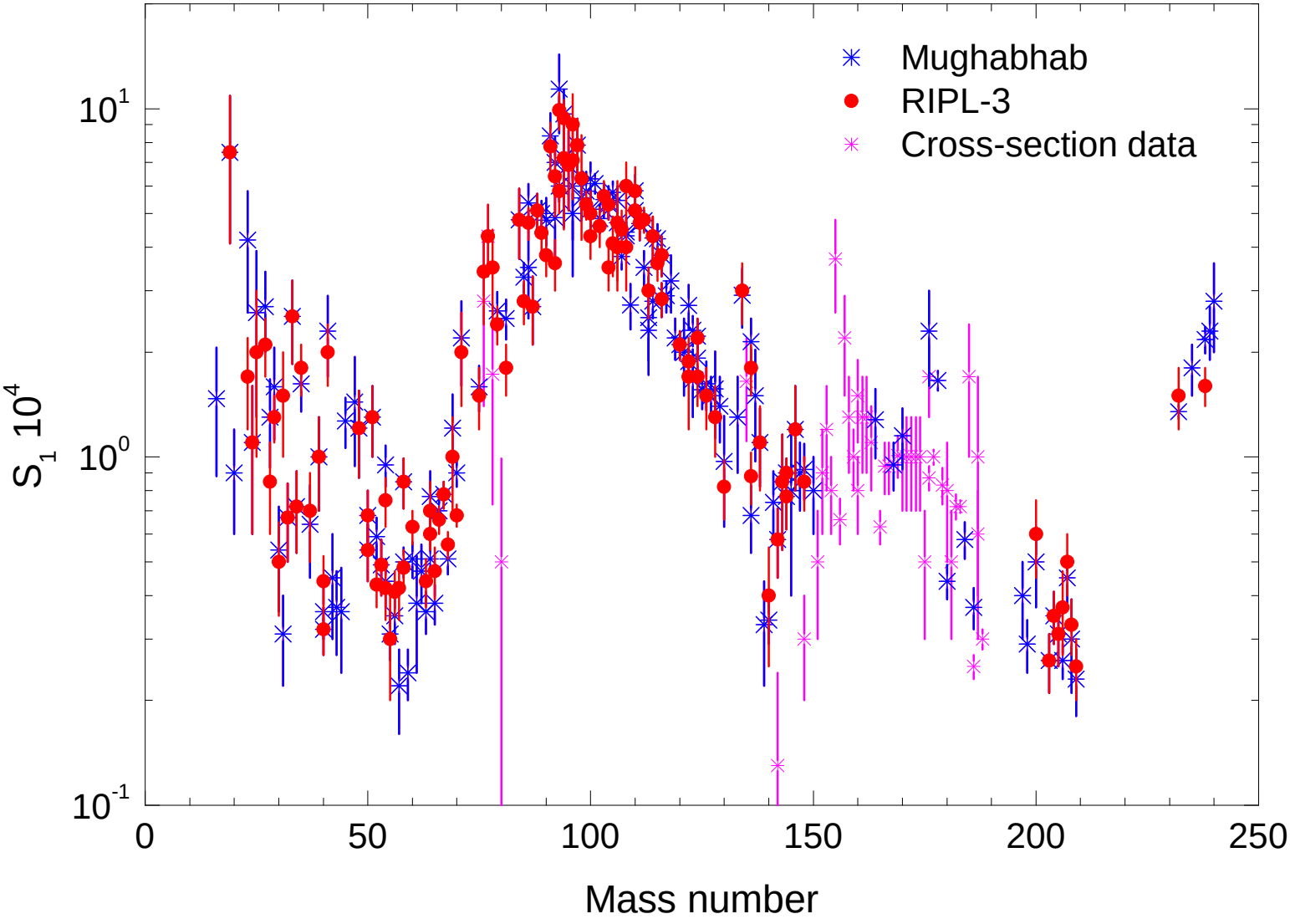
Neutron strength functions

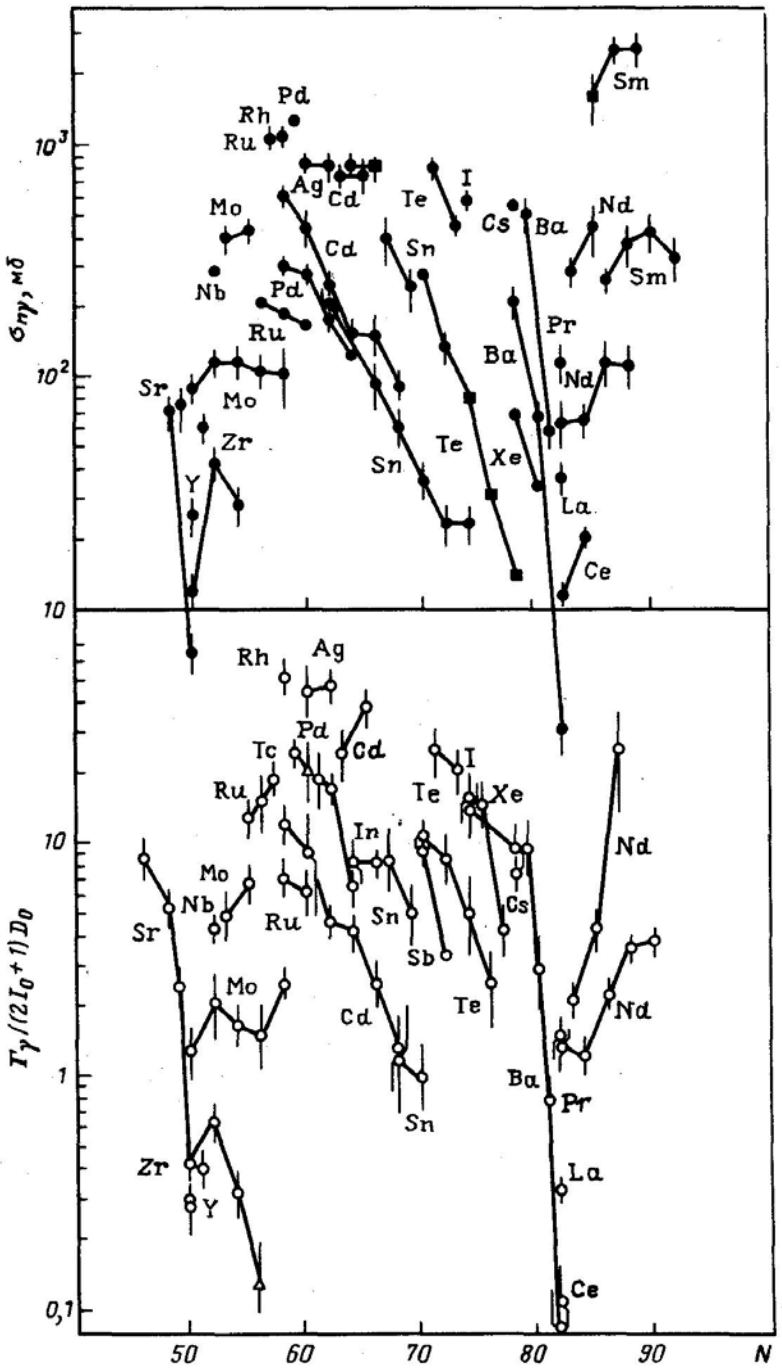
As a rule, there are no essential contradictions between the RIPL-3 and Mughabghab estimations (Atlas, 2006) . Nevertheless, it should be remarked that the RIPL-3 values were obtained from a consistent fit of the Porter-Thomas distribution of resonance widths in a carefully selected energy interval, while the Mughabghab estimations are based mainly on the analysis of widths over wide energy intervals including in many cases the results of the neutron capture cross-section analysis for the region of unresolved resonances.

Strength functions for s-wave neutrons



Strength functions for p-wave neutrons





Capture cross sections for 30 KeV neutrons are correlated strongly with the ratios of $\Gamma\gamma/(2Io+1)Do$. The statistical calculations of the cross sections are sensitive to the p-wave neutron strength functions too. So, a consistent estimations of the neutron strength functions from the capture cross-section analysis is possible for cases only when the total radiative widths and the resonance spacings are known with a rather high accuracy.

Nuclear level densities

Some of the most important concepts upon which our current understanding of the structure of low-lying nuclear levels is based are shell effects, pairing correlations and collective phenomena. All these concepts have been incorporated into the generalized superfluid model developed by many authors over the last 60 years. Most consistently all these properties are taken into account in microscopic versions of the model, but phenomenological versions of the model – convenient for the analysis of experimental data – have also been developed during the previous decades. All relations required for practical calculations are presented in details in the RIPL-1, RIPL-2, and RIPL-3 reports (See summary in Nuclear Data Sheets, 110 (2009), 3107-3214).

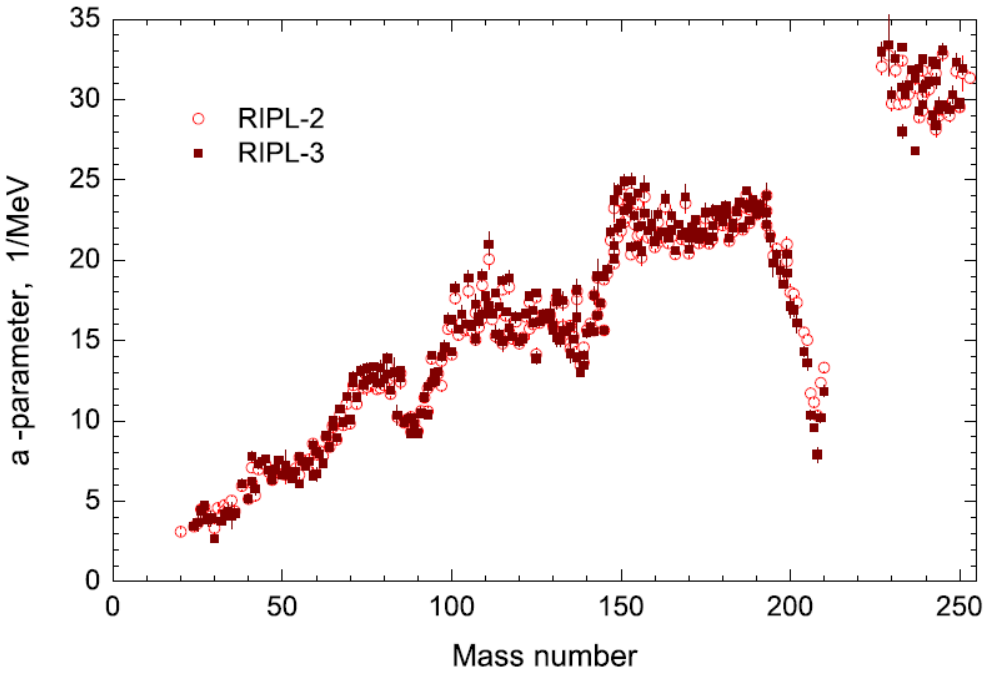
We should distinguish between two types of phenomenological approaches depending upon whether collective effects are explicitly accounted for or not. The simplest approach: the Composite Gilbert-Cameron Model (CGCM) and the Back-Shifted Fermi Gas Model (BSFGM) – do not take into consideration explicitly any collective enhancement of the level densities. These models are based on simple but easy to use analytical expressions with few parameters, which hopefully reduces the uncertainty of the model.
On the contrary, both the Generalized Superfluid Model (GSM), the Enhanced Generalized Superfluid Model (EGSM) and all microscopic models explicitly deal with collective effects but at the price of introducing more complicated expressions.

