

# Shell Model applications to neutron capture studies

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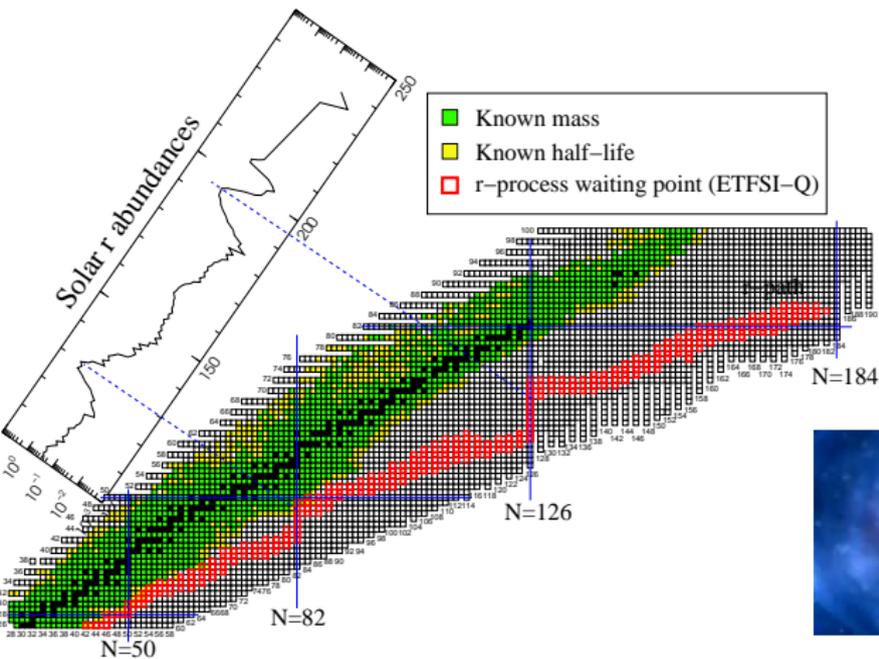
Institut Pluridisciplinaire Hubert Curien, Strasbourg



KTH, 23-25.05.2022

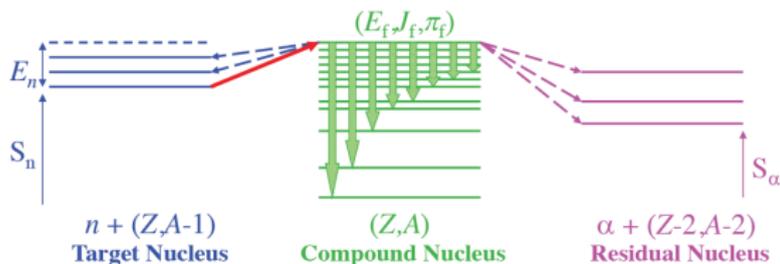
# R-process nucleosynthesis

- Nuclear models are needed to provide input for r-process simulations: masses, *level densities* ( $\rho$ ),  $\beta$  half-lives,  $\gamma$ -Strength Functions ( $f_{\chi L}$ ), fission barriers...



B. Metzger, G. Martinez-Pinedo et al., *Monthly Notices of the Royal Astronomical Society*. 406, 2650 (2010)

# Radiative neutron capture: resonant capture



$$\sigma_{(n,\gamma)}^{\mu\nu}(E_i, n) = \frac{\pi \hbar^2}{2M_{i,n} E_{i,n}} \frac{1}{(2J_i^\mu + 1)(2J_n + 1)} \sum_{J,\pi} (2J + 1) \frac{T_n^\mu T_\gamma^\nu}{T_n^\mu + T_\gamma^\nu}$$

for  $E_n \sim \text{keV}$   $T_n^\mu \gg T_\gamma^\nu \rightarrow \sigma^{\mu\nu} \sim T_\gamma^\nu$

$E_{i,n}, M_{i,n}$  - center-of-mass energy, reduced mass of the system

$J_n = 1/2$  - neutron spin

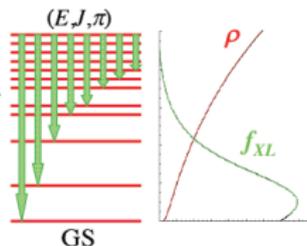
$T_n^\mu = T_n(E, J, \pi; E_i^\mu, J_i^\mu, \pi_i^\mu)$   $T_\gamma^\nu = T_\gamma(E, J, \pi; E_\gamma^\nu, J_\gamma^\nu, \pi_\gamma^\nu)$  - transmission coefficients

