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NUCLEAR MODEL PARAMETER TESTING FOR NUCLEAR DATA EVALUATION (Reference Input Parameter Library: Phase II)

Summary Report of the Second Research Co-ordination Meeting

Varenna, Italy 12 - 16 June 2000

Prepared by

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September 2000

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Abstract

This report summarizes the results and recommendations of the second Research Coordination Meeting on testing and improvement of the Reference Input Parameter Library: Phase II. A primary aim of this meeting was to review progress in the CRP work, to review results of testing the library, to establish the RIPL-2 format and to decide on the contents of the library. The actions were agreed with an aim to complete the project by the end of 2001.

September 2000

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SUMMARY OF THE MEETING

The Reference Input Parameter Library (RIPL) is a collection of input parameters for theoretical calculations of nuclear reaction cross sections. It is targeted at users of nuclear reaction codes and, in particular, at nuclear data evaluators. The first phase of the project completed in 1998, produced a Starter File and related documentation (TECDOC-1034). In 1999 the second phase was initiated in order to test the RIPL-1 data and produce interfaces between RIPL and commonly used nuclear reaction codes.

The second Research Coordination Meeting of the RIPL-2 CRP was held in Varenna (Italy), 12 - 16 June 2000. It was attended by 10 CRP participants and local organizer E. Gadioli, University of Milan. The IAEA was represented by the Head of Nuclear Data Section D. W. Muir and M. Herman who served as a scientific secretary. Phil Young (Los Alamos) was elected chairman of the meeting.

The participants reviewed the status of the work within the CRP. Library testing, interfaces to the reaction model codes, additions to the library and retrieval/presentation tools were discussed. In particular, issues related to level densities and shell corrections were debated in details. The participants agreed to undertake efforts in order to assure internal consistency and completeness of the library. Only those files which fulfill these two conditions will be accepted for the final version of the RIPL-2 library. In particular, this will lead to a substantial modification of the segments containing discrete levels and level density parameters. One of the major issues considered in details was the RIPL-2 format. The discussion resulted in the formulation and adoption of the homogenous RIPL-2 format for all the segments. The RIPL-1 recommended files that are accepted for the RIPL-2 will be converted into the new format. The same format will also be used for new submittals. The actions and relative time-schedule were agreed aiming in the completion of the RIPL-2 library by the end of 2001 and its release early in 2002.

In the following the status of work and recommendations in regard to RIPL-2 contents, format and testing are summarized.

SEGMENT 1: MASSES

(Coordinator: S. Goriely)

RIPL-2 will simplify and reformat (see Section "General RIPL-2 Format Specifications") the data contained in Segment 1 of RIPL-1. Original files will be reworked in order to provide data of relevance without duplicating the same information. In particular, the audi.dat file will not be kept, the experimental masses being transferred to the FRDM and ETFSI files. The beijing.dat file does not contain data which are not already included in other files (masses are in FRDM, half-lives and spin in the Level segment, abundances will be provided in a separate file) and will consequently not be kept in RIPL-2. The jaeri-deformation.dat file will be kept but extended and moved to the Optical Segment. Segment 1 will be therefore reduced to:

- frdm95.dat file including experimental masses and FRDM predictions of masses, microscopic corrections and β deformations. The FRLDM and ε-deformations will not be kept;
- etfsi00.dat file including experimental masses and ETFSI-2 predictions of masses, shell corrections, β deformations and nuclear matter density distributions;
- expdef.dat file including the experimental β^2 deformations of Raman et al. (1987);
- abundance.dat file with the terrestrial abundances to be provided by A. Koning following the Wallet Cards;
- dz.f fortran code which will provide RIPL-2 with the systematics to be used if requested masses are missing in the frdm95.dat and etfsi00.dat files.

In addition, a clear definition of the shell and microscopic corrections will be added to the TECDOC. No other shell corrections, even if required in the Nuclear Level Density Segment (for example Myers & Swiatecki (1966)), will be given in Segment 1.

SEGMENT 2: LEVELS

(Coordinator: T.Belgya)

All files actually present in the Segment 2 of RIPL-1 will be removed and replaced by a new recommended file. The preliminary version of this file has been presented during the Meeting. Contents of the file can be found in the format description later in this section. The file has been checked for multipolarity of γ -rays and for consistency of transition energies with γ -ray energies. Also, sums of the decay branchings were checked. Additional checking by the CRP participants is in progress.

A new method of constant temperature fit has been used to determine cutoff energies for 641 nuclei that have more than 30 levels within a band of +-4 mass units around the valley of stability. This procedure yields nuclear temperatures consistent with the values reported in the level density segment of RIPL-1 (bombay_gc.dat) except discrepancies around mass numbers 58 and 150 (for details see contribution by T. Belgya in Appendix 4). In addition, level density parameters a, extracted from the analysis of cumulative plots using Gilbert-Cameron matching condition were compared and proved consistent with those listed in the bombay_gc.dat file.

After thorough discussion the CRP participants suggested following changes/extensions to the preliminary file:

- To flag the worst fits (X>0.05) of the cumulative plots.
- To derive Nmax and Nc (for definition see the format below), as well as related level energies, for all nuclei using Gilbert-Cameron matching procedure or mass dependent systematics for nuclear temperature T(A).
- To include total transition probabilities, γ-emission probabilities and electron conversion coefficients (ECC) for all nuclei and transitions. Exponential format will be used for γ-emission probabilities and ECC to avoid zero for small values.
- To calculate ECC's if these are not provided by the ENSDF. In the case of mixed E2/M1 transitions the conversion coefficient will be taken to be that of M1 for odd-odd and odd-even nuclei and E2 for even-even nuclei.

• To use F5.1 format for spin, F10.6 for level energy [MeV], and I3 for parity according to general RIPL-2 format specifications.

The formulae for calculation of transition probabilities for all decay modes will be provided. The file containing results of fitting the cumulative plots will be reformatted according to the general RIPL-2 format specifications and will include T, U0, Nc, Nmax, Umin, and Uc. These data will be checked in co-operation with Ignatyuk and Capote with the GC formula using systematics.

Checking of the internal consistency of the Segment will continue and eventual problems in the ENSDF file will be reported to BNL evaluators.

Format

The format of the Segment 2 will be close to the format of the preliminary file. Minor modifications will be proposed by Belgya in order to account for the additional quantities and to assure compatibility with the general RIPL-2 format specifications. The following FORTRAN 90 code was used to create the output for a single isotope in the preliminary file:

```
write(2,'(a5,6i5,2f12.3)') &
                 symb, &
                 A, &
                Ζ, &
                nlev, &
                ngam, &
                nmax. &
                nc, &
sn, &
                 sp
j=0
do i=1,nlev
        write(2,'(i3,1x,f10.3,1x,f5.1,f4.0,1x,(1pe10.2),i3,1x,a1,1x,a4,1x,a18,i>
                 i, &
                 e_lev(i), &
                 jsmy_lev(i), &
                 jpmy_lev(i), &
                 t_lev(i), &
                 nog_lev(i), &
                 jpestimate_lev(i), &
                 uncertain_lev(i), &
                 jptext_lev(i), &
                 nobr_lev(i), &
                 (pfix_lev(i,m),dpercent_lev(i,m),dmodes_lev(i,m),m=1,nobr_lev(i>
                 do k=1,nog_lev(i)
                         i=i+1
                         write(2,'(39x,i4,1x,f10.3,1x,f8.3,1x,f8.3)') &
                         final_gam(j), &
                         e_gam(j), &
                         ri_gam(j), &
                         cc_gam(j)
                 enddo
enddo
```

Meaning of variables and fields:

1) Isotope identification record						
symb: Mass number and isotope symbol						
A: Mass number	Mass number					
Z: Charge number	Charge number					
nlev: Total number	nlev: Total number of levels.					
ngam: Total number	of γ rays.					
nmax: Ordinary num	ber of level up to which the level scheme is complete.					
is relayed Situ	ution like $(5+)$ is accepted as $5+$ unique spin and parity					
Sn. Neutron separ	ation energy in (keV)					
Sp: Proton separat	ion energy in (keV).					
2) loval nacond						
2) level recora	Ordinary number of level					
$e_{i} = e_{i} (i)^{2}$	level energy in (keV)					
$c_{ismv} lev(i)$	Calculated unique spin. Value -1.0 means undetermined spin					
ipmy lev(i):	Calculated unique parity. Value 0.0 means undetermined parity.					
JF	1.0 positive, and -1.0 means negative parity.					
t_lev(i):	Lifetime of the level in seconds. Value -1.0 means stable.					
nog_lev(i):	Number of γ rays that are de-exciting the level.					
jpestimate_lev(i):	It can have 4 different values. Letter "u" means					
	unique, "c" chosen from a set of value (either it was given in					
	ENSDF or limited from γ transitions), "n" means that it					
	was determined from the spin distribution determined from					
	known values, " " means that no value is given.					
uncertain_lev(i):	If not empty it shows that the level energy is relative					
:	to an unknown value. Its value can be X+, Y+ etc.					
jptext_lev(1):	Figure and the second to adjust the spin parity values by					
	hand					
nobr lev(i)	Number of different decay modes. It can have values up to 10					
	O means that it may decay by y ray, but other decay mode					
	is not expected.					
m:	Index for the decay modes.					
pfix lev(i,m): Prefix	- as it was found in the ENSDF file - that modifies					
	the value given after it. Possible values are, =, >, <, LT, AP,					
	GT, LE, GE, SY, ?. The last two needs explanation:					
	SY means value is from systematic, "?" means unknown %,					
	but expected or seen decay mode.					
dpercent_lev(i,m):	Percentage of the given decay mode. In some cases it					
	adds up more than 100%. If the percentage is small the sum					
	should be re-normalized. If the decay mode is one from					
	'%ECP', %ECA', %B+P', %B+2P', %B-N', %B-2N' then					
	the % before it should be taken as β delay particle emission					
	trom the 100% β decay. I.e. This part leads to particle					
	unstable levels.					

dmodes_lev(i,m):	Its value can be one of these: '%P', '%N', '%G', '%EC+%B+',
	'%EC','%A','%B-','%IT','%SF','%3HE','%ECP','%ECA',
	'%B+P', '%B+2P', '%B-N', '%B-2N'. Some minor
	possibilities like 20Ne decay is neglected.

2) Gamma record	;	is a	running	index i	of the .	vravs
υ,	ounina record	, J	is u	running	тиел в	j me	ruys –

final_gam(j):	Ordinary number of the final level.
e_gam(j):	γ-ray energy in (keV).
ri_gam(j):	Relative γ -ray branching. The strongest being 100. In the
	reaction calculations it needs to be normalized by the user.
cc_gam(j):	Internal conversion coefficient, that should be taken into
	account when intensity balance is made. Given in ENSDF only
	when measured. Thus despite of its 0.0 value it may differ from 0.

SEGMENT 3: RESONANCES

(Coordinator: A. Ignatyuk)

The average resonance parameters of RIPL-1 were tested by the Brussels and Obninsk groups and the following points were noted:

- Chinese evaluation of D_o includes about 60 nuclei not available in the recommended Obninsk file. It is necessary to clarify the origin of these data and eventually to include them in the recommended file. The data for 34-S, 209-Pb and 142-Ce should be checked and, probably, corrected;
- New evaluations of the average parameters for p-wave neutron resonances prepared by the Obninsk group will be included into the RIPL-2 as an additional recommended file;
- New compilation of the neutron resonance parameters prepared by S.Sukhoruchkin et al. and published by Springer Verlag could be useful for updating the recommended parameters. Unfortunately this compilation is not available to most users. It is recommended that IAEA-NDS purchase this publication in order to reanalyze average resonance parameters for those cases in which the number of reported resonances differs strongly from the Mughabhabg compilation. Obninsk group is ready to perform such an analysis and to update corresponding recommended files.
- The recommended file will be reformatted by the Obninsk group following general RIPL-2 format specifications.

The Beijing group is strongly encouraged to contribute to these activities.

SEGMENT 4: LEVEL DENSITIES

(Coordinator: A. Ignatyuk)

Total Level Density

Contradictions between the average resonance spacings in the beijing.dat file and the average resonance spacings calculated with the Back Shifted Fermi Gas (BSFG) and Gilbert-Cameron (GC) models were noted by the Beijing group. General discussion of the recommended and others files included in this Segment indicates the need for a more complete definition of all model parameters used in the experimental data fitting. A necessity to supplement the recommended level density parameters with the corresponding systematics for all nuclei was confirmed by all the participants.

It was decided that RIPL-2 will include recommended (and only recommended) files for the three accepted models and microscopic level densities in the tabular form.

- For the Generalized Superfluid Model (GSM) the recommended reformatted file, together with the related systematics, will be prepared by the Obninsk group.
- For the BSFG and GC models similar files will be prepared in collaboration by the Beijing and Obninsk groups. The contradictions of D_o evaluated by these groups should be clarified and removed wherever possible. The level density parameter systematics will be provided for the BSFG and GC models. These will be supplemented with the detailed formulas or tables for the shell corrections, pairing parameters and other relevant quantities.
- Tables of microscopic nuclear level densities, based on a HF+BCS single-particle schemes and including collective effects, will be provided by Goriely. Testing of these level densities has already been initiated (comparison with the average neutron resonance spacings).

Consistency checking of the recommended GC level density parameters with discrete levels in Segment 2 has been initiated and will continue (see also discussion of Segment 2).

Fission

The theoretical fission barriers will be supplied for all heavy nuclei by the Brussels group and will be included in the RIPL-2. The experimental fission barriers available in the RIPL-1 will be extended to lighter nuclei and reformatted in accordance with the accepted general RIPL-2 format specifications. The description of the level density for fission channels will be modified in collaboration with V. Maslov to reflect changes in the recommended experimental and theoretical fission barriers.

Partial level densities

The two methods for determining partial level densities (PLD) in pre-equilibrium model calculations were described in the RIPL-1 Handbook (TECDOC-1034). The first one consists of closed formulae using the equidistant spacing model. The second is a semimicroscopic one, which employs single-particle level schemes contained in the RIPL-1 and relies upon combinatorial counting of the states. Limited testing of the both methods has been carried out. Good agreement between closed formulae and microscopic PLD was demonstrated for the deformed nuclei. However, large shell energy shifts that appear for nearmagic nuclei can not be taken into account by any closed formula. In order to facilitate selection and use of PLD in nuclear model calculations recommended subroutines for PLD calculations will be extracted from the AVRIGEANU.FOR code. The microscopic PLD's for one, two and three particle-hole configurations can be calculated with the microscopic code already included in RIPL-1 using either Nix-Moeller or ETFSI single-particle level schemes. In RIPL-2 the latter two files will be split into elemental files. Appropriate interface code for reading these files and the updated code for the PLD calculations will be provided by Capote.

SEGMENT 5: OPTICAL

(Coordinator: O. Bersillon)

Many optical model parameter sets were collected for RIPL-1. Only those which cover a broad energy range are useful for production of nuclear data files since combining different sets results in the undesired discontinuities in cross sections. Therefore, it was decided to split the present selection into an archival part (containing essentially monoenergetic sets) and a users part, which will contain only global potentials. Moreover the most recent developments for neutron and proton o.m.p. at Bruyeres will be included in RIPL-2 after their release. This may require some extensions to the current format of Segment 5. The global o.m.p. for neutrons and protons on spherical nuclei as proposed by the Petten group will be introduced into RIPL-2 after its release. In addition, 88 o.m.p. sets compiled in Beijing will be added. The RIPL-1 collection of o.m.p. will be extended by the compilation of o.m.p. for complex particles (up to α -particle) that will be provided by the Bombay group.

Where there are not enough experimental data to define precisely the o.m.p. one has to resort either to global phenomenological parameterization or to new more microscopic approaches. Such semi-microscopic approach developed at Bruyeres (revisited JLM) will be submitted to RIPL-2 starting with the case of spherical nuclei.

Coupled Channels and Distorted Wave Born Approximation calculations require the so called experimental deformations for excited states. In order to satisfy this need it was decided to include in the RIPL-2 the compilation of experimental deformations published by Raman et al. in 1987. In addition, Fukahori will combine and submit to RIPL-2 experimental deformation used in various evaluation projects. For the purpose of identification these files will reproduce discrete level record from the Segment 2.

SEGMENT 6: GAMMA

(Coordinator: M. Herman)

The RIPL-1 file *kopecky.dat* containing γ -strength functions has been reformatted by Plujko into computer readable form. It will be further reformatted by Herman according to general RIPL-2 format specifications. Also, the Beijing file with GDR parameters will by reformatted to conform with the new specifications. These parameters will be supplemented with the shell-dependent GDR width provided by Goriely. Additional systematics for M1 and

E2 isovector Giant Multipole Resonances (GMR) will be provided by Fukahori. Obninsk group will supply new systematics for the parameters of E1, E2, and M1 GMR's.

The code $fE1_vs_A$ for for calculation of E1 γ -strength functions in the frame of the SLO, EGLO and TPA (Thermodynamic Pole Approximation) models has been provided by Plujko and will be included in RIPL-2.

Participants decided that GDR compilation by Varlamov will be available from RIPL-1 only.

SEGMENT 7: ANGULAR

(Coordinator: M. Herman)

No changes with respect to RIPL-1 are foreseen.