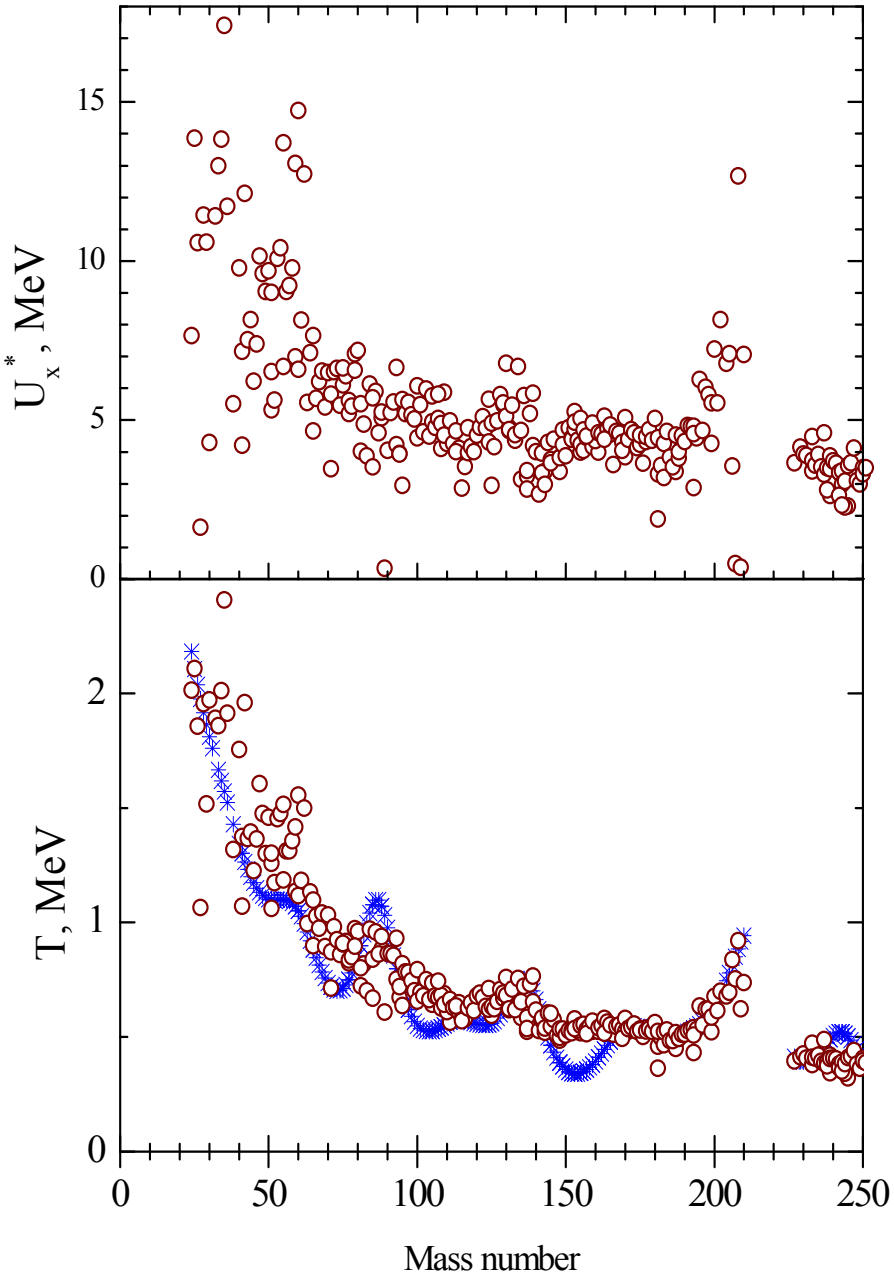
Composite Gilbert-Cameron model

To obtain the level density for the whole range of excitation energies, Gilbert and Cameron [1965] proposed to combine the low-energy region (constant temperature) with the high-energy dependence predicted by the Fermi gas model. The pairing correction was taken as

$$\Delta = 12nA^{-1/2},$$

where n=0, 1, 2 for odd-odd, odd A, and even-even nuclei.





Composite Gilbert-Cameron model (cont.)

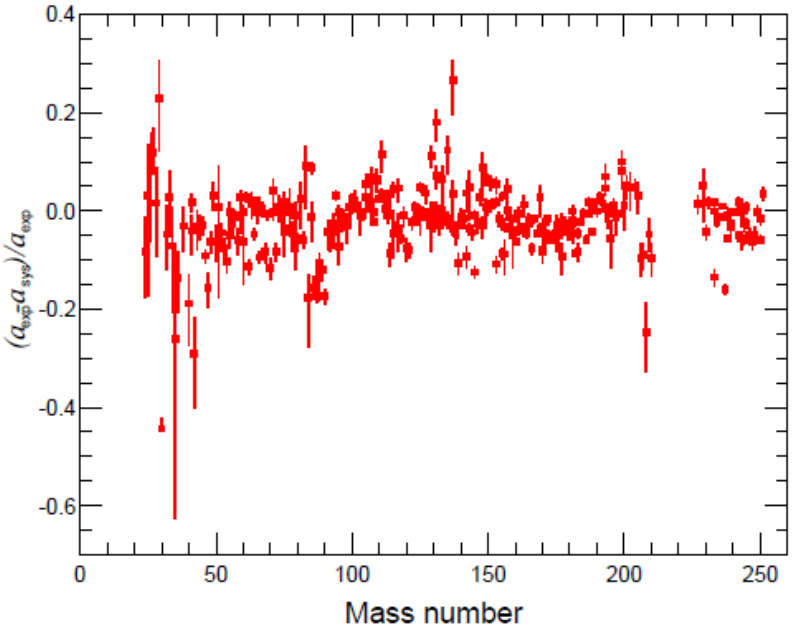
To take into account the shell effect damping, the level density parameters should be energy dependent. This dependence may be approximated by the formula

$$a(U) = \tilde{a}\{1 + \delta E_0[1 - \exp(-\gamma U)]/U\}$$

where δE_0 is the shell correction and $\tilde{a}$ is the asymptotic level density value obtained when all shell effects are damped. The asymptotic level density parameter and the damping parameter is usually selected in the form: $\tilde{a} = \alpha A + \beta A^{2/3}$ $\gamma = \gamma_0 A^{-1/3}$

From a fit of the CGCM *a*-parameters with the Myers-Swiatecki shell corrections the following coefficients have been obtained (in MeV^{-1}):

$$\alpha = 0.0692559, \quad \beta = 0.282769, \quad \gamma_0 = 0.433090.$$

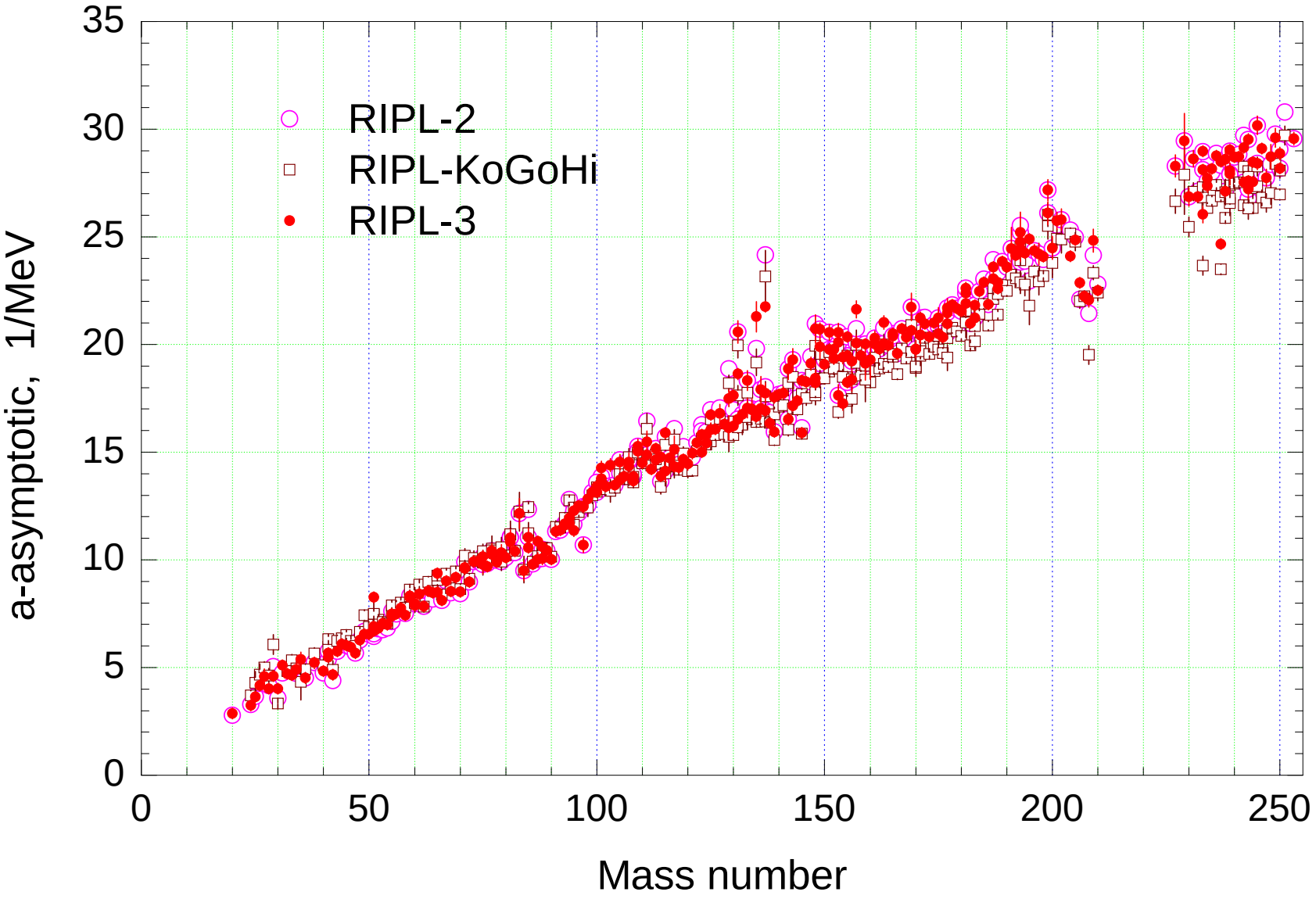


The root mean square deviation factor f_{rms} can be used to estimate the overall deviation with respect to the experimental data :

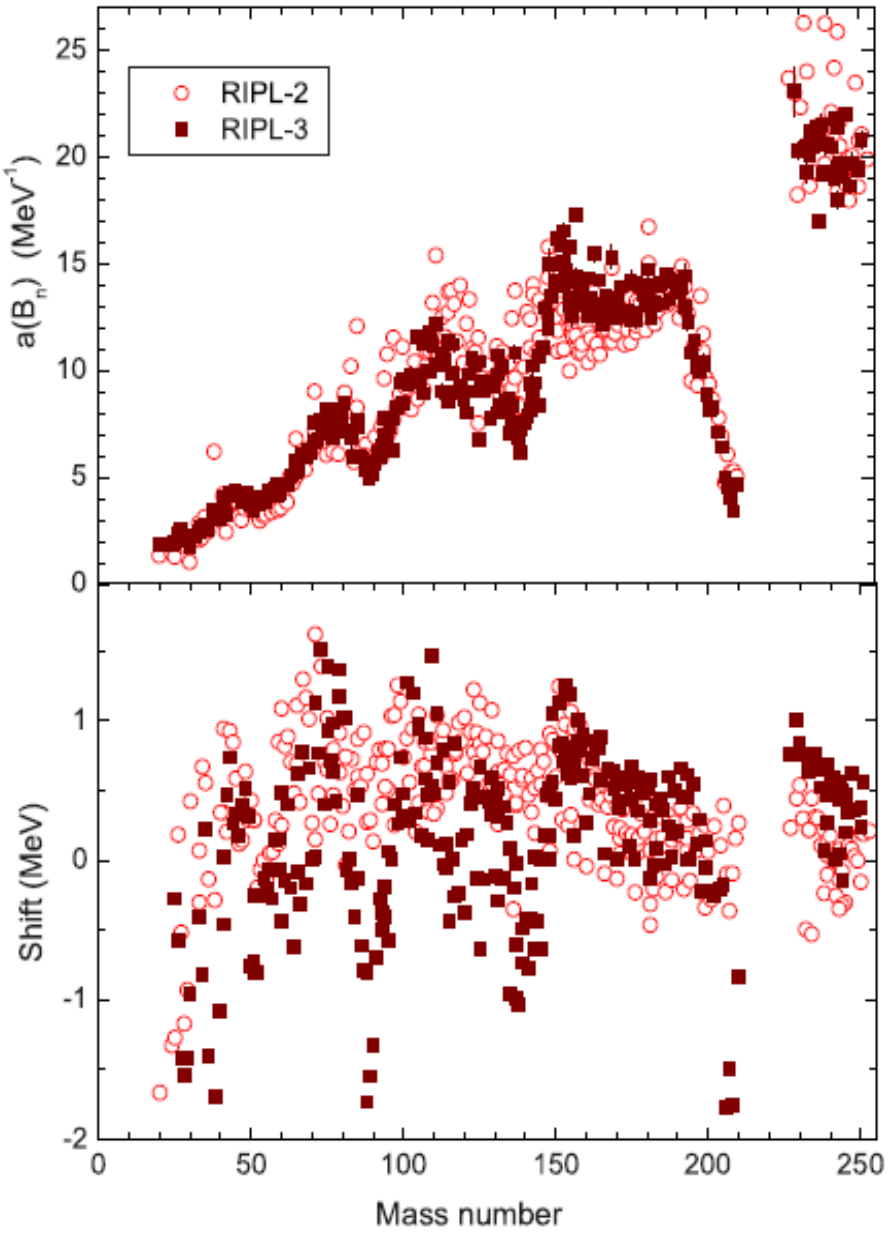
$$f_{rms} = \exp\left[N^{-1} \sum_{i=1}^{N} \ln^2 \frac{D^i_{th}}{D^i_{\exp}} \right]^{1/2}$$

With the above global parameters, the f_{rms} deviation with respect to the experimental resonance spacings is $f_{rms} = 1.76$. This means that the global systematics describes the available *a*-parameters with one-sigma uncertainty of 6.1%.

