Large-scale calculations of excited states of heavy nuclei

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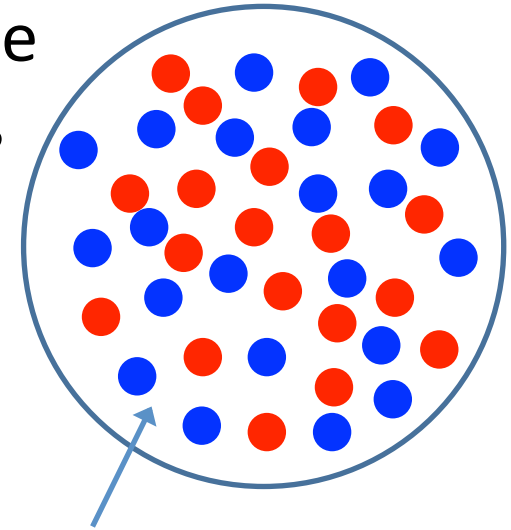
1. Physics
   – strength functions and energies
2. Computational matters
   – a few details of my calculation

1. Physics

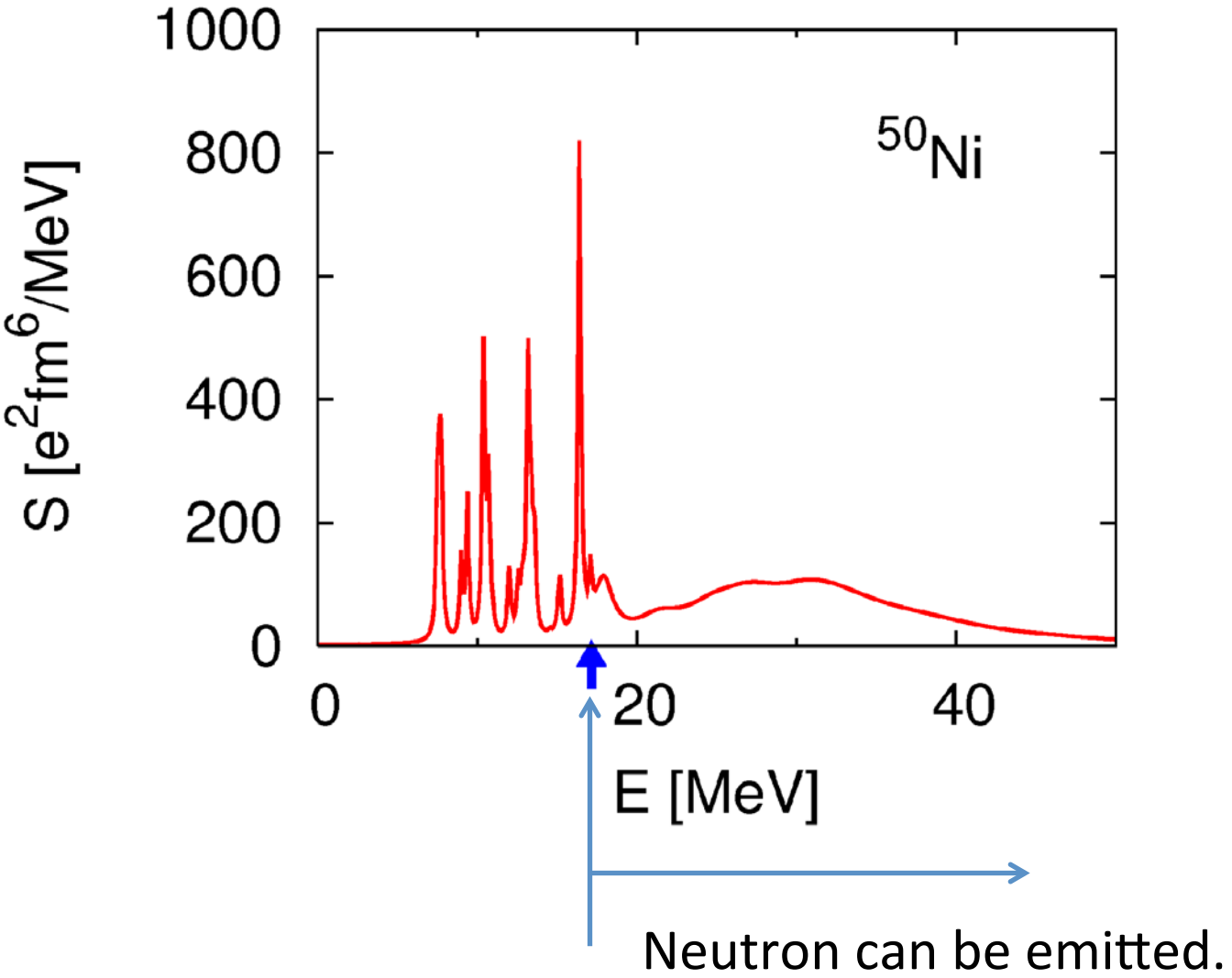
A simplified picture of atomic nucleus



For some combinations of the proton and neutron numbers, the system becomes bound.

The lowest-energy state – ground state
Those having more energy – excited state
What excited states are there of nuclei?

Isoscalar 1^- strength functions by QRPA

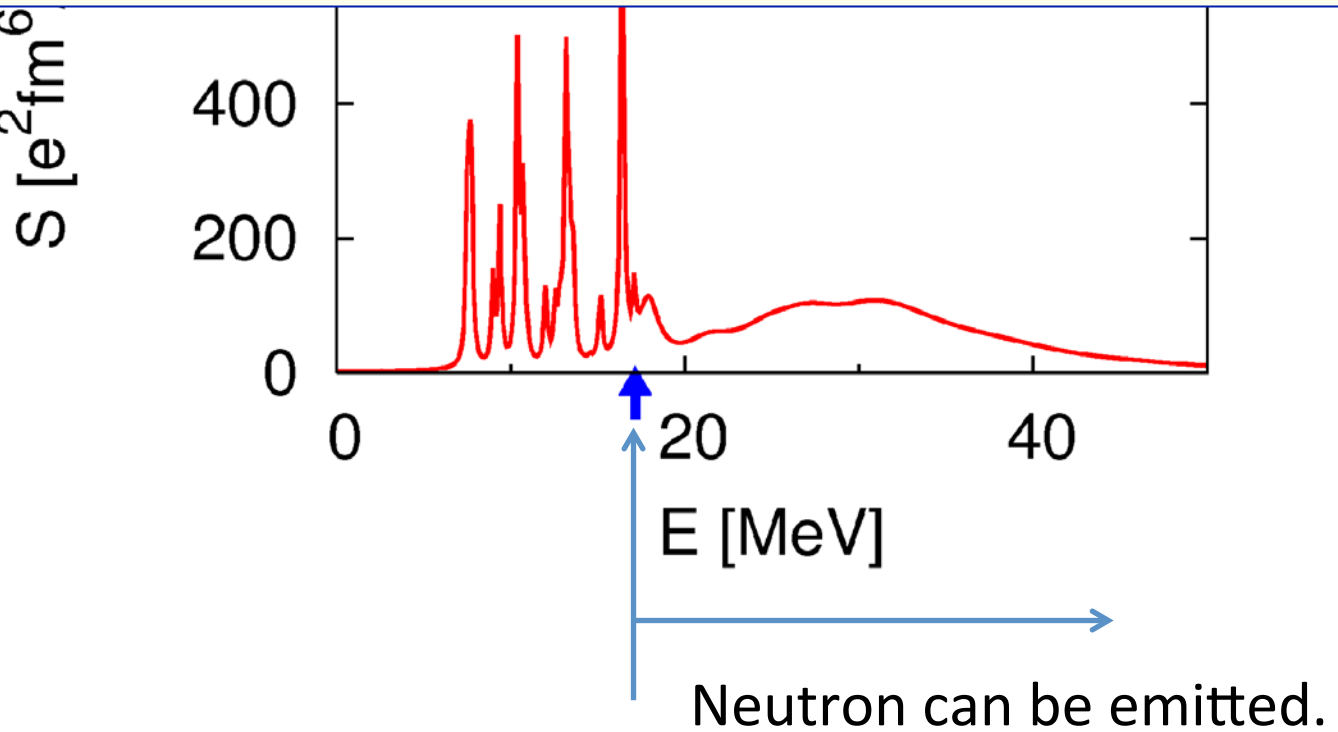


T. et al. Phys. Rev. C **74**, 044301 (2006)

Its meaning:

How efficiently the ground state is changed to the excited state of the energy (horizontal axis), when that energy is given from the environment to the nucleus.

Experimental observable → test of theory

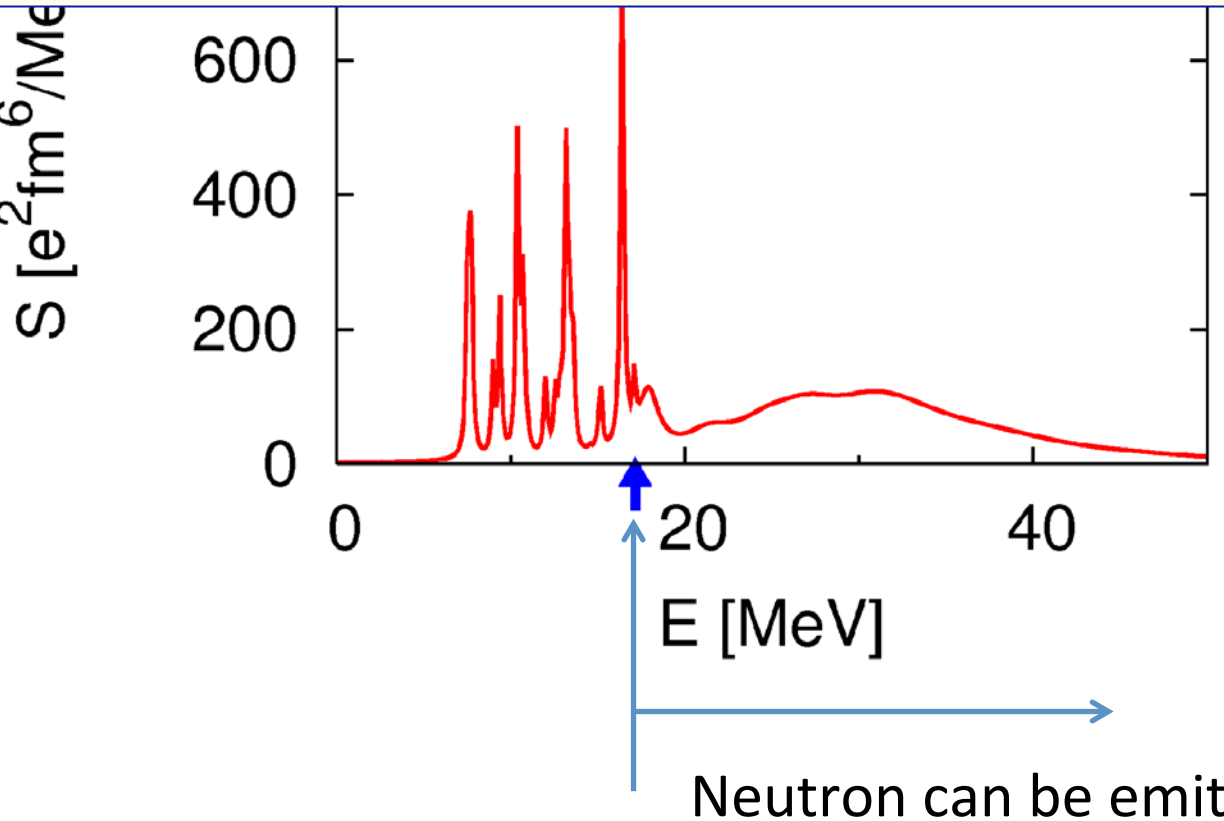


T. et al. Phys. Rev. C **74**, 044301 (2006)

Its meaning:

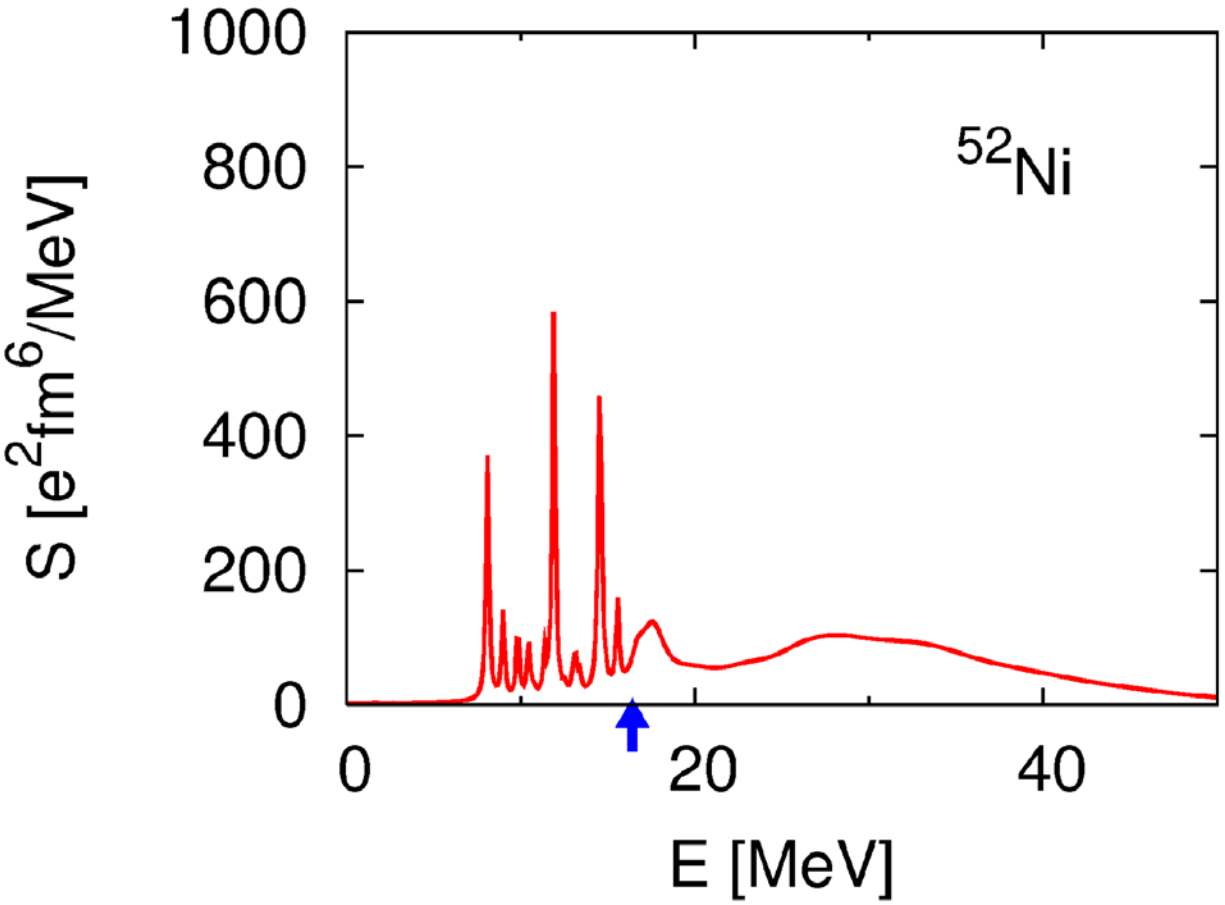
The abundance of elements in the universe is affected.

A part of the history of the universe depends on the strength functions of nuclei.