SYSTEMATICS

The role of systematics for nuclear model parameters was recognized by the participants of the Meeting. Actually, even relatively simple calculations on a stable isotope at moderate energies involve nuclei for which there are no experimental data allowing for the determination of the parameters. In such cases one has to resort to systematics or more microscopic approaches. The RIPL-2 will attempt to address both possibilities. There are quantities which are difficult or impossible to systematize (such as masses, observed spacings of neutron resonances or shell corrections). For those (except D0) calculated numerical data will be provided in a tabular form for all nuclei between the two drip lines. For all others appropriate systematics will be constructed. Each Segment in the TECDOC will contain at the very end a section with relevant systematics. In addition to the systematics already contained in the RIPL-1 following systematics will be included:

- energies of 2+ levels for the GSM.
- energies of 3- levels for the GSM.
- all level density parameters for GC, BSG, and GSM models. These will be compared with the recommended D0 values and cumulative plots of levels.
- Γ_γ from D.G. Gardner "Methods for calculating neutron capture cross sections and γ-ray energy spectra", in Neutron Radiative Capture, OECD/NEA series on Neutron Physics and Nuclear Data in Science and Technology, Volume 3, Pergamon Press, pp. 62-118 (1984).
- Obninsk systematics for E1, E2, and M1 GMR parameters.
- Duflo&Zuker subroutine for calculation of nuclear masses.

The quality of the systematics will be assessed by the plot of differences between systematics and experimental values (wherever available) in function of mass number. The resulting average standard deviation will serve as a global quality indicator. In the case of level densities these will be supplemented by the comparison with the physical quantities as stated above.

GENERAL RIPL-2 FORMAT SPECIFICATIONS

Besides the quality of the scientific content of the files, for which the specialists of each Segment are being responsible, it is very important that various files can be accessed easily. The following items will be taken into account when constructing the RIPL-2 database:

- Each file should be readable by a FORTRAN (77 or 90) nuclear model code.
- The format of the files should be unified as much as possible.
- For each file it should be clear whether something has been done to supply missing information (e.g., unknown spins and parities in the discrete level file).
- Each file should be 'human readable'.

The RIPL-2 format will aim to reach the best possible combination of these four aspects.

It was agreed that most of the parameter sets will remain in single dedicated files. The three exceptions are:

- discrete levels
- single particle states (s.p.s.)
- microscopic level densities.

These three parameter sets will each be placed in the dedicated sub-directories. The names of the sub-directories will define their contents. Each sub-directory will contain about 100 files, where each individual file will represent a nuclear element and will have the name zZZZ.dat where ZZZ is the charge number of the element (e.g., z012.dat for ¹²Mg). Thus, one file will contain information for all the isotopes of an element. The I3.3 format can be used to fill in the correct charge number for ZZZ (i.e., to print 012 rather than 12).

Apart from the three cases mentioned above all other files will be organized columnwise. Each file will start with 4 lines containing descriptive information. The first character of these 4 lines will be a "#". The 4 lines will contain the quantities, their units and a separation line. If only 3 lines are used the first one should be left blank (except of # sign). Typical example reads:

#							
#	Z	А	El	D0	dD0		
#				[meV]	[meV]		
# -						 	

The information in each file will be given in order of increasing Z and per each Z in order of increasing A.

Each new nuclide will start with Z, A, and elemental symbol in the format (2i4, 1x, a2). The symbol will be left justified in the "a2" field and will always start with a capital (e.g. Fe).

Blanks in the file are allowed, but only in fields where a data value of zero cannot occur. In such cases blanks indicate that systematics should be applied. The use of blanks should be clearly explained in the manual. Special care is required for the 12-C mass, shell

corrections and deformation parameters as their physical value might be zero. For this reason the discrete levels file (Segment 2) will not contain blank fields.

A few rules uniformly apply throughout all the files:

- spins will be given in (f5.1) format
- level energies will be given in (f10.6) format
- parities will be given in (i3) format, with possible values: -1 (negative), 1 (positive) or 0 (unknown)
- following units will be used (unless common practice imposes other choice, e.g., D0 is normally given in meV):
 - energy in MeV,
 - time (half-lives) in seconds
 - length in fm
- Most important quantities should appear to the left.

A single file must contain *all* the parameters necessary for determination of a physical quantity and refer to one specified model. Thus, for example, level density parameters for GC and BSG models should be given in separate files and not mixed together.

RIPL-2 RETRIEVAL TOOLS

(Coordinator: T. Fukahori)

Web pages for retrieval of recommended masses, discrete levels (also in the GNASH format) and optical potential parameters based on RIPL-1 starter file have been prepared by Fukahori and made available at:

http://wwwndc.tokai.jaeri.go.jp/RIPL/RIPL_mass.html and http://wwwndc.tokai.jaeri.go.jp/RIPL/wripl/index.html

Retrieval of the optical model parameters is coupled with optical model code which allows for on-line calculation of elastic angular distributions, total and absorption cross sections, S-matrix elements, and transmission coefficients. Plots of angular distributions, optical model potentials, and cumulative plots of discrete levels can be requested. These retrieval tools will be expanded so that the final Web interface will include (items within square brackets are tentative):

Masses:

• Audi, FRDM, ETFSI, and abundances (numerical data)

Levels:

- levels and decay data (numerical data and cumulative plots)
- Nmax (numerical data)

Resonance:

• D0 (numerical data)

Optical:

- index of optical potentials,
- cross sections: single energy, total, elastic, nonelastic, (numerical data)
- transmission coefficients (numerical data),
- S-matrix (numerical data)
- angular distributions (numerical data and plots)
- potential shape (plot)
- volume integral (plot)
- [total, elastic, and nonelastic cross sections in function of energy (numerical data and plots, comparison with TOTELA systematics above 20 MeV)]
- deformation parameters (numerical data)

Density:

Total and Fission:

- (numerical data, [plots including comparison with cumulative number of discrete levels and various level density formulae])
- microscopic (ETFSI) level densities (numerical data)
- D0 calculated using given model parameters and/or systematics (numerical data) **Partial**:
- link to the codes

Gamma:

- GMR parameters according to Beijing and Goriely (numerical data)
- [GDR shape using different parameterizations (plot)]
- link to the codes.

Angular:

• link to the codes.

TESTING OF RIPL-1

Testing of the RIPL library concentrated mostly on the level density segment. Following tasks have been carried out by Capote:

- Software package for level density calculations within BSFG and GSM model were written and tested using RIPL-1 recommended parameters. Phenomenological level density code OBNINSK_BCS.FOR distributed with RIPL-1 was also tested.
- Microscopical code OBNINSK_MICRO.FOR, distributed with RIPL-1, was compared with microscopical Monte Carlo state density calculations using Nix-Moeller single particle levels.
- Phenomenological level density code OBNINSK_BCS.FOR, distributed with RIPL-1, was tested against Monte Carlo calculations mentioned above.
- Collective enhancement factors in the GSM formulation were compared with semimicroscopical calculation using Interacting Boson Model (IBM) for vibrational, rotational and transitional nuclei. The impact of negative parity states on the enhancement factor was evaluated for samarium and thorium isotopes.
- Microscopical particle-hole state densities calculated with the CAPOTE_MICRO.FOR code using Nix-Moeller single particle levels were compared with the results of AVRIGEANU's phenomenological code.

All microscopical codes in RIPL-1 proved to be complete. No strong dependence on the used single particle level scheme was observed in microscopical calculations. More work on the collective enhancement of the level densities is needed to improve currently used phenomenological recipes. It was shown that phenomenological closed formulae for particlehole state density fails to describe microscopical calculation for magic nuclei. For deformed nuclei, like Sm-152, the agreement of Williams closed formulae using Kalbach pairing correction with microscopical calculations was very good.

In addition, a comprehensive testing of the level density parameters was performed by the Beijing group. The level densities were calculated for 303 nuclei using GC and BSG approaches and compared against experimental D0's and cumulative plots of discrete levels. Generally, better agreement was found for the GC approach but there is a clear need for improvement.

CODE INTERFACES

Progress has been made in preparing interfaces between RIPL and selected nuclear reaction codes. This work will continue being facilitated by the adopted common RIPL-2 format. Status of the interfaces is summarized below (note that most interfaces will need adjustments due to the new RIPL-2 format):

- ECIS interface to prepare ECIS input from the RIPL library was coded by Young for the case of rotational nuclei. Further work is needed to include vibrational cases.
- SCAT2 two interfaces were prepared independently by Young and Capote. Both authors will agree on a single recommended version
- GNASH interface to GNASH optical model transmission coefficient file (tape10) for the RIPL-1 library has been completed with the optical model parameter retrieval code reported here. Similarly, implementation of a mass/spin-parity table (tape13) has also been implemented. Final interface will be based on the existing PREGNASH code after modification to the RIPL-2 format. Interface to the discrete levels (Segment 2) will be coded separately. RIPL-1 discrete levels in the GNASH format are already available on the WEB at: http://wwwndc.tokai.jaeri.go.jp/RIPL/wripl/index.html).

Development of the software package for the generalized superfluid level density model using RIPL parameters is under way (Ignatyuk and Young).

- ALICE95 interface has been prepared by Fukahori but needs adjustment to the new format
- SINCROS interface has been prepared by Fukahori but needs adjustment to the new format
- **EMPIRE-2** the code will be modified to access RIPL-2 library directly without any additional interface. Actually, EMPIRE-2.13 already makes use of certain data contained in RIPL-1 (Ilijnov data, GDR systematics, and masses). Future releases will fully rely on RIPL-2 data (except EMPIRE specific level densities that will not be included in the official RIPL-2 version).
- UNF the basic structure of the unified UNF code has been fixed and support for RIPL-2 will be developed.

- **STAPRE** this code has been dropped from the list of supported codes due to lack of interest among the participants and to the fact that there is no reference version publicly available. It was also noted that the code is not capable of treating energies considerably higher than 20 MeV. However, Herman will inform Avrigeanu about RIPL-2 development and in case appropriate interfaces are produced they will be included in RIPL-2.
- **TNG** this code is not on list but Herman will inform P. Fu about RIPL development. In case appropriate interfaces are produced they will be included in RIPL-2.

TECDOC

Participants agreed that the RIPL-2 TECDOC should follow the structure of its predecessor. The theoretical descriptions for each Segment in TECDOC-1034 will be carried over to the new document with appropriate modifications reflecting changes and extensions in the new library. New section with the description of the Web interface will be written by Fukahori. Coordinators of the Segments will be responsible for drafting appropriate chapters prior to the final RIPL-2 CRP meeting, as detailed below under ACTIONS.

UPLOADING NEW FILES

The RIPL2 area has been set up on the NDS-Alpha server running under VMS operating system for uploading and downloading new RIPL-2 files. It is accessible (only to the RIPL participants) via ftp to:

iaeand.iaea.or.at user: reserved to the RIPL-2 participants

The directory structure is the same as the one of RIPL-1 but there is no distinction between recommended and other files:

- masses
- levels
- resonances
- optical
- densities
 - total
 - fission
 - partial
- gamma
- angular
- PRELIMINARY (the same structure as above but contains preliminary files in nonstandard format supplied before the Meeting)

The files should be stored in the appropriate directories. The name of the file should start with the contributor's name followed by additional specification. For example, Mengoni's file with Gilbert-Cameron parameters (originally named *mengoni_gc.dat* in RIPL-1) when reformatted by Capote should be named as *capote-mengoni_gc.dat*

The 'reformatter' name will be removed in the final version. If a file is a new entry its name should start with the contributor's name and necessary specification (e.g., bcs, micro, def, ...). The directory name should not be repeated (masses, levels, etc.) in the filename. The general structure of the filename should be:

[reformatter-]origin[_specification].dat

with items within square brackets being optional. Be aware that VMS accepts only one dot in the filename so anything like *capote.mengoni.gc.dat* will **NOT** work. Each file must be accompanied by the related 'readme' file containing description of the data. These files should have the same root-name as 'data' files but *.dat* extension should be replaced by *.readme* extension. The style of *.readme* files should follow an example in Appendix 5.

Related FORTRAN coding for reading the file is recommended for more complicated (non column-oriented) structure.

NEW (OR REFORMATTED) ENTRIES IN THE RIPL-2 LIBRARY

(AS OF JUNE, 2000)

A number of new or reformatted files have been uploaded by the CRP participants into the RIPL-2 area at the NDS server before the Meeting. These files do not conform to the new RIPL-2 format specifications and are intended as working files to be used by the CRP participants only. The following files are placed in the *PRELIMINARY* directory:

- Masses
 - KONING-ABUNDANCE.README
 - KONING-ABUNDANCE.DAT
 - KONING-AUDIMOLLER.README
 - KONING-AUDIMOLLER.DAT
 - GORIELY-ETFSI2.README
 - GORIELY-ETFSI2.DAT
 - GORIELY-MOLLER.README
 - GORIELY-MOLLER.DAT
- Levels
 - KONING-MOLNAR.README
 - KONING-MOLNAR.DAT
 - BELGYA.README
 - BELGYA
 - Z_xxx.DAT (110 files with levels for Z=0 through Z=109)
 - •
- Resonances
 - KONING-IGNATYUK.README
 - KONING-IGNATYUK.DAT

• Optical

•

- CNDC_OMPARAMETER.DAT
- YOUNG_OMFORMAT.README
- YOUNG_OMFORMAT.DAT
- YOUNG_OMPARAMETER.README
- YOUNG_OMPARAMETER.DAT
 - YOUNG_OMINPUT_FOR
 - OMINPUT.README
 - OMINPUT.FOR
 - OMINPUT.CMB
 - OMINPUT.INP
 - EC96.INP
 - SC2.INP
- KONING-DEFORMATION.README
- KONING-DEFORMATION.DAT
- YOUNG_GS-MASSSP.README
- YOUNG_GS-MASSSP.DAT
- GORIELY-RAMAN.README
- GORIELY-RAMAN.DAT
- FUKAHORI-DEFORM_Q.DAT
- FUKAHORI-DEFORM_Q.FOR (code to extract data from ENSDF)
- FUKAHORI-DEFORM_BE2.DAT
- FUKAHORI-DEFORM_BE2.FOR (code to extract data from ENSDF)
- FUKAHORI-DEFORM_BE3.DAT
- FUKAHORI-DEFORM_BE3.FOR (code to extract data from ENSDF)
- FUKAHORI-DEFORM_BE2W.DAT
- FUKAHORI-DEFORM_BE2W.FOR (code to extract data from ENSDF)
- FUKAHORI-DEFORM_BE3W.DAT
- FUKAHORI-DEFORM_BE3W.FOR (code to extract data from ENSDF)
- FUKAHORI-DEFORM_BE2R.DAT
- FUKAHORI-DEFORM_BE3R.DAT
- densities
 - total
 - GORIELY-NLD.README
 - GORIELY-NLD.DIR
 - *GE_ZHIGANG-PLOTS.DIR*
 - GCBS.DOC
 - 51 PostScript files with plots
 - fission
 - partial
 - GORIELY-SPLETFSI2.README
 - GORIELY-SPL.DIR
 - Z_xxx.SPL (90 files with s.p.s. for Z=15 through Z=104)

- gamma
 - KONING-BEIJING.README
 - KONING-BEIJING.DAT
 - PLUJKO-KOPECKY.DAT
 - PLUJKO-FE1_VS_A
 - FE1_VS_A.README
 - FE1_VS_A.FOR
 - FE1_VS_A.EXE
 - FE1_VS_A.BAT
 - GNUPLOT.EXE
 - GNUPLOT.INI
 - KOPECKY.DAT (the same as PLUJKO-KOPECKY.DAT above)
 - PAR_DEF.DAT
 - PAR_DENS.DAT
 - BEIJING.DAT
- angular

ACTIONS

The participants agreed upon the following tasks and their relative deadlines:

Belgya

Deigju	
• Reformat the level file and flag high χ^2	09/2000
• Send one sample case with levels to Koning	07/2000
• Check consistency of the recommended Nmax with the level density files	
(with Capote nad Ignatyuk)	04/2001
• Provide updated and consistent version of the levels file	06/2001
• Write first draft of the TECDOC Segment 2 (Levels)	09/2001
Bersillon	
• Define the format necessary for the semi-microscopic parameterization	
(matter distribution)	10/2000
• Provide the interface code between matter distribution file and ECIS	12/2000
• Introduce new Koning's global optical model parameters	12/2000
Introduce new Koning's particular optical model parameters	03/2001
• Introduce available phenomenological optical model parameters	
from Bruyeres	06/2001
• Write first draft of the TECDOC Segment 5 (Optical)	09/2001
Capote	
• Submit Nix_Moeller s.p.s. splitted into elemental files and properly renamed	07/2000
• Submit routine for reading new s.p.s. files	07/2000
• Extract single recommended subroutines from the Avrigeanu code	03/2001
• Check consistency of the recommended GC parameters with the	
level file (with Belgya and Ignatyuk)	04/2001
• Write first draft of the TECDOC Segment 4 (Densities - partial)	09/2001