For a given multipolarity

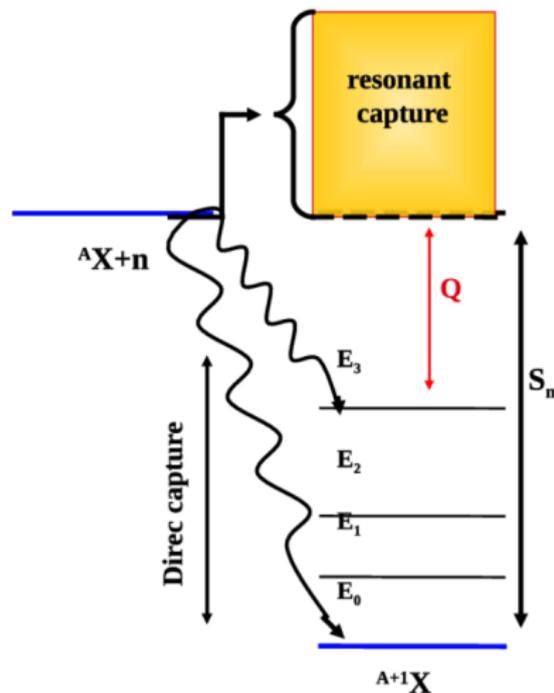
$$T_{XL}(E, J, \pi, E_\gamma^\nu, J_\gamma^\nu, \pi_\gamma^\nu) = 2\pi E_\gamma^{2L+1} f_{XL}(E, E_\gamma)$$

Test, using SM, the key ingredients of Hauser-Feshbach calculations:

- description of  $\gamma$  emission spectra
- Brink-Axel hypothesis



# Radiative neutron capture: direct capture



*Xi. Yu and S. Gorieli, Phys. Rev. C86 (2012) 045801*

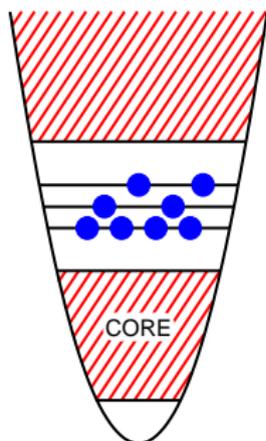
$$\sigma^{DC}(E) = \sum_{f=0}^x S_f \sigma_{dis}(E) + \langle S \rangle \int_{E_x}^{S_n} \sum_{J_f, \pi_f} \rho(E_f, J_f, \pi_f) \times \sigma_f^{cont} dE_f$$

If no experimental data available:

- use combinatorial model for the level density with  $\langle S \rangle = \text{const}$
- ☞ The key ingredients: low-energy levels and spectroscopic factors
- ☞ Validate theoretical approximations (HFB) in exotic nuclei using SM predictions

# Shell model: generalities

Shell model relies on the possibility of diagonalizing the Hamiltonian matrix and deriving (constraining empirically) a suitable effective interaction.

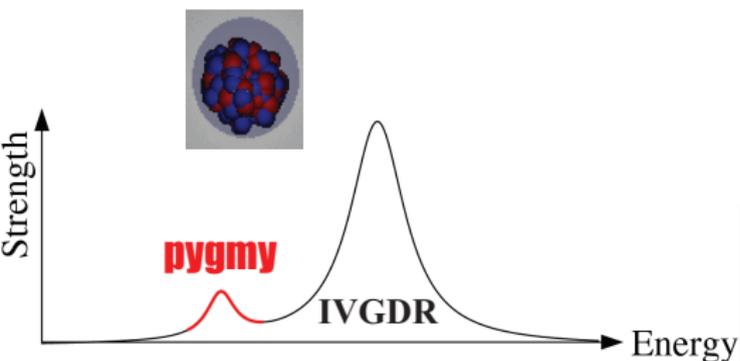


$$H_{eff}|\Psi_{eff}\rangle = E|\Psi_{eff}\rangle$$

- **Direct capture:** knowledge of the lowest-lying levels (energies and spectroscopic factors) → **quality of the effective Hamiltonian**
- **Resonant capture:** knowledge of statistical properties (energies and transitions in nuclear continuum) → **possibility of computing of hundreds of nuclear levels**

- Tests of the Brink-Axel hypothesis in the PDR region
- Upbend of decay  $\gamma$ -strengths : origin, global trends, consequences for global models
- Shell-model benchmarks of global models for direct neutron capture calculations
- Influence on neutron-capture rates and consequences for astrophysics

# Pygmy-dipole resonance



- the pygmy part impacts astrophysical reaction rates and resulting abundances in the r-process