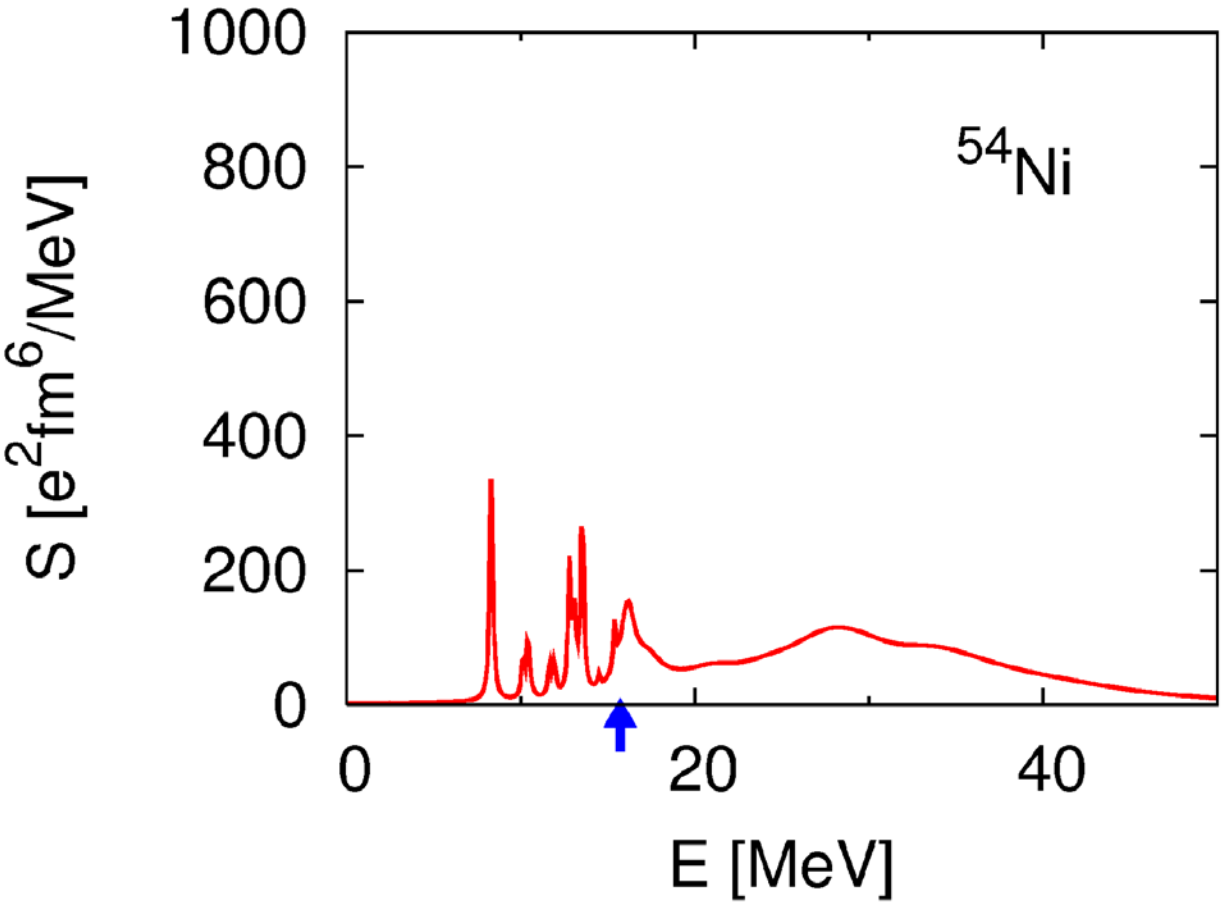


T. et al. Phys. Rev. C **74**, 044301 (2006)

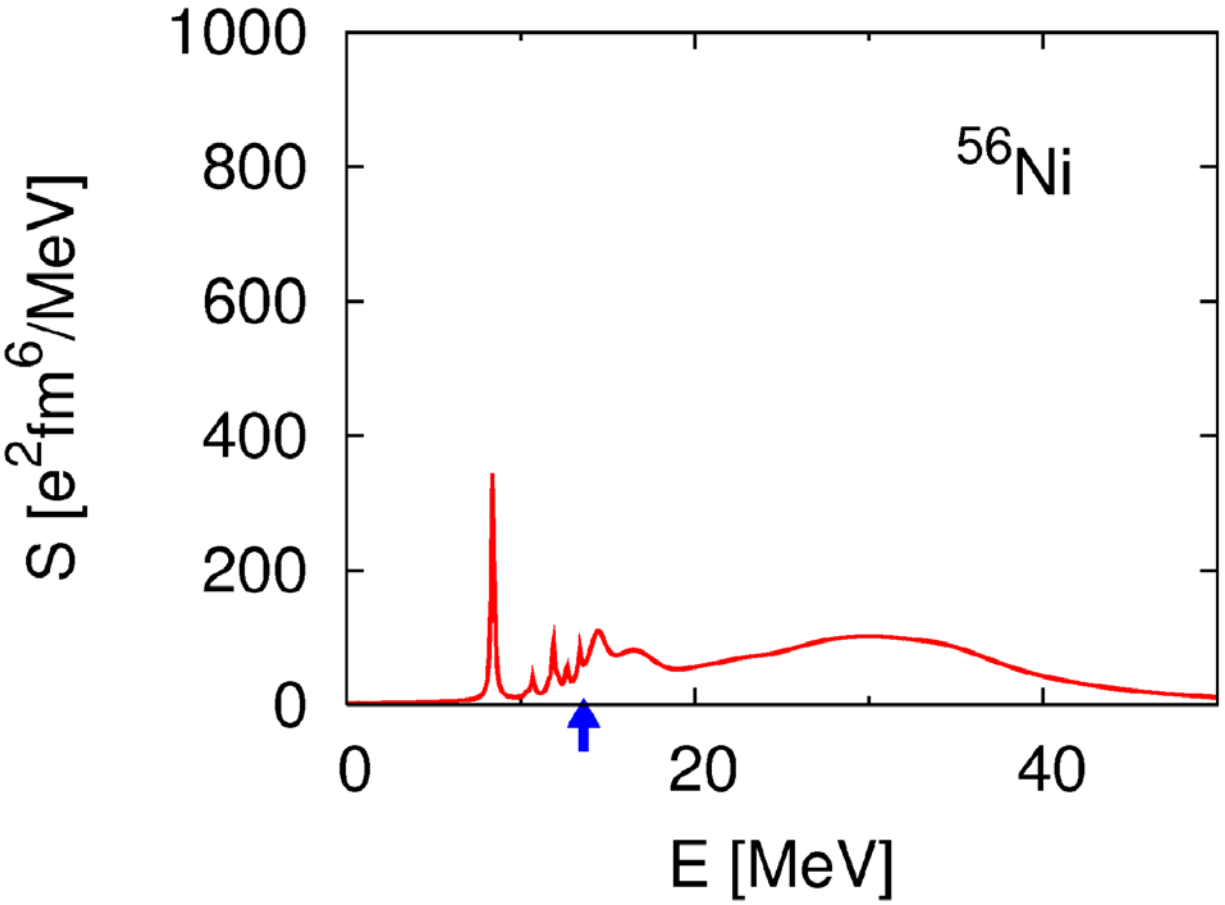
Isoscalar 1^- strength functions



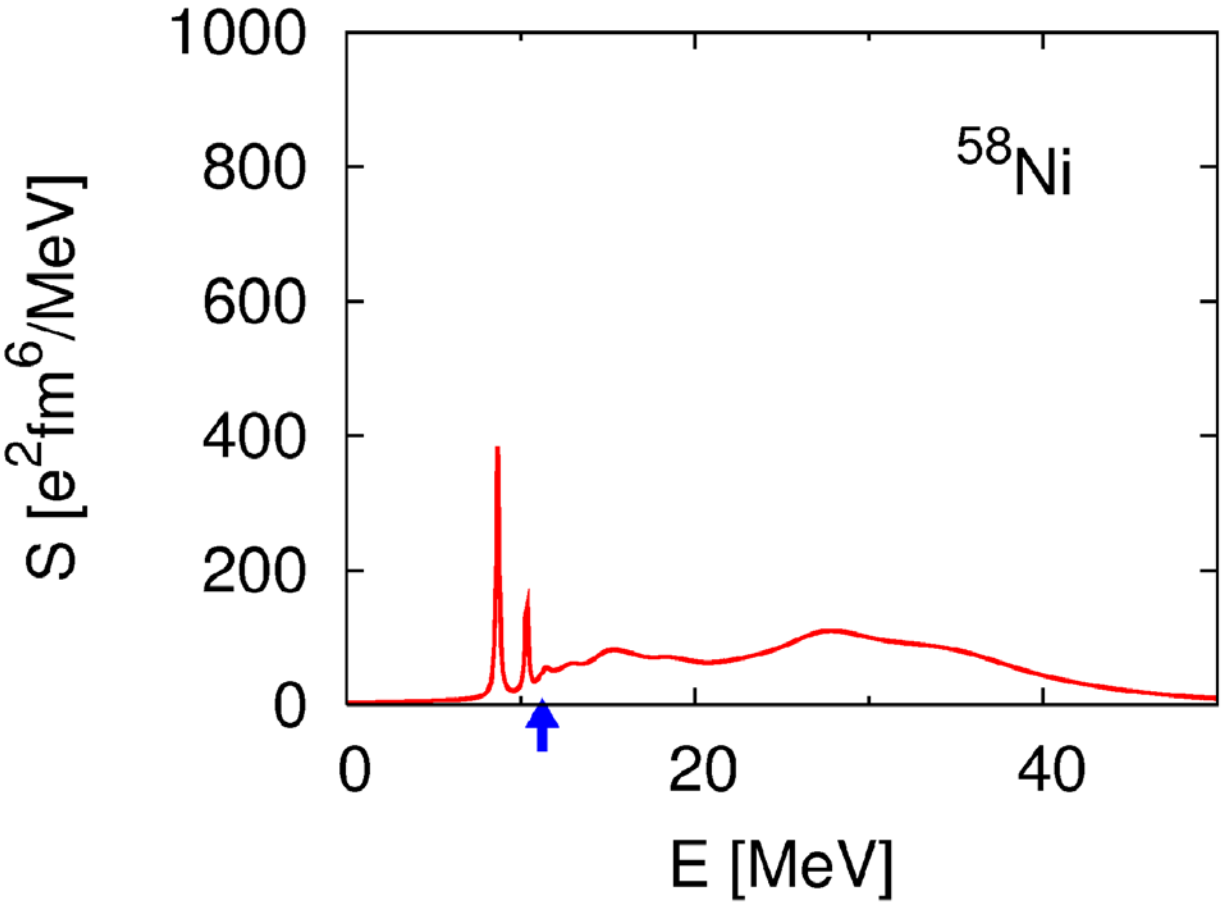
Isoscalar 1^- strength functions



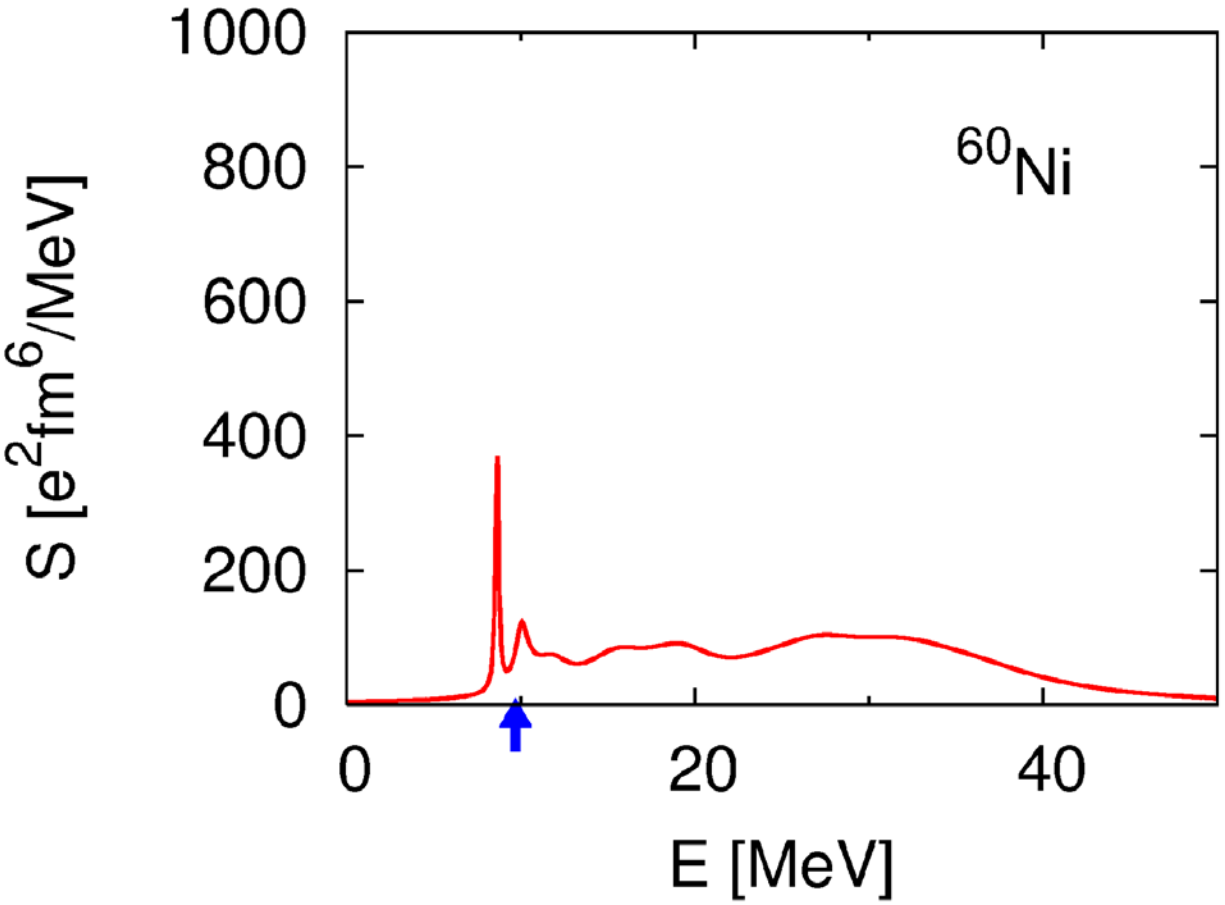
Isoscalar 1^- strength functions



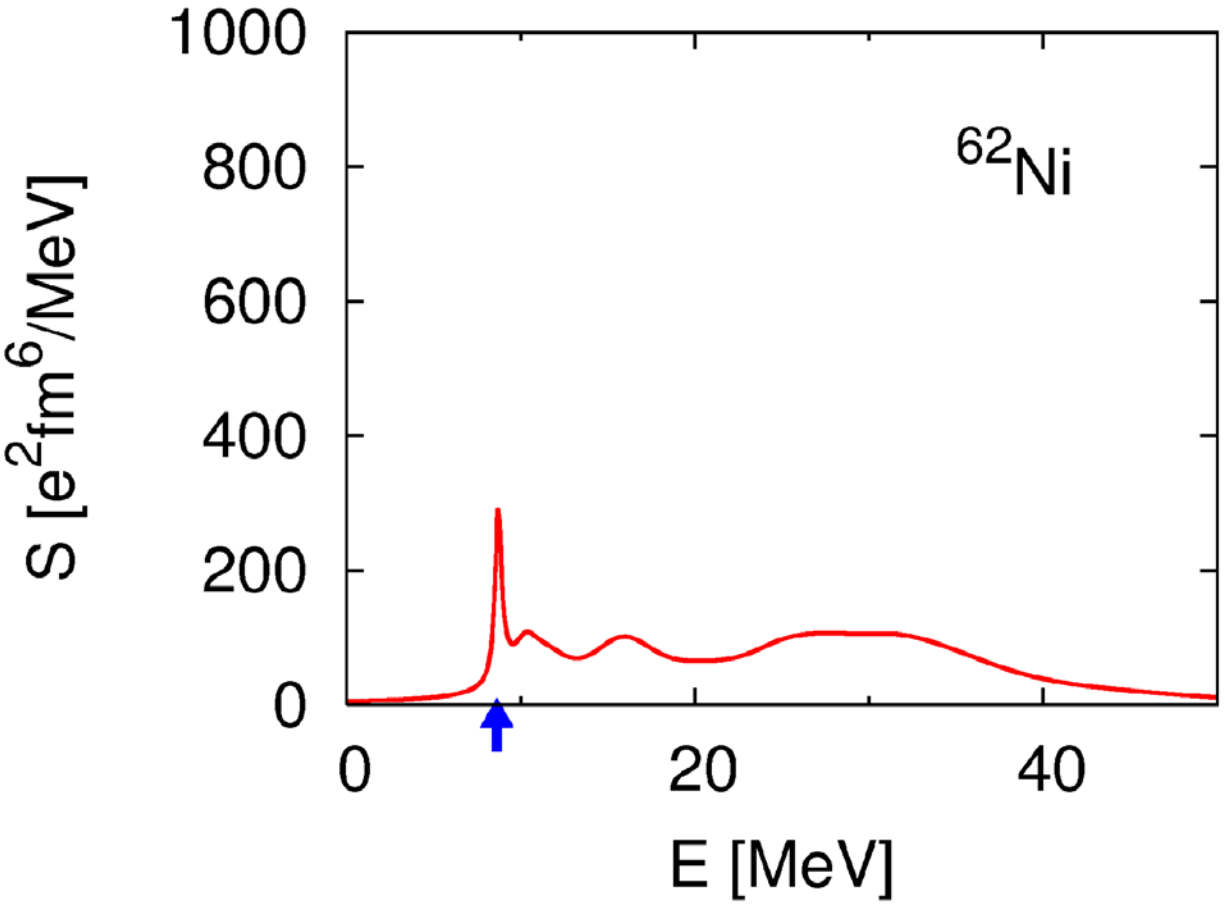
Isoscalar 1^- strength functions