Fukahori

•	Submit TOTELA code with JAERI systematics and contribution to the	
	meeting	06/2000
•	Combine experimental deformation parameters	12/2000
•	Provide additional systematics for M1 and E2 isovector GMR	03/2001
•	Develop Web retrieval tools according to section "RIPL-2 Retrieval Tools"	09/2001
•	Write first draft of the TECDOC chapter on Web intrfaces	09/2001
G	Zhigang	
•	Investigate the origin of additional data in the Beijing file and provide	
	additional data to Ignatyuk or provide reformatted file.	09/2000
•	Provide new 88 o.m.p. sets obtained by Beijing group	08/2000
•	Investigate contradictions of experimental and theoretical D0 for BSFG and	
	GC models and provide reformatted files or inform Ignatyuk about the results	12/2000
•	Perform a detail testing of Koning's global potential on selected nuclei	
	including other reliable global optical potentials	04/2001
•	Prepare the UNF code for physical testing of RIPL-2	10/2001
G	oriely	
•	Provide reformatted files with ETFSI s.p.s.	09/2000
•	Reformat all files of Segment 1 according to the agreed specifications	10/2000
٠	Provide ETFSI fission barriers	10/2000
•	Provide Duflo-Zuker fortran code	10/2000
٠	Provide shell dependent GDR table	03/2001
•	Provide hybrid formula for E1 strength function	03/2001
•	Provide tables of microscopic level densities up to 150 MeV and J=30	
	including parallel and perpendicular spin cut-off parameters	03/2001
•	Provide BSFG systematics with all required input, preferentially	
	consistent with RIPL-2	09/2001
•	Write first draft of the TECDOC Segment 1 (Masses)	09/2001
H	erman	
٠	Provide ICC code to Belgya	07/2000
٠	Investigate the possibility of buying Suchoruchkin book and providing	
	new data to Ignatyuk	09/2000
•	Coordinate Segment 6 (Gamma)	
٠	Write first draft of the TECDOC introduction	09/2001
٠	Write first draft of the TECDOC Segment 6 (Gamma)	09/2001
•	Write first draft of the TECDOC Segment 7 (Angular)	09/2001
Ig	natyuk	00/2000
•	Provide Obninsk systematics for E1, E2, and M11 GMR parameters	09/2000
•	Reformat Opinisk resonance file and add p-wave resonance parameters	10/2000
•	Communicate with Masiov with regard to fission parameters for light	10/0000
	Preacunide and naevy transplutonium isotopes	12/2000
•	Redo parameterization of the BCS level density parameters and shell	06/0001
	corrections of Myers Swiatecki for 8000 nuclei (as in Nix-Moller)	06/2001

• Provide routines for calculation of level densities using GC, BSFG,	
and GSM models (with Capote)	06/2001
• Check consistency of the recommended BSFG and GC parameters with the	
level file (with Capote and Belgya)	04/2001
• Writing down first draft of the TECDOC resonances and level density total	
and fission	09/2001
• Write first draft of the TECDOC Segment 3 (Resonances)	09/2001
• Write first draft of the TECDOC Segment 4 (Densities - total and fission)	09/2001
• Test new data from Suchoruchkin, analyse differences, and update	
recommended file	10/2001
Kailas	
• Extend omp to complex light (up to α) particles.	03/2001
• Investigate influence of the level density parameterization on particle spectra.	06/2001
• Test recommended BSFG and GC parameters	06/2001
Vening	
Drovide abundance file according to Wallet Cards	00/2000
• Provide a buildance file according to water Cards • Provide Γ from Cardner book	09/2000
 Provide new global optical model parameters 	12/2000
 Provide PEGNASH code with capability of reading the CDP parameters 	12/2000
to Young	08/2000
 Prenare experimental deformation file reproducing discrete level record 	08/2000
along with deformation B2 and B3 and send it to Eukahori	00/2000
 Provide new particular optical model parameters 	03/2000
	03/2001
Young	
• Incorporate optical model retrieval of RIPL potential into PREGNASH	10/0000
code of Koning	10/2000
• Help Bersilion in splitting optical model library into user and archival part	10/2000
• Expand format of the optical potential library as needed	10/2000
for new potentials (with Bershion)	10/2000
Develop interface cound for linking KIPL-2 level file with GNASH Introduce the 8% of mini cette collected of Decising	11/2000
Introduce the 88 0.111.p. sets confected at Beijing	12/2000
• Install new optical model potentials into library as needed	06/2001

CONCLUSIONS

Presentations and discussions during the Meeting showed good progress of the CRP work. Participants agreed that main emphasis should be given to internal consistency and reliability of the library. In particular, consistency between level densities, discrete levels and shell corrections must be assured. For each quantity full information must be provided in order to avoid ambiguities in its use (e.g., level density parameters must be accompanied by relevant shell corrections used for their derivation). It was noted that providing computer codes for calculation of certain physical quantities from the RIPL-2 parameters might be beneficial to the users and would prevent misuse of the library. Standardization of the format will make RIPL-2 more user friendly and will facilitate preparation of interfaces to nuclear reaction codes. The new RIPL-2 library will contain less files compared to RIPL-1. As a rule only recommended, and well tested, files will be retained. On the other hand, RIPL-2 will be

extended to comprise quantities that were missing or not adequately represented in RIPL-1 (such as abundances and 'experimental' deformations). More attention will also be dedicated to various systematics with the ultimate goal to provide data for any nucleus between neutron and proton drip lines. A considerable amount of new data resulting from the ETFSI model will be included. These semi-microscopic data are particularly attractive because of their internal consistency, wide range of nuclei, and quality comparable to the phenomenological ones. Considerable progress is expected in the optical model segment with the inclusion of new global parameterizations, semi-microscopic approaches and additional potentials for light complex particles. This new features should make RIPL-2 a unique and reliable tool for guiding theoretical calculations at incident energies up to 200 MeV needed for development of modern nuclear data.

ACKNOWLEDGMENTS

Participants wish to express their gratitude to Prof. E. Gadioli for dedicating his time to the organization of the Meeting and for providing such a stimulating surrounding.

Appendix 1

International Atomic Energy Agency

Second Research Coordination Meeting on

Nuclear Model Parameter Testing for Nuclear Data Evaluation (Reference Input Parameter Library: Phase II)

Varenna, Italy

12 - 16 June 2000

AGENDA

Monday, 12 June

- 09:00-10:00 Opening Session
 - Opening, election of chairman, adoption of Agenda
 - RIPL-2 and other IAEA services to nuclear data evaluators (Muir)
- 10:00-12:00 Presentations and Status Reports (Meeting participants)
- 14:00-17:00 Presentations and Status Reports (cont.)
- 17:00-18:00 Nuclear Data and Model Needs for Evaluation of Heavy Ion Reactions (Gadioli)

Tuesday, 13 June

09:00-12:00 Contents and Organization of the RIPL-2

- Shell corrections
- Nuclear deformations
- New quantities (abundances, ETFIS data, ...)
- Level density segment
- Resonance segment
- Systematics

14:00-18:00 Contents and Organization of the RIPL-2 (cont.)

- Interfaces to nuclear reaction codes
- Testing
- Retrieval tools, Web

<u>Wednesday, 14 June</u>

- 09:00-12:00 RIPL-2 Format
 - General principles (Koning)
 - masses (Goriely)
 - levels (Belgya)
 - resonances (Ignatyuk)

14:00-18:00 RIPL-2 Format (cont.)

- optical (Bersillon)
- densities
 - total (Capote)
 - fission (Ignatyuk)
 - partial (Capote)
- gamma (Fukahori)
- angular

Thursday, 15 June

- 09:00-10:00 Discussion of the TECDOC layout (assignment of tasks and deadlines for drafts)
- 10:00-12:00 Drafting the Meeting Report
- 14:00-18:00 Drafting the Meeting Report

<u>Friday, 16 June</u>

- 09:00-12:00 Discussion of the Meeting Report
- 14:00-17:00 Concluding Session
 - Adoption the Meeting Report
 - Final discussion, possible future developments

Appendix 2

International Atomic Energy Agency

Second Research Coordination Meeting on

Nuclear Model Parameter Testing for Nuclear Data Evaluation (Reference Input Parameter Library: Phase II)

Varenna, Italy

12 - 16 June 2000

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Appendix 3

EXAMPLE OF THE README FILE

> S. Goriely Universite Libre de Bruxelles (Belgium) M. Pearson Universite de Montreal, Quebec (Canada) F. Tondeur Institut Superieur Industriel de Bruxelles (Belgium)

> > 12 June 2000

<u>Contents</u>

The data file contains the predictions of the ground state properties obtained within the Extended Thomas-Fermi plus Strutinsky Integral(ETFSI) method, a semi-classical approximations to the Hartree-Fock methat that includes full Strutinsky shell corrections. BCS corrections are added with a delta-force. The present data represent the predictions obtained with the second ETFSI version based on the SkSC18 Skyrme force [1]. The eight active parameters of the underluing Skyrme and delta-function pairing forces are fitted to all the 1719 (A>35, |Z-N|>1) experimental mass data; the rms error of the fit is 709keV.

The present ETFSI-2 compilation include all nuclei with A>35, Z<=110 between the proton and neutron driplines. In addition to the calculated masses, we include the deformation parameters, density distribution parameters, pairing gaps and (pairing-independent) shell correction energies.

<u>Format</u>

Each record of the file contains Z, N, A, M, beta2, beta4, rn, an, rp, ap, D0n,D0p, dWn, dWp defined as follows:

z :	charge number				
EL :	element symbol				
A :	mass number				
M :	the atomic mass excess in MeV				
beta2:	the beta2 deformation parameter				
beta4:	the beta4 deformation parameter				
rn :	the radius of the neutron density distribution in fm				
an :	the diffuseness of the neutron density distribution in fm				
rp :	the radius of the proton density distribution in fm				
ap :	the diffuseness of the proton density distribution in fm				
Dn :	the neutron pairing gap in MeV				
Dp :	the proton pairing gap in MeV				
Wn :	the neutron shell correction energy in MeV (pairing				
	independent)				
Wp :	the proton shell correction energy in MeV (pairing independent)				

The corresponding fortran format is (3i4, f10.3, 10f8.3)

<u>References</u>

- [1] S. Goriely (2000), in Proc. of the 10th International Symposium on
- Capture Gamma-ray Spectroscopy and Related Topics, (Santa-Fe) in press
- [2] R.C. Nayak and J.M. Pearson, Phys. Rev. C52 (1995) 2254
- [3] Y. Aboussir, J.M. Pearson, A.K. Dutta and F.Tondeur, At. Data and Nucl. Data Tables 61 (1995) 127
- [4] Y. Aboussir, J.M. Pearson, A.K. Dutta and F.Tondeur, Nucl. Phys. A549 (1992) 155
- [5] J.M. Pearson, Y. Aboussir, A.K. Dutta, R.C. Nayak, M. Faine and F. Tondeur, Nucl. Phys. A528 (1991) 1
- [6] F. Tondeur, A.K. Dutta, J.M. Pearson and R. Behrman, Nucl. Phys. A470 (1987) 93

APPENDIX 4

Technical input

1.	Los Alamos Progress Report for RIPL-II P.G. Young, M.B. Chadwick and P. Möller	35
2.	General Developments in the Los Alamos Nuclear Physics Group (T-16) P.G. Young and M.B. Chadwick	37
3.	Status of Japanese Contribution to RIPL-2 and some Suggestions T. Fukahori	41
4.	The Completeness of Nuclear Level Schemes T. Belgya	47
5.	Activities Related to "Nuclear Model Parameter Testing for Nuclear Data Evaluation" (RIPL: Phase II) at CNDC Ge Zhigang, Zhang Jingshang, Sun Zhengjun	53
6.	On the Need of Nuclear Data and Codes for the Evaluation of Heavy Ion Reaction Cross Sections E. Gadioli, M. Cavinato, E. Fabrici and E. Gadioli Erba	63
7.	Testing of the Level Density Segment of the RIPL R. Capote R. Capote	73
8.	At Last, Competitive Microscopic Predictions of Nuclear Masses and Nuclear Level Densities S. Goriely	79
9.	Work Report S. Goriely	87
10.	Program TOTELA Calculating Basic Cross Sections in Intermediate Energy Region by Using Systematics T. Fukahori and K. Niita	97

Readers, please note: The attachments were prepared by CRP members before the meeting – subsequent discussions have resulted in modifications to recommendations that are NOT relected in these texts.

LOS ALAMOS PROGRESS REPORT FOR RIPL-II

P.G. Young, M.B. Chadwick and P. Möller 1 June 2000

Summary

Since the last RIPL-II CRP meeting, we have developed a code that prepares inputs from the RIPL-I optical model parameter data base for the SCAT2 and ECIS96 computer codes. We have also made limited corrections to the optical model parameter file, and have made minor extensions to the format for optical potentials. We have implemented mass information from the RIPL-I mass library into the ground-state mass/spin/parity file (Tape13) used in GNASH and other codes. Additionally, we have developed software for using the generalized superfluid level density model on SUN computers at LANL, ultimately for use of the RIPL-I level density information in the GNASH code.

Optical Model Parameter File (RIPL-I)

The format for compiling optical model potentials in the RIPL-I library was modified to include flags to indicate cases where relativistic calculations should be used and to indicate the use of dispersive model parameterizations. Corrections were made to the entry in the parameter library for the Madland Semmering potential (the imaginary part of the spin-orbit potential was inadvertently omitted from the original library). The revised format description and parameter data file are in the IAEA RIPL-II file (OPTICAL area) as young_omformat.dat and young_omparameter.dat.

Retrieval Code for RIPL-I Optical Parameters

A new code, OMINPUT, is being developed for retrieving optical model potentials from the RIPL-I optical model parameter library and formatting the potentials for input into either the SCAT2 or ECIS96 optical model codes. The input required for the code is the energy grid for the calculations (or a default grid can be used), the Z and A of the target nucleus, and the optical model potential number in the RIPL-I library. In addition to the RIPL-I optical parameter file, the ground-state mass/spin/parity file that is described below is required, and appropriate subroutines are included for reading these files. At present the code works for spherical and rotational band potentials but is only partially complete for vibrational potentials. Additionally, the code needs further testing to make certain it works for all cases. A working version (preliminary) of the code is included in the IAEA RIPL-II file (OPTICAL area) as young_ominput.for.

Development of a New Ground-State Mass/Spin/Parity Table Based on the RIPL-I Library for Use in the GNASH Code.

An updated version of the ground-state mass/spin/parity file (tape13) used with the GNASH code has been constructed using the 1995 Audi experimental mass file and the Möller-Nix calculated mass file in RIPL-I. The algorithm used in building the file is to incorporate experimental masses when available and to only use calculated masses in cases where experimental masses are unavailable. Ground-state spins and parities are taken from the Wallet Card compilation by the National Nuclear Data Center at Brookhaven National

Laboratory. The new file contains entries for 9151 nuclei, approximately twice our previous file (3846 entries). [The algorithm used to retrieve masses uses an approximation by Duflo in cases where there is no mass entry in the file.]

The present file is preliminary and needs to be updated for the year 2000 Wallet Card spins and parities that have just been issued. A working file entitled young_gs-masssp.dat is included in the IAEA RIPL-II file (MASS area).

Other Developments

We are developing a code to transform discrete energy level information from the ECN TALYS library (and possibly RIPL-II format) into a GNASH formatted file. This effort will be completed when a new RIPL-II discrete level library is available.

We have developed and tested a software package for the generalized superfluid level density model, ultimately to be implemented in the GNASH code. We have also made a number of improvements and corrections of the GNASH code and have performed extensive calculations with it (see T-16 progress report). A new version of the code will be available soon from the code centers.
GENERAL DEVELOPMENTS IN THE LOS ALAMOS NUCLEAR PHYSICS GROUP (T-16)

P.G. Young and M.B. Chadwick 1 June 2000

Summary

Nuclear physics activities in support of nuclear data development by the newly formed "Nuclear Physics" group (T-16) at Los Alamos are summarized. Activities such as the development of a new Hauser-Feshbach/preequilibrium reaction theory code, improvements to and reissue of the existing GNASH reaction theory code, nuclear cross section evaluation in the context of ENDF/B-VI, development of a new medium-energy optical model potential, new fission neutron spectrum calculations with the Los Alamos model, and development of new 6-group delayed neutron constants for ENDF/B-VI are described.

Formation of New T-16 Group

A new group, "Nuclear Physics" (T-16), was formed in March at Los Alamos from the previous groups "Nuclear Theory and Applications" (T-2) and "Medium Energy Theory" (T-5). The new group has some 20 permanent scientific staff members and postdoctoral fellows, as well as a number of affiliates and consultants. For the present, activities of the new group are not expected to deviate much from those of the two previous groups.

Development of a New Hauser-Feshbach/Preequilibrium Code, McGNASH (Chadwick)

At LANL, significant progress has been made in developing a new and modern version of GNASH, known as McGNASH. The code is being written in a modular fashion, using Fortran90. Over 4000 lines have been written. Significant testing/validation has been accomplished, through checks against GNASH predictions. (This has also led to identifying and removing some approximations in GNASH too). In Hauser-Feshbach validation tests (we focused on 20 MeV n+58Ni, allowing n,p,d,t, α , γ ejectiles in sequential decay processes), we find agreement with GNASH to the better-than 0.2% level.

We have also completed a first version of a Hybrid Monte Carlo preequilibrium module. A collaboration with Oblozinsky at BNL has begun in this area.

Development of 150-MeV Libraries for ENDF/B-VI System (Chadwick)

New evaluations for incident neutrons and protons from 20 to 150 MeV were completed using the GNASH code, with the calculations optimized to available experimental data and systematics, especially for nonelastic cross sections. For the neutron evaluations experimental data were utilized for the total cross sections. The neutron evaluations were combined with existing ENDF/B-VI evaluations, and both the proton and neutron evaluations have been accepted for ENDF/B-VI and are included in Release 6. Target nuclei in the evaluations are: ^{1.2}H, ¹²C, ¹⁴N, ¹⁶O, ²⁷Al, ^{28,29,30}Si, ³¹P, ⁴⁰Ca, ^{50,52,53,54}Cr, ^{54,56,57}Fe, ^{58,60,61,62,64}Ni, ^{63,65}Cu, ⁹³Nb, ^{182,183,184,186}W, ^{206,207,208}Pb, and ²⁰⁹Bi.

Modifications and Corrections of the Original GNASH Code (Young, Chadwick)

We of the original **GNASH** are preparing to issue a new version Hauser-Feshbach/preequilibrium code to the RSIC and NEA Data Bank code centers. The new code includes a number of minor improvements and one important correction in the way multiple reaction channels are buffered for high-energy calculations. The latter deficiency leads to inaccuracies of the order of 30% at 150 MeV in neutron production cross sections for structural materials but is substantially less important for heavy targets and decreases as the incident energy is lowered.