*S. Goriely, E. Khan and M. Samyn, Nucl. Phys. A739 (2004) 331*

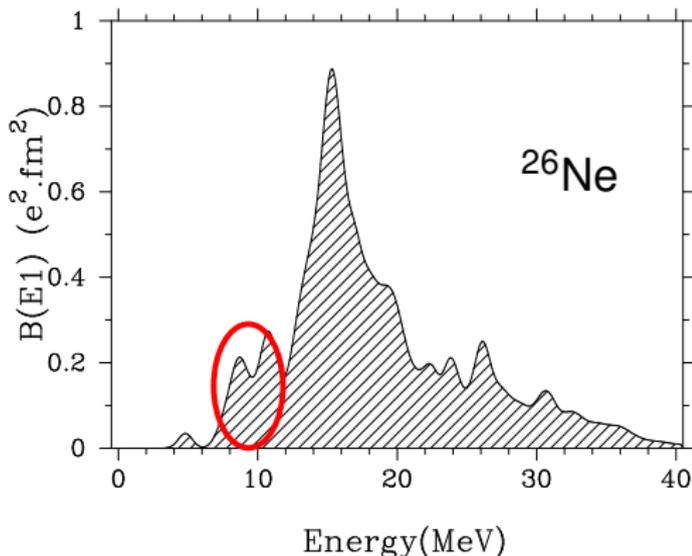
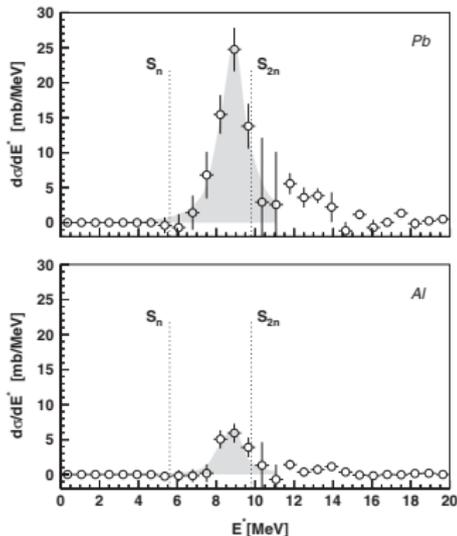
*E. Litvinova et al., Nucl. Phys. A823 (2009) 26*

- in stellar environments finite temperatures => reactions on excited states => Brink-Axel hypothesis becomes crucial
  - SM: only weak violation for E1 sum rules with initial energy *C. Johnson, Phys. Lett. 750 (2015) 72*
  - TCQRPA: different shapes of photoabsorption strength functions with increasing temperature *E. Litvinova and N. Belov, Phys. Rev. C88 (2013) 031302*
  - Phonon-dumping model: violation of BA with temperature *N.Q. Hung, N.D. Dang, L.T.Q. Huong, Phys. Rev. Lett 118 (2017) 022502*

# Motivation: E1 excitations in nuclei

EXP:  $\sum B(E1)=0.49 \pm 0.16 \text{ e}^2\text{fm}^2$  (6-10MeV)  
5% of TRK sum rule

THEO:  $\sum B(E1)=0.485 \text{ e}^2\text{fm}^2$  (0-10MeV)



*J. Gibelin et al., Phys. Rev. Lett. 101 (2008) 212503*

Low peaks structure:  $\nu s_{1/2}^{-1} p_{3/2}^1$ ,  $\nu s_{1/2}^{-1} p_{1/2}^1$

SM: Complex wave functions

(major contributions  $\leq 30\%$ )

QRPA main contribution: 70% of  $\nu s_{1/2}^{-1} p_{3/2}^1$

SM from Strasbourg (unpublished)

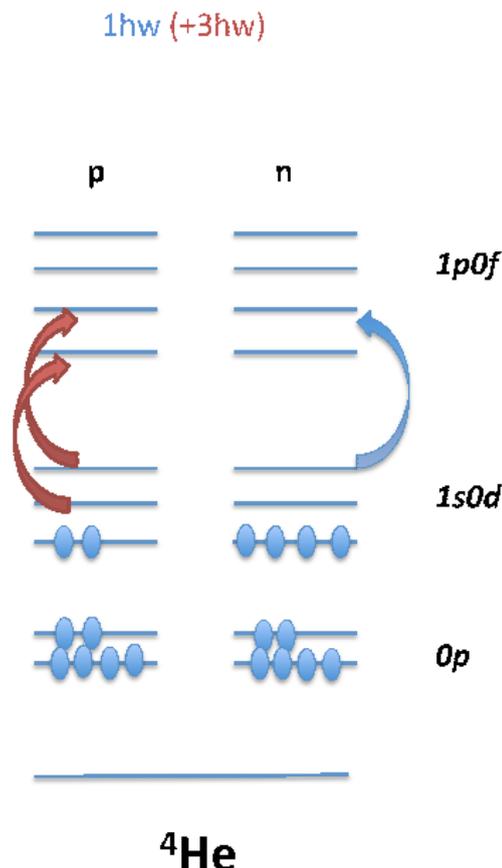
QRPA study *M. Martini, S. Péru, and M. Dupuis, Phys. Rev. C 83, 034309 (2011)*

Evolution of photoabsorption strength with energy (spin)

# E1 calculations in psdpf space

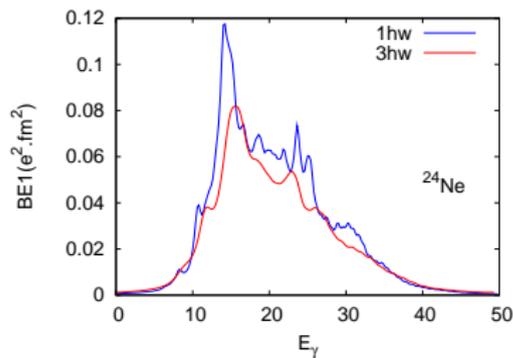
$$Q_{\mu}^{\lambda=1} = \frac{Z}{A} e \sum_{k=1}^N r_k Y_{1\mu}(r_k) - \frac{N}{A} e \sum_{k=1}^Z r_k Y_{1\mu}(r_k)$$