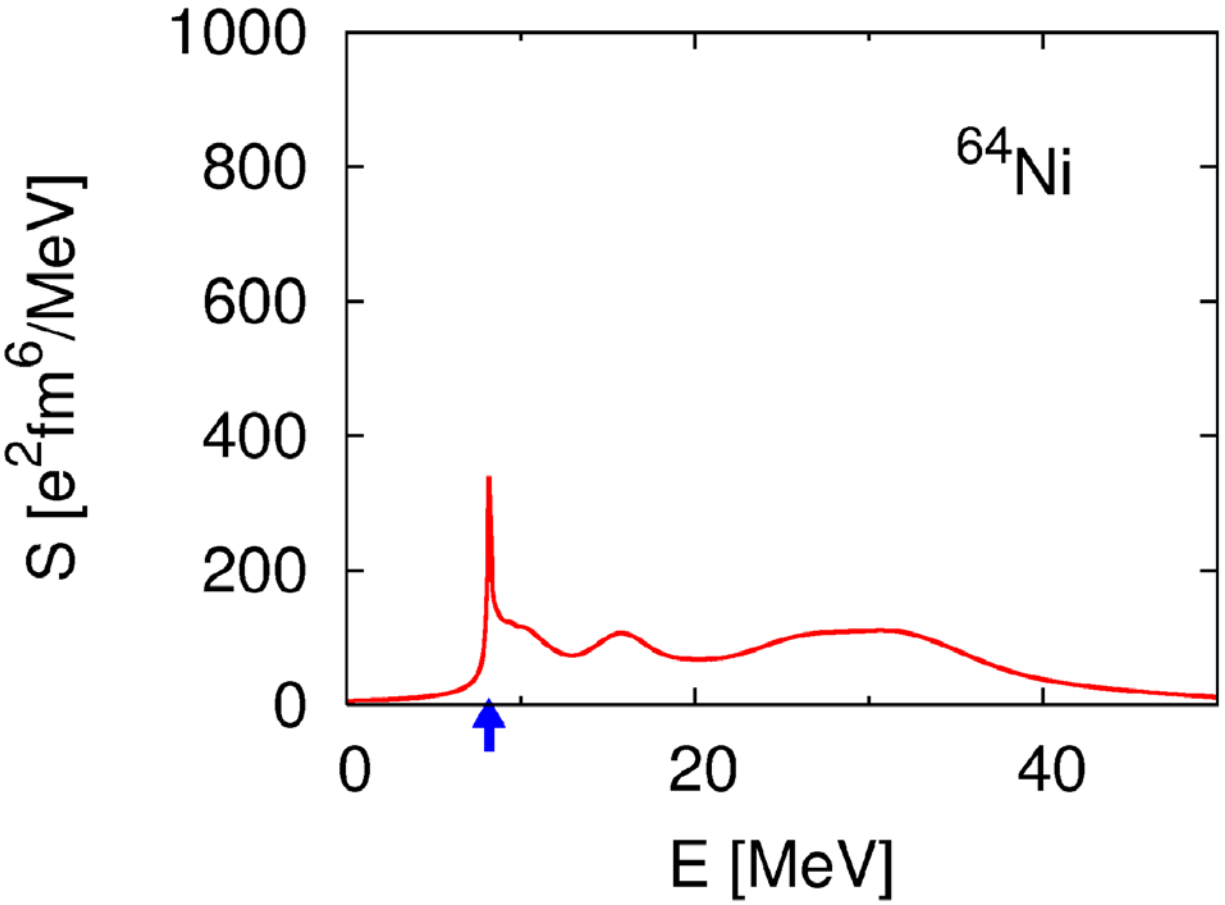
Isoscalar 1^- strength functions



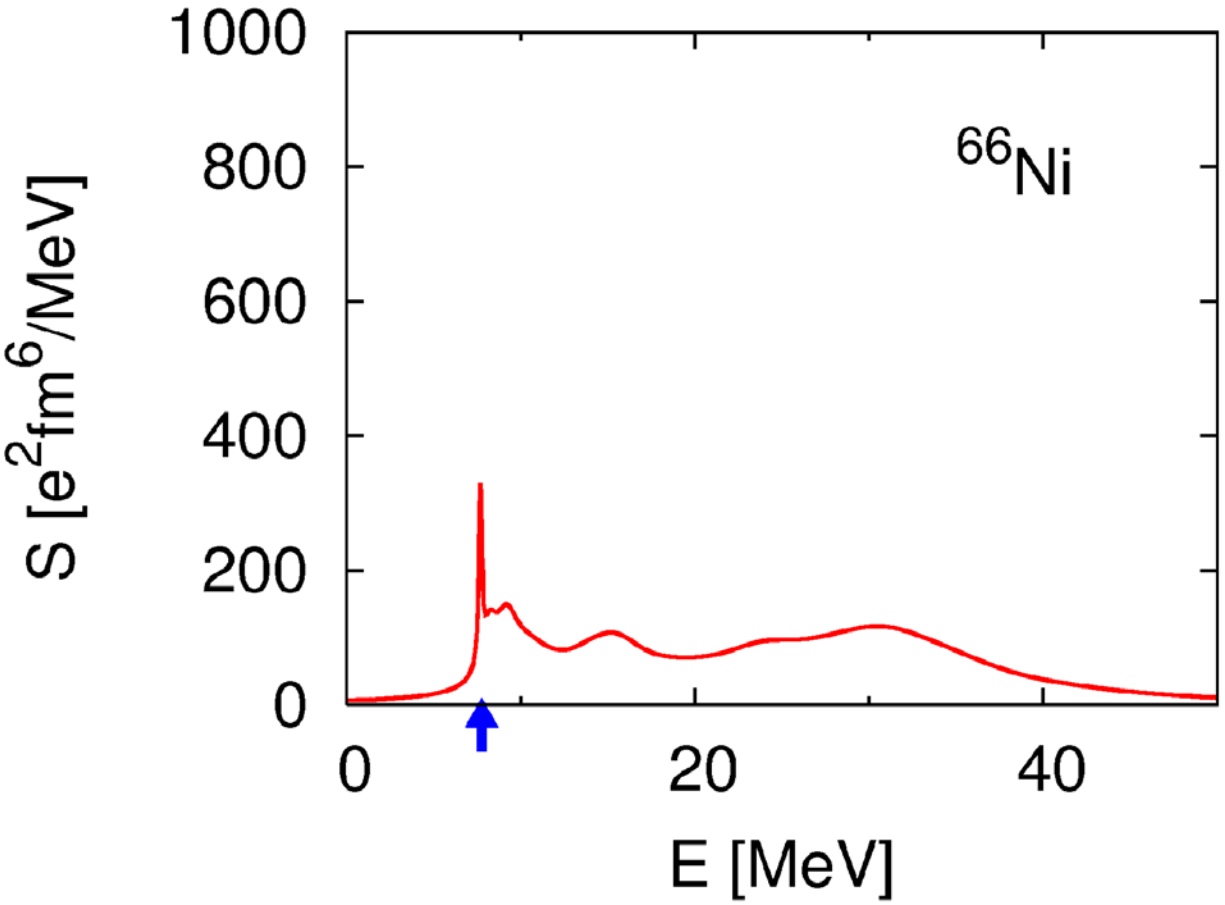
Isoscalar 1^- strength functions



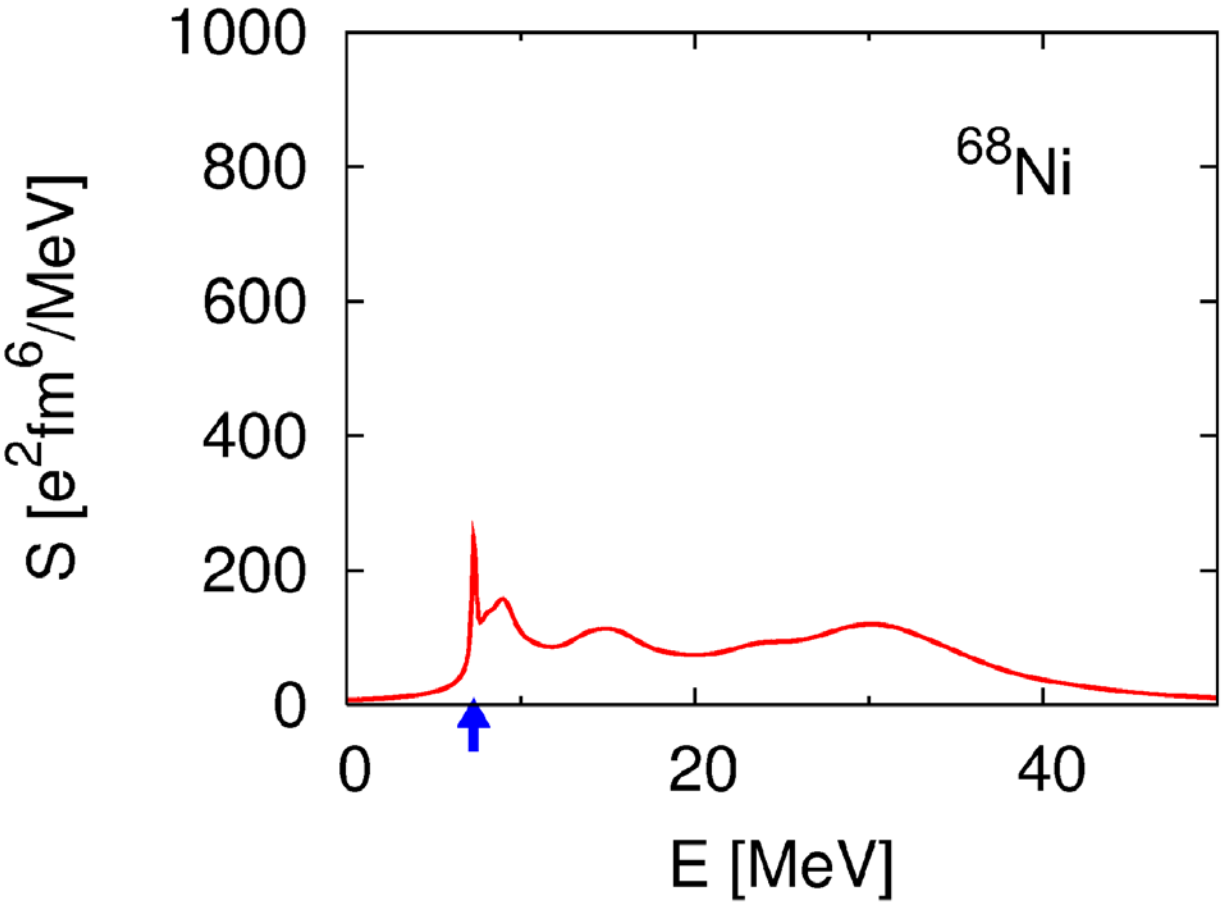
Isoscalar 1^- strength functions



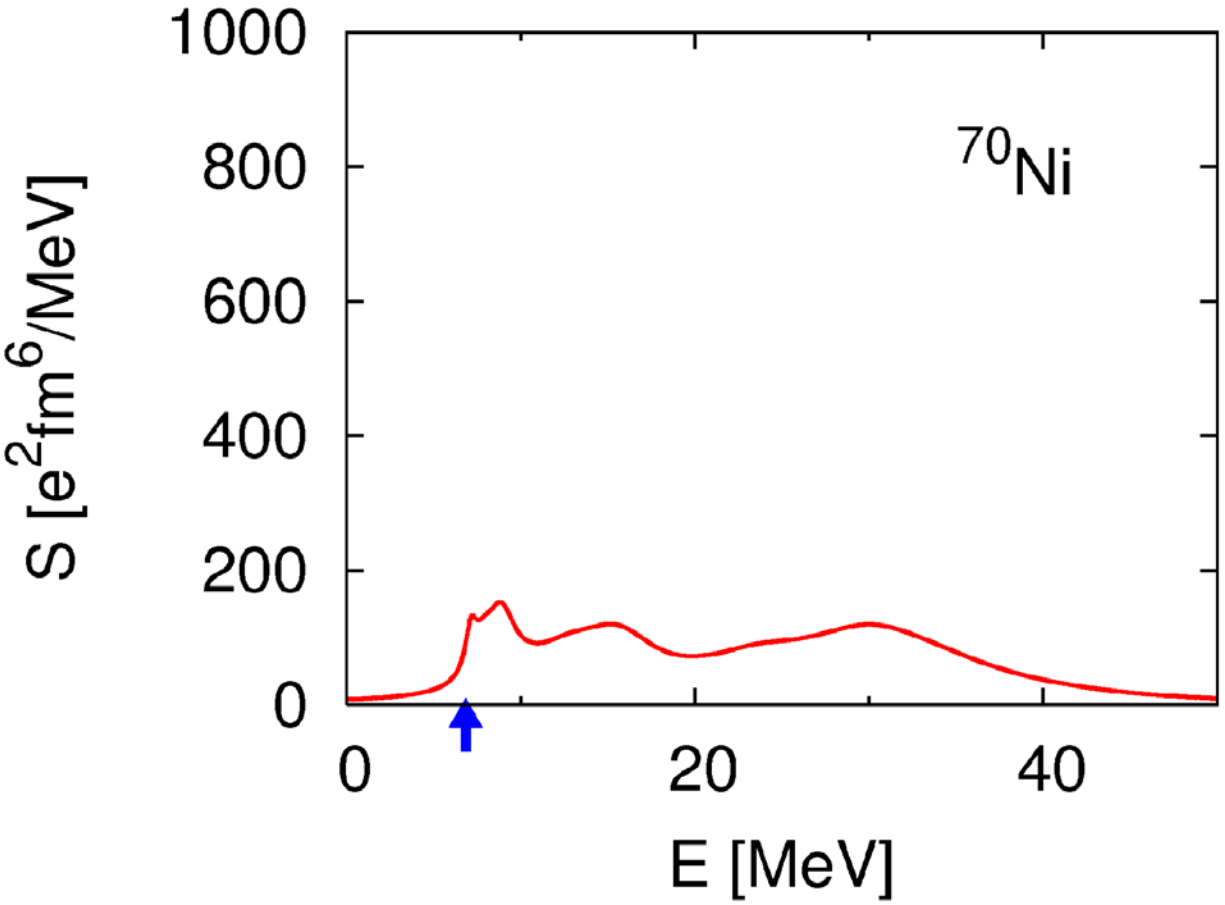
Isoscalar 1^- strength functions



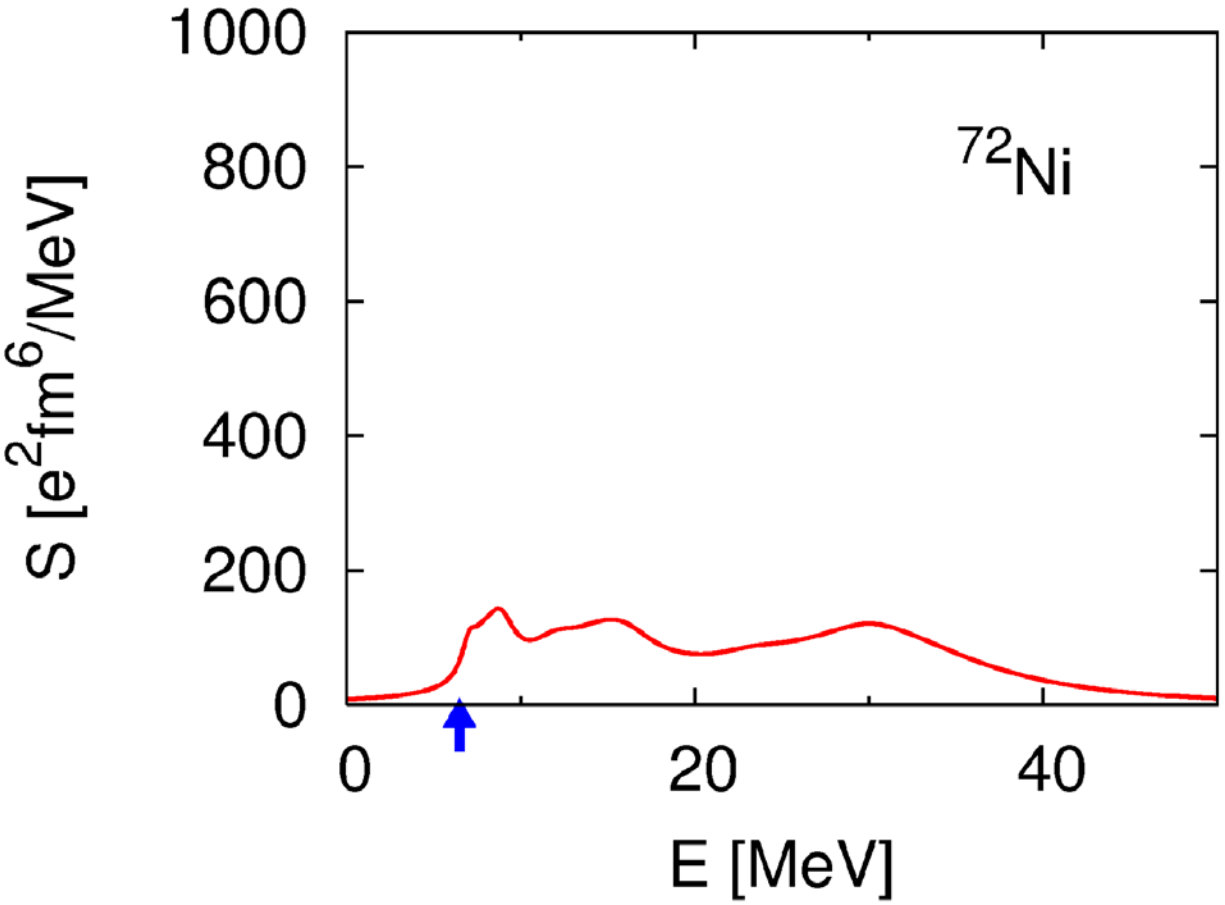
Isoscalar 1^- strength functions