Light Element Studies with R-Matrix Theory (Hale)

Much of our light-element R-matrix activity has been directed to reactions of importance in astrophysics. We have been looking at important helium-burning reactions, such as ${}^{12}C(\alpha,n){}^{16}O$ and ${}^{13}C(\alpha,n){}^{16}O$, for the past several years. We are also beginning a systematic study of the big-bang nucleosynthesis reactions, starting with n+p capture. Astrophysical interests have also motivated us to investigate fully quantum-mechanical calculations of screened reaction rates. In keeping with the strong interest in the nature of fundamental hadronic interactions in our combined group, we have continued our studies of the lightest systems (A=3,4) with particular attention to evidence for three-body nuclear forces in the experimental data. We also anticipate that additional R-matrix work on the systems containing the light-element standard cross sections will begin soon in support of the newly proposed Standards CRP.

Miscellaneous Evaluation Work (Young)

New evaluations have been completed for neutron-induced reactions on ¹⁶O, ³⁵Cl and ³⁷Cl. The ¹⁶O evaluation spans the energy range 10^{-5} eV to 30 MeV, where it is joined with the existing 150-MeV evaluation. New measurements of ¹⁶O(n,x γ) discrete γ -ray angular distributions for E_n = 4 – 200 MeV were available from LANSCE and provided a major new evaluation input. The new data permit much more reliable determination of (n,n') cross sections [not to mention (n,x γ) cross sections] than was previously possible.

The ³⁵Cl and ³⁷Cl evaluations extend to 20 MeV and are based largely on GNASH calculations matched to the available experimental data, with resonance parameters and inelastic angular distribution taken from JENDL evaluations. New evaluations by Frankle and Reedy of thermal-neutron radiative capture photon production data were incorporated into the ³⁵Cl and ³⁷Cl evaluations. Additionally, the new evaluations by Frankle and Reedy of thermal-neutron photon production have been incorporated into existing ENDF/B-VI evaluations for ⁹Be, ¹⁴N, ¹⁹F, ²³Na, ²⁷Al, ⁴⁵Sc, ^{50,52,53,54}Cr, ⁵⁵Mn, ^{54,56,57,58}Fe, ^{58,60,61,62}Ni, ^{63,65}Cu, and natural K and Mg. These results will be made available for a future update of the ENDF/B-VI file.

New Medium-Energy Nucleon-Nucleus Optical Model Potential (Madland, Sierk)

A global medium-energy nucleon-nucleus optical model potential is under development. The objective is to construct a potential with the following properties: (1) applicable to spherical (or approximately spherical) nuclei in the mass number range $16 \le A \le 209$; (2) simultaneous treatment of proton and neutron projectiles (explicit isospin dependence): (3) energy range of

(perhaps) 20 MeV $\leq E_{proj} \leq$ 2000 MeV; (4) predict very accurate integral observables: σ_R , σ_{tot} ; and, (5) phenomenological approach guided by results/conclusions from microscopic approaches. The two formalisms that are being use are the relativistic Schrödinger formalism and a Dirac formalism. With the relativistic Schrödinger formalism, a second-order reduction of the Dirac equation is formally identical with the non-relativistic Schrödinger equation provided the potential is multiplied by a momentum-dependent factor. In the Dirac formalism, an extended Walecka model is applied in the mean field approximation. The "extended" here means the introduction of isospin and corresponding isovector-scaler and isovector-vector mean fields in addition to the two isoscalar fields. This approach yields a relativistic generalization of the Lane model to allow simultaneous treatment of proton and neutron scattering.

Fission Neutron Spectra Calculations (Madland)

The Los Alamos model has been used to calculate a new prompt fission neutron spectrum matrix for the $n + {}^{235}U$ system. Energy-dependent compound-nucleus formation cross sections for the inverse process were used throughout. The matrix includes first-, second-, and third-chance fission components and also includes the neutrons evaporated prior to fission in second- and third-chance fission. It has been calculated for 19 incident neutron energies ranging from 0 to 15 MeV. The nuclear level-density parameters used in the calculations were determined in least-squares adjustments to the measured differential spectra assembled by N. Kornilov and P. Staples. The matrix is considered complete except for the following: the measurements of the thermal-neutron-induced spectrum are not in agreement. This means that the calculated thermal spectrum depends upon which measurement, or measurements, is used to determine the nuclear level-density parameter for this case. Fortunately, 30 integral cross section measurements have been made in the thermal field. These measurements will assist in determining the correct thermal spectrum.

Fission Product and Decay Data (Wilson, England)

Delayed neutron group parameters have been recalculated with the CINDER'90 code using revised decay data and improved fission yields, with the eventual goal of replacing the values currently in ENDF/B-VI. Beta decay spectra, Pn values, and other decay data are greatly improved relative to those used earlier for ENDF/B-VI, and 60 new fission-yield data sets have replaced the 50 older sets used in the previous calculations. As part of this work, the use of 8 groups with constant exponential (lambda) values for all fission nuclides was compared to the traditional use of 6 groups with lambdas determined by a least squares fitting code. No advantage was observed in the use of 8-group fits with fixed lambdas relative to conventional 6-group fits with variable lambdas. This outcome is important because it means that reactor codes that have traditionally been used do not need to be modified.

STATUS OF JAPANESE CONTRIBUTION TO RIPL-2 AND SOME SUGGESTIONS

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1. Deformation Parameter Retrieve from ENSDF and Literature

The deformation parameters have been retrieved from ENSDF and literature. They are summarized in Table 1. The deformation parameters, such as quadrupole moment (Q), BE2, BE3, BE2W and BE3W have been pick up from ENSDF. The deformation parameter, β_2 , was derived from Q by using the equation;

$$Q = Q_0 \frac{3K^2 - I(I+1)}{(I+1)(2I+3)}$$
(1)

$$Q_0 = \frac{3}{\sqrt{5\pi}} Z R_0^2 \beta (1 + 0.16\beta + ...)$$
(2)

$$\boldsymbol{R}_{0}^{2} = 0.0144 \boldsymbol{A}^{2/3} \text{ [b]}$$
(3)

where K, I were assumed to be equal to ground and excited state spins, and Z, A are atomic and mass numbers, respectively.

The deformation parameters, $B(E2;0^+ \rightarrow 2^+)$ and $B(E3;0^+ \rightarrow 3^-)$, were compiled from the Ref. [1,2]. The parameters can be converted to β_2 and β_3 by using appropriate equations [1,2];

$$\boldsymbol{B}(\boldsymbol{E}2) \uparrow = \left(\frac{3}{4\pi} \boldsymbol{R}_0^2 \boldsymbol{Z} \boldsymbol{e} \boldsymbol{\beta}_2\right)^2 \ [\mathrm{e}^2 \mathrm{b}^2 \text{ or } \mathrm{W.U.}] \tag{4}$$

$$B(E3) \uparrow = (\frac{3}{4\pi} R_0^3 Ze\beta_3)^2 \ [e^2b^3 \text{ or } W.U.]$$
(5)

However, only the parameter Q was converted at the moment.

Parameters	Sources	File Name	Amount [recodes]	Amount [kB]
Q, β_2	ENSDF	deform_q.dat	834	67
BE2	ENSDF	deform_be2.dat	208	17
BE3	ENSDF	deform_be3.dat	100	9
BE2W	ENSDF	deform_be2w.dat	110	9
BE3W	ENSDF	deform_be3w.dat	16	2
$B(E2;0^+ \rightarrow 2^+)$	Ref. [1]	deform_be2r.dat	276	6
$B(E3;0^+\rightarrow 3^-)$	Ref. [2]	deform_be3r.dat	154	3

 Table 1 Retrieved Deformation Parameters

2. WWW Page Preparation

We have initiated the work on WWW page related to the RIPL Starter File. The pages for masses, discrete levels and optical potentials were prepared. The samples of these pages are shown in Figs. 1-3.

3. Suggestions

RIPL-2 File Format

- 1) The format should be fixed and never changed.
- 2) The column for strings of like '56fe' had better to be moved to the beginning of the line.
- 3) The large amounts of blanks should be removed to reduce the space.
- 4) The empty fields should be filled with some character or symbol, in order to be easily treated by the C or PERL languages.
- 5) In the discrete level file, something should be placed at the beginning of the record of identify nuclide for easy retrieval.
- 6) The deformation parameters should be placed in the same files as discrete levels.
- 7) The E-format is better for the unification of the format.
- 8) Possibly, the units should be unified (eV, barn, fm, sec, etc.). If difficult, the unit (and definition of the value) should be written in each file and unified at least in each segment.
- 9) It is recommended to use the comment record.

WWW page preparation,

- 1) The cgi-bin scripts are basically developed in PERL. Thus point 4 above is very important.
- 2) The pages for level density, deformation, GDR, average resonance spacing parameters will be prepared by Japanese group, as well as those for mass, discrete level and optical potential parameters.
- 3) Possibly, the angular distribution segment will also be prepared.

Miscellaneous,

- 1) In the GDR segment, the GDR parameters compiled by Varlamov for the IAEA/CRP on Photonuclear Data should be included.
- 2) The reports will be prepared for the Integrated Nuclear Data Evaluation System (INDES). The UNIX version of INDES is under development.

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Fig. 1 The example of "Mass Page"



Fig. 2 The example of "Discrete Level Page"



Fig. 3 The example of "Optical Model Page"

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Abstract: A new fitting method was developed to determine the completeness of nuclear level schemes. The method was used to fit 641 nuclei with constant temperature model with temperature being a function of the mass number. The obtained temperatures are compared with those determined from Gilbert-Cameron fits. The advantage of the method is that it can be used for nuclei for which level densities at neutron binding energies are not known.

Introduction

The knowledge of completeness of discrete level schemes is important for nuclear reaction calculations. It is determined, by the last level (U_{max} and N_{max} are its energy and the corresponding level number) up to which the discrete level scheme is complete. Due to the nature of its definition, there is no simple way to determine it. It depends very much on the variety of nuclear reactions used to study the nucleus in question. One way to obtain an estimate of the completeness is to use the Gilbert-Cameron (GC) procedure [Gil65].

It has been observed that at low energies the cumulative number of nuclear levels (CNL) can be well described by the constant temperature formula [Hug72, Gil65, Ign85, Ripl-I98],

$$N(E) = \exp\left(\frac{U - U_0}{T}\right),\tag{1}$$

where U_0 and the nuclear temperature T are parameters that can be determined from a fit of N(E) to the CNL of a given nucleus. It is assumed that all neutron resonances in a narrow spin window (J=J_{gs}±1/2 for J_{gs}>0 and j=1/2 for J_{gs}=0) above the neutron binding energy can be determined experimentally without any losses. The obtained neutron resonance density is then used in the GC procedure to adjust the slope of the constant temperature formula [Hug72] at lower energies to fit both the cumulative number of levels at low energies and the density of levels around the binding energy at the same time. However the GC type of fit has a severe drawback. It is restricted to nuclei with experimentally determined neutron resonance spacing, see e.g. [Ilj92, Ripl-I98]. Thus a new method is needed to fit the CNL for a larger number of nuclei.

The new method

By studying the plots of cumulative number of levels [Bel97] and nuclear temperature plots vs. mass number [Ripl-I98], it was observed that the nuclear temperature changes regularly with the mass number. This observation suggested the idea of fitting the temperature T, taken as a function of mass number, simultaneously for a large number of nuclei. After several attempts it became clear that nuclei around the valley of stability could be fitted in such a way.

Below, I briefly present the method, which will be published in more detail later [Bel00]. In the selection of nuclei a natural requirement is that the number of levels has to exceed a certain value N_0 , then for the fitting the following method was used. First the fit already used in the first phase of the Ripl project [Bel97] was done for the selected nuclei. This provided an initial value for N_{max} . The initial values for the lowest level number N_{min} were set to 7 for even-even or odd-even, and 14 for odd-odd nuclei. Then for all of the nuclei a common temperature function T(A) was fitted. Free parameters were the U_0 for each nucleus. Then the values of N_{max} and N_{min} (with the above restrictions) were changed in the meanwhile the distance between them was kept larger than a minimum value. Finally the procedure was repeated until the N_{max} and N_{min} values did not change. The result of the fit is shown in Fig. 1. The nuclei inside a mass band of ± 4 around the valley of stability were included if they had more then $N_0=30$ known excited levels. The result is based on the CNL's for 641 nuclei.



Figure 1 Nuclear temperature as a function of the mass number

The levels used to construct CNL's were taken from ENSDF II [Fir98]. The corresponding U_0 parameters are shown in Fig 2. It is also important that for the first time reliable uncertainty for T and U_0 could be determined.

The paring and shell effects are mainly absorbed in the U_0 parameters, although the temperature function also shows shell effects to some extent. It should be kept in mind that the input data is affected by unknown experimental uncertainties, thus the fit for individual nuclei might not be 'perfect'. A good example is the ²⁰⁸Pb nucleus for which the latest experimental results show that 11 levels out of 58 below 5 MeV should be removed [Bel00a] from the recent compilation [Mar86].



Figure 2 U_0 as a function of mass number A.

Validation and checking of the fit results

The quality of the fits has been checked visually for all the 641 nuclei and, in general, it seemed satisfactory. The results were then checked in two ways. First, the T(A) function was compared with data obtained from a GC fit by the Bombay group [Ripl-I98]. This comparison is shown in Fig. 3.



Figure 3 Comparison of the T(A) function with the results of the Bombay group using Gilbert-Cameron type fits.

As it can be seen, the fitted T(A) function runs close to the GC values, however there are some discrepancies around mass numbers 58 and 150. Around the former mass region GC data show an enhanced shell effect, while in the latter case the opposite is true – GC results do not reflect the rapid structural changes in the transitional and deformed region. This later feature, although less pronounced, can be seen in the transitional regions around mass 74 and 100. The reason for these discrepancies can be partly due to the non-uniform handling of the data in the GC procedure and due to the less complete data available by the time these fits were performed.

The second check was a GC like extrapolation that did not use the level density at the neutron binding energy. In this procedure the Fermi gas model parameters a and the matching parameters U_x were determined through the usual matching conditions introduced by GC. These provide two equations that completely determine the parameters a and U_x for each nucleus. Here, there was no need to determine the pivot point [Gil65], because the T and U_0 parameters have already been determined as described above. A comparison to the GC results of the Bombay-group is show in Fig 4. As it can be seen, the data show exactly the same discrepancies that have been already observed for the temperature function T(A). The enhanced level densities in the transition regions do not show up in the GC fit of the Bombay group. The a values obtained in this work seem to be much closer to the values obtained by the JAERI group (see Fig. 5.1 in [Ripl-I98]). The increase in the value of level density parameter a relative to the Bombay results around the transition regions is the same in amplitude and size to the present values.



Figure 4 Comparison of Gilbert-Cameron like extrapolated values of Fermi gas parameter a (diamond) with Gilbert-Cameron values (triangle) of the Bombay group

Details of these calculations will also be published [Bel00].

Extension of the method to wider region

The possibility of extension of the method to nuclei further from the stability valley was investigated. However, due to the rapid decrease of experimental data for these nuclei and to the possible structural changes outside the considered region contradictory results in respect to the present fit were observed. New shell closure like bumps appear in the extended fit with much larger uncertainty on the T(A) function. Thus, it seems necessary to include charge or neutron numbers, in addition to the mass numbers, if the fit is to be extended over a wider mass band around the valley of stability.

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ACTIVITIES RELATED TO "NUCLEAR MODEL PARAMETER TESTING FOR NUCLEAR DATA EVALUATION" (REFERENCE INPUT PARAMETER LIBRARY: PHASE II) AT CNDC

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Introduction

The objectives of the RIPL CRP Phase II^[1] are to test thoroughly all segments of the Starter File of the Reference Input Parameter Library, focusing on optical model parameters and nuclear level density parameters. The nuclear level density calculations for 303 nuclei with the two recommended parameter sets have been performed. 88 sets of optical potential parameters are prepared for RIPL-2. A nuclear model code UNF is being prepared at CNDC for the physical testing of RIPL.

1. The basic test of total level density parameters with G-C and Back-Shifted models

There are many sets of level density parameters for three kinds of level density models (Gilbert-Cameron, Back-Shift and GSM) in the RIPL Starter File. They have been used widely in the nuclear reaction model calculations and studies. Relibility of these parameters requires basic testing. The level density calculations for 303 nuclei (from ²⁴Na to ²⁵⁰Cf) for the Gilbert-Cameron model and Back-Shift model with the recommended parameters have been performed. The resulting cumulative number of levels were plotted (Fig. 1) together with the cumulative plots given in the Segment 2 of the Starter File. The users can judge the quality of both parmaterizations and related models. The calculations for Generalized Superfluid Model and the related recommended parameters should also be performed, but the recommended file does not provide all the parameters needed for the GSM model. For example, the energy of quadrupole vibrations and quadrupole deformations that define the vibrational and rotational enhancement of the nuclear level density are missing.

The average resonance spacings D_o for the nuclei region mentioned above have been calculated within the GC and BS level density models. The calculated results and related data of Segment 3 are showed in Fig. 2.

2. The extention of the RIPL-1 optical model parameter set

88 sets of optical model parameters for incident neutron energy region of 0-20 MeV were obtained in course of evaluation activities at Chinese Evaluated Nuclear Data Library (Version 3, CENDL-3). They have been transformed into the format designed by P.G.Young for the Segment 4 of the RIPL starter file and are ready for inclusion RIPL-2. List of available sets is presented in Table 1.