Composite Gilbert-Cameron model (cont.)



Generalized superfluid model (GSM)



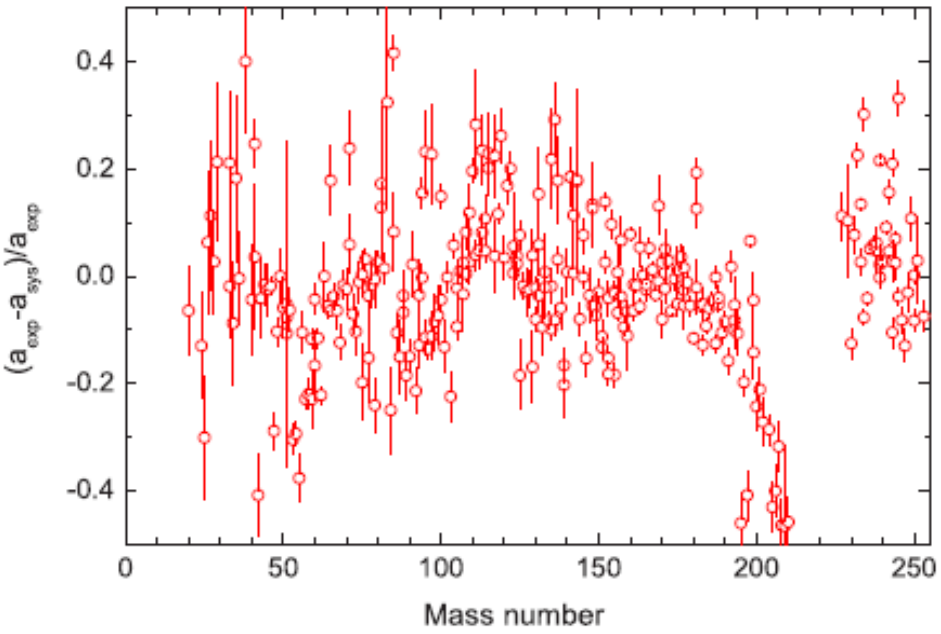
$$\rho(U) = \rho_{qp}(U) K_{vibr} K_{rot}$$

$$K_{rot}^{adiab} = \begin{cases} 1 & \text{for spherical nuclei,} \\ \Im_{\perp} t & \text{for deformed nuclei.} \end{cases}$$

$$a(U,Z,A) = \begin{cases} \tilde{a}(A)\left\{1 + \delta E_0 \dfrac{f(U^*)}{U^*}\right\} & \text{for U} \geq U_{cr} \\ a_{cr}(U_{cr}, Z, A) \; for \; U < U_{cr} \end{cases}$$

GSM resembles the CGCM to the extent that the model distinguishes between a low energy and a high-energy region, although for the GSM this distinction follows naturally from the theory and does not depend on specific discrete levels that determine a matching energy. To take into account possible shortcomings of the global systematics of the enhancement coefficients, an additional shift of the excitation energy δ_{shift} is introduced in the GSM.

Generalized superfluid model (cont.)



$$a(U,Z,A)=\begin{cases}\tilde{a}(A)\left\{1+\delta E_0\dfrac{f(U^*)}{U^*}\right\} & \text{for } U \geq U_{cr}\\ a_{cr}(U_{cr},Z,A) & \text{for } U < U_{cr}\end{cases}$$

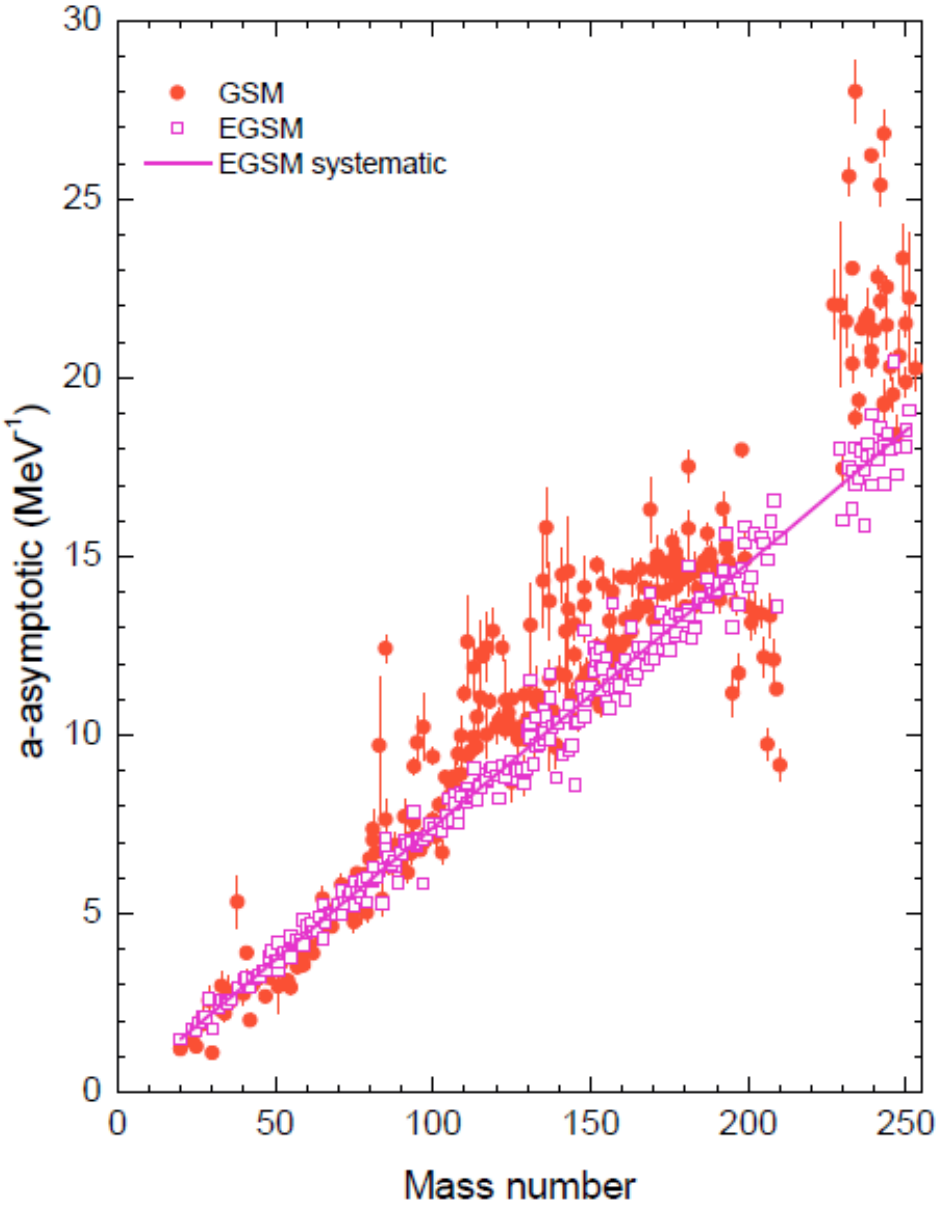
Using the Myers-Swiatecki shell corrections and the collective enhancement coefficients described in RIPL-2, for the asymptotic a-parameters have been obtained from a GSM least-squares fit of data the following parameters (in MeV^{-1}):

$\alpha = 0.093 \pm 0.004$, $\beta = 0.105 \pm 0.014$, $\gamma_0 = 0.375 \pm 0.015$, and $\delta_{shift} = 0.617 - 0.00164A$ MeV.

The standard deviation for the *a*-parameters is equal to 0.169 and the equivalent factor frms = 1.98.

From a more careful analysis of significant deviations an impression arises that the main deviations occur for near-magic nuclei for which the shell effects are so strong that their consistent description is only possible by using microscopic models. Important deviations exist also for transitional nuclei in which the structure of collective excitations is intermediate between vibrational and rotational. A more accurate estimation of collective enhancements is certainly required for transitional nuclei to avoid the adiabatic separation of vibrational and rotational effects.

Enhanced generalized superfluid model (EGSM)



EGSM includes a more accurate treatment of high angular momenta, which are important for heavy-ion induced reactions. The rotational energy is subtracted from the intrinsic excitation energy. The collective enhancement of the level densities arising from nuclear rotation is taken into account in the non-adiabatic form. The vibrational collective enhancement is calculated in the adiabatic approach, but the vibrational energies are estimated from the liquid drop model assuming surface oscillations of the liquid drop.

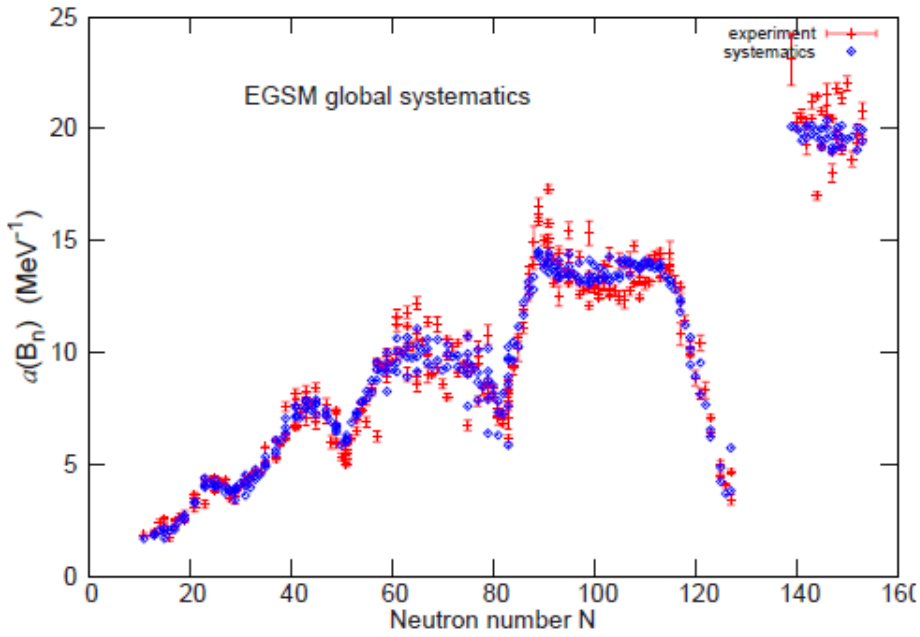
The resulting global EGSM systematics is represented by the set of parameters (in MeV^{-1}): $\alpha = 0.0741$, $\beta = 0.0003$, $\gamma_0 = 0.5725$. These parameters yield $f_{rms} = 1.70$.