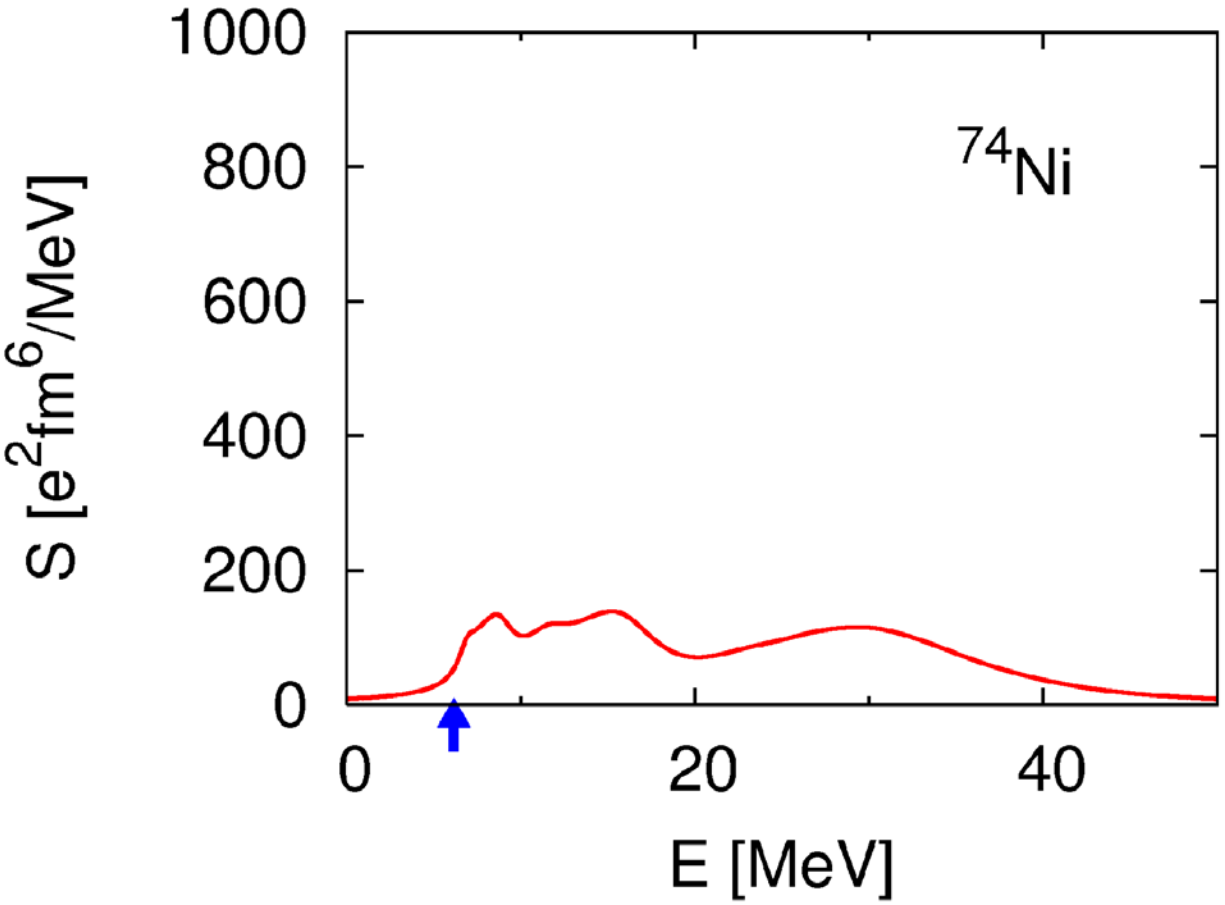
Isoscalar 1^- strength functions



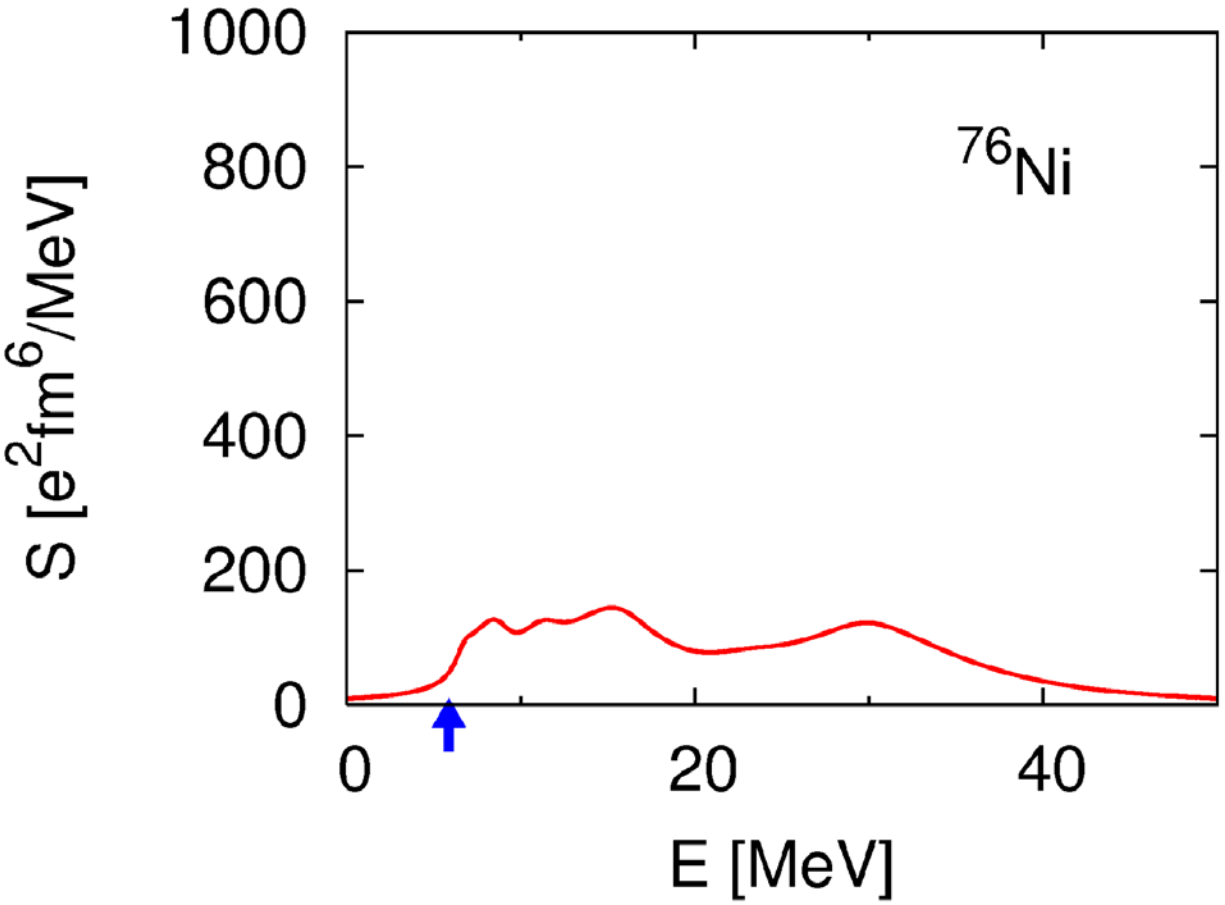
Isoscalar 1^- strength functions



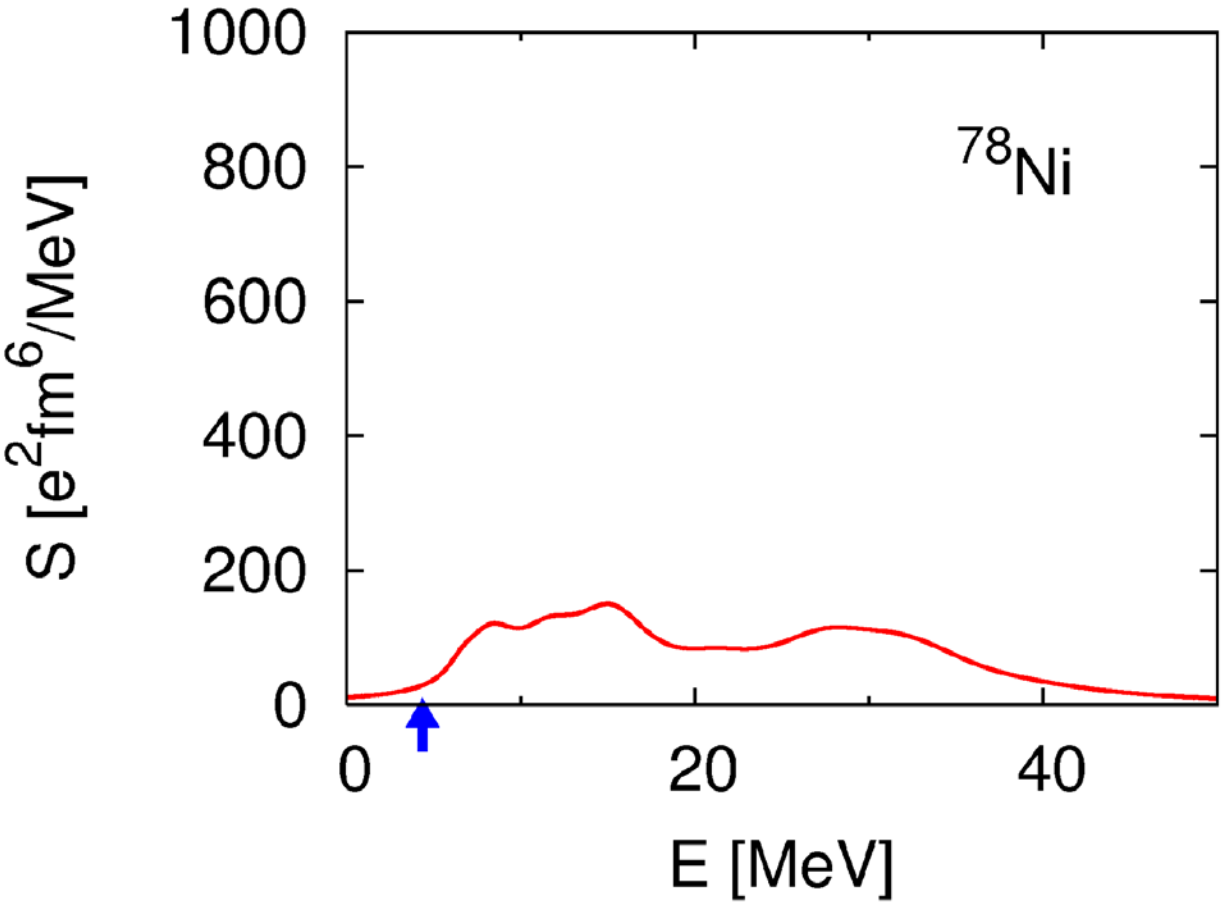
Isoscalar 1^- strength functions



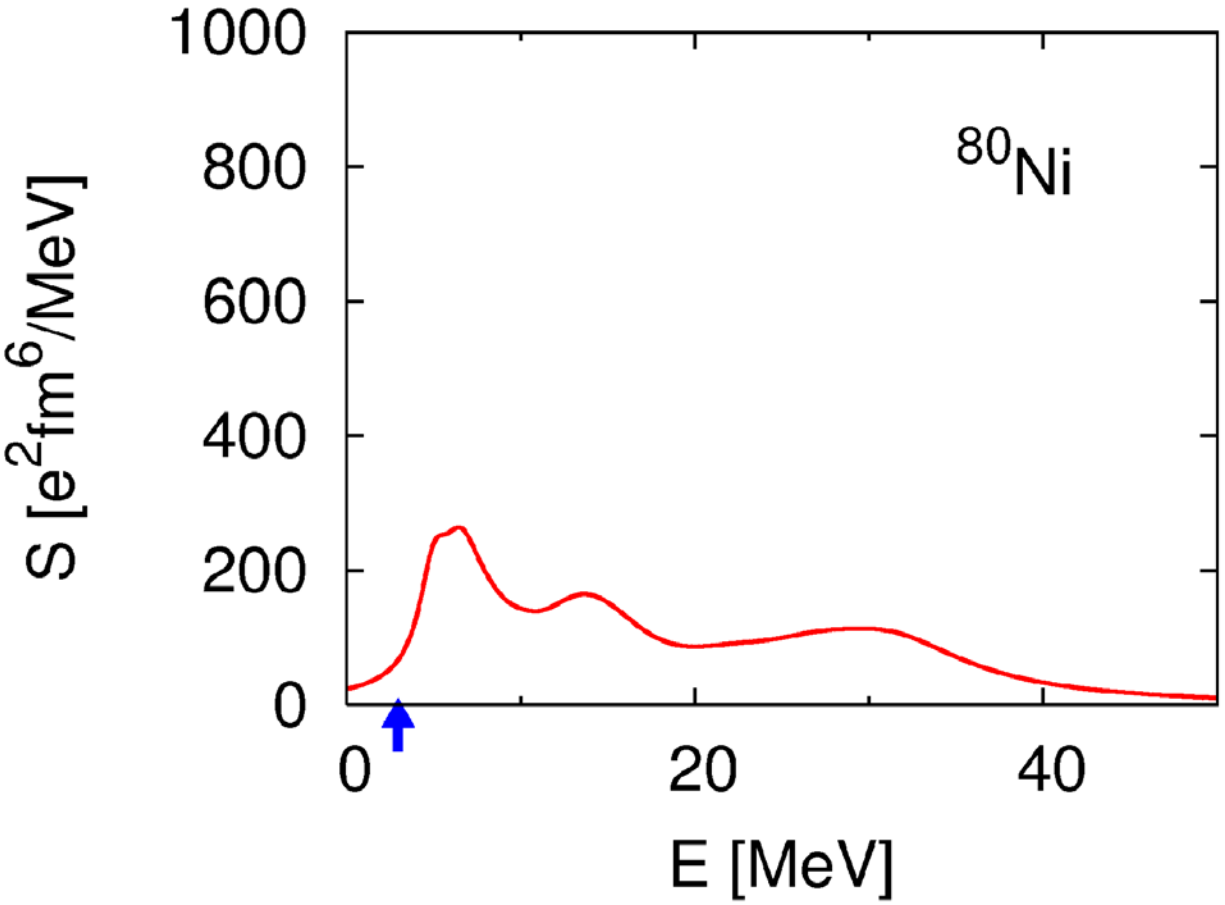
Isoscalar 1^- strength functions



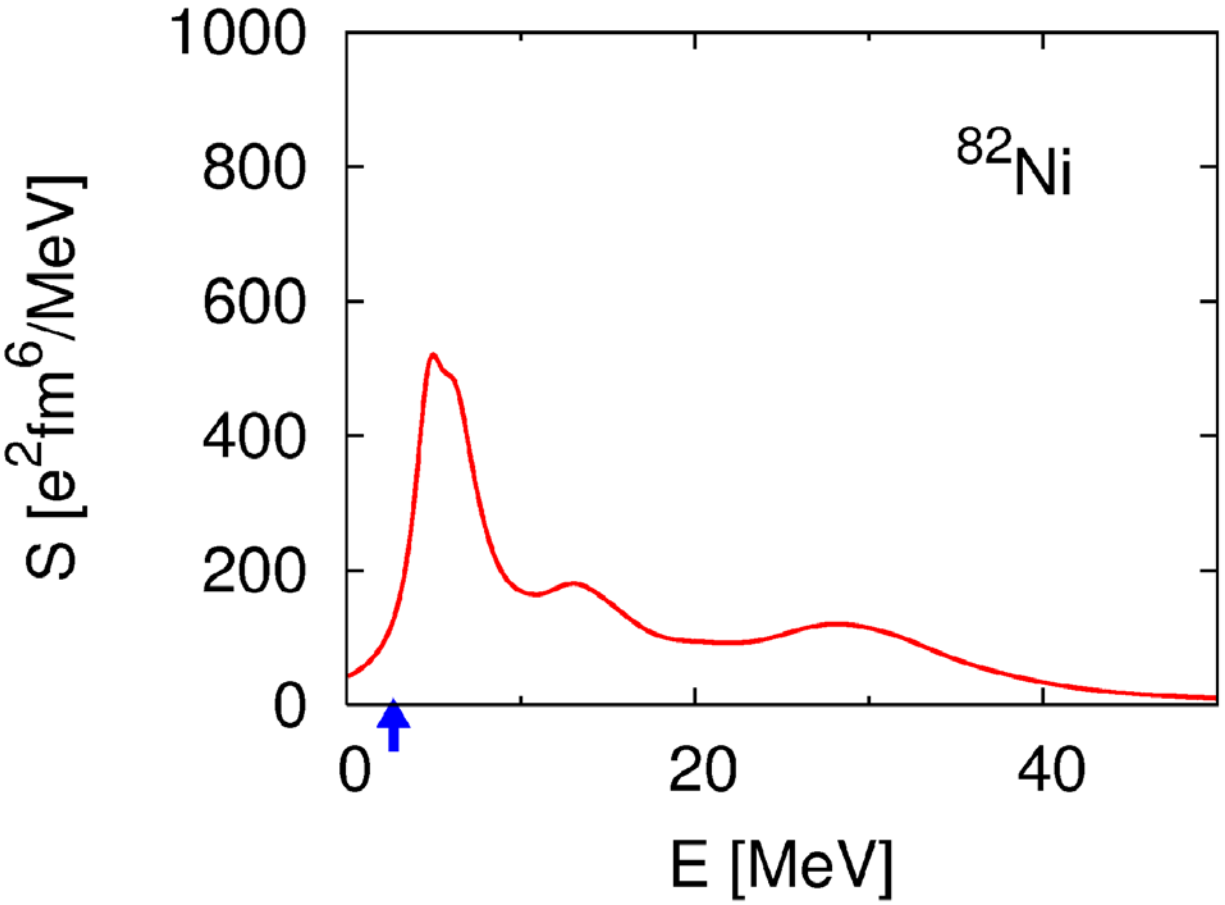
Isoscalar 1^- strength functions