- full *sd* diagonalization + full  $1\hbar\omega (+3\hbar\omega)$  excitations
- Exact removal of COM components
- Interaction: PSDPF  
*M. Bouhelal, F. Haas, E. Caurier, F. Nowacki and A. Bouldjedri, Nucl. Phys. A864 (2011) 113.*
- 500 Lanczos iterations to get distributions
- Lorentzian smoothing with  $\Gamma/2 = 500\text{keV}$

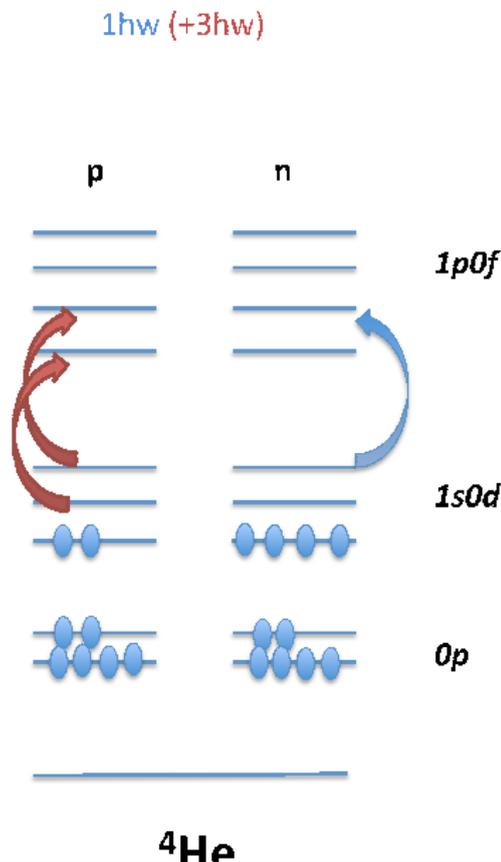


# E1 calculations in psdpf space

- $1\hbar\omega$  calculations  
 $0\hbar\omega$  for positive parity states  
 $1\hbar\omega$  for negative parity states
- $3\hbar\omega$  calculations  
 $0 + 2\hbar\omega$  for positive parity states  
 $1 + 3\hbar\omega$  for negative parity states

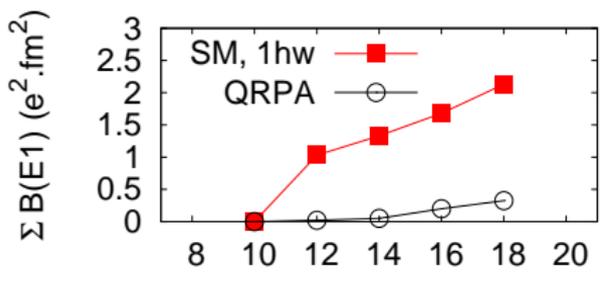
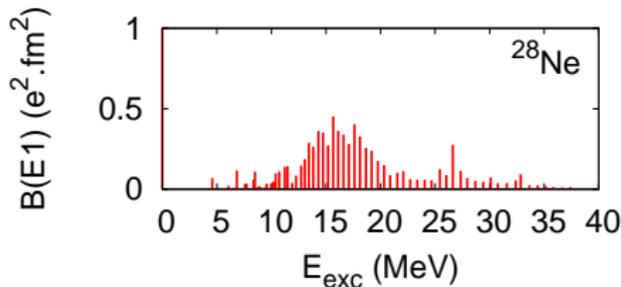
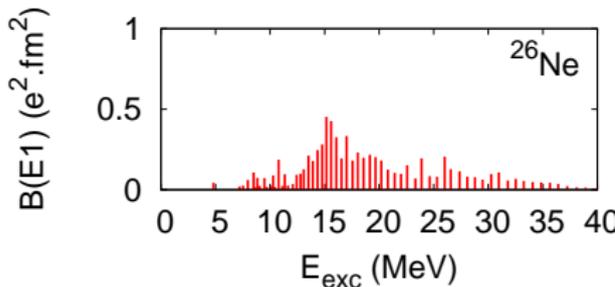
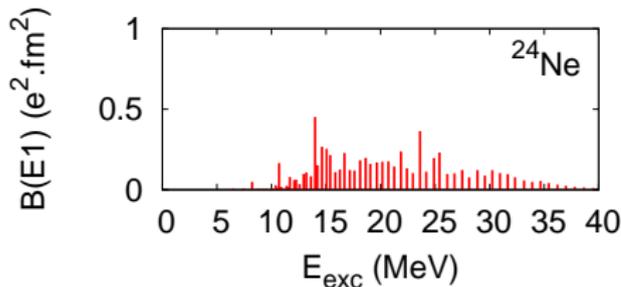
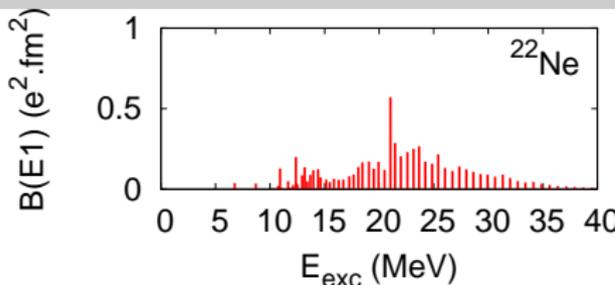
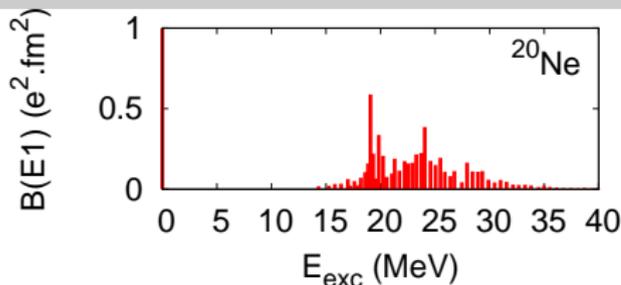