These optical model parameters were obtained fitting experimental data (total cross section, nonelastic cross section and elastic scattering angular distribution) using an optical model code APMN. The experimental total cross sections are well reproduced. Fig. 3 shows the comparisons of experimental total cross sections with the theoretical calculations for some nuclei. As an example, the calculated elastic scattering angular distributions of ${}^{56}Fe(p, p){}^{56}Fe$ are presented by Fig. 4. One can see that the calculated results are in pretty good agreement with the experimental values in a wide energy range.

The code APMN can be used for incident neutron, proton, α , d, t and ³He, in the energy region up to 300 MeV. The APMN can automatically search for optimal optical potential parameters for 1~40 nuclei at a time. The adjustment of the parameters is automatically performed by computer by minimization of χ^2 , which represents the deviation of calculated total and nonelastic cross sections and elastic scattering angular distributions from the experimental values.

3. The preparation of the UNF code for physical testing of RIPL

The UNF series of codes play a key role in the model calculations for CENDL-3, similarly to the GNASH, ECIS and TNG in the ENDF and JENDL. The UNF series have been used for nuclear data model calculations for most of the nuclei (more than 120) in CENPL-3 along with auxiliary codes (Optical Model Code APOM94 and APMN and Direct Reaction Code WUCK).

The UNF code contains the Hauser-Feshbach and the exciton models as the limiting cases. The unified treatment of equilibrium and pre-equilibrium reaction processes includes the introduction of composite particle formation factors in calculations of pickup-type composite particle emissions. A method to calculate the double-differential cross sections for all kinds of particles is based on the leading particle model.

The UNF was developed for calculation of fast neutron data with incident energies from a few keV to 20 MeV. The code can handle a decay sequence up to the (n, 3n) reaction channel, including 14 reaction channels. The physical quantities calculated by the UNF contain the following:

- 1. cross sections of total, elastic scattering, compound elastic scattering, nonelastic scattering, and all reaction channels including emission to discrete levels and to continuum
- 2. angular distributions of elastic scattering both in the center-of-mass system and in the laboratory system
- 3. the energy spectra of particles emitted in all reaction channels
- 4. double-differential cross sections for all kinds of particle emissions (neutron, proton, α particle, deuteron, triton, and ³He), as well as for recoil nuclei
- 5. kinetic energy released (kerma factors)
- 6. γ production data (γ spectra, γ production cross section, and multiplicity) and the isomeric ratios
- 7. total double-differential cross sections of emitted particles from all reaction channels.

If the direct inelastic scattering data and direct reaction data are available from other codes, one can input these data so that the results include direct process effects. The output is in the ENDF/B-VI format.

We already have accumulated a lot of experience for nuclear data calculations with the UNF series of codes. We hope that the UNF can be selected for a physical testing of RIPL. For this propose, a unified UNF code, which contains the all the functions of the UNF series currently used at CNDC, is being developed and the initial version has been completed.

The related interface between the unified UNF code and the RIPL will be developed, and all documents regarding the unified UNF will be provided to the NEA/DATA BANK before the start of the physical testing of RIPL.

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Fig. 1



Fig. 2



Fig. 3-1 ⁸⁹Y total, elastic and nonelastic cross sections energies of incoming neutron in L-frame (MeV)



Fig. 3-2 ^{88,89,90}Sr total, elastic and nonelastic cross sections



Fig. 4 56 Fe(p, p) 56 Fe elastic scattering angular distribution

Tabla	1
Lane	J

Lib. No. ~	Inc. Part.	Model Type	Z-Range	A-Range (MeV)	E-Range No.	Ref. First Author
500	n	spher.	31-31	69- 69	0.1-20.0	1 Zhang
501	n	spher.	36-36	83- 83	0.1-20.0	2 Cai
502	n	spher.	36-36	86- 86	0.1-20.0	3 Cai
503	n	spher.	37-37	85- 85	0.1- 20.0	2 Cai
504	n	spher.	38-38	88- 88	0.1- 20.0	2 Cai
505	n	spher.	39-39	89- 89	0.1-20.0	2 Cai
506	n	spher.	39-39	91-91	0.1-20.0	4 Cai
507	n	spher.	41-41	93-93	0.1-20.0	5 Rong
508	n	spher.	41-41	95- 95	0.1-20.0	5 Rong
509	n	spher.	42-42	95- 95	0.1-20.0	6 Cai
510	n	spher.	42-42	97- 97	0.1-20.0	7 Cai
511	n	spher.	42-42	98- 98	0.1-20.0	7 Cai
512	n	spher.	42-42	100-100	0.1-20.0	3 Cai
513	n	spher.	43-43	99- 99	0.1-20.0	4 Cai
514	n	spher.	44-44	99- 99	0.1-20.0	8 Zhang
515	n	spher.	44-44	100-100	0.1-20.0	8 Zhang
516	n	spher.	44-44	101-101	0.1-20.0	9 Zhang
517	n	spher.	44-44	102-102	0.1-20.0	8 Zhang
518	n	spher.	44-44	103-103	0.1-20.0	9 Zhang
519	n	spher.	44-44	104-104	0.1-20.0	8 Zhang
520	n	spher.	44-44	105-105	0.1-20.0	8 Zhang
521	n	spher.	45-45	103-103	0.1-20.0	8 Zhang
522	n	spher.	45-45	105-105	0.1-20.0	8 Zhang
523	n	spher.	46-46	105-105	0.1-20.0	10 Zhang
524	n	spher.	46-46	108-108	0.1-20.0	10 Zhang
525	n	spher.	48-48	113-113	0.1-20.0	11 Zhang
526	n	spher.	49-49	115-115	0.1-20.0	11 Zhang
527	n	spher.	51-51	121-121	0.1-20.0	11 Zhang
528	n	spher.	51-51	123-123	0.1-20.0	11 Zhang
529	n	spher.	52-52	130-130	0.1-20.0	10 Zhang
530	n	spher.	53-53	127-127	0.1-20.0	10 Zhang
531	n	spher.	53-53	135-135	0.1-20.0	10 Zhang
532	n	spher.	54-54	123-123	0.1-20.0	12 Shen
533	n	spher.	54-54	124-124	0.1-20.0	12 Shen
534	n	spher.	54-54	129-129	0.1-20.0	13 Shen
535	n	spher.	54-54	131-131	0.1-20.0	13 Shen
536	n	spher.	54-54	132-132	0.1-20.0	13 Shen
537	n	spher.	54-54	134-134	0.1-20.0	13 Shen
538	n	spher.	54-54	135-135	0.1-20.0	13 Shen
539	n	spher.	54-54	136-136	0.1-20.0	13 Shen
540	n	spher.	<u> </u>	133-133	0.1-20.0	8 Zhang
541	n	spher.	55-55	134-134	0.1-20.0	8 Zhang
542	n	spher.	55-55	135-135	0.1-20.0	8 Zhang
543	n	spher.	55-55	137-137	0.1-20.0	8 Zhang
544	n	spher.	30-30 56 56	133-135	0.1-20.0	o Zhang
545	n	spher.	20-20 56-50	130-130	0.1-20.0	8 Zhang
546	n	spher.	30-30 56 56	137-157	0.1-20.0	ð Zhang
547	n	spher.	50-50 57 57	138-138	0.1-20.0	o Zhang
548	n	spher.	51-57	139-139	0.1-20.0	8 Zhang
549	n	spher.	28-28 59-58	140-140	0.1-20.0	8 Zhang
550	n	spher.	28-28	141-141	0.1-20.0	8 Zhang

551	n	spher.	58-58	142-142	0.1-20.0	8 Zhang	
552	n	spher.	58-58	144-144	0.1-20.0	8 Zhang	
553	n	spher.	59-59	141-141	0.1-20.0	12 Shen	
554	n	spher.	60-60	142-142	0.1-20.0	12 Shen	
555	n	spher.	60-60	143-143	0.1-20.0	12 Shen	
556	n	spher.	60-60	144-144	0.1-20.0	12 Shen	
557	n	spher.	60-60	145-145	0.1-20.0	12 Shen	
558	n	spher.	60-60	146-146	0.1-20.0	12 Shen	
559	n	spher.	60-60	147-147	0.1-20.0	12 Shen	
560	n	spher.	60-60	148-148	0.1-20.0	12 Shen	
561	n	spher.	60-60	150-150	0.1-20.0	12 Shen	
562	n	spher.	61-61	147-147	0.1-20.0	12 Shen	
563	n	spher.	61-61	148-148	0.1-20.0	12 Shen	
564	n	spher.	61-61	149-149	0.1-20.0	12 Shen	
565	n	spher.	62-62	144-144	0.1-20.0	12 Shen	
566	n	spher.	62-62	147-147	0.1-20.0	12 Shen	
567	n	spher.	62-62	148-148	0.1-20.0	12 Shen	
568	n	spher.	62-62	149-149	0.1-20.0	12 Shen	
569	n	spher.	62-62	150-150	0.1-20.0	12 Shen	
570	n	spher.	62-62	151-151	0.1-20.0	12 Shen	
571	n	spher.	62-62	152-152	0.1-20.0	12 Shen	
572	n	spher.	62-62	154-154	0.1-20.0	12 Shen	
573	n	spher.	63-63	151-151	0.1-20.0	14 Ge	
574	n	spher.	63-63	153-153	0.1-20.0	14 Ge	
575	n	spher.	63-63	154-154	0.1-20.0	14 Ge	
576	n	spher.	63-63	155-155	0.1- 20.0	14 Ge	
577	n	spher.	64-64	152-152	0.1-20.0	12 Shen	
578	n	spher.	64-64	154-154	0.1-20.0	12 Shen	
579	n	spher.	64-64	155-155	0.1-20.0	12 Shen	
580	n	spher.	64-64	156-156	0.1-20.0	12 Shen	
581	n	spher.	64-64	157-157	0.1-20.0	12 Shen	
582	n	spher.	64-64	158-158	0.1-20.0	12 Shen	
583	n	spher.	64-64	160-160	0.1-20.0	12 Shen	
584	n	spher.	66-66	164-164	0.1-20.0	15 Ge	
585	n	spher.	69-69	169-169	0.1-20.0	15 Ge	
586	n	spher.	71-71	174-174	0.1-20.0	16 Han	
587	n	spher.	71-71	175-175	0.1-20.0	16 Han	

ON THE NEED OF NUCLEAR DATA AND CODES FOR THE EVALUATION OF HEAVY ION REACTION CROSS SECTIONS

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Abstract

The main purpose of this report is to show that past and present research does not always provide the systematic and quantitative information which is needed to allow the accurate evaluation of heavy ion cross sections.

1. Introduction

The last forty years have witnessed an increasing interest in the investigation of heavy ion interactions. Actually, many laboratories throughout the world provide heavy ion beams and a large number of the experiments are made to study the heavy ion reactions and the nuclear structure. This huge amount of work has greatly increased our knowledge of nuclear physics, because in these interactions unusual states of matter are produced such as highly deformed nuclei in very high spin states or nuclei with neutron to proton ratios very different from those of the nuclei near the bottom of the valley of β stability which are produced in light particle induced reactions. This led to important discoveries such as those of the superdeformed nuclei, of the nuclei near the proton drip line and of the superheavy nuclei, just to quote only a few remarkable examples.

However, when one considers all these results and one asks if a systematic investigation of the nuclear properties has been pursued in heavy ion physics and a systematic knowledge has been gained, one has the impression that while the studies of nuclear structure have indeed provided such type of knowledge, the studies of heavy ion dynamics are still fragmentary and sparse. It is undeniable that they have greatly added to our knowledge, however there does not exist a systematic information comparable to that which is deemed to be necessary in light particle induced reactions (as, for instance, in the case of the slow neutron resonances or the neutron induced fission).

In fact even the most basic information is often lacking. Just to give an example: systematic measurements of reaction cross sections are quite rare and little is know about the elastic scattering of most ions so that even in the case of a basic reaction model such as the Optical Model one does not know much about the best parameters to use. Certainly when one consider the heavy ion reactions the enormous number of ion combinations is discouraging, but one has the impression that a real and systematic effort has not been made to clarify this matter. Most of the present experiments look for discovering new phenomena neglecting the fact that a knowledge of the basic processes is invaluable to understand the more complex ones.

Another point that should be stressed is that, contrary to what has been made in the case of light particle induced reactions, often one does not look for a complete knowledge of the two-ion interaction which one investigates preferring to study exclusive processes which however important provide only a partial information. A complete information is necessary both for understanding in all its complexity the two-ion interaction and to have a really significant information to be used in trans-disciplinary fields to the development of which nuclear physics may greatly contribute. Thus, while the study of the exclusive spectrum of the particles emitted in a given process may prove to be of invaluable importance in order to understand a particular aspect of the two-ion interaction, one must keep in mind that all processes occur in nature and the knowledge of the particle inclusive spectra is necessary. The same consideration holds for many other observables such as the cross-section for residues' formation, the residue's momenta, the total γ ray yield, and so on....

It would be unfair to say that an information of this type is absolutely lacking. However one must admit that it is only partial and not easy to find, making it highly advisable to undertake a systematic search of what has been published in heavy ion dynamics collecting this information in a systematic and easy to access form.

Similar considerations hold for the theoretical models which have been proposed, selecting the best fitting parameters to be used and comparing their predictions when many of them can be used to describe a given reaction. It must be also remarked that many analyses of data used very simplistic models or not proven assumptions which often lead to unjustified conclusions. Examples of this type of analyses will be discussed later.

Heavy ion reactions are much more complex than light ion induced reactions because two heavy ions may interact in many different ways which depend on their structure, their relative energy and angular momentum. Thus the fusion of two heavy ions to produce a compound nucleus with full energy, mass and charge may be forbidden by the fact that this compound nucleus would be unstable: in the case of light compound nuclei because these rotate with such high angular velocities to be unstable against centrifugal forces, in the case of heavy nuclei because the high relative angular momentum induces a deformation which makes the compound nucleus unstable against fission. Instead of fusion other interaction modes may come into play. An ion may break up into two fragments only one of which may fuse with the other ion, or the two ions may form an intermediate di-nuclear system exchanging mass and energy and further separating again producing projectile-like and target-like residues.

There is a continuous interplay between mean field and nucleon-nucleon interactions. The first are mostly responsible of the processes which occur, the second greatly contribute to the damping of the two ion relative motion and by means of them the initial orderly energy of the two ions transforms into random thermal energy. The value of all physical observables depends on both these two interaction modes, often indicated as the one-body and the twobody interaction mechanisms. Even when one expects that one of the two interaction modes may have a greater influence on what one observes, one must necessarily consider the consequences of the assumed mechanism on the further evolution of the system which one investigates. Thus, if one measures the spectrum of particles which has been produced in an early stage of the interaction the calculation used to reproduce this spectrum must give the information necessary to predict the further evolution of the system: that is the mass, charge, energy, angular momentum distributions of the nuclei which are produced after the emission of the particle. As we will see later not often this happens. After these general remarks we will discuss a few items concerning the interactions of very light heavy ions (A<20) with nuclei which are representative, at low and intermediate energies, of the questions which we must confront in order to get a quantitative knowledge of heavy ion dynamics.

2. Low energy reactions

The study of the reactions occurring in the interaction of two low energy heavy ions reveals a large variety of contributing mechanisms and has greatly contributed to our knowledge of nuclear dynamics. These studies clarified the role of angular momentum in nuclear interactions and showed that high relative angular momenta lead to a dramatic increase of γ -ray emission and to dynamical instability toward fission (see, for instance [1-5]). This lead

to the recognizion of the existence of the yrast states [6,7] and of a large variety of phenomena which range from complete and incomplete fusion processes and deep inelastic collisions to distant interactions [8-11]. Also the existence of angular momentum windows for the occurrence of these processes was clearly recognized [12-17]. The interaction of low energy heavy ions has also greatly increased our knowledge of nuclear structure through the investigation, by means of the in-beam γ -ray spectroscopy, of giant resonances [18] and nuclear deformation and super-deformation [19-21].



Fig. 1 Double differential cross sections of the ⁸Be_{gs} fragments observed at the indicated angles in the interaction of 100 MeV ¹²C ions with ⁵⁹Co. The open points are the experimental results [26], the full line histograms the predicted spectra [26].

The complete fusion of the two ions is usually the dominant process at low energy, however, as mentioned before, even at energies only slightly greater than the Coulomb barrier incomplete fusion and deep inelastic processes are far from being negligible. Contrary to a widespread opinion the complete fusion itself may not produce immediately an equilibrated compound nucleus. On the way to the equilibrium the emission of pre-equilibrium ejectiles from the intermediate composite nucleus created in the two-ion fusion may be not negligible. From its study one may deduce important information on both the two ion mean field interaction and the intranucleon interaction cascade through which the composite nucleus equilibrates.

In order to study these processes a large variety of experimental techniques, which include particle spectroscopy and in- and off-beam γ -ray spectroscopy, has been used. In particular nuclear activation studies have demonstrated the presence of incomplete fusion reactions in light ion induced reactions. For instance, in the case of reactions induced by ¹²C or ¹⁶O ions on heavy nuclei one observes the production with quite high cross sections of residues with charge only two units higher than that of the target nucleus. These residues could be produced only with negligible cross sections in the decay of the composite nuclei created in complete fusion reactions [22-24]. They also have a forward recoil range which is considerably smaller than that of the nuclei produced in complete fusion reactions. This is to be expected in incomplete fusion processes where there is a small transfer of the projectile linear momentum to the composite nucleus. These residues also recoil at considerably larger angles than those of the complete fusion reaction [25].