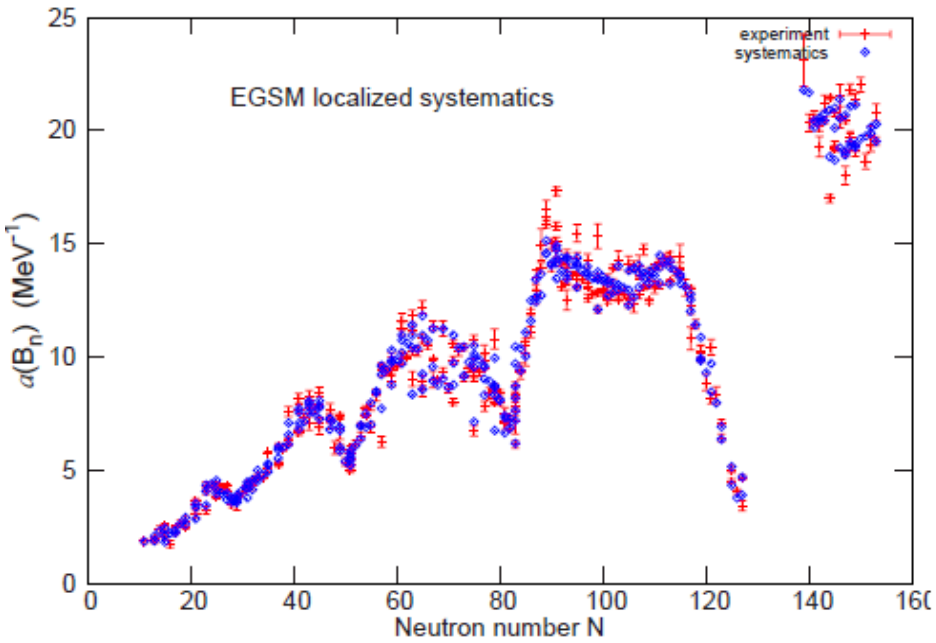
Left: Mass dependence of the asymptotic level density parameter *ã* for the EGSM and the GSM.

Enhanced generalized superfluid model (cont.)

Contrary to other level density models considered in RIPL-3, the EGSM global systematics does not account for discrete levels. Instead, the adjustment is performed automatically by the EGSM code (provided in RIPL-3) when level densities are calculated. A shift is applied to the excitation energy to reproduce the cumulative number of levels at the energy corresponding to the highest level considered in the calculations. **This shift is linearly decreased with increasing energy in such a way as to reach zero at the neutron binding energy.**

The global systematics can be improved by applying normalization factors defined for each element for which experimental a(Bn) are available (right panel below). The localized systematics accounts for an unknown Z-dependence that is either not considered in the shell corrections or included improperly.

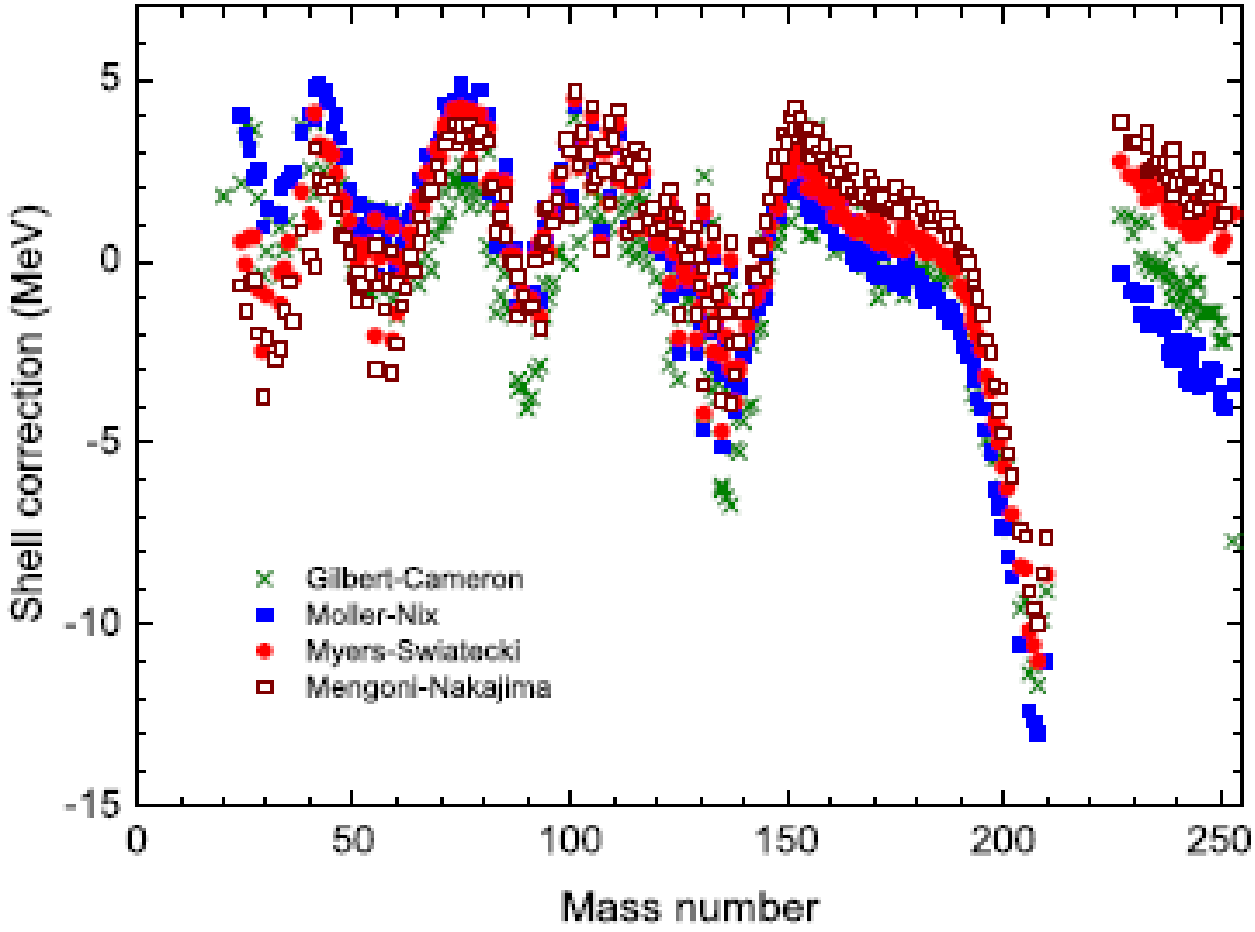




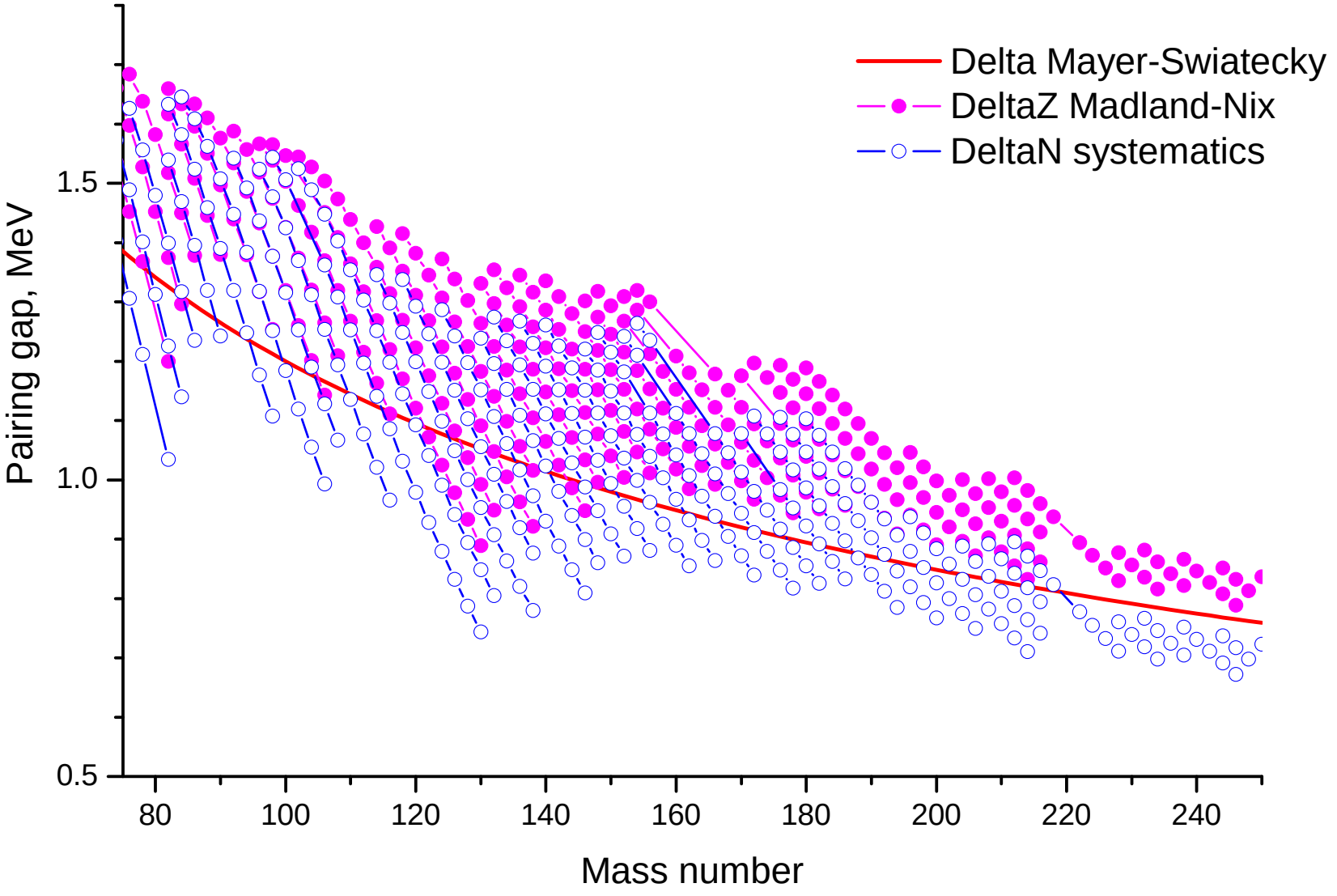
Shell corrections

Microscopic corrections to the binding energy are quantities of fundamental importance in the derivation of many physical properties affected by shell, pairing or deformation effects. The most common one defines the various microscopic corrections as follows:

$$E_{tot}(Z, A, \beta) = E_{mac}(Z, A, \beta) + E_{shell}(Z, A, \beta)$$

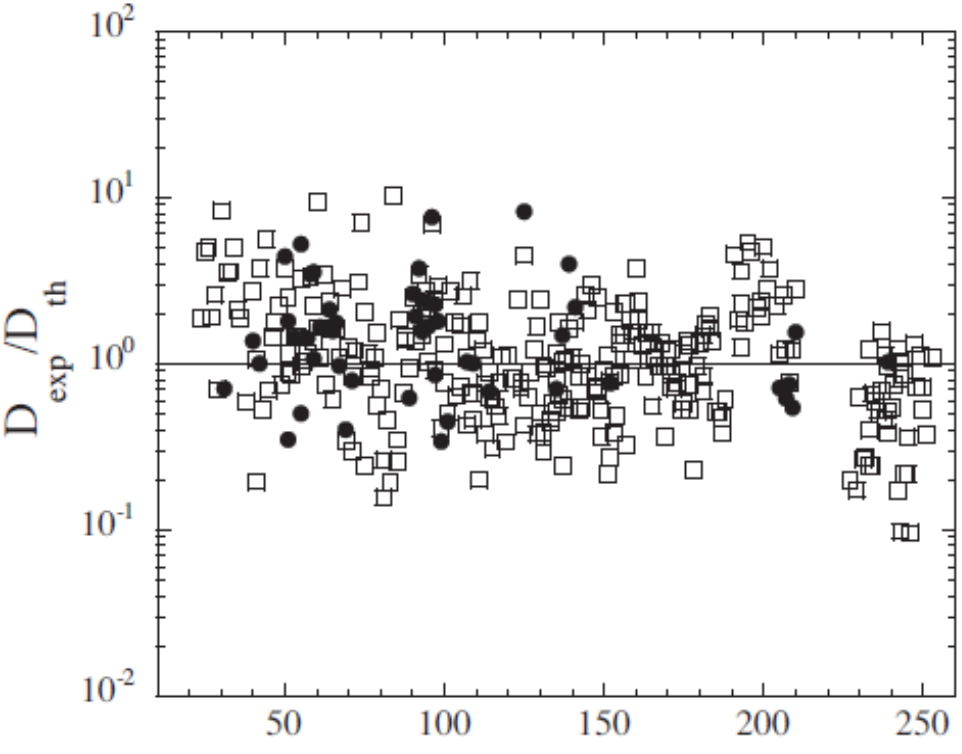


Even-odd effects



Microscopic level densities (cont.)