$1\hbar\omega$ : sufficient for low-energy strength  
 $3\hbar\omega$ : correlations suppress  $E1$  strength

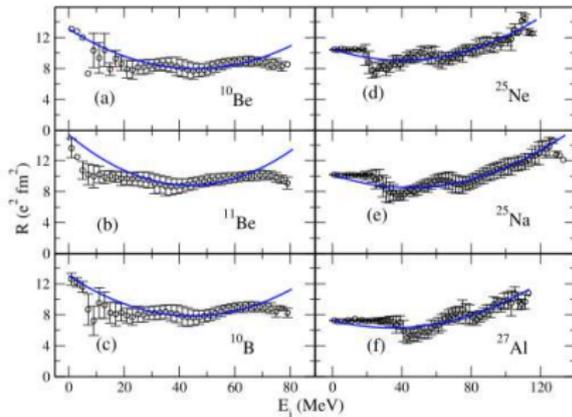
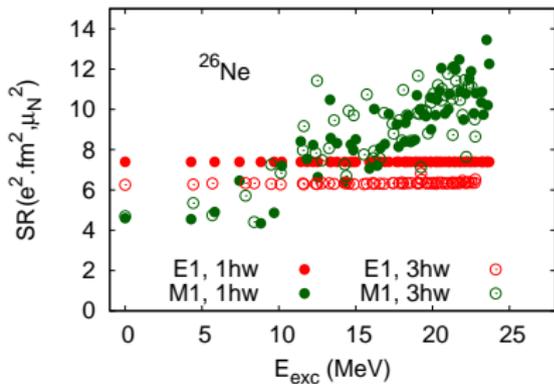
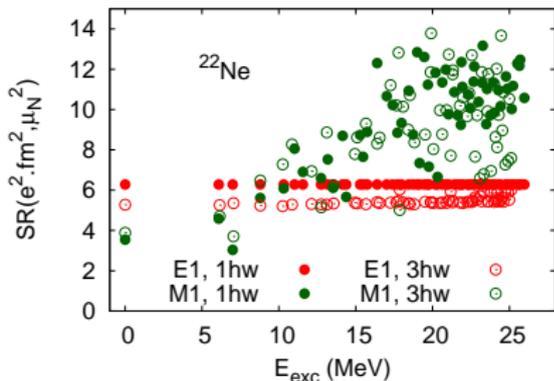


$^4\text{He}$

# E1 strength in even neon isotopes



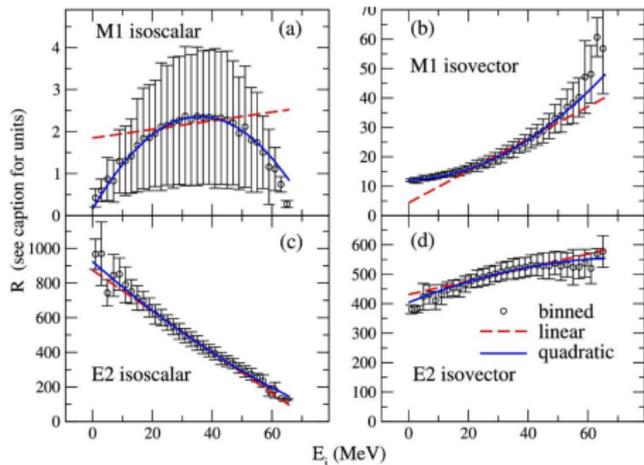
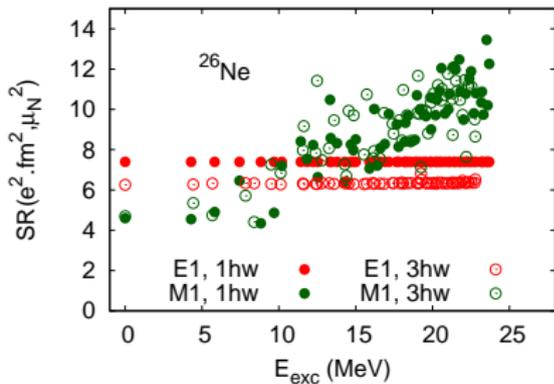
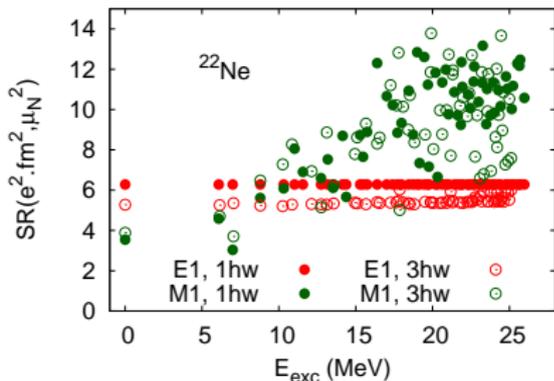
# E1 and M1 sum rules dependence on initial state