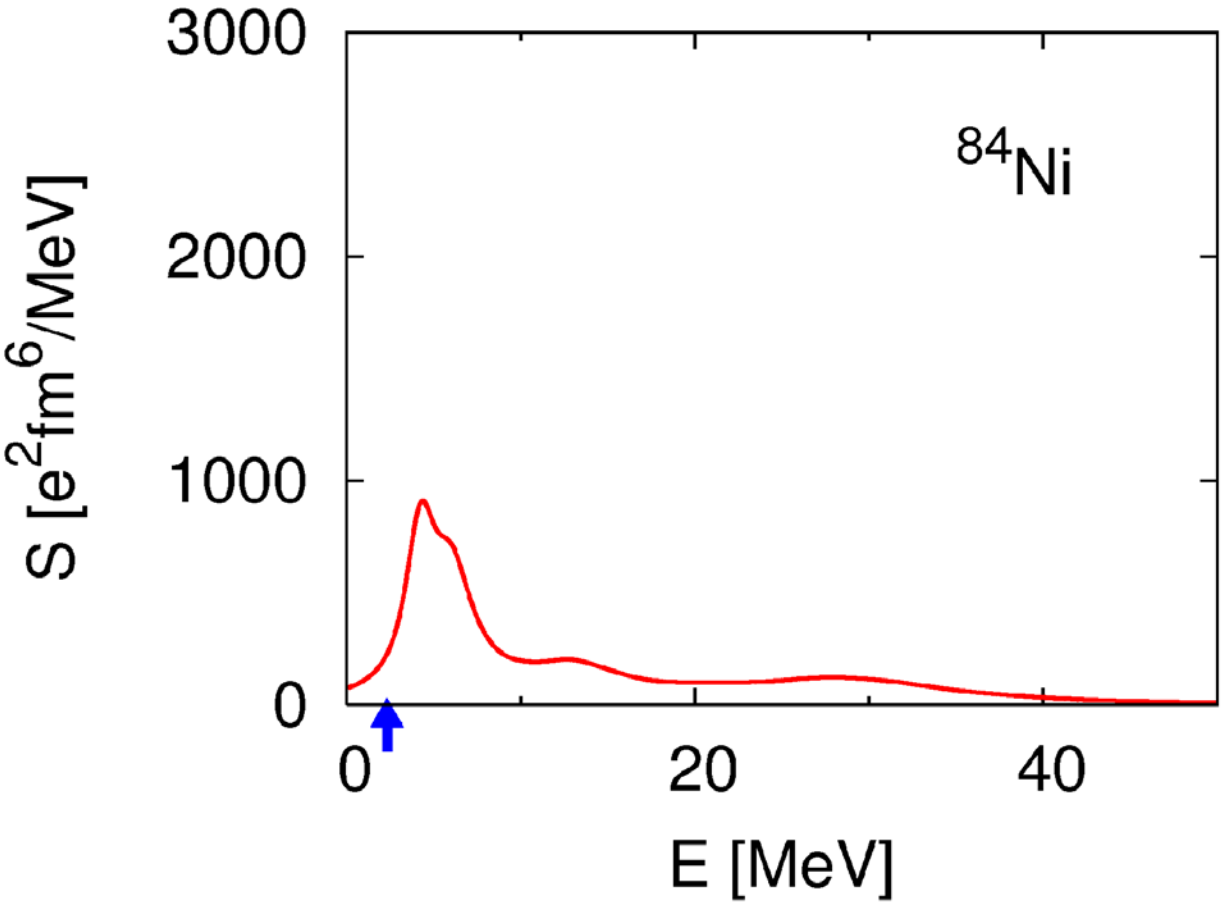
Isoscalar 1^- strength functions



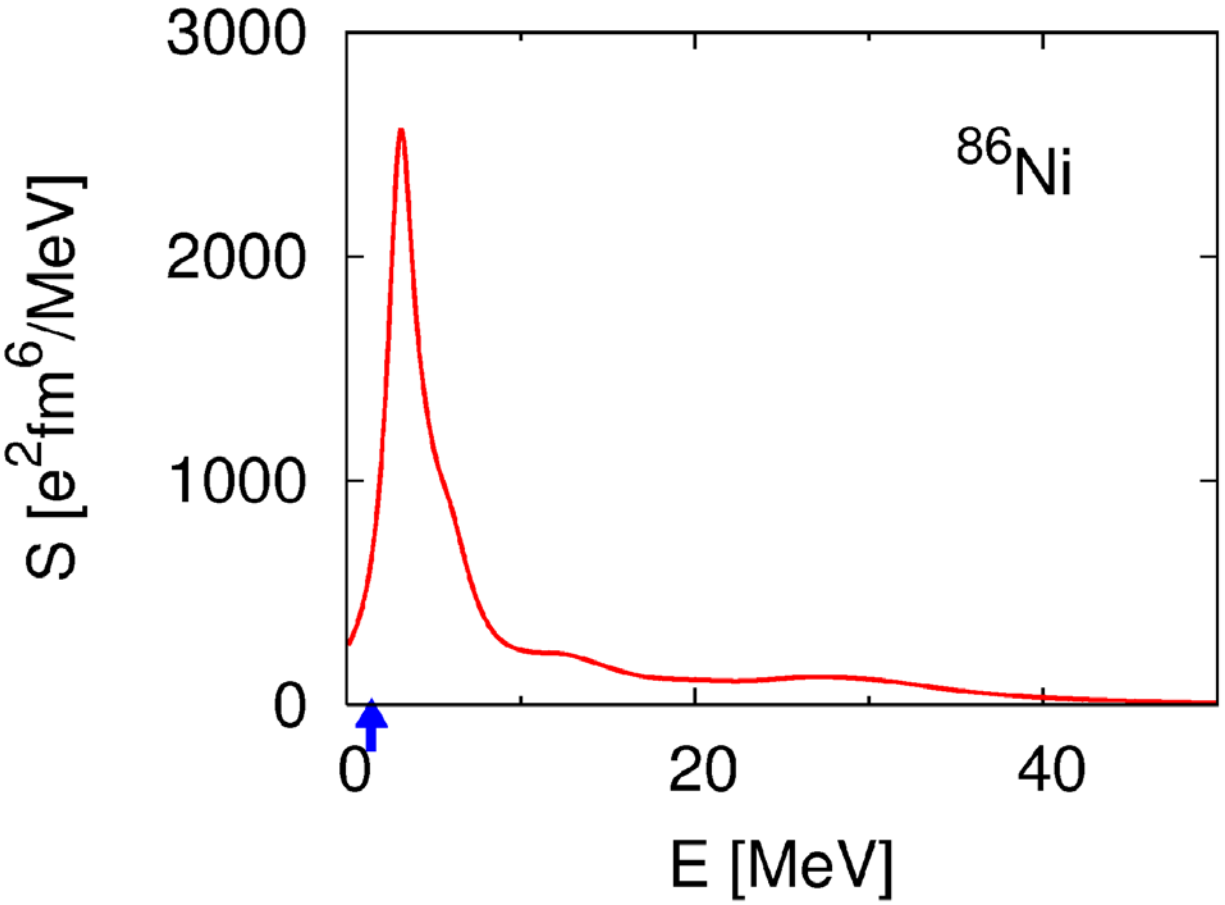
Isoscalar 1^- strength functions



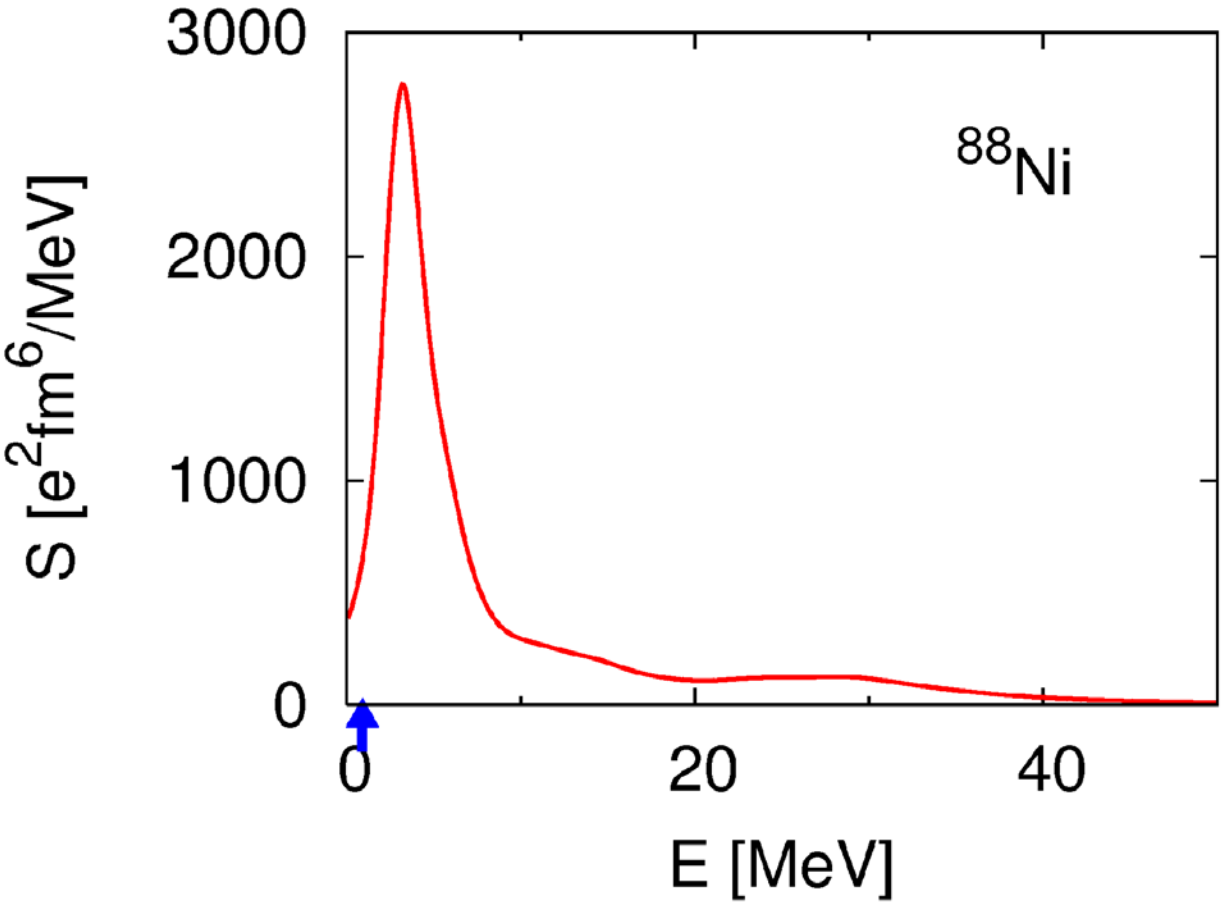
Isoscalar 1^- strength functions



Isoscalar 1^- strength functions



Isoscalar 1^- strength functions



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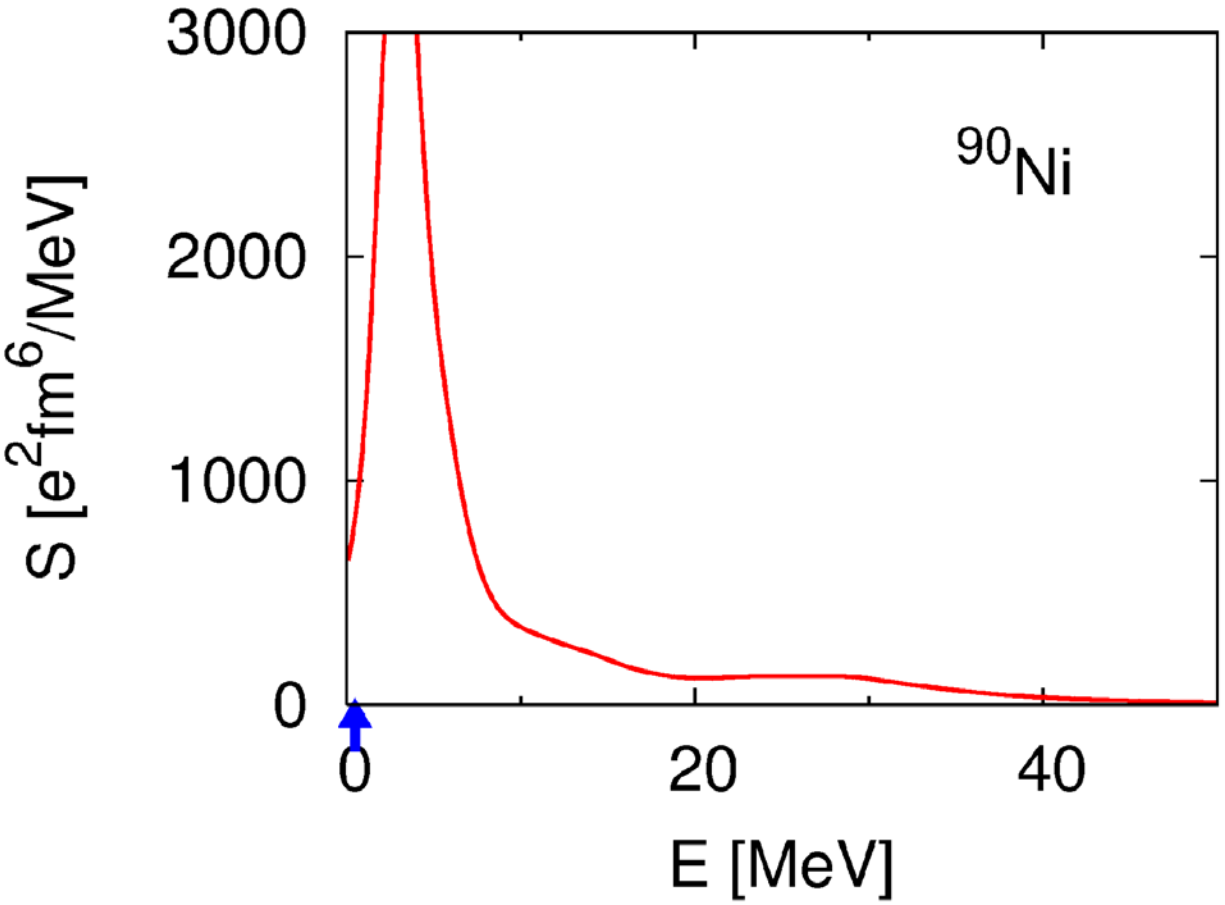