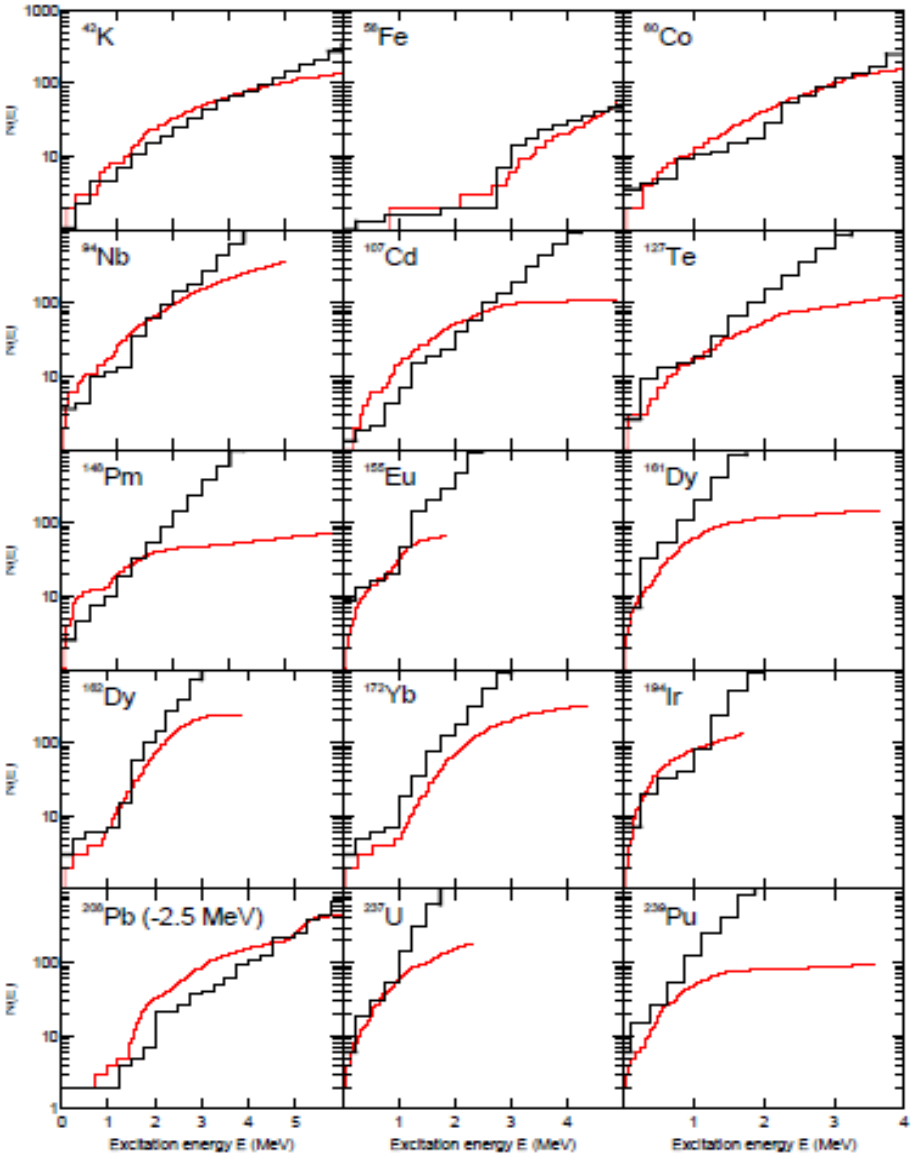
A microscopic combinatorial approach was developed during the RIPL-3 stage to include in the level density calculations both collective effects and all possible particle-hole excitation with an improved treatment of the pairing interaction. This method consists of using single-particle level schemes obtained from the constrained axially symmetric HFB method with the BSk14 effective Skyrme force to construct incoherent particle-hole level densities as functions of the excitation energy U, the spin projection M on the intrinsic symmetry axis, and the parity π. Once all particle-hole state densities are determined, the collective effects should be added. The choice of multiplying the level densities by the phenomenological vibrational enhancement factor was made after accounting for rotational motion, if necessary (i.e. for deformed nuclei).



To improve the phenomenological treatment of vibrational effects the boson partition function was added to combinatorial calculations [2008Gor]. The quadrupole, octupole, and hexadecapole collective excitations were taken into consideration. The calculated vibrational state densities were than folded with the incoherent particle-hole state densities to obtain the total state density. Three coupled phonons folded in with particle-hole configurations results in a fairly good reproduction of $D_0(B_n)$, as shown in the figure on the left.

Microscopic level densities (cont.)

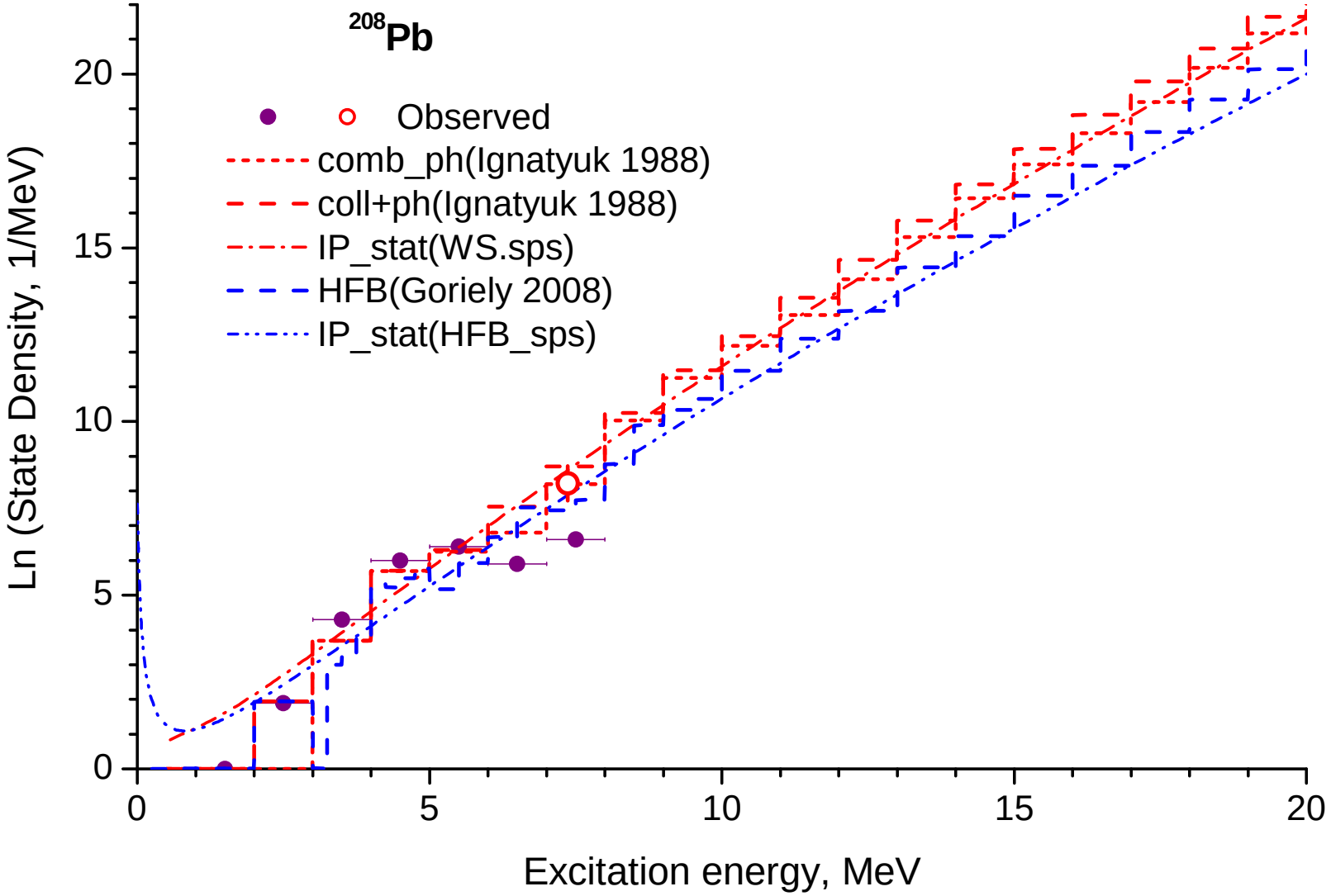
Globally, the D_0 values are predicted within a factor of two. The value of the factor f_{rms}= 2.3 found with the present approach including both the *s*- and *p*-wave resonance spacing data.



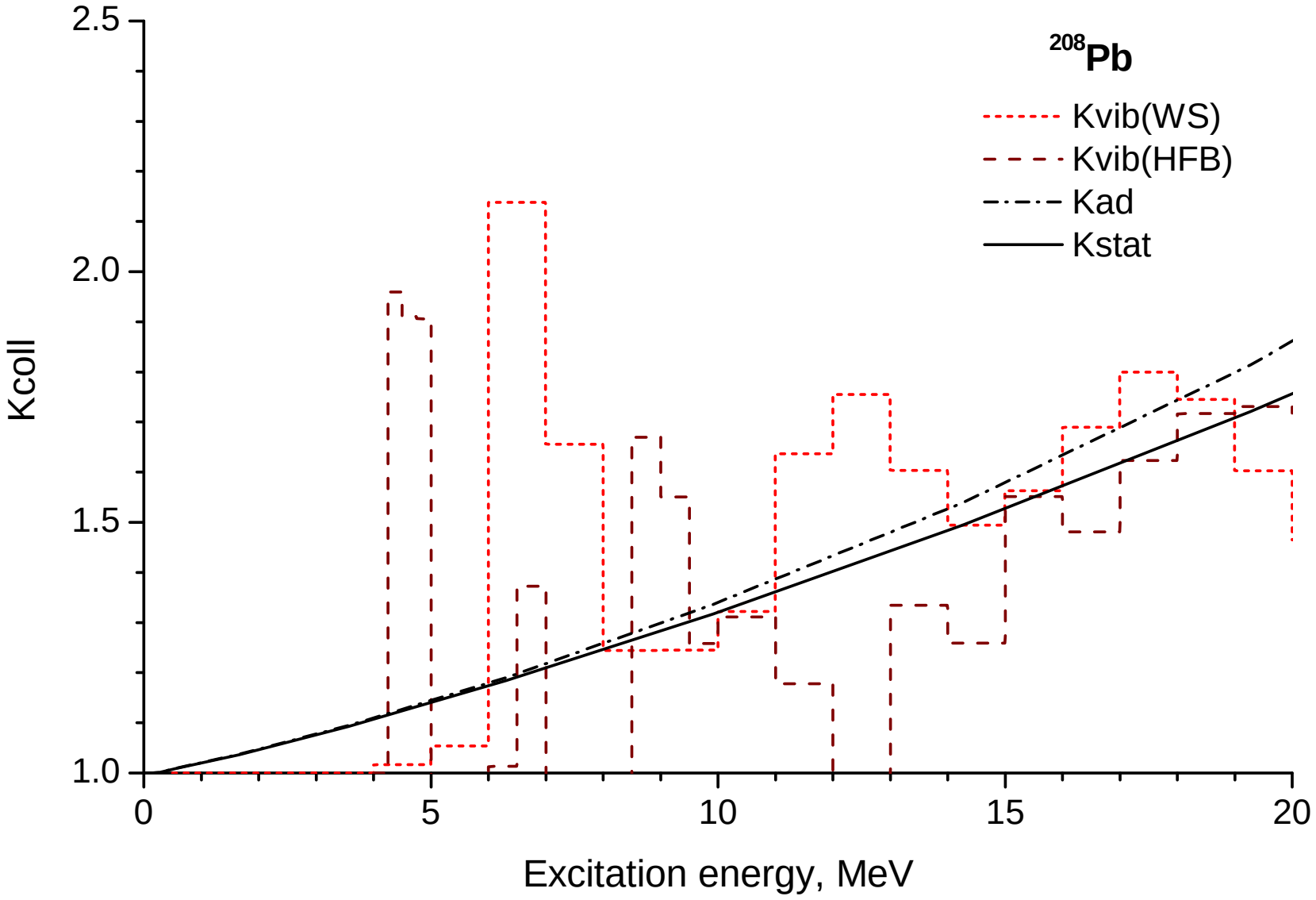
The HFB combinatorial model also gives satisfactory extrapolations to low energies. As an example, the predicted cumulative number of levels $N(U)$ are compared in the left-side plot with the experimental data on low-lying levels for 15 nuclei including spherical as well as deformed species.

The level density overestimations for deformed nuclei seen at low energies (rare-earth and actinide nuclei) are a direct consequence of using the rigid-body moment of inertia in calculations of the rotational enhancement of the level density. The experimental values of the moment of inertia for low-lying rotational bands correspond to about three times lower values. So, a more accurate approximation of the moments of inertia could substantially improve the description of the experimental data for low-lying levels.