*C. Johnson, Phys. Lett. 750 (2015) 72*

- $3\hbar\omega$  correlations reduce  $E1$  sum rule up to 15%
- $E1$  sum rule stays constant within energy/spin range
- good agreement with previous SM studies

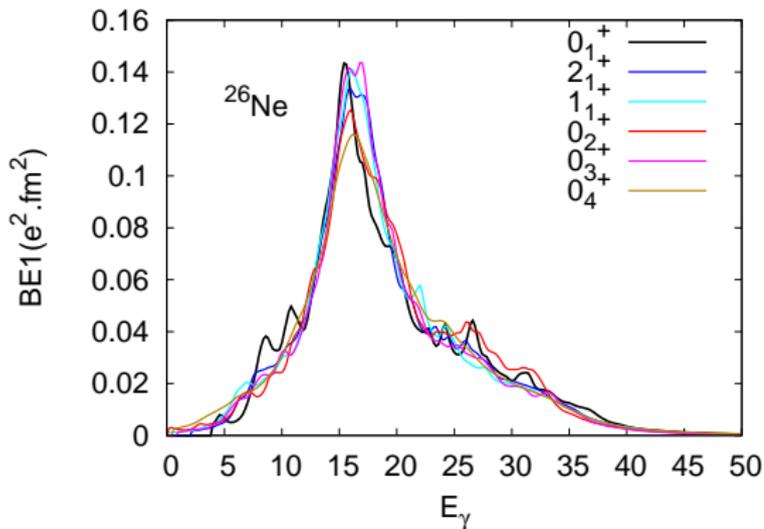
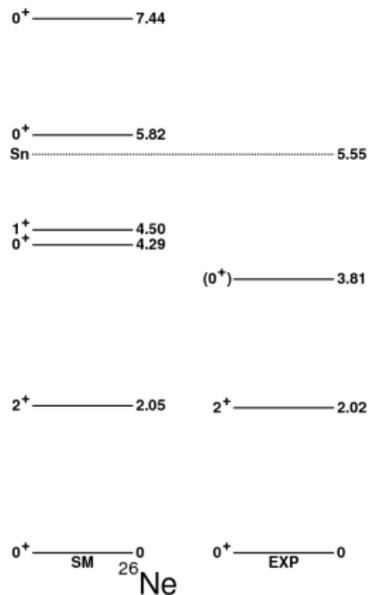
# E1 and M1 sum rules dependence on initial state



*C. Johnson, Phys. Lett. 750 (2015) 72*

- no distinct trend with correlations
- M1 sum rules vary with energy/spin range
- good agreement with previous SM studies

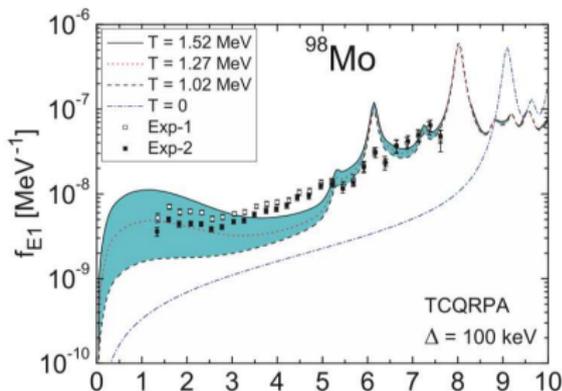
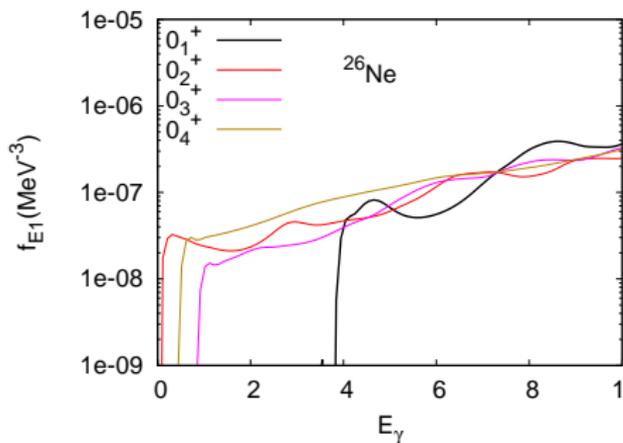
# E1 strength functions on excited states