While experimentally the occurrence of incomplete fusion processes is clearly demonstrated, we are not aware of a satisfactory model for predicting the absolute value of the incomplete fusion cross section at such low energies. A recent study of the fragments produced in the projectile break-up suggests to describe these reactions as a break-up fusion process because this hypothesis allows one to reproduce accurately the spectra of the fragment which did not fuse with the target. As an example, Fig. 1 shows the spectra of ⁸Be_{gs} emitted at forward angles in the interaction of ¹²C with ⁵⁹Co at an incident energy of 100 MeV [26]. The energy and angular dependence of these spectra are accurately reproduced by the break-up theory in the Serber approximation [27-30]. However the absolute cross section, integrated over the angle and the energy (≈ 50 mb) is much larger than that expected on the basis of a generalization of the critical distance model which seems to work at considerably higher energies [15, 30-32].

As mentioned before, the study of low energy heavy ion interactions also revealed that the emission of pre-equilibrium particles from the excited nuclei created in complete fusion reactions may be far from negligible. In absolute terms this emission is small in comparison with particle evaporation, so that it may be not easily revealed by measuring the emitted particle spectra. However it may explain the production of evaporation residues with mass only slightly smaller than the compound mass which are formed with cross sections of several mb at energies where an evaporative calculation predicts a value which is orders of magnitude smaller [33]. The consequences of pre-equilibrium emissions are in several respects similar to those due to the hindrance of the particle emission and to the enhancement of the γ -emission for high angular momenta at excitation energies not greatly larger than the yrast state energy of the decaying nucleus. This is discussed in [23,25,33] where it is shown that when the angular momentum of the composite nucleus is rather small, and thus the emission of γ -rays is not enhanced, pre-equilibrium emissions may still explain the observed production of residues which could not be produced in the compound nucleus evaporation. This occurs in the case of reactions induced on heavy targets where composite nucleu with high angular momenta fission with a very high probability. In general both pre-equilibrium emission and enhanced γ -ray emission must be taken into account in heavy ion interactions, however a systematic study of their competition in the decay of high angular momentum states has not been made. It must be also noted that the probability of pre-equilibrium emission sensibly depends on the initial mean field interaction of the two heavy ions which may be investigated through a careful study of this de-excitation mechanism [33,34].

Other arguments which should be systematically studied include the level density of highly deformed nuclei which could be produced in these interactions, the dependence of the shell correction to the fission barrier on the nucleus angular momentum, and the transition from incomplete fusion to massive mass transfer in deep inelastic collisions.

3. Intermediate energy reactions.

This is a field which has been widely investigated. However, in most cases the experimental data provide only a partial information on the reactions which may occur, and an accurate and consistent quantitative analysis of the data is not made. On the contrary, one often follows empirical and not justified procedures. Just to give an example, one of the most accurately studied reaction mechanisms is that of the processes which occur when the two nuclei make a central collision. This produces an initial composite nucleus in a state far from statistical



Fig. 2 Spectra of neutrons emitted in the interaction of ⁴⁰Ar with Ni, ⁹²Mo and ¹²²Sn at an incident energy of 26 MeV/nucleon in coincidence with residues emitted at an angle of 8.1°±1.6° with about the CM velocity. The symbols give the experimental data [35], the histograms the result of the calculation. Starting from the top the spectra are progressively scaled down by a factor ten.

equilibrium with the full linear momentum and energy carried in by the projectile. We will call these processes complete fusion reactions even if, before reaching an equilibrium state, a considerable number of pre-equilibrium emissions may occur. The emission of these preequilibrium particles is often studied by measuring their spectra in coincidence with an heavy residue emitted at a very forward angle with the Centre of Mass velocity. One typical example are the spectra of the neutrons emitted in the interaction of ⁴⁰Ar with Ni, ⁹²Mo and ¹²²Sn at an incident energy of 26 MeV/amu in coincidence with residues emitted at angles between 6.5° and 9.7° with the CM velocity [35]. These spectra which are given by the black and open symbols in Fig. 2, clearly show that many neutrons have an energy considerably larger than that of the neutrons evaporated by the equilibrated compound nucleus with the full projectile energy. These spectra were parametrized in terms of the thermal moving source model [36] by assuming that the neutrons are isotropically emitted by two sources with a definite temperature and a definite velocity. The lowest energy part of the spectra, which corresponds to neutrons emitted after the composite nucleus has achieved the thermal equilibrium, is due to the emissions from the *fusion* source. The highest energy part of the spectra which correspond to "neutron emission before the whole system has reached thermal equilibrium" is due to the emissions from the pre-equilibrium source. The use of a definite temperature for this source seems to imply that at least part of the composite nucleus has reached a state of thermal equilibrium. This procedure, almost universally adopted because it allows one to reproduce very easily the data, presupposes an excitation/de-excitation mechanism which has never been satisfactorily explained. One should also explain how energy is transferred from the hotter to the cooler source. On the other hand, the same data may be satisfactorily reproduced, as shown in Fig. 2 by the histograms, by evaluating the time evolution of the occupation probability of the composite nucleus states and the emission of particles in the course of the cascade of nucleon-nucleon interactions by means of which the orderly initial energy of the two colliding ions transforms into random thermal energy. This is obtained by solving a set of coupled Boltzmann master equations [37]. We will not discuss here such calculations which are based on a theory which is explained in several published papers [38-43] but we wish to mention that, according to this theory, during the approach to the equilibrium the nucleus has not a constant temperature, the pre-equilibrium particles are not isotropically emitted in the decaying nucleus reference frame and the equilibrated nuclei have not a unique mass, charge, energy and angular momentum. If these calculations are correct one must question the validity of the information which is obtained by previous procedure. In particular, we think that it could be hardly used to prove that high temperature nuclear matter has been created.

Another case worth discussing is that of the analyses of the cross-sections for production of radioactive residues measured by the activation technique. In spite of well known deficiencies (the possibility of identifying only part of the residues which are produced, which often are also produced in a cumulative way, that is both *directly* in the reaction and through decay of precursors of shorter lifetime) these measurements, allowing to identify with absolute certainty the residues which are produced, provide a quite unique information. The analysis of these data provides useful informations on the reaction mechanisms, as shown for instance in [31,32]. Unfortunately, in most cases, also these data were analyzed using empirical prescriptions or over-simplified models and one cannot really trust many of the estimates given in literature of physical quantities of major importance such as the total reaction crosssection or the average linear momentum transferred in the interaction. For instance, most authors base their analyses on the hypothesis that the percentage charge distribution (PCD) of the produced isobars may be accurately represented by a quasi-Gaussian distribution, around a



Fig. 3 Percentage charge distributions (PCD) of the residues produced in the interaction of 45 MeV/amu ¹²C on natural copper. The values predicted by our model are given by the open and full symbols, the values given by the expression proposed by [45] are given by the full line. Z_p is the most probable charge for each PCD.

most probable charge Zp, almost independent on their mass and on the total cross-section for their production, as first indicated by Rudstam [44] by analysing a large number of reactions induced by light ions. This dependence is used to deduce the values of the cross-section for production of unobserved residues. We made detailed calculations of the PCD distributions in the case of the reactions induced by 45 MeV/amu ¹²C ions on natural copper considering the main reaction mechanisms which are expected to contribute. Fig. 3 shows the comparison of the calculated residue's PCD (open and full symbols) of two different groups of residues, with, respectively, 39<A<50 and 51<A<65, and the empirical Rudstam type distribution suggested by [45] (full lines). One may see that for $|Z-Z_n| \leq 2$ (the interval considered by these authors) the calculated PCD are quite similar to the ones obtained empirically. In particular they are nearly the same for all the isobars irrispective of their total production cross section. However, the PCD of the isobars of higher masses shows, at low and high charges, wings which are not reproduced by the proposed PCD expression. What seems to be more relevant for the use which is usually made of the PCD is the fact that, there are quite considerable local fluctuations in the values of the calculated cross sections which are not accounted for by an analytical expression. So the estimated total isobar cross sections

(the cross section for production of all the residues of a given mass) obtained by using analytical expressions for the PCD and the measured cross-section of only one or two residues, as it happens in most cases, may lead to an incorrect estimate of the yield of unobserved residues. Thus, one cannot be surprised if the total cross section estimated with such procedure considerably differs from that measured in beam attenuation experiments [46] (in this particular case it is considerably smaller).

One could give other examples of analyses of data which should be considered with some suspicion, but we wish instead to discuss a point which is of major importance for the evaluation of heavy ion cross-sections. Due to the enormous complexity of the heavy ion interactions is it reasonable to try to provide a comprehensive description of the whole of the processes which may occur when two nuclei interact? While, at the moment, a formal comprehensive theory seems to be beyond our possibilities, it may be possible that phenomenological approaches have some success. We are investigating such a possibility since many years in the case of the interaction of ¹²C and ¹⁶O with nuclei. Our experience, for this particular case, may be summarized as follows. To get a comprehensive description one must first of all analyze a large and significant set of experimental data. One could be tempted to say a large set of "independent" experimental data, but in reality this is not correct, because according to our experience all the observables which one may measure are related. For instance, the emission of high energy particles in very short times has a great influence on the further decay of the excited nuclei which are produced. The initial interaction of the two ions is responsible of the further evolution of the system and thus every time one assumes a particular reaction mechanism to explain a particular phenomenon one must consider its consequences. In short: in order to be really acceptable a calculation must be able to evaluate all the chain of processes which may occur.

One related question is: may the data reported in literature provide the comprehensive set of data which is needed? In most cases not. What is needed in principle is a set of data which allows one to study the interaction of a particular ion with nuclei as a function of the target mass and charge and the relative energy. Possibly a few target nuclei may be sufficient. Even if the target nucleus structure may be important to correctly describe a particular process, the general features one observes change rather weakly with the target and one may thus hope to reach meaningful conclusion by carefully analysing a rather limited set of sample cases. The energy (and implicitly the angular momentum) dependence of the cross sections is a factor of much greater importance. The initial two ion interaction and the subsequent processes depend and change appreciably with the two ion relative energy. For this reason, one cannot use limited sets of data taken at different energies and try to get from them sensible conclusions. In practice we found necessary to measure the data which we deemed necessary. Every time we collected new data we learnt something new which obliged us to re-analyse all the previously collected data. Though we are still far from being satisfied and in spite of the many open problems which require further consideration we succeded in reproducing a large set of cross sections, particle spectra, residue recoil ranges and angular distributions with an accuracy comparable to that which is generally obtained in the analysis of the same quantities in nucleon induced reactions [22-26,30-34,38-43]. This is encouraging and we feel that this is the way one must follow if one wishes to obtain a quantitative understanding of the heavy ion interactions.

Summary and conclusions

In this report we have tried to show that if one wishes to evaluate with a reasonable accuracy heavy ion reaction cross sections one must make a very extensive and co-ordinated effort which includes the selection and the classification of the rather confused information which has been collected during the years. Many worthwhile experimental data which have been analysed using simplistic and not justified models may require a considerable re-evaluation. A large number of new experimental and systematic investigations is also required. All this requires a huge effort which however it is essential if one wish to transform our knowledge of heavy ion reactions from essentially qualitative to quantitative.

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Figure Captions

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TESTING OF THE LEVEL DENSITY SEGMENT OF THE RIPL

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ABSTRACT

A comparison between RIPL phenomenological state density parameterizations and microscopical state density (SD) codes was performed for nickel and samarium isotopes. All the codes were shown to be complete. More work is needed on calculation of the collective enhancement of the level densities to improve currently used phenomenological recipes. It was shown that phenomenological closed formulae for particle-hole state density fails to describe microscopical calculation for magic nuclei. For deformed nuclei, like Sm-152, the agreement of Williams closed formulae considering Kalbach pairing correction with microscopical SD calculations was very good.

This work was devoted to the testing of microscopical level density codes contained in the RIPL library and comparison of the phenomenological parameterizations recommended by RIPL with the results of microscopical calculation. The back-shifted Fermi gasⁱ(BSFG) and the generalized superfluid^{ii,iii,iv}(GSM) models were employed as phenomenological parameterizations of the level and state densities. Microscopical OBNINSK_MICRO^v and CAIN^{vi} codes were used for total state density calculation. The former is a statistical microscopical code included in the RIPL, the second one is the Monte Carlo code for state density calculations, subroutines extracted from the AVRIGEANU^{vii} package (also included in the RIPL) were used and compared with the results of the RIPL microscopical CAPOTE_MICRO code^{viii}. This is a preliminary report of the work done.

Three papers on related subjects were presented by a collective of authors, including myself, in Varenna and Bologna Conferences in May-June 2000 and will be published in the Proceedings of these conferences. The titles of these contributions are:

- "Damping of the collective enhancement of the level density for thorium isotopes"
- "Realistic intrinsic state densities for deformed nuclei"
- "On the collective enhancement of level densities of transitional nuclei"

We are going to present some figures to highlight the most important conclusions.

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Figure 1. Comparison of phenomelogical and microscopical total LD codes from RIPL for Sm-148

The BSFG and GS model parameters from RIPL were using to calculate the total state density for spherical nucleus Sm-148. Good agreement between these phenomenological approaches is observed. Also are shown the results of microscopical calculations of the same magnitude using OBNISNK-MICRO RIPL code. Nix-Moeller single particle level (SPL) schemes^{ix} were used in this calculation. The intrinsic state density is well below the phenomenological curves showing the importance of the collective enhancement. However the phenomenological collective enhancement model included in the OBNISNK_MICRO code seems to overestimate the vibrational enhancement for this nucleus.



Figure 2. Comparison of phenomelogical LD parameters from RIPL with MC LD code for Sm-152

The BSFG and GS model parameters from RIPL were using to calculate the total state density for well-deformed nucleus Sm-152. The agreement is worse, than for Sm-148, showing that GSM will predict much lower level density at energies higher than 40 MeV. Also are shown the results of microscopical calculations of the same magnitude using CAIN^{vi}, a Monte Carlo code for state density calculations recently developed in our group. Nix-Moeller single particle level (SPL) schemes were used in this calculation. Again the calculated intrinsic state density is below the phenomenological curves till 20 MeV, showing then similar behaviour. It is evident the importance of the collective enhancement for a proper description of the state densities in the whole energy range.

PARTICLE-HOLE STATE DENSITIES

In figure 3 one-particle-one hole and two particle-two holes state densities were calculated for a nickel proton system, featuring a magic number of protons equal to 28. The Williams formula's^x values obtained with conventional single-particle level density g=A/13 is shown together with the results for g calculated from a value of level density parameter a given by a BSFG model. Also are shown the results of microscopical calculations using RIPL CAPOTE_MICRO code, a combinatorial code for particle-hole state density calculations. Nix-Moeller single particle level (SPL) schemes were used in this calculation. As can be seen, especially for the two-particles-two holes case, the threshold behaviour of the microscopical calculations can not be reproduced by any closed formulae, no matter what parameter value you are using. On the other hand, well above the threshold (from 9 MeV for 2p-2h densities) agreement between microscopical and closed formulae results is improved when using phenomenological derived value for the single-particle level density.



Figure 3. Particle-hole state densities calculation for nickel (Z=28)

In figure 4 one-particle-one hole and two particle-two holes state densities were calculated for a samarium 152 neutron system, featuring a number of neutrons equal to 62. The Williams formula's^x values considering Kalbach's pairing correction^{xi} are shown together with the results of microscopical calculations using RIPL CAPOTE_MICRO code. Nix-MoellerError! Unknown switch argument. and ETFSI^{xii} single particle level (SPL) schemes were used in this calculation. The agreement between results from different SPL schemes is very good. Only slight difference in the first energy bin exists, probably because not exactly the same pairing treatment was used in each calculation. As can be seen the Williams closed formula considering Kalbach's pairing correction gives an excellent description of the microscopical calculations for this non-magic well-deformed neutron system.



Figure 4. Particle-hole state densities calculation for samarium-152 (N=62)

CONCLUSIONS

All the microscopical RIPL codes were shown to be complete. No dependence on the used SPL scheme was observed in microscopical calculations. More work is needed on calculation of the collective enhancement of the level densities to improve currently used phenomenological recipes. It was shown that phenomenological closed formulae for particle-hole state density fails to describe microscopical calculation for magic nuclei. For deformed nuclei, like Sm-152, the agreement of Williams closed formulae considering Kalbach pairing correction with microscopical SD calculations was very good.

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At last, competitive microscopic predictions of nuclear masses and nuclear level densities

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1 A microscopic HF-BCS mass formula

Until recently the atomic masses were calculated on the basis of one form or another of the liquid-drop model, the most sophisticated version of which is the "finite-range droplet model" (FRDM) [1]. Despite the great empirical success of this formula (it fits the $Z \ge 8$ 1887 masses with an rms error of 0.689 MeV), there is still an obvious need to develop a mass formula that is more closely connected to the basic nuclear interactions. Two such approaches can reasonably be contemplated at the present time, one being the nonrelativistic Hartree-Fock (HF) method (e.g [2]), and the other the relativistic Hartree method, also known as the relativistic mean-field (RMF) method (e.g. [3]). Recently, only modest progress has been made in the HF method or of the RMF method. In neither case has the basic parameter set been fitted to the masses of more than ten or so nuclei, presumably because of the computer-time limitations that arose in the past with deformed nuclei. However, using parameter sets determined in this way, the masses (and some other properties) of more than a thousand nuclei have been calculated in both the HF [4] and RMF [3] approaches. Unfortunately, in both cases the rms errors in the resulting mass predictions for nuclei of known mass were well in excess of 2 MeV, which is far from reaching the level of precision found by droplet-like models (around 700 keV); moreover, both sets of calculations were limited to even-even nuclei.