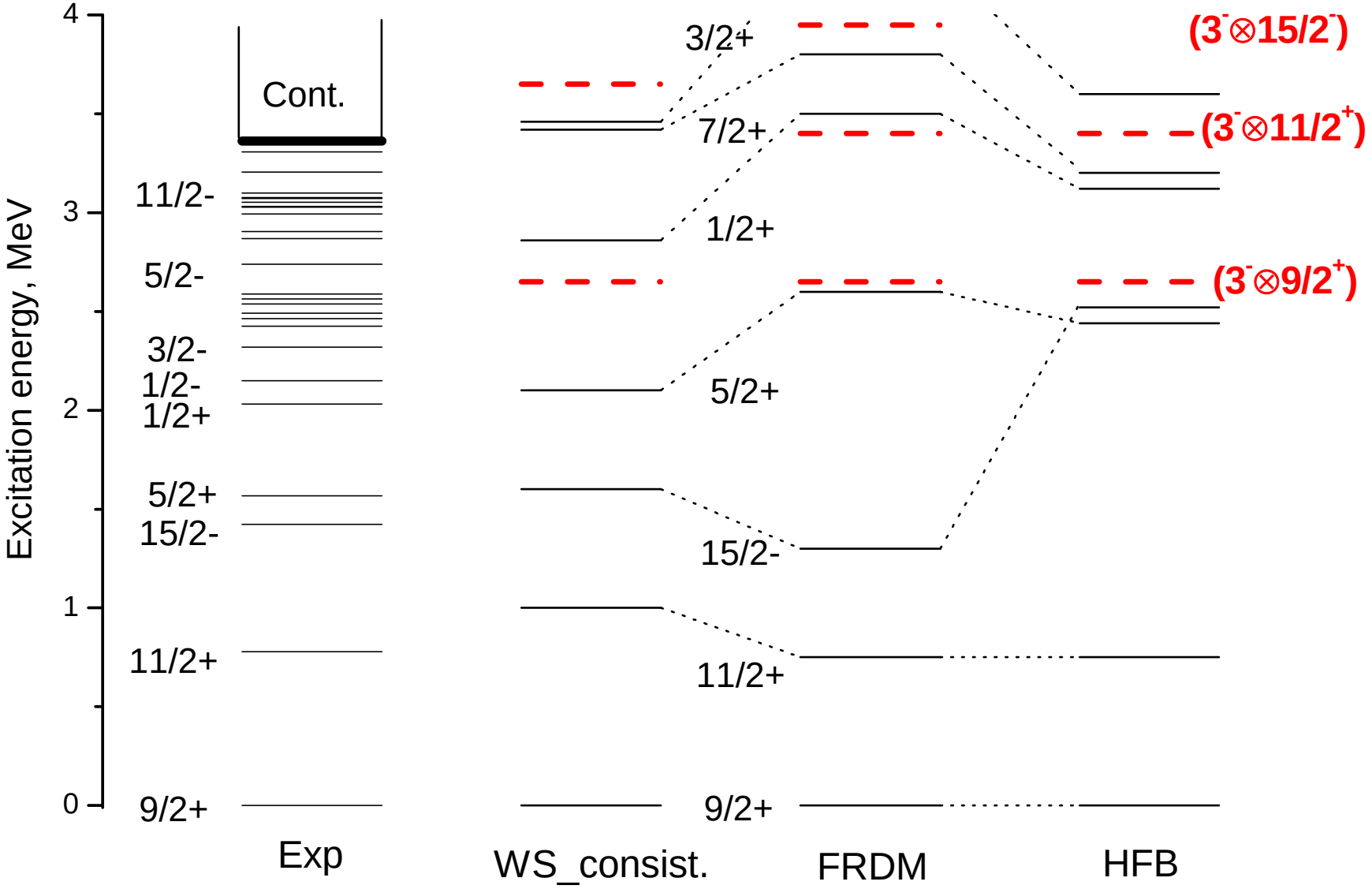
Combinatorial and statistical calculations of the level densities



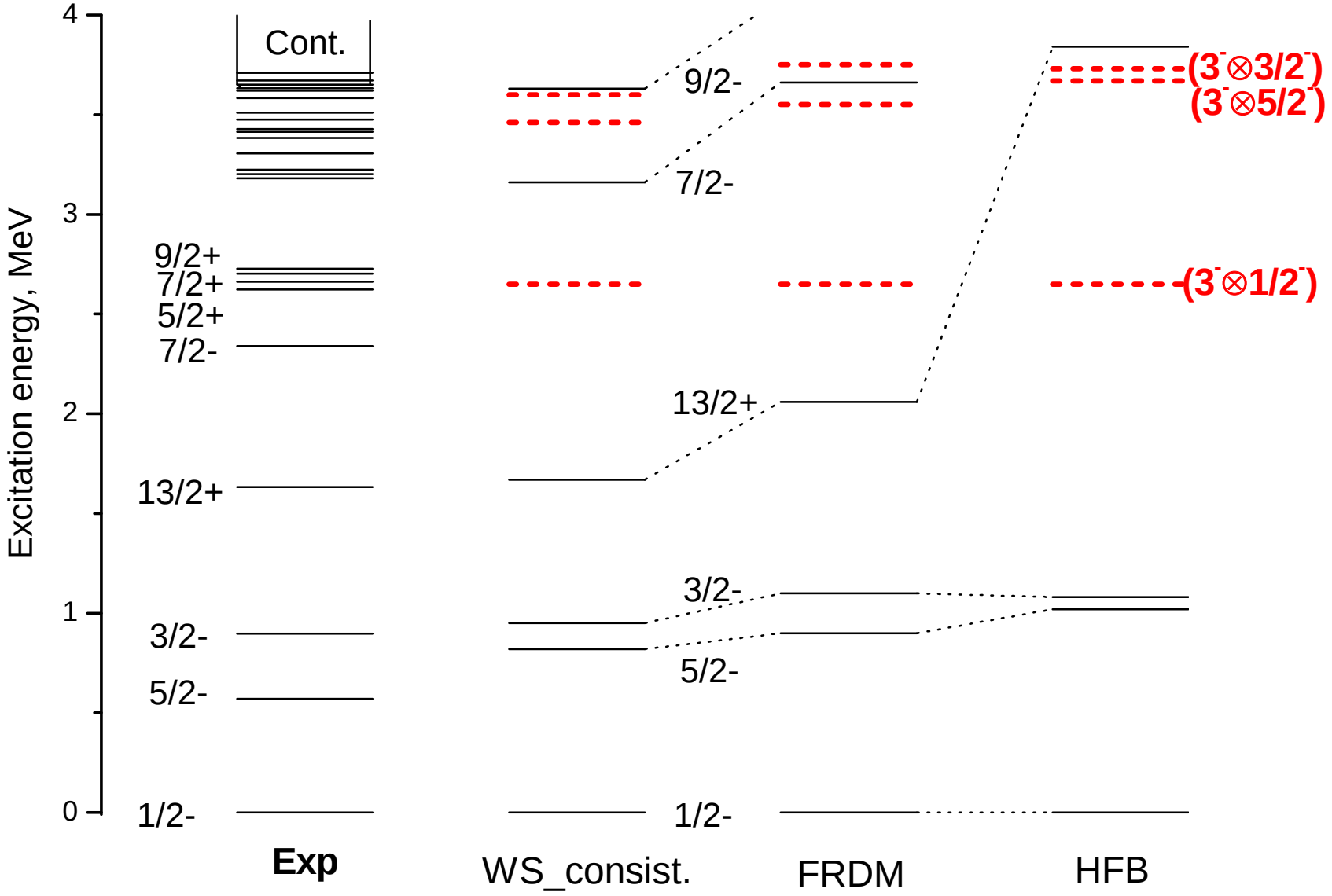
Collective enhancement coefficients



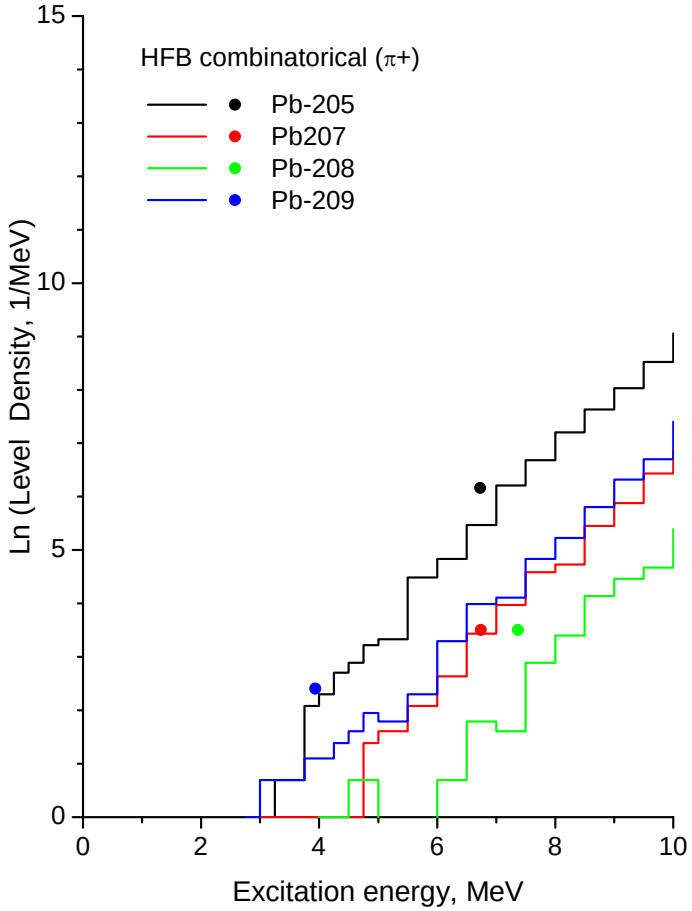
Low-lying levels of Pb-209 and the corresponding single-particle + collective excitations

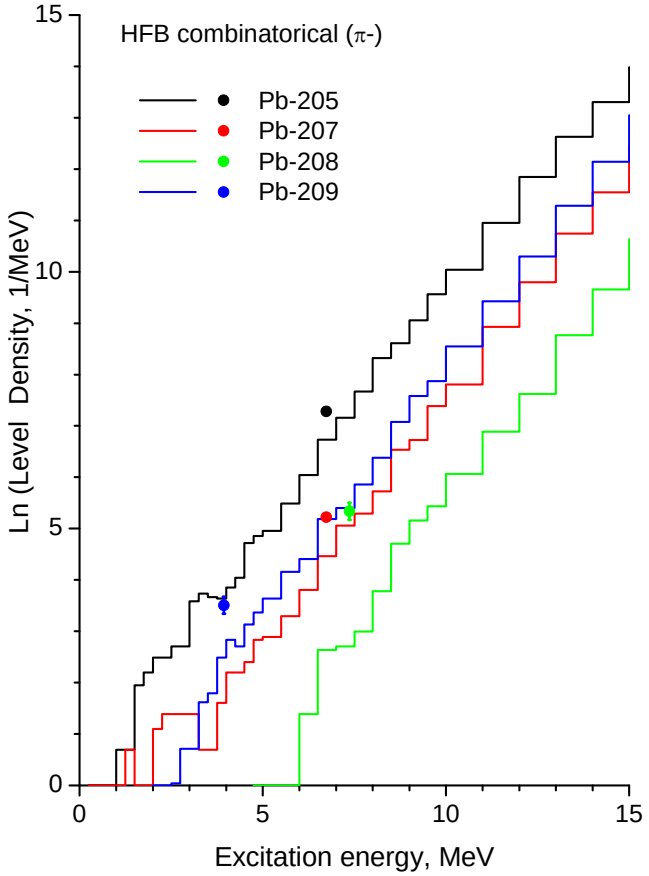


Low-lying levels of Pb-207 and the corresponding single-particle + collective excitations



Combinatorial calculations (solid histograms) compared with the neutron resonance densities (symbols) for lead isotopes