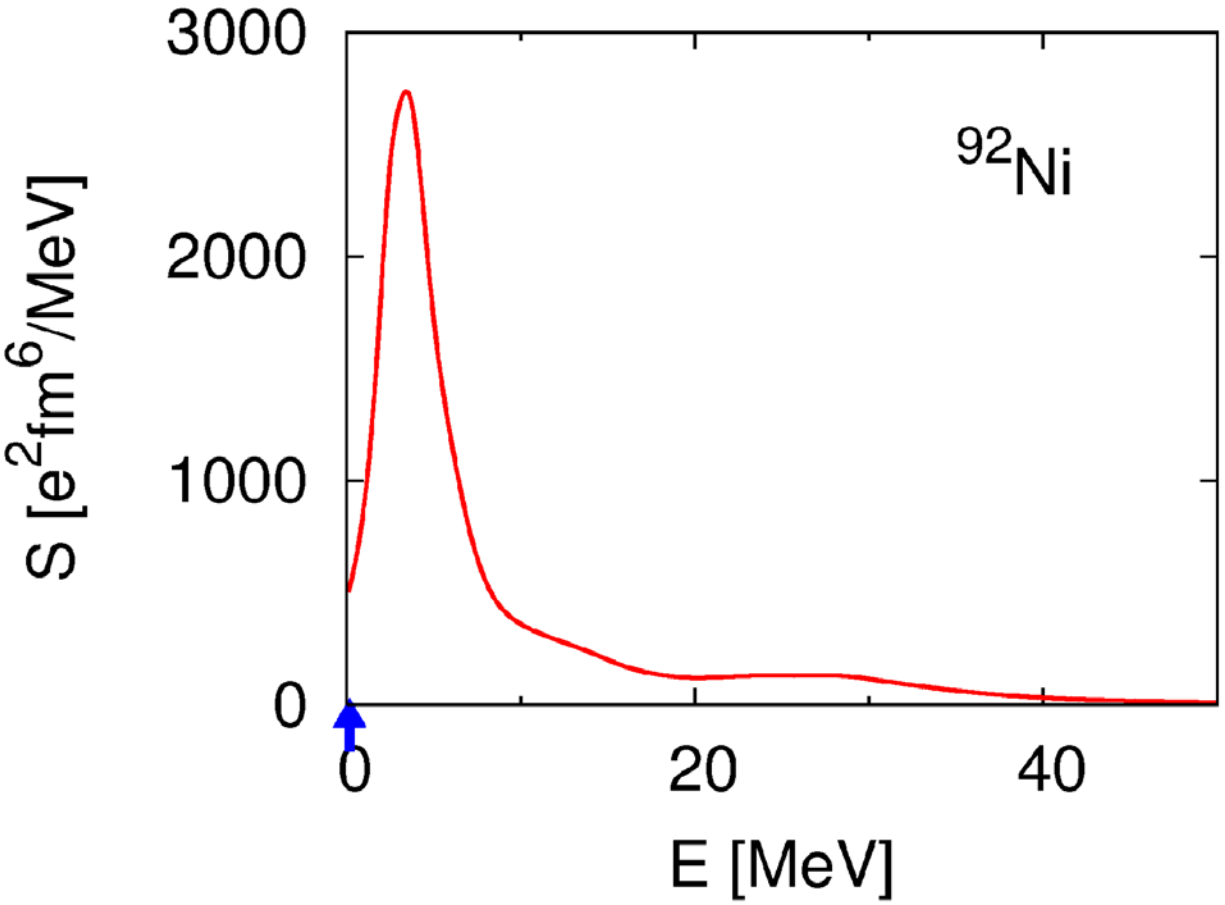
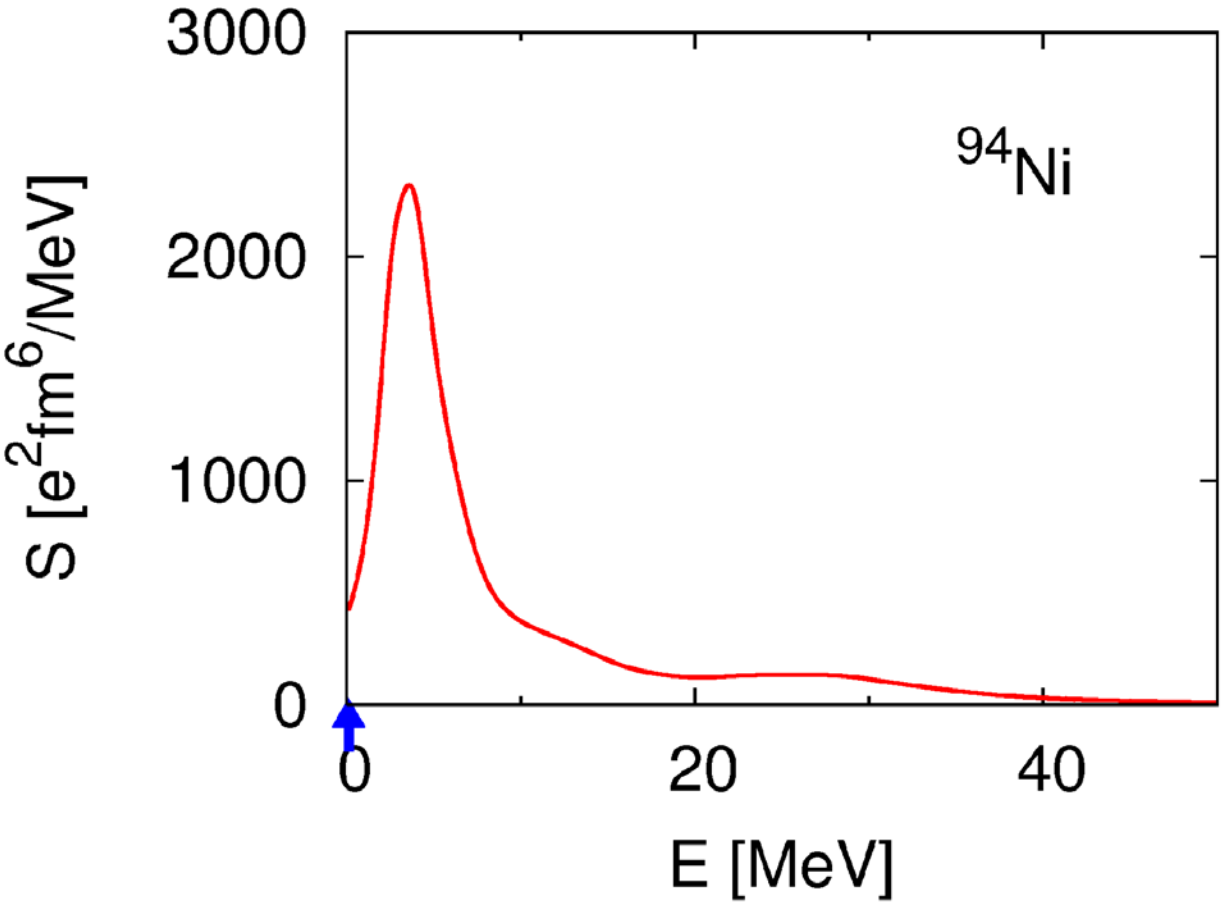


Isoscalar 1^- strength functions



Isoscalar 1^- strength functions



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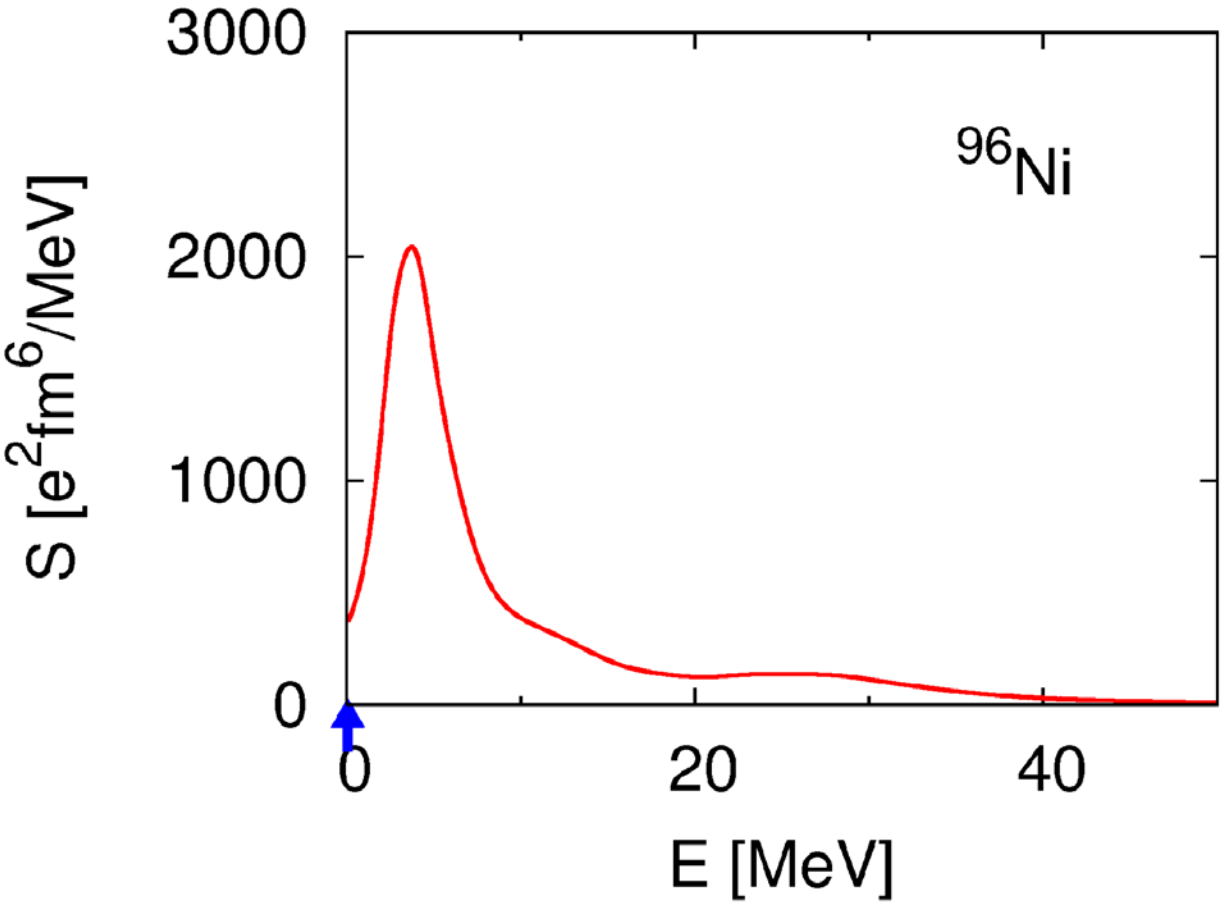
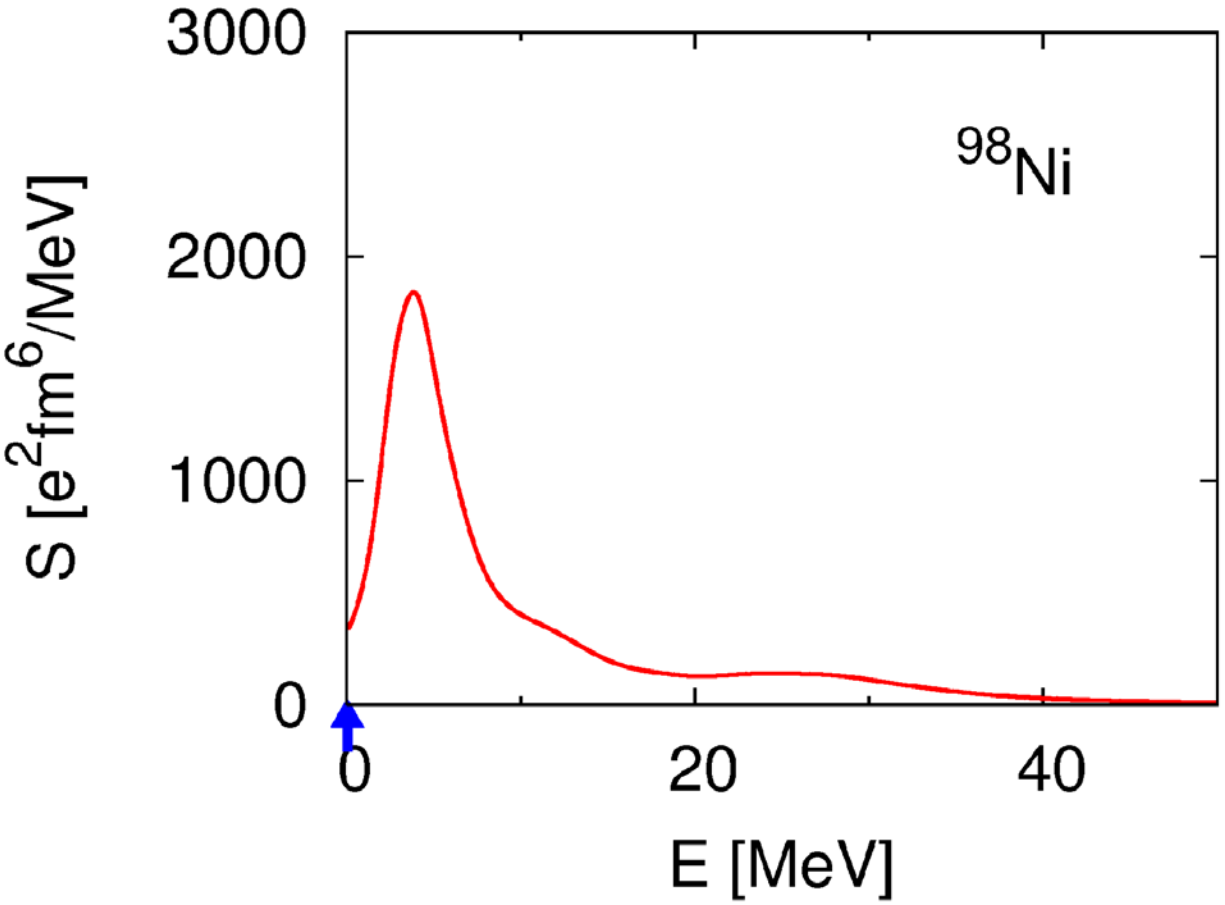
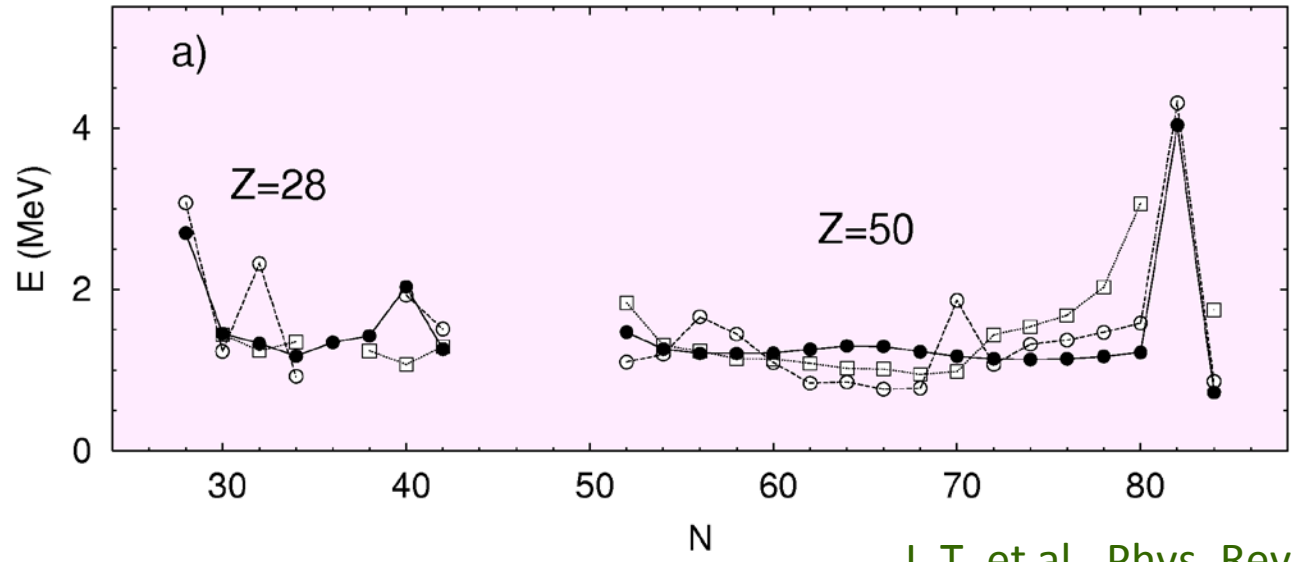
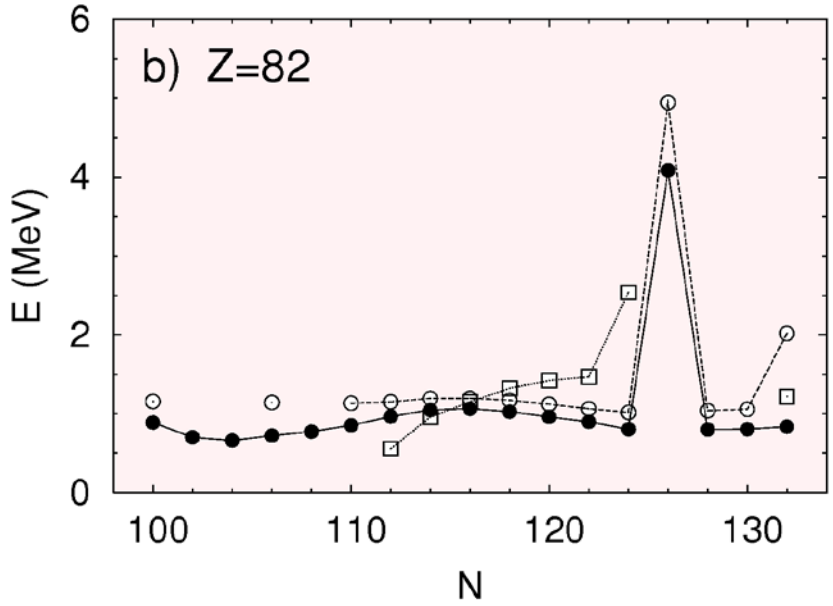