The result is that the most microscopically founded mass formulas of practical use were till now those based on the so-called ETFSI (extended Thomas-Fermi plus Strutinsky integral) method. The ETFSI method is nothing else than a high-speed high-quality macroscopic-microscopic approximation to the HF method based on Skyrme forces, with pairing correlations generated by a δ -function force that is treated in the usual BCS approach (with blocking). The macroscopic part consists of a purely semi-classical approximation to the HF method, the full fourth-order extended Thomas-Fermi method, while the second part, which is based on what is called the Strutinsky-integral form of the Strutinsky theorem, constitutes an attempt to improve this approximation perturbatively, and in particular to restore the shell corrections that are missing from the ETF part. For full details of this method see Refs. [5] and reference therein. Eleven parameters are found to reproduce the 1719 experimental masses of the $A \geq 36$ nuclei with an rms deviation of 701keV [6]. The precision of ETFSI mass table is therefore comparable with the one obtained by the droplet-like formula. Nevertheless, the ETFSI model remains a macroscopic-microscopic approximation to the HF method and a logical step towards improvements obviously consists in considering now the HF method as such. We demonstrated very recently [8, 9] that HF-BCS calculations in which a Skyrme force is fitted to essentially all the mass data are not only feasible, but can also compete with the most accurate mass droplet-like formulas available nowadays.

The best force that we found, labelled MSk7, is a conventional 10-parameter Skyrme force. The Msk7 parameters are determined along with the pairing parameters by fitting the 1719 measured masses of nuclei with $A \ge 36$ (with the exception of the $|N-Z| \le 1$ nuclei subjected to the Wigner anomalies). All the details can be found in [8, 9]. It should be stressed that the best fit is obtained for an effective nucleon mass slightly larger than one $(M^* = 1.05M)$ and a symmetry coefficient J = 28 MeV. Note that the choice of J is subject to the constraint that the neutron matter does not collapse at nuclear and sub-nuclear densitites. A compromise between a good fit to experimental masses of finite nuclei and the stability of neutron matter at nuclear densities leads to the value of J = 28 MeV. The chosen value of $\gamma = 1/3$ in the MSk7 force leads to a nuclear-matter incompressibility coefficient $K_v = 231.2$ MeV in excellent agreement with the experimental value of 231 ± 5 MeV. The Fermi momentum is fixed to the value of $k_F = 1.326$ fm⁻¹ giving an rms charge radius of ²⁰⁸Pb in close agreement with the experimental value of 5.50 fm. The remaining Skyrme and pairing parameters are determined by fitting to the full data set of 1719 masses. The pairing correlations are taken into account in the BCS approach (with blocking) using a δ -function pairing force. We allow the pairing strength to be different for neutrons and protons, and also to be slightly stronger for an odd number of nucleons than for an even number, i.e the pairing force between neutrons, for example, depends whether N is even or odd.

In order to describe the $|N - Z| \leq 1$ nuclei, a phenomenological Wigner correction term of the form

$$E_W = V_W \exp(-\lambda |N - Z|/A) \tag{1}$$

is added to the total HF-BCS binding energy. The two parameters V_W and λ are determined by fitting to a new data set of 1772 masses, consisting of the original 1719 nuclei plus the 53 measured nuclei with $N = Z, Z \pm 1$ and $A \ge 36$ that were originally excluded, even though they are given in the 1995 compilation.

The data set of 1772 measured masses to which the force MSk7 and the two Wigner parameters were fitted was restricted to nuclei with $A \ge 36$, the point being that the HF-BCS method is expected to work less well for very light nuclei. Nevertheless, the new mass table gives all nuclei with $Z, N \ge 8$, of which 1888 have measured masses appearing in the 1995 compilation [7]. The rms error for the set of 1888 masses is 0.738 MeV, as compared with 0.683 MeV for the set of 1772 nuclei with $A \ge 36$. A slightly smaller rms error for the 1888 masses might have been found if we had refitted the force on adding the 116 light nuclei, but this would have been at the expense of a worse fit to the heavier nuclei, for which the HF-BCS method is more appropriate. Fig. 1 plots the errors of our fit for this same data set of 1888 nuclei. For the same set of 1888 masses the rms error given by the FRDM predictions [1] is 0.689 MeV.

Other quantities, such as deformations and rms charge radii are also predicted in close agreement with experimental data. The rms charge radius is defined as

$$R_{ch}^2 = \int \rho_p(\mathbf{r}) r^2 d^3 \mathbf{r} \quad , \tag{2}$$

where $\rho_p(\mathbf{r})$ represents the HF proton density with a correction for the finite size of the proton (whose charge distribution is supposed to have a Gaussian form of rms radius 0.8 fm). Comparison with the measured charge radii of the 143 nuclei listed in the 1994 data



Figure 1: Comparison of the theoretical HF-BCS mass predictions with the 1888 $(Z, N \ge 8)$ measured masses.

compilation of Nadjakov *et al* [10] shows an rms error of only 0.019 fm. We stress that this good agreement has been achieved without any further parameter adjustment, all our parameters being determined by fitting exclusively to the mass data. This is a sensitive test of the overall reliability of the present mass formula. Concerning the deformation parameters, the HF-BCS predictions were compared and found in good agreement with the experimental compilation of [11]. The rms error to the 274 experimental β_2 -deformations is 0.100, to be compared with the FRDM [1] figure of 0.121.

2 Microscopic predictions of nuclear level densities

In a similar way as for the nuclear ground state description, until recently only classical or semi-classical analytical models of nuclear level densities (NLD) were used for most of the practical applications. Although reliable microscopic models (in the statistical and combinatorial approaches) have been developed in the recent years, the back-shifted Fermi gas model (BSFG) approximation-or some variant of it- remains the most popular approach to estimate the spin-dependent NLD, particularly in view of its ability to provide a simple analytical formula. However, it is often forgotten that the BSFG model essentially introduces phenomenological improvements to the original analytical formulation of Bethe, and consequently none of the important shell, pairing and deformation effects are properly accounted for in such a description. Drastic approximations are usually made in deriving analytical formulae and often their shortcomings in matching experimental data are overcome by empirical parameter adjustments. In particular, it is well accepted that the shell correction to the NLD cannot be introduced by neither an energy shift, nor a simple energy-dependent level density parameter, and that the complex BCS pairing effect cannot be reduced to an odd-even energy back-shift (e.g [12]). A much more sophisticated formulation of NLD than the one used in BSFG approach is required if one pretends to describe the excitation spectrum of a nucleus analytically, especially because of the very high sensitivity of NLD to the different empirical parameters. For these reasons, large

uncertainties are expected in the BSFG prediction of NLD, especially when extrapolating to very low (a few MeV) or high energies ($U \gtrsim 15$ MeV) and/or to nuclei far from the valley of β -stability.

Several approximations used to obtain the NLD expressions in an analytical form can be avoided by quantitatively taking into account the discrete structure of the singleparticle spectra associated with realistic average potentials (e.g.[13]). This approach has the advantage of treating in a natural way shell, pairing and deformation effects on all the thermodynamic quantities. The computation of the NLD by this technique corresponds to the exact result that the analytical approximation tries to reproduce, and remains by far the most reliable method for estimating NLD (despite some inherent problems related to the choice of the single-particle configuration and pairing strength). A level density formula based on the ETFSI ground state properties (single-particle level scheme and pairing strength) has already been proposed by [12]. Though it represents the first global microscopic formula which could decently reproduce the experimental neutron resonance spacings, some large deviations, for example in the Sn region, were found.

A new NLD formula within the microscopic statistical approach and based on the above-described HF-BCS method has been constructed. Some improvements concern the NLD description only, regardless of the quality of the HF-BCS input used. In particular, the formula makes use of a phenomenological deformation damping function which takes two specific effects into account. First, an energy-dependent part describes the transition from deformed to spherical shapes at increasing excitation energies. At energies above the deformation energy $E_{def} = E_{sph} - E_{eq}$ (where E_{eq} is the energy at the equilibrium deformation and E_{sph} the energy in the spherical configuration) the nucleus is assumed to become spherical. No shape barriers is assumed in this simple picture. Second, the unphysical sharp transition in the NLD formula from deformed to spherical shapes is avoided by including in the damping function a smooth deformation-dependent transition.

In contrast to our previous approach [12], the spherical approximation to the NLD is now estimated with the use of a spherical single-particle level scheme, while the deformed NLD is derived from the deformed scheme at the equilibrium deformation. Another improvement is brought to the $T \rightarrow 0$ behaviour of the total NLD. To avoid the unphysical divergence at low temperatures, the traditional formula is corrected by the asymptotic limit given by [16].

All nuclear structure properties, i.e the single-particle energies ε_q^k up to an energy cut-off $\epsilon_{\Lambda} = \hbar\omega_0$, the pairing strength G and the deformation parameters β_2 , β_4 are derived from the HF-BCS model based on the MSk7 Skyrme force. However, the constant-G strength is obtained by imposing taht the pairing energy calculated with the MSk7 δ -pairing force and a cut-off energy of $\epsilon_{\Lambda} = \hbar\omega_0$ be the same as in the constant G-approximation with the constant cut-off energy $\epsilon_{\Lambda} = 20$ MeV. This increase of the cut-off energy from $\hbar\omega_0$ to 20 MeV leads to a global decrease of the pairing energy in the NLD application compared with the value derived in the HF-BCS mass predictions. This increasing treatment of the pairing strength is found necessary to ensure an accurate fit to the experimental data on s-neutron resonance spacings, as shown in Fig. 2. We define the rms deviation as

$$f_{rms} = \exp\left[\frac{1}{N_e} \sum_{i=1}^{N_e} \ln^2 \frac{D_{th}^i}{D_{exp}^i}\right]^{1/2} \tag{3}$$

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where $D_{th}(D_{exp})$ is the theoretical (experimental) resonance spacing and N_e is the number of nuclei in the compilation. The rms deviation found with the present microscopic HF-BCS formula is $f_{rms} = 2.14$ on the 344 experimental data [14] which is comparable with the



Figure 2: Ratio of theoretical D_{th} to experimental D_{exp} [14] s-neutron resonance spacings.

value of $f_{rms} = 2.04$ obtained with the phenomenological BSFG formula [15] on the same data set. The microscopic NLD formula can also be shown to give reliable extrapolation at low energies where experimental data on the cumulative number of levels for which the set is complete can be estimated.

The NLD formula described in the present paper has been applied to the calculation of the spin-dependent NLD for more than 8000 nuclei ranging from Z=8 to Z=110 and tabulated in an energy and spin grid (U = 0.25 to 100 MeV and the lowest 15 spins). The corresponding table can be found at the website http://www-astro.ulb.ac.be.

Appendix: Summary of the microscopic NLD formula

The density of levels with spin J at an excitation energy U in a nucleus (Z, A) is given by

$$\rho(U,J) = \left[1 - f_{dam}(U)\right]\rho_{sph}(U,J) + f_{dam}(U)\rho_{def}(U,J)$$
(4)

where the damping function is divided into an energy damping part and a transitional deformation part given by

$$f_{dam}(U) = \frac{1}{1 + e^{(U - E_{def})/d_u}} \left[1 - \frac{1}{1 + e^{(\beta - \beta^*)/d_\beta}} \right]$$
(5)

where the deformation energy $E_{def} = E_{sph} - E_{eq}$ is estimated within the HF-BCS method with the Msk7 Skyrme force. E_{eq} is the energy at the equilibrium deformation and E_{sph} the energy in the spherical configuration. The parameters are taken as $d_u = 2$ MeV, $\beta^* = 0.15$ and $d_\beta = 0.02$.

The J-dependence of the level density is obtained from the relation

$$\rho_{sph}(U,J) = \frac{2J+1}{2\sqrt{2\pi}\sigma^3} e^{-\frac{J(J+1)}{2\sigma^2}} \omega(U)$$
(6)

$$\rho_{def}(U,J) = f_{as} \frac{1}{2} \sum_{K=-J}^{J} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\left[\frac{J(J+1)}{2\sigma_{\perp}^2} + \frac{K^2}{2} \left(\frac{1}{\sigma^2} - \frac{1}{\sigma_{\perp}^2}\right)\right]} \omega(U)$$
(7)

where $f_{as} = 2$ for axially symmetric shapes and to 1 for mirror and axially symmetric shapes.

The J-independent level density is given by

$$\omega(U) = \frac{e^{S(U)}}{(2\pi)^{3/2} \sqrt{D(U)}}$$
(8)

or equivalently, for a reliable description at low temperatures [16]

$$\frac{1}{\omega(U)} = (2\pi)^{3/2} \left[\frac{\sqrt{D(U)}}{e^{S(U)}} + \frac{1}{\omega_0(T)} \right]$$
(9)

where

$$\omega_0(T) = \frac{(2\pi)^2 e}{12} [a_n(T) + a_p(T)] e^{a_{red}(T)U(T)}$$
(10)

The reduced parameter $a_{red}(T) = 4a_n a_p/(a_n + a_p)$ is obtained from the *T*-dependent parameter $a_q = S_q(T)/2T$. The *T*-dependent entropy *S* and excitation energy *U* are derived from the summation on the doubly degenerate single-particle levels ε_q^k (with blocking effect for odd nucleon systems)

$$S(T) = 2 \sum_{q=n,p} \sum_{k} \ln \left[1 + \exp(-E_q^k/T) \right] + \frac{E_q^k/T}{1 + \exp(-E_q^k/T)}$$
(11)

$$U(T) = E(T) - E(T = 0)$$
(12)

where the total energy is given by

$$E(T) = \sum_{q=n,p} \sum_{k} \varepsilon_{q}^{k} \left[1 - \frac{\varepsilon_{q}^{k} - \lambda_{q}}{E_{q}^{k}} \operatorname{tanh}(\frac{E_{q}^{k}}{2T}) \right] - \frac{\Delta_{q}^{2}}{G}$$
(13)

and $E_q^k = \sqrt{(\varepsilon_q^k - \lambda_q)^2 + \Delta_q^2}$ is the quasi-particle energy.

The lengthy expression for the determinant D(T) can be found in [17].

The BCS equations determine the gap parameter Δ_q and the chemical potential λ_q as a function of the pairing strength G_q

$$N_{q} = \sum_{k} \left[1 - \frac{\varepsilon_{q}^{k} - \lambda_{q}}{E_{q}^{k}} \tanh(\frac{E_{q}^{k}}{2T}) \right]$$
(14)

$$\frac{2}{G_q} = \sum_k \frac{1}{E_q^k} \tanh(\frac{E_q^k}{2T})$$
(15)

The parallel spin cut-off parameter for axially-deformed nuclei is obtained from the summation on the projection on the symmetry axis of the single-particle angular momentum ω_q^k

$$\sigma^2(T) = \frac{1}{2} \sum_{q=n,p} \sum_k \omega_q^{k^2} \operatorname{sech}^2(\frac{E_q^k}{2T})$$
(16)

and the perpendicular spin cut-off parameter is

$$\sigma_{\perp}^{2}(T) = \sum_{q=n,p} \frac{\mathcal{I}_{q}^{rig}}{\hbar^{2}} \left[1 - g\left(\frac{\delta\hbar\omega_{0}}{2\Delta_{q}}\right) \right] T\left(1 + \frac{1}{3}\delta\right)$$
(17)

$$g(x) = \frac{\ln(x + \sqrt{1 + x^2})}{x\sqrt{1 + x^2}}$$
(18)

where the rigid-body value of the moment of inertia is

$$\frac{\mathcal{I}_q^{rig}}{\hbar^2} = \frac{2}{5} \frac{\mathrm{m}R^2}{\hbar^2} N_q \tag{19}$$

and

$$\hbar\omega_0 = 41 A^{-1/3} \, [\text{MeV}]$$
 (20)

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Work Report

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1 Improvements and extensions

1.1 Segment 1: Masses and deformations

New files have been added to Segment 1 in agreement with the Vienna meeting (1998, INDC(NDS)-389). These concern

- goriely-etfsi2.dat and goriely-etfsi2.readme: ETFSI (version 2) ground state properties (masses, deformations, density distribution, pairing gaps and shell correction energies).
- goriely-raman.dat and goriely-raman.readme: experimental deformations from Raman et al. (1987).
- goriely-moller.dat and goriely-moller.readme: updated files where all recommended experimental masses from the Audi & Wapstra (1995) compilation have been included in the corresponding column of the moller.dat file.
- goriely-fission.dat and goriely-fission.readme: ETFSI Fission barriers still need to be supplied after publications.

Improvements could also be brought through a more homogeneous format among all the files. However, this would imply modifying original files from the authors and suppressing some useless or redundant data. Some suggestions (to be discussed) could be

- 1. providing all files including masses in a common format starting in the first columns with (Z,A,Mass excess) in a common format (2i4,f10.3).
- 2. simplifying the recommended moller.dat file by including FRDM masses, experimental masses and the β -deformations only. The FRLDM masses and ε -deformations could be transferred to the Other_files directory. The Myers & Swiatecki (1995) masses could be included in the same file.
- 3. simplifying the recommended audi.dat file to include principally the mass excesses and the binding energy for given (Z,A).
- 4. reducing the beijing.dat file to the original data it includes, i.e the data not found in other files like the spin and parity, and eventually the β -decay half-life, or merging it with the experimental mass file of Audi & Wapstra (1995). The merged

abundance/half-life column is not in an easy-to-read fortran format (half-life given in terms of s,d,yr or of level width in ev,keV,MeV)

5. the jaeri_deform.dat file could be transferred to Segment 2 dealing with excitation levels, the ground-state deformation being now included in a specific file (goriely-raman.dat).

Obviously, these are only suggestions for a greater homogeneity in the Library and are open to further discussions.