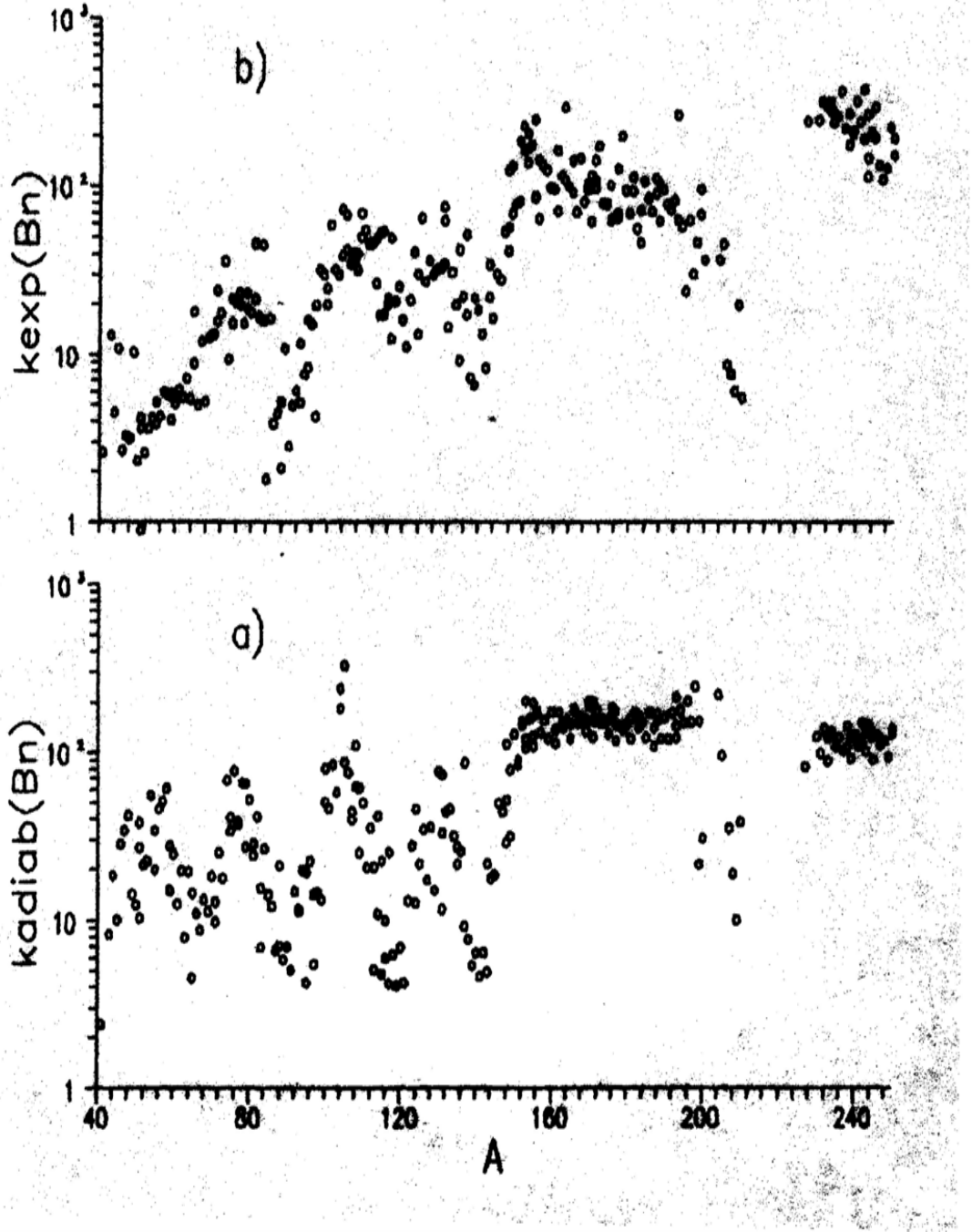




Statistical estimations for the ratio of Ds/Dp are about 3 for even-even target and ~2.25 for odd ones:

Ds/Dp	Pb-205	Pb-207	Pb-208	Pb-209
Exp.	3.04	5.55	6.25	-
Calc.	2.37	2.93	1.11	5.70

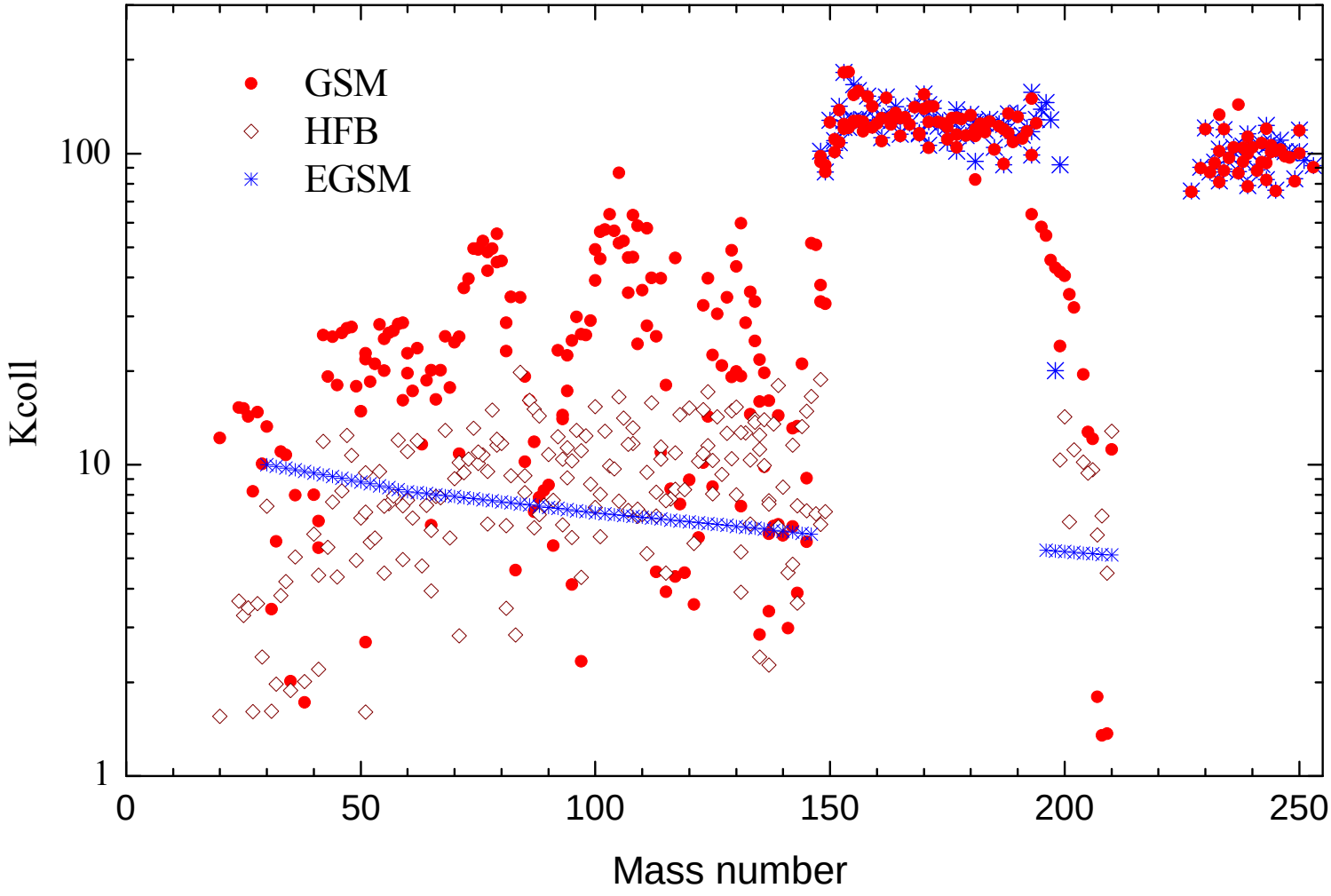
Collective enhancement of the level densities

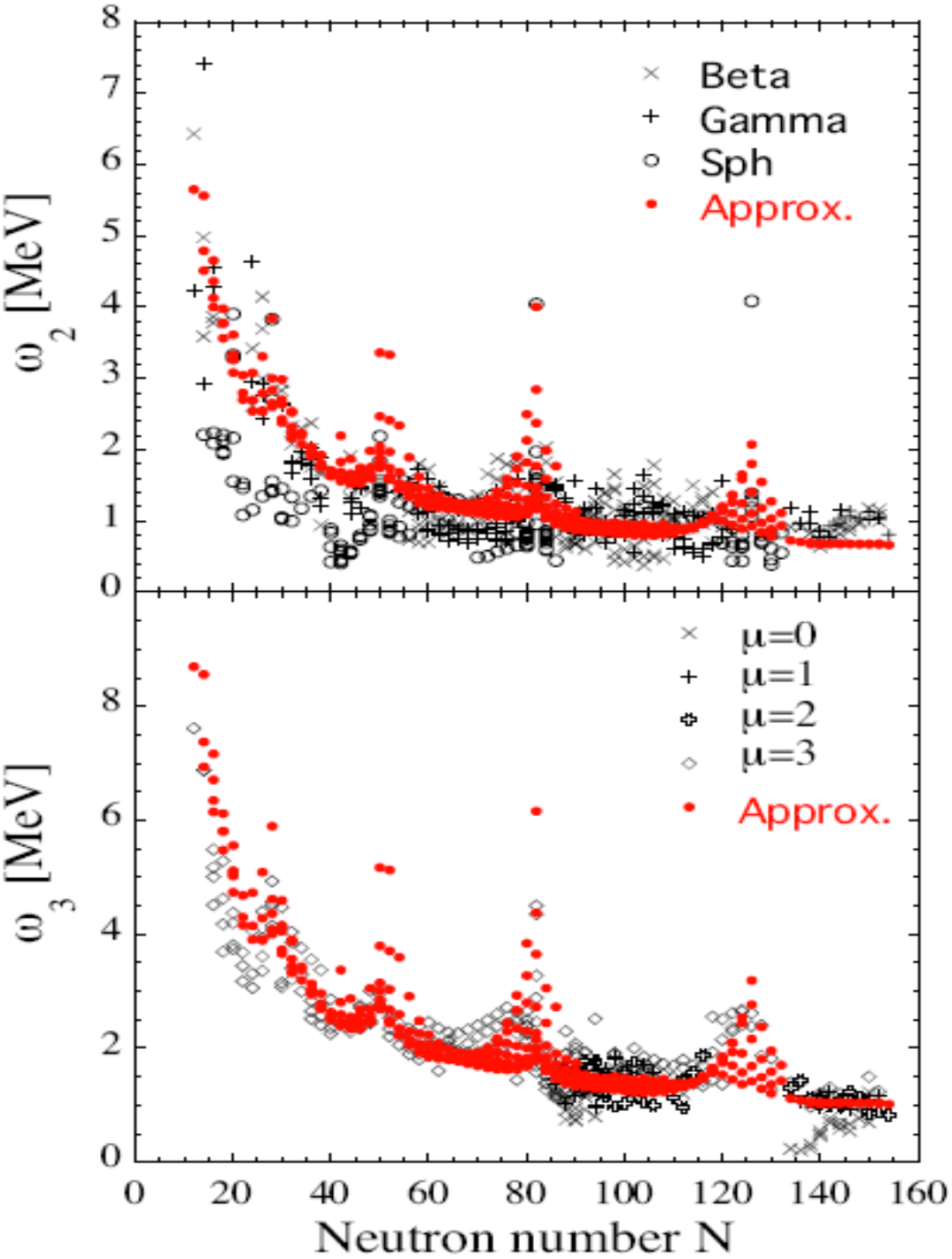


Nowadays almost everybody is agree that the collective levels should be added to quasiparticle excitations at the level density calculations.
However, the estimated coef-ficients of the corresponding level density enhancements differ rather strongly in various publications.

Left: Old Russian estimations of such coefficients [~1980] for spherical (open symbol) and deformed nuclei (closed ones).