SM predicts 135 levels below 10MeV of both parities (13 levels below  $S_n$ )

- Similar strength distributions leading to similar total SR values
- BA-hypothesis holds for  $E1$  resonances

# E1 strength functions on excited states

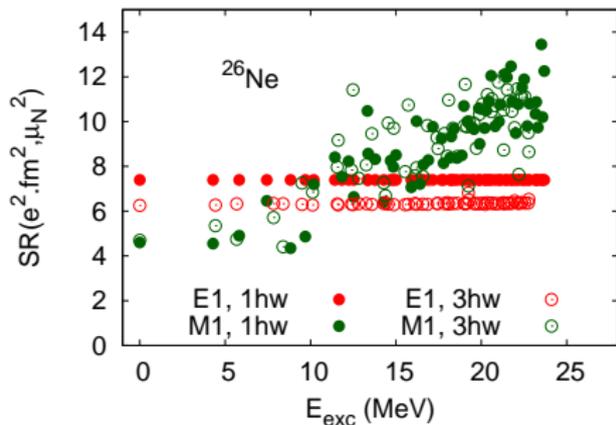
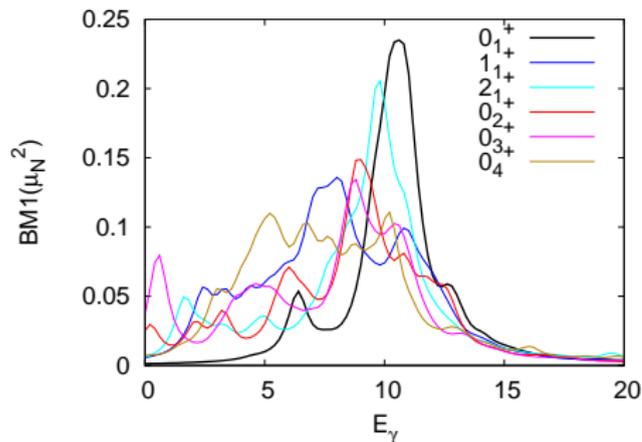


*E. Litvinova and N. Belov, Phys. Rev. C88 (2013) 031302*

$J^{\pi}$	E (MeV)	EWSR (0-10MeV)
$0^+$	0.0	3.96
$0^+$	4.29	3.06
$0^+$	5.82	3.35
$0^+$	7.44	3.31

- Different behavior at low energy in SM and TCQRPA
- Benchmark of many-body theories needed
- Larger deviations for g.s. strength function

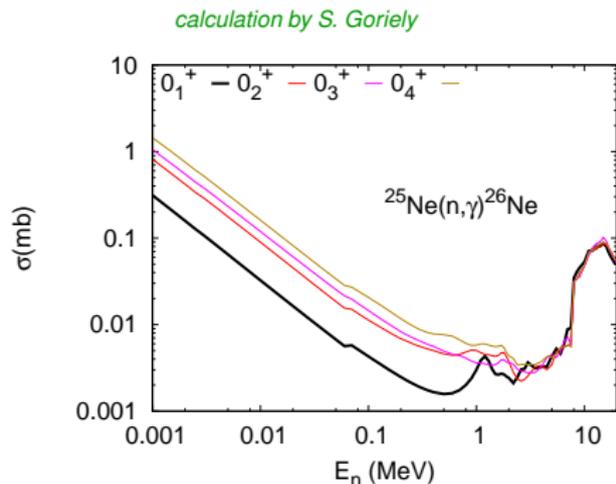
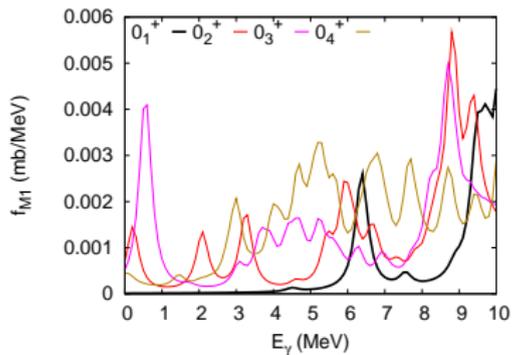
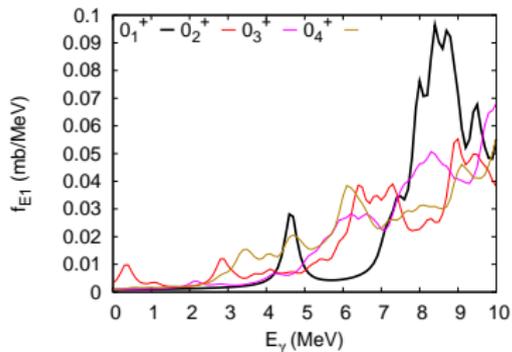
# M1 strength functions on excited states



$J^\pi$	E (MeV)	EWSR (0-10MeV)
$0^+$	0.0	8.90
$0^+$	4.29	8.91
$0^+$	5.82	20.73
$0^+$	7.44	19.38

- Deviations from BA-hypothesis for  $M1$  photoabsorption strength functions
- Impact on neutron capture?