Isoscalar 1^- strength functions



Systematics of lowest 2+ states

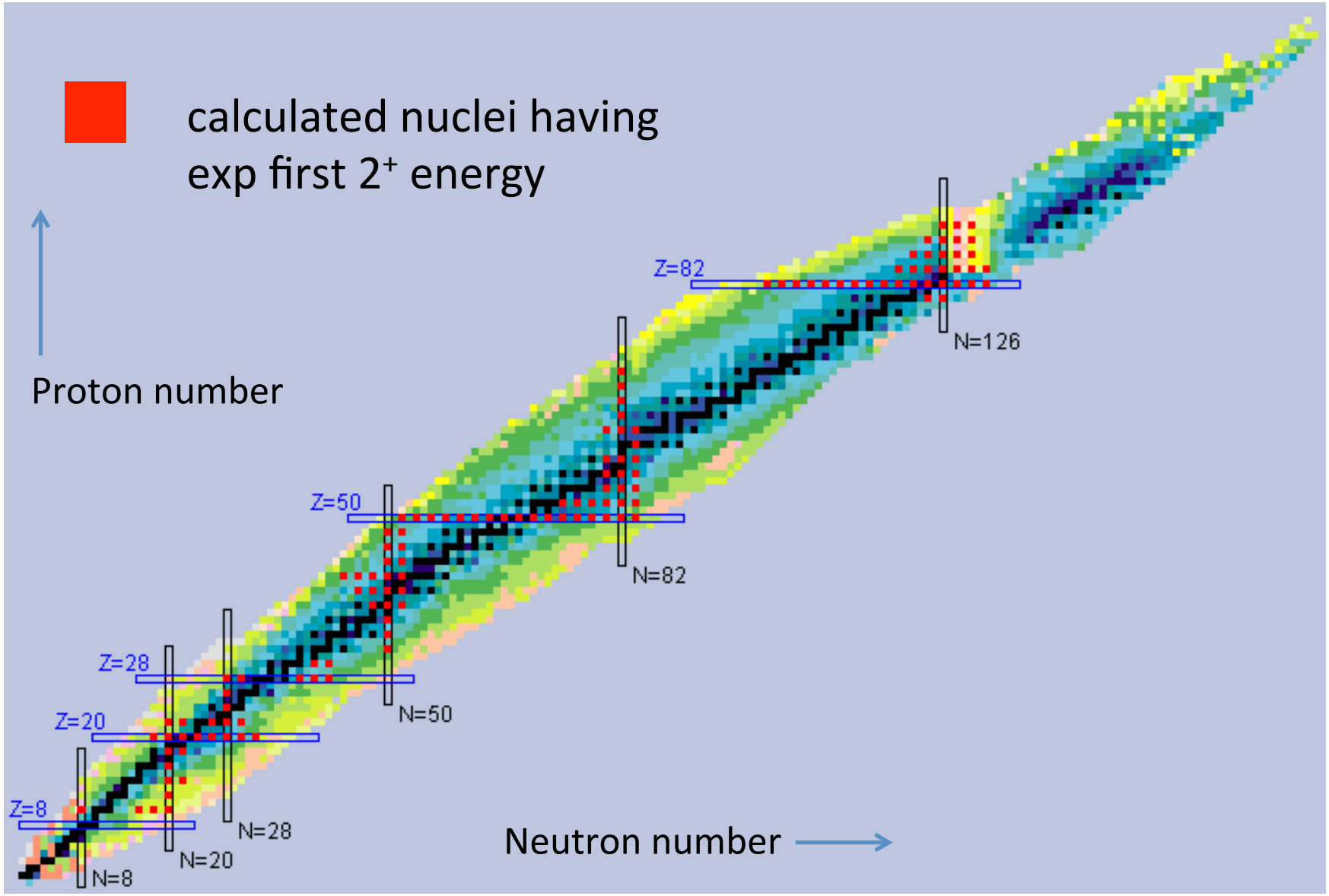




J. T. et al., Phys. Rev. C **78**, 044311 (2008)

- ● Exp.
- ○ QRPA(SkM*)
- □ GCM-5DCH(Gogny)

Exp:
S. Raman et al., At. Data Nucl. Data Tables **78**, 1 (2001).