Collective enhancement coefficients corresponding to the observed resonance spacings in different models





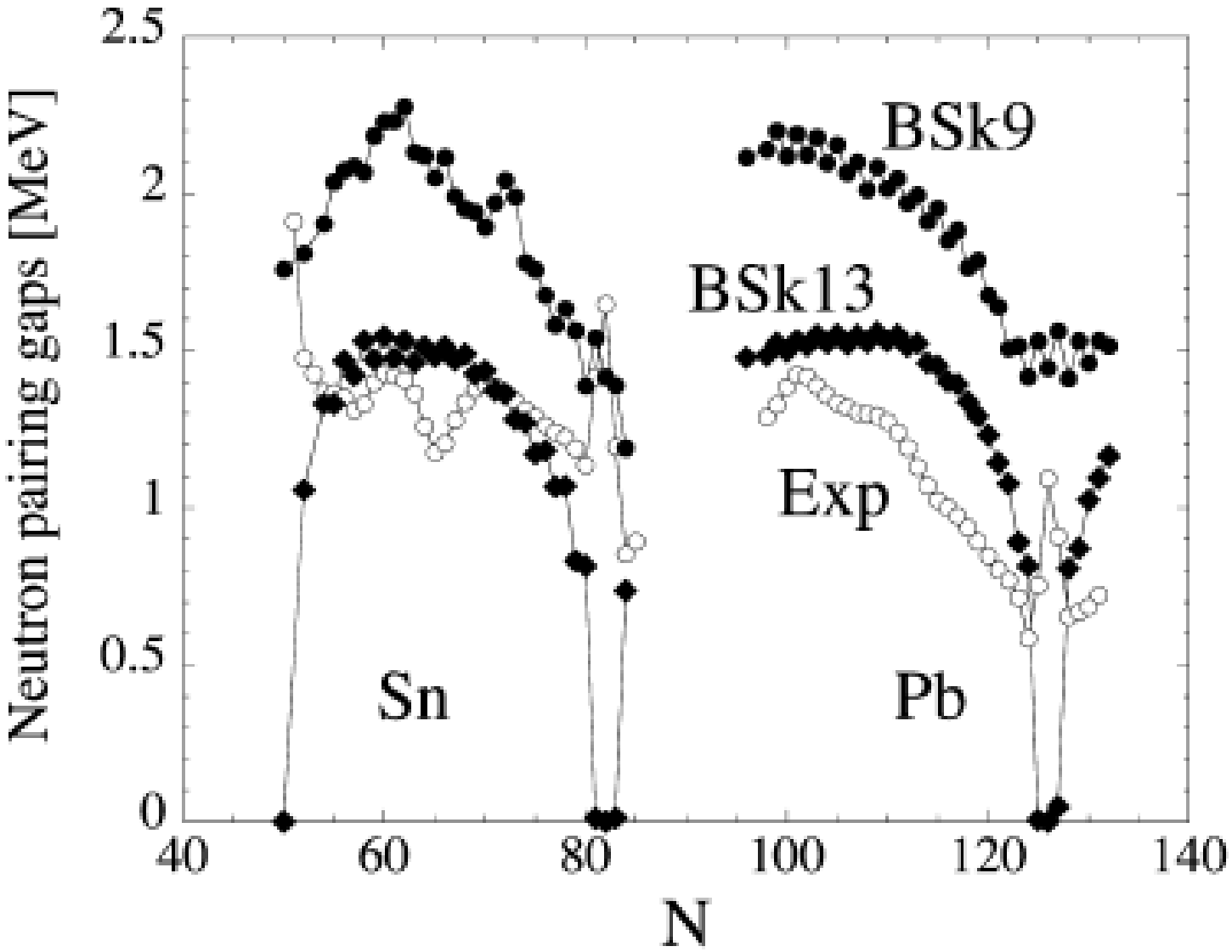
Three analytical expressions based on sets of experimental data on the vibrational levels have been tabulated in order to provide the boson partition function with the quadrupole, octupole, and hexadecapole phonon energies. These expressions are as follow:

$$\omega_2[\mathrm{MeV}] = 65A^{-5/6}/(1+0.05E_{shell}),$$

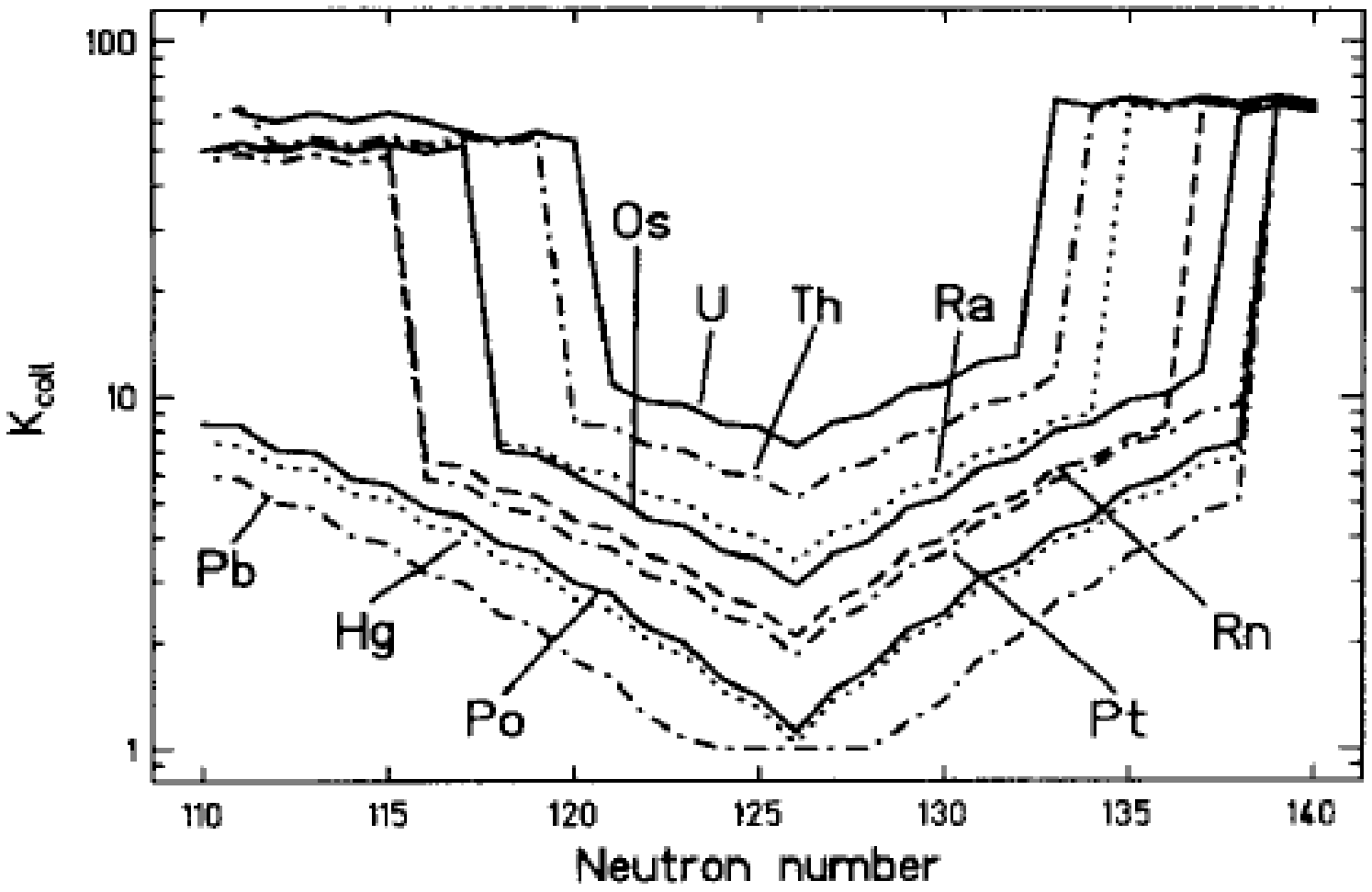
$$\omega_3[\mathrm{MeV}] = 100A^{-5/6}/(1+0.05E_{shell}),$$

$$\omega_4[\mathrm{MeV}] = 160A^{-5/6}/(1+0.05E_{shell}).$$

Comparison for the Sn and Pb isotops of the theoretical neutron pairing gaps and the experimental gap (open symbol). The theoretical spectral gaps are shown for the force BSk9 (full dots) and BSk13 (diamonds).



The collective enhancement for even-Z isotopes obtained from the analysis of the survival probability against fission of excited compound nuclei at an excitation energy of 10 MeV



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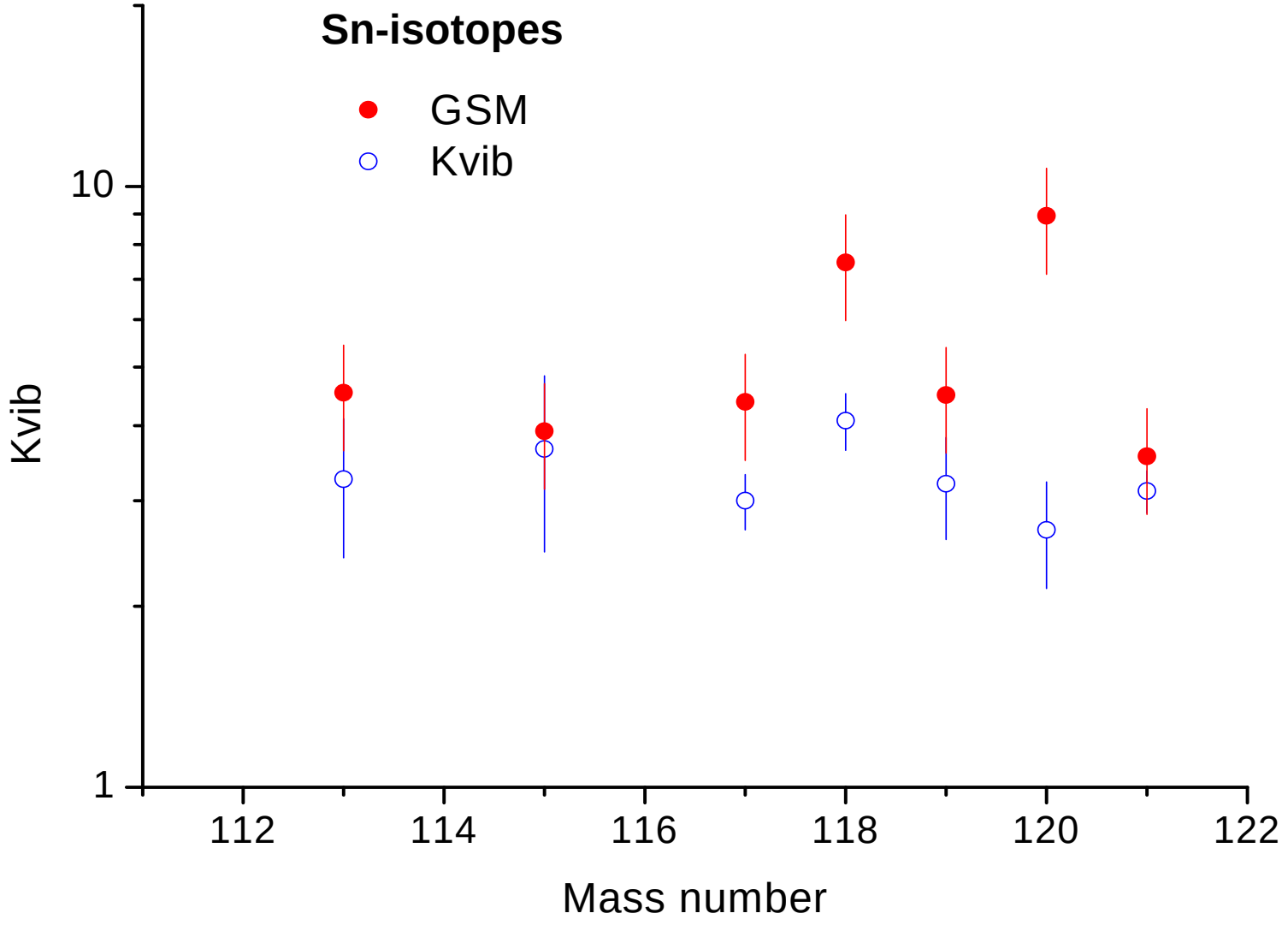
Collective enhancement for Sn- isotopes obtained for the GSM systematics and the microscopic calculations with WS-potential



Conclusion

IAEA has undertaken an extensive coordinated effort to develop a library of evaluated and tested nuclear-model input parameters.

Nuclear data evaluators around the world have emphasized and recognized the importance of the IAEA RIPL databases, and have continued to stress their full reliance on the IAEA RIPL-2 and -3 databases for reaction cross section calculations in many publications and conference presentations.

There are still large uncertainties in modelling important nuclear reactions, where insufficient experimental data for guidance exist – e.g. fission and nuclear reactions on excited states, and isomer production, to mention a few. These outstanding issues should be the subject of further activity, and could lead to further improvements in practical calculations.

Last but not least, we would like to stress that the IAEA Nuclear Data Section will maintain in the foreseeable future both the RIPL coordination activities and the compilation of input parameters, including updates to the released RIPL-3 database.