1.2 Segment 5: Densities

- nld.zxxx and goriely-nld.readme: Nuclear Level Densities derived for some 8000 nuclei (with $8 \le Z \le 110$ and lying between the neutron and the proton driplines) from the microscopic statistical approach based on a HF+BCS single-particle level scheme. The nuclear level densities are given in a table format (one file per isotopic chain Z) for excitation energies from $0.25 \le U[MeV] \le 100$ and for spin ranging from J=0 (1/2) to J=15 (31/2).
- Z_xxx.SPL and spl.readme: ETFSI single-particle level scheme including for about 8000 nuclei the deformation and for both the neutron and proton systems, the pairing strength and cut-off energies, and the single-particle level scheme (energy, parity, spin). All the data files are provided in a format identical to the files including the FRDM single-particle levels.

2 Testing

Some comments on new problems encountered in the use of the RIPL-1 data. We will not mention here the problems already discussed during the Vienna meeting in November 1998 and summarized in the INDC(NDS)-389 report. However, we would like to stress the diversity found in the format of the "README" files. I would propose a standardisation of the files, which would include title, authors, abstract of the content, definition of symbols (with fortran format) and references. I would also propose that when possible the data files include a first title line. This standard format for the whole library should be coordinated by one person.

2.1 Segment 2: Levels

A systematic testing of the cumulative number N_m up to the energy U_{max} could be achieved a posteriori by estimating N_m by global NLD formulae, like GSM, BSFG or microscopic formulae. We did such a test on the RIPL-1 file making use of BSFG and the microscopic HF-BCS formula (see above). In many cases, the ratio between global prediction of N_m and the compiled value can be huge, for example ¹⁶⁹Ta it amounts 10^5 at $U_{max} = 4$ MeV. This means that, if we believe in the predictive power of the theoretical formulae, in these cases, the set of excited levels is far from being complete, though it looks like complete in its exponentially increasing pattern at low energies. This defect was already raised by A. Ignatyuk in Novembre 1998 who proposed to check the consistency with the Gilbert-Cameron formula. We would also suggest considering the use of global and robust NLD formulae, to avoid the completely parametric character of the Gilbert-Cameron approach.

It remains difficult to test the determination of the number of cumulative levels in the new compilation (Belgya_paramsl.dat) on a few nuclei only ! However, the large difference between the minimum (N_{min}) and maximum (N_{max}) number of levels for which the level scheme is complete clearly shows the difficulty of the task. For practical applications, it might be difficult to make use of the data if no recommended value is provided. It might also be of interest to associate the experienced chinese group (CENPL) to such an ambituous work.

The Ripl-2 compilation (cf. belgya-par-30_20_-4_4.dat file) on N_{max} , the maximum number of level up to which the level scheme is predicted to be complete, has apparently been achieved by imposing a unique temperature T within a given isobaric chain (i.e T is the same for a given A). The physical reasons for such an assumption is obscure. Regions of different deformations, pairing or shell effects might be met within an isobaric chain. This approach presents at least the advantage of avoiding spurious predictions as mentioned above for ¹⁶⁹Ta. This time, on the 641 entries, the N_{max} predicted by the BSFG of Rauscher et al. (1997) or the microscopic HF-BCS formula remains within a factor of roughly 10 with respect to the Ripl2 data (some larger deviations by a factor of a few hundreds are found in particular for ²¹⁴Fr). Nevertheless, many fits present large χ^2 -values, and predictions with $\chi^2 > 0.05$ can hardly be considered as reliable. The major difficulty of the approach might be related to the fact that the constant-T formula is simply not adequate to fit the low-energy data.

Also note that the Figs 2.2-2.5 given in the Ripl-1 publication seem to correspond to even or odd values of (A, Z) and not (Z, N), as traditionnally defined. A clear definition of a even-even, even-odd, odd-even or odd-odd nucleus should be given in order not to mislead the readers.

2.2 Segment 3: Resonances

- 1. The Ripl-1 resonance spacings D_0 for ³⁴S and ²⁰⁹Pb included in the obninsk.dat file are drastically different when compared with other compilations. In the case of ³⁴S, the D_0 and δD_0 values seem to have been erronously multiplied by a factor of 10. The ²⁰⁹Pb values are "strange" compared with beijing.dat or Iljinov et al. (1992) and do not include error bars.
- 2. Most of the data in the obninsk.dat file refers to the references [3.20] or [3.32] (1996 and 1997, Ignatyuk, RIPL-1 CRP meeting). It would be important to make this reference available on the web, since it contains most of the results presented in the obninsk.dat file. The users have no means to check the consistency or origin of the experimental data (like in the ²⁰⁹Pb case mentioned above).
- 3. Most of the data in the beijing.dat file refers to Huang Zhongfu et al. (1996, to be published). Other data have no references, so there is no possibility to check the origin of the data. For example, ¹⁴²Ce is characterized by a D_0 -value much smaller (by a factor of about 20-30) than predicted by global NLD formulae. A direct communication with Dr. Su Zongdi from the chinese group taught us that the revisited experimental resonance spacing of ¹⁴²Ce is $D_0 = 0.83 \pm 0.08$ keV, i.e about 23 times the value in the RIPL-1 compilation.

Data are also provided for some exotic nuclei, like 94 Y ($T_{1/2} = 18.7$ min). It would be of general interest to have more documentation on the origin of the experimental data, if possible.

The set of resonance data compiled by the chinese group is much larger than all other existing sets (62 more nuclei than in obninsk.dat). It would be worth updating the RIPL data with the updated chinese library CENPL-98 data, if available, and give the users more information about CENPL.

2.3 Segment 5: Level Densities

- 1. Many different compilations based on the same level density formula with the same input parameters are provided by RIPL. For example, the BSFG formula of Dilg et al. (1973) is found in the beijing and bombay compilations. The shell-dependent BSFG model with Myers & Swiatecki (1967) shell correction is included in the Iljinov (1992) and Mengoni et al. (1994) compilations. The GSM approach is provided by the obninsk and beijing compilations. The need to duplicate the same input files compiled by different groups is questionable for a reference library.
- 2. As already pointed out during the Vienna Meeting, there is an obvious confusion and incoherence between the shell (or microscopic) correction to be applied to the NLD formula and the shell correction to the binding energies defined in Segment 1. See note below. Some input data (shell corrections, but also pairing strength for the microscopic approach) are not provided. The corresponding NLD formula might never be used.

3 The shell correction energy

3.1 the microscopic corrections to the binding energy

There is in the literature a great confusion about what is referred to as the shell correction energy. Different definitions exist. The most common one defines the various microscopic corrections (e.g Moller et al. 1995) as follows:

The total nuclear binding energy is written as

$$E_{tot}(Z, A, \beta) = E_{mac}(Z, A, \beta) + E_{s+p}(Z, A, \beta)$$
(1)

where β charaterizes the nuclear shape at equilibrium, i.e the shape which minimizes the total binding energy. $E_{s+p} = E_{shell} + E_{pair}$ is the shell-plus-pairing correction energy¹. Defining a macroscopic deformation energy by the difference in the macroscopic energy between the equilibrium and spherical shape,

$$E_{def}(Z, A, \beta) = E_{mac}(Z, A, \beta) - E_{mac}(Z, A, \beta = 0)$$
⁽²⁾

the total nuclear binding energy can now be expressed as

$$E_{tot}(Z, A, \beta) = E_{mac}(Z, A, \beta = 0) + E_{mic}(Z, A, \beta)$$
(3)

with the microscopic correction

$$E_{mic}(Z, A, \beta) = E_{shell}(Z, A, \beta) + E_{pair}(Z, A, \beta) + E_{def}(Z, A, \beta).$$
(4)

Another frequent definition of the shell energy considers the experimental energy $E_{exp}(Z, A)$, when available, instead of the total binding energy:

$$\delta E_0 = E_{exp}(Z, A) - E_{mac}(Z, A, \beta)$$
(5)

$$\simeq E_{shell}(Z, A, \beta) + E_{pair}(Z, A, \beta) = E_{s+p}(Z, A, \beta)$$
(6)

Should the mass formula be exact, $\delta E_0 = E_{s+p}(Z, A, \beta)$.

Each mass model calls for specific theoretical backgrounds to estimate the macroscopic part, as well as the shell, pairing and deformation energies. The most common approaches to derive

- the macroscopic part are the droplet-like models, the most popular of which is the FRDM model (Moller et al., 1995), the Thomas-Fermi approach (e.g Myers and Swiatecki 1995) or the Extended-Thomas-Fermi approach (Aboussir et al., 1995).
- the shell correction energy is the Strutinsky theorem applied with the standard averaging procedure or the semi-classical integral method.
- the pairing correction energy are the BCS or Lipkin-Nogami models using a constant-G strength or a δ -pairing force.

¹note that we define here the pairing correction for even-even nuclei and do not consider the odd-even effect also attributed to the pairing interaction

The parameters of each of these ingredients in the mass formula are determined by a fit to about 1800 experimental masses. The quality of the mass model is traditionnally estimated by the root mean square deviation to the expertimental data and the number of parameters required to achieve the fit. Depending on the approach followed to derive the smooth macroscopic part of the binding energy (droplet, TF, ETF, ...), the microscopic corrections can take relatively different values.

The shell corrections in the standard averaging procedure can be expressed by

$$E_{shell}(Z, A, \beta) = E_{s.p.} - \dot{E}_{s.p.}$$
(7)

$$= \sum_{i=1}^{N} \epsilon_{i} - \int_{-\infty}^{\bar{\lambda}} \epsilon \ \tilde{g}(\epsilon) \ d\epsilon \ . \tag{8}$$

The smooth sum can in some conditions be obtained by the Strutinsky Integral method. Nevertheless, it should be noted that the so-defined shell correction is pairing independent, the summation covering all single-particle energies, and not the quasiparticle energies.

The pairing correction, also known as the condensation energy, represents the difference in the binding energy between the systems with or without pairing interactions. It reads for a constant-G pairing interaction

$$E_{pair}(Z, A, \beta) = \sum_{i} v_i^2 \epsilon_i - \sum_{i=1}^N \epsilon_i - \frac{\Delta^2}{G} - \frac{1}{2} G\left[\sum_{i} v_i^4 - N\right]$$
(9)

where v_i^2 are the well-known occupation probabilities. A smooth pairing contribution needs to be subtracted from E_{pair} if already included in the smooth macroscopic part. This is the case for the FRDM-type mass model, but not of the TF or ETF methods (where the macroscopic part is derived from an effective nuclear interaction independently of the pairing interaction). In the macroscopic-microscopic approach,

$$E_{pair}^{mic-mac} = E_{pair}(Z, A, \beta) - \tilde{E}_{pair}(Z, A, \beta)$$
(10)

where the smooth average \tilde{E}_{pair} is derived making use of a smooth single-particle level density in the vicinity of the Fermi surface.

3.2 the microscopic corrections to the nuclear level density

The nuclear level density is also affected by microscopic corrections, i.e by the shell, pairing and deformation effects. The temperature-dependent microscopic corrections can be related to the ground state corrections in a phenomenological way. However, we should remain extremely careful about the meaning of the microscopic corrections considered in the specific level density formula used. To illustrate the different possible definitions, we will consider here different expressions of the popular Back-Shifted Fermi Gas (BSFG) model (or some variant of it) and discuss the impact of the microscopic corrections on the entropy (i.e on the *a*-parameter) and not on the back-shift δ .

• The non-corrected BSFG:

The most widely used expression of the total level density reads

$$\rho(U) = \frac{\sqrt{\pi}}{12\tilde{a}^{1/4}(U-\delta)^{5/4}} e^{2\sqrt{\tilde{a}(U-\delta)}}$$
(11)

where both parameters \tilde{a} and δ are energy-independent and determined by a direct fit to the low-lying spectrum and the neutron s-wave spacings D_0 (e.g Dilg et al. 1973). The \tilde{a} and δ parameters can hardly be connected to any ground-state corrections since they correspond to temperature-dependent parameters estimated at an excitation energy $U \simeq S_n$. No reliable systematics can be derived from this formula.

• The spherical shell-dependent BSFG:

The same expression as Eq. (11) is used, but the *a*-parameter is now considered to be energy-dependent:

$$a(U) = \tilde{a}[1 + \delta W f(U)] \tag{12}$$

where f(U) is a decreasing function with increasing U (e.g Ignatyuk et al. 1995; Goriely 1996). Neither the collective enhancement, nor the pairing correction are included explicitly in such a BSFG formula. The pairing correction is reduced to an odd-even shift in energy, but the T-dependent entropy is not affected by the pairing correlation. In this case, the correction energy δW includes all non-smooth effects and is thus an approximation of the microscopic ground-state correction $\delta W \simeq E_{mic}$. It includes shell, pairing and deformation effects. The 3 effects are known to disappear with increasing excitation energies, though not at the same threshold energy in contrast to the approximation (12). Such an approximation corresponds for example to the Rauscher et al. (1997) formula with the use of the FRDM microscopic correction $\delta W = E_{mic}$, the Mengoni et al. (1994) formula with the droplet corrections of Myers & Swiatecki (1967), or the .

• The deformed shell-dependent BSFG:

Some BSFG formulas take into account vibrational and rotational enhancements explicitly through the expression

$$\rho(U) = K_{vib} K_{rot} \frac{\sqrt{\pi}}{12a^{1/4}(U-\delta)^{5/4}} e^{2\sqrt{a(U-\delta)}}$$
(13)

where a(U) is given by Eq. (12). Since the deformation effects due to the collective degrees of freedom are considered separately in the rotational K_{rot} and vibrational K_{vib} factors, it should not be included anymore in the *T*-dependent *a*-parameter. In this case, $\delta W = E_{s+p}$, the shell-plus-pairing correction. This expression corresponds, for example, to the BSFG of Iljinov et al. (1992) with collective enhancement.

Note, however, that another complication arises when considering the transition from deformed to spherical shape at increasing excitation energies. The ground state shell correction energy E_{shell} is deformation-dependent, so that at increasing energies when the sphericity of the nuclear surface is recovered, a spherical shell-correction energy should theoretically be considered. This effect has never been taken into account in analytical formula yet.

• the deformed shell- and pairing-dependent Fermi gas:

In this case, the shell correction due to the non-equidistant pattern of the singleparticle level scheme is treated as above in Eq. (12), but in the approximation of independent particles, the impact of the pairing interaction on the entropy and excitation energies being considered explicitly on top of the mean field produced by the non-interacting particles. We are dealing now with quasi-particles. Analytical approximations of the ground-state BCS pairing with a constant G-force are widely available. T-dependent BCS pairing has been estimated analytically by Ignatyuk (1985) and Goriely (1996). At low energies, the fermion system is in the so-called supraconducting phase, while at excitation energies higher than the critical energy, the system enters the normal phase. In this normal phase, the pairing correlation affects the excitation energy by a simple energy shift equal to the condensation energy (i.e $\delta = E_{pair}$), but does not affect the *a*-parameter at all. On the other hand, in the supraconducting phase (below the critical energy), the complicated temperature-dependent *a*-parameter can be expressed by

$$a_{supra}(T) \simeq F(\Delta/T) \ a(T)$$
 (14)

where Δ is the *T*-dependent BCS pairing gap and *F* a gaussian-like function (Goriely 1996) and a(T) is the pairing-independent *a*-parameter for the non-interacting system, given for example by Eq. (12). In this case, $\delta W = E_{shell}$. The pairing effect is included in the *F*-dependence (14) and the deformation effect in the collective enhancement factors.

This deformed shell- and pairing-dependent Fermi gas is found in the generalized superfluid model (GSM) of Ignatyuk (1985) or the semi-classical approximation (SCA) of Goriely (1996).

In summary, depending on the NLD formula considered, the microscopic correction to the *a*-parameter (12) can include very different effects. When the different parameters $(\tilde{a}, \delta, \delta W)$ are not determined by a direct fit to experimental data, but rather from systematics, we recommend the following microscopic correction, for the

- GSM formula: $\delta W = E_{shell}$
- Mengoni et al (1994) BSFG: $\delta W = E_{mic}$
- Rauscher et al. (1997) BSFG: $\delta W = E_{mic}$
- Iljinov et al. (1992) BSFG without collective enhancement: $\delta W = E_{mic}$
- Iljinov et al. (1992) BSFG with collective enhancement: $\delta W = E_{s+p}$

The various ground-state corrections E_{shell} , E_{pair} and E_{def} can be obtained by the FRDM or ETFSI mass model, for example. The Myers & Swiatecki (1967) liquid drop or von Groote et al. (1976) droplet models only provide E_{s+p} and E_{def} . However, the microscopic corrections depend on the macroscopic part used in the mass model, and can consequently differ in a non-negligible way between different prescriptions. When dealing with NLD, for a given set of microscopic corrections, the systematic \tilde{a} -parameter must be adjusted accordingly by a fit to experimental data.

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Program TOTELA Calculating Basic Cross Sections in Intermediate Energy Region by Using Systematics

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Program TOTELA can calculate neutron- and proton-induced total, elastic scattering and reaction cross sections and angular distribution of elastic scattering in the intermediate energy region from 20 MeV to 3 GeV The TOTELA adopts the systematics modified from that by Pearlstein [1] to reproduce the experimental data and LA150 evaluation better. The calculated results compared with experimental data and LA150 evaluation are shown in figures in following pages. The TOTELA results can reproduce those data almost well. The TOTELA was developed to fill the lack of experimental data of above quantities in the intermediate energy region and to use for production of JENDL High Energy File. In the case that there is no experimental data of above quantities, the optical model parameters can be fitted by using TOTELA results. From this point of view, it is also useful to compare the optical model calculation by using RIPL with TOTELA results, in order to verify the parameter quality.

Input data of TOTELA is only atomic and mass numbers of incident particle and target nuclide and input/output file names. The output of TOTELA calculation is in ENDF-6 format used in the intermediate energy nuclear data files. It is easy to modify the main routine by users. Details are written in each subroutine and main routine.

Reference [1] S. Pearlstein: Nucl. Sci. Eng. <u>95</u>, 116 (1987).




















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