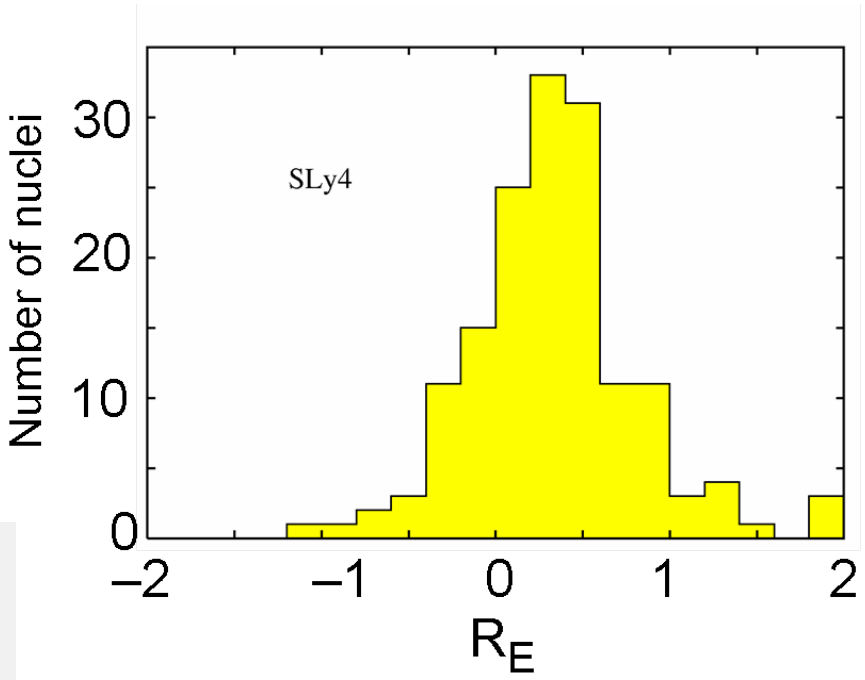


original figure: http://www.nndc.bnl.gov/chart/

Energy

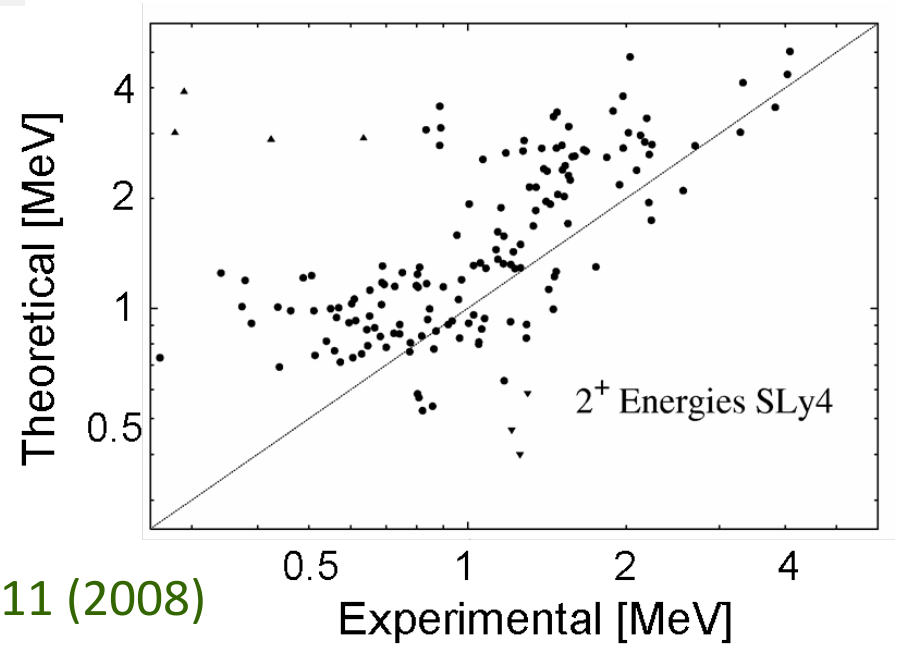
Histogram of

$$R_E = \ln \frac{E_{\text{cal}}}{E_{\text{exp}}}$$



ln1.1 = 0.095
ln2.0 = 0.693

Distribution of $(E_{\text{exp}}, E_{\text{cal}})$

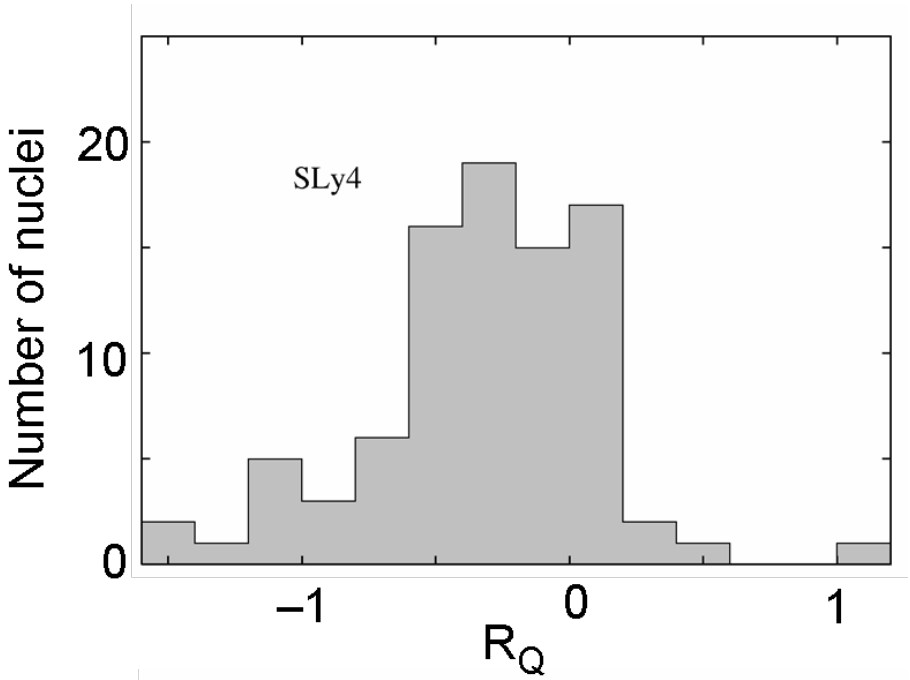


J. T. et al., Phys. Rev. C **78**, 044311 (2008)

Transition strength

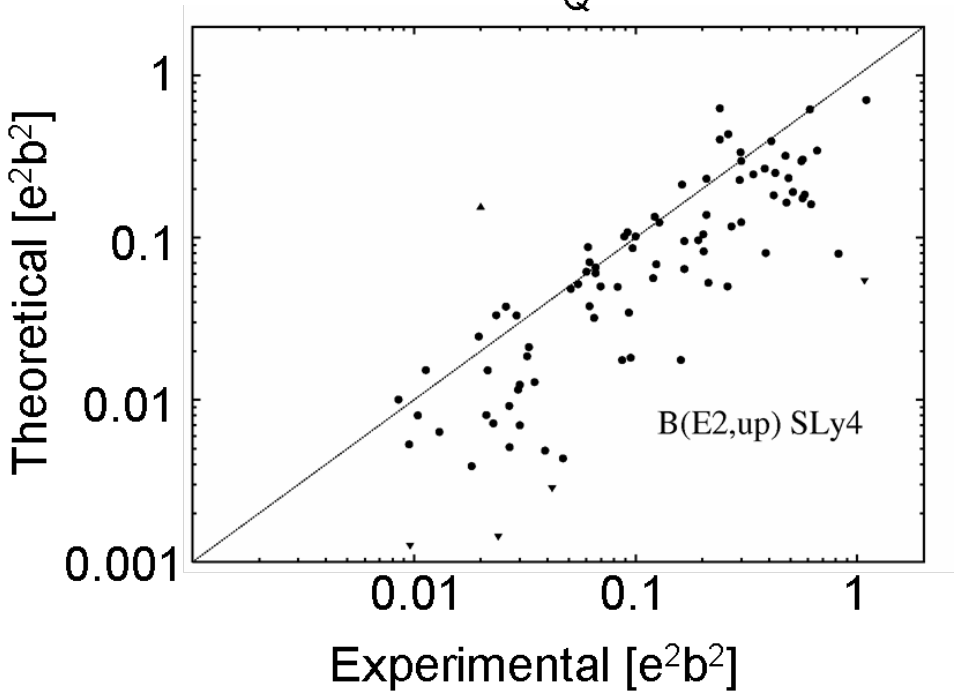
Histogram of

$$R_Q = \ln \sqrt{\frac{B(E2)\uparrow_{cal}}{B(E2)\uparrow_{exp}}}$$



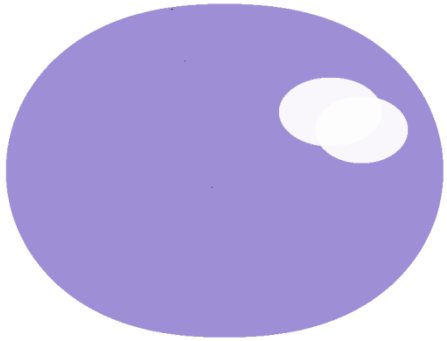
Distribution of

$(B(E2)\uparrow_{exp}, B(E2)\uparrow_{cal})$



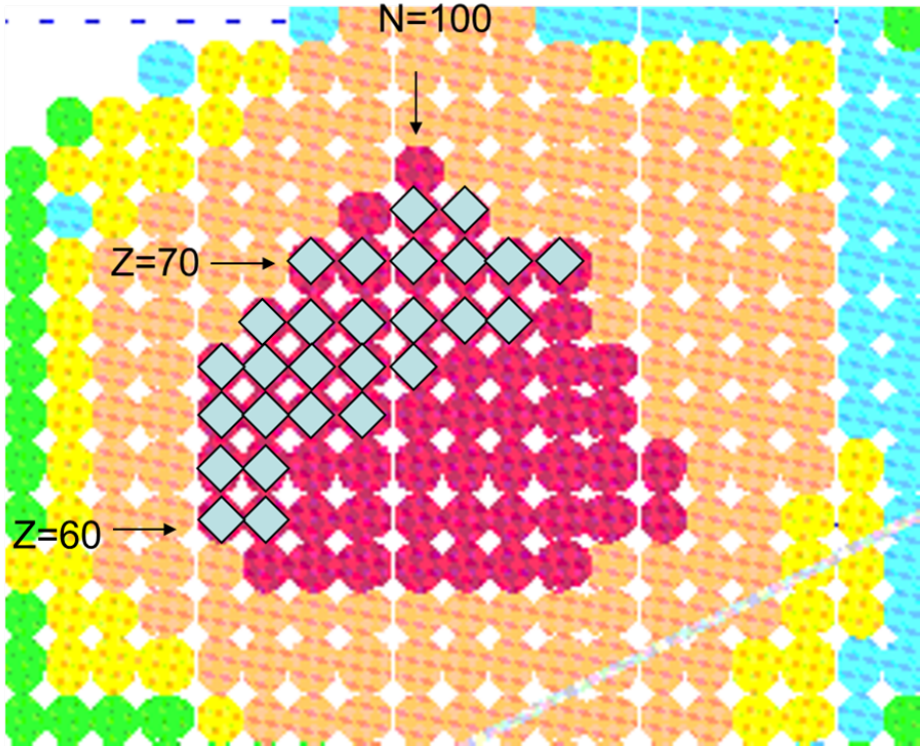
Deformed nuclei

Code breaking the rotational symmetry was developed.



Quadrupole deformation $\beta = 0.3$
Well deformed

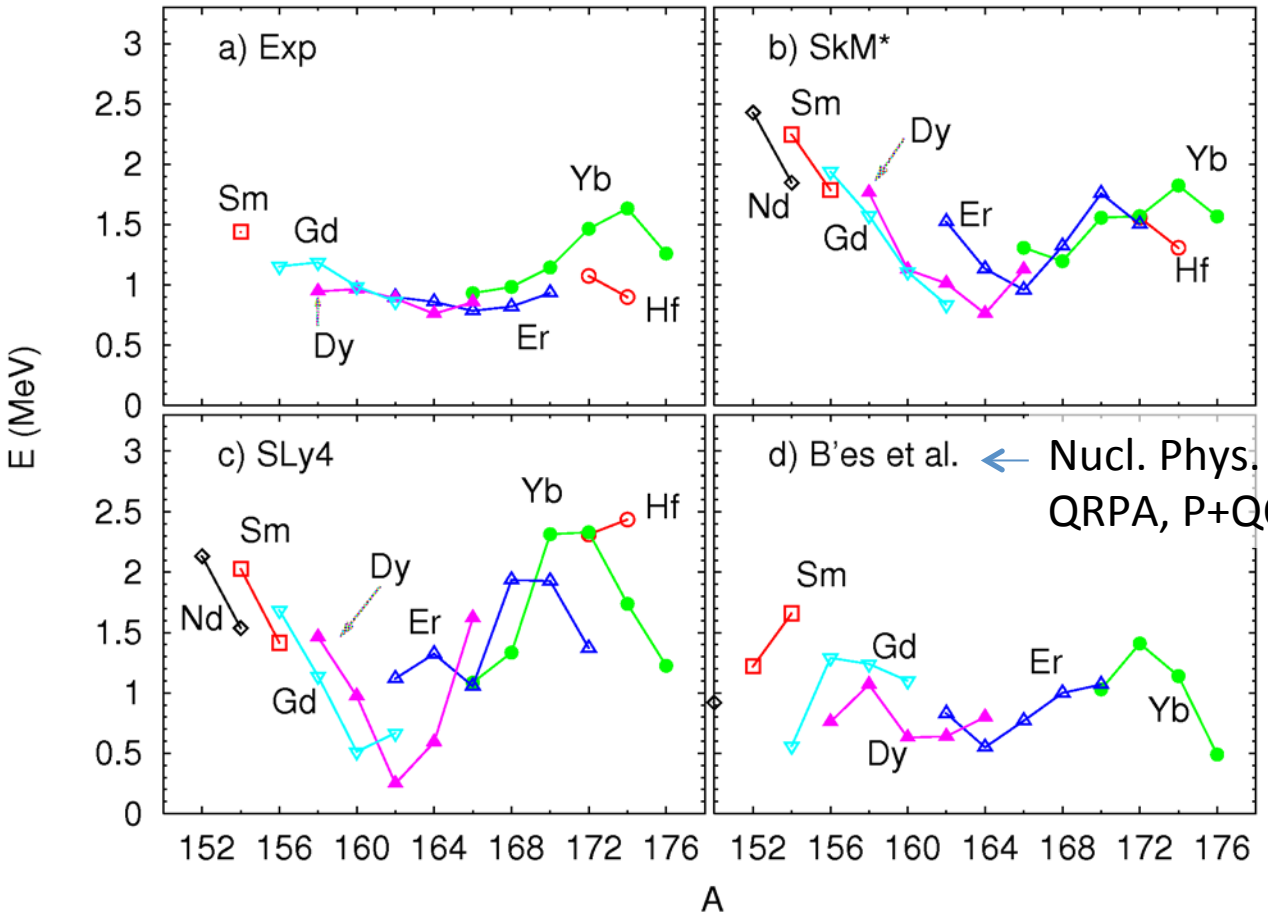
Deformed nuclei calculated



β > 0.3, (SkM*)

Gamma-vibrational states measured

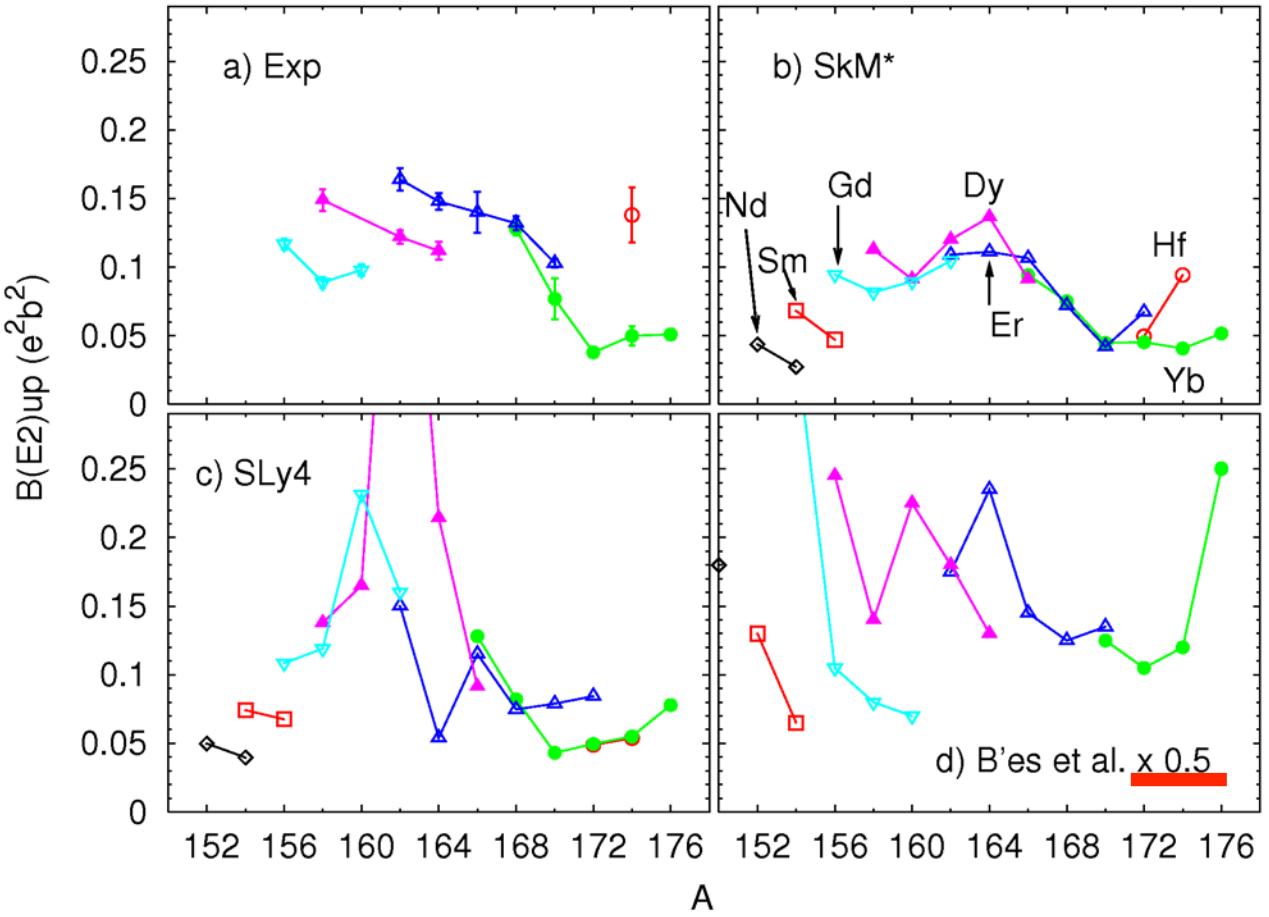
Energy of Gamma-vibrational states



← Nucl. Phys. **65**, 1(1965)
QRPA, P+QQ

J. T. and J. Engel, Phys. Rev. C **84**, 014332 (2011)

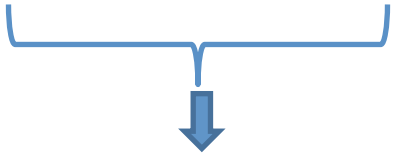
B(E2)↑ of Gamma-vibrational states



2. Computational matters

Eigen equation to obtain wave function expressed by B-splines (for the ground states).

$$\sum_j \hat{H}_0(r_i, r_j) w_j \psi(r_j) = E\psi(r_i)$$

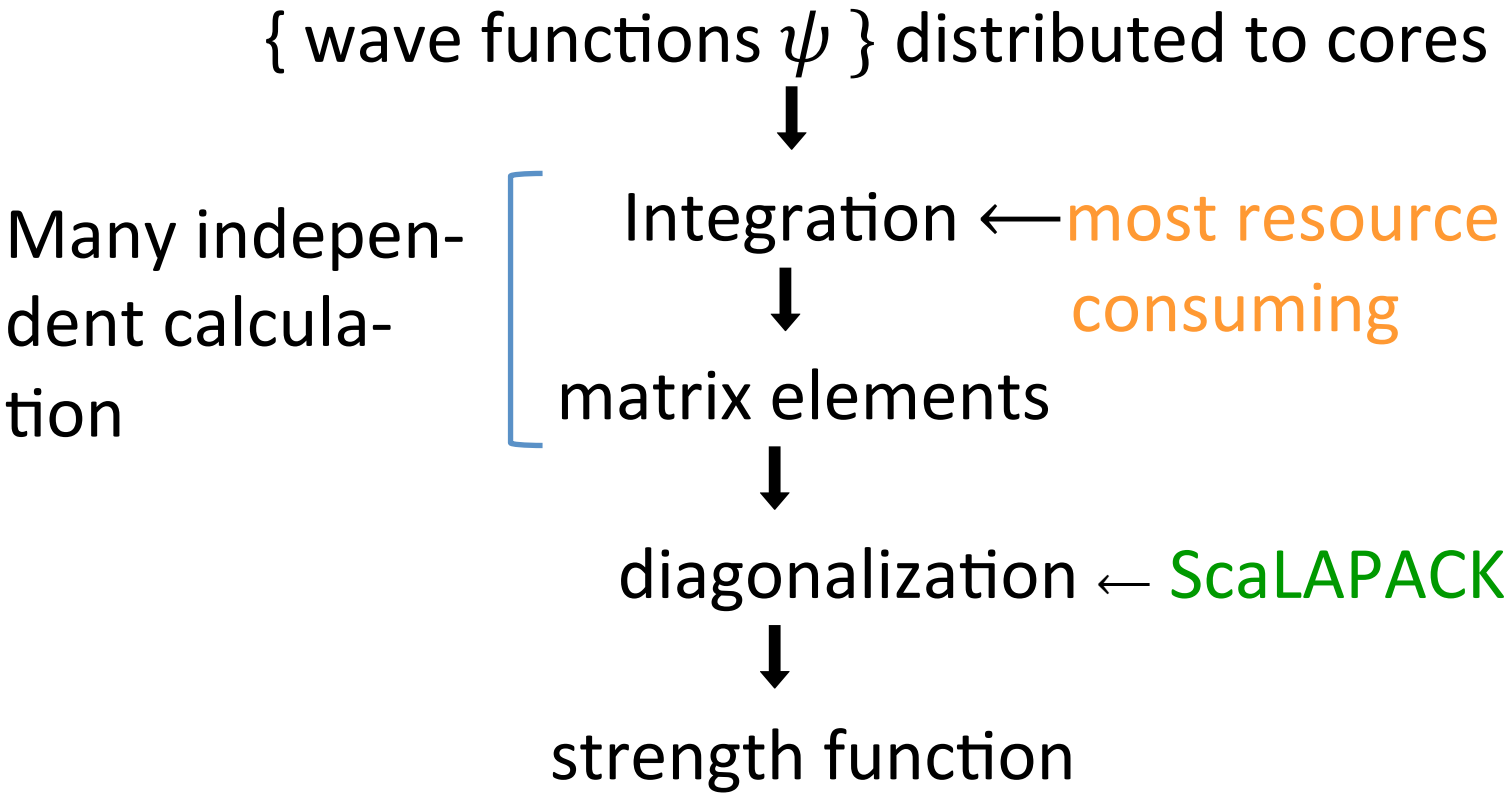


not Hermite. – no ScaLAPACK routine for this

A LAPACK subroutine is used for the diagonalization.

Hopefully, the parallel subroutine is constructed soon by HPCI strategic project.

Calculation of excited states



Efficiency of the calculation of the matrix elements

	#core	#matrix elements	Wall-clock time (h)	Core-sec/ mat. el.
A	20,000	7.8×10^{8}	1.5	0.14
B	80,000	3.5×10^{9}	2.0	0.16

Parallel efficiency of cal. B to cal. A
= core-hour of cal. A/ core-hour of cal.B adjusted
=1.12

Potential problems in the case of larger-scale calculations

- The same set of $\{\psi\}$ is copied to all cores.
  Partitioning of the set and storage of a subset by a core
  —not good

- Calculation time of the matrix elements is not uniform.
  ⟶ waiting time in some cores
  shuffling of the assignment of the matrix elements
  to core ⟶ extra time for calculation of the shuffling

Summary

- Strength functions have been shown of many nuclei. Comparison has been made between the experimental and theoretical values.
  Our aim : to develop reliable theoretical methods to describe more than hundreds of nuclei correctly for knowing the history of the universe.

- Parallelization is not so much complicated, but still there are a few thing I want to improve.