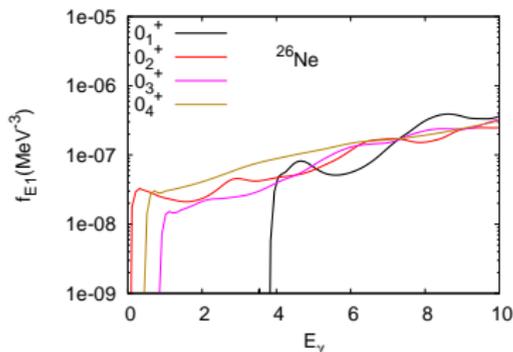
# Impact on neutron capture



- factor 5 difference between cross sections
- M1 impact minor
- similar cross sections for  $E_n \geq 1$  MeV

# Photoabsorption vs $\gamma$ -decay

photoabsorption (PSF)



- Lanczos Strength Function method with a large number of iterations
- folded with a Lorentzian of  $\Gamma/2$  width

## SM studies of M1 upbend:

*R. Schwengner et al., PRL111 (2013) 232504*

*B.A. Brown and A.C. Larsen, PRL113 (2014) 252502*

*K. Sieja, Eur. Phys. J. Web of Conf.146 (2017) 05004*

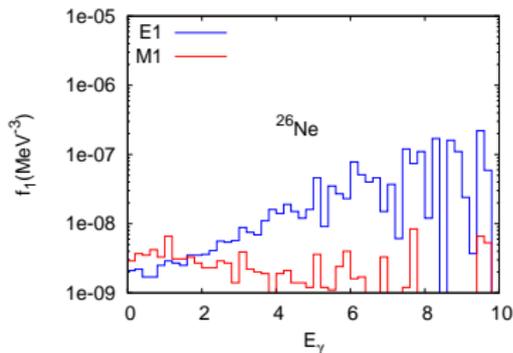
*S. Karampagia et al., Phys. Rev. C95 (2017) 024322*

*R. Schwengner et al., Phys. Rev. Lett. 118 (2017) 092502*

*K. Sieja, Phys. Rev. C98 (2018) 064312*

*J. Midtbo et al., Phys. Rev. C98 (2018) 064321*

$\gamma$ -decay (RSF)



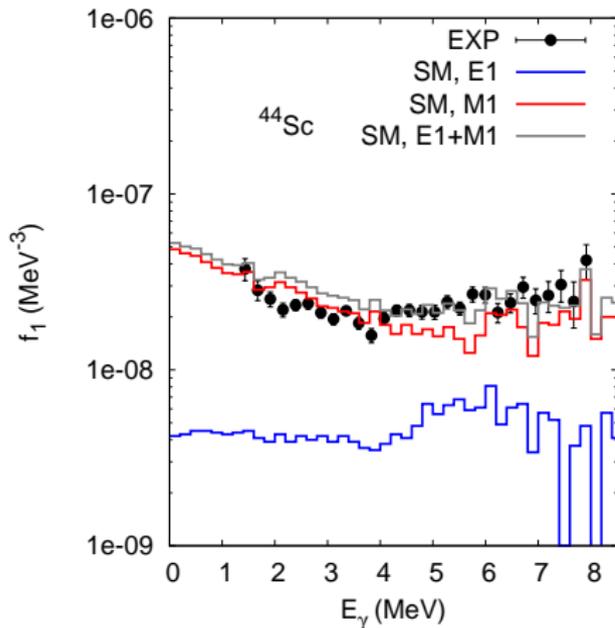
- calculate desired number of low lying states using standard SM diagonalization techniques
- obtain the averages and radiative strength functions from relations:

$$f_{M1/E1}(E_{\gamma}) = 16\pi/9(\hbar c)^3 S_{M1/E1}(E_{\gamma})$$
$$S_{M1/E1} = \langle B(M1/E1) \rangle \rho_i(E_i)$$

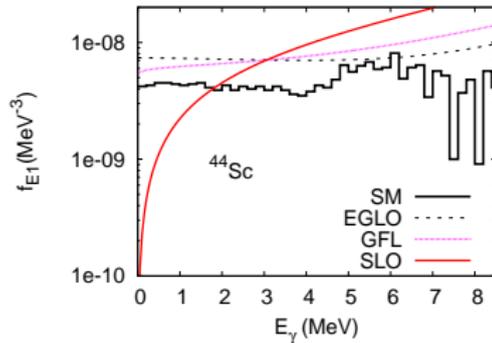
*R. Schwengner et al., Phys. Rev. C105 (2022) 014303*

*R. Schwengner et al., Phys. Rev. C105 (2022) 034335*

# Dipole strength in $^{44}\text{Sc}$ : theory vs exp



-all states below  $S_n \sim 10\text{MeV}$   
-86642  $M1$  matrix elements  
-65670  $E1$  matrix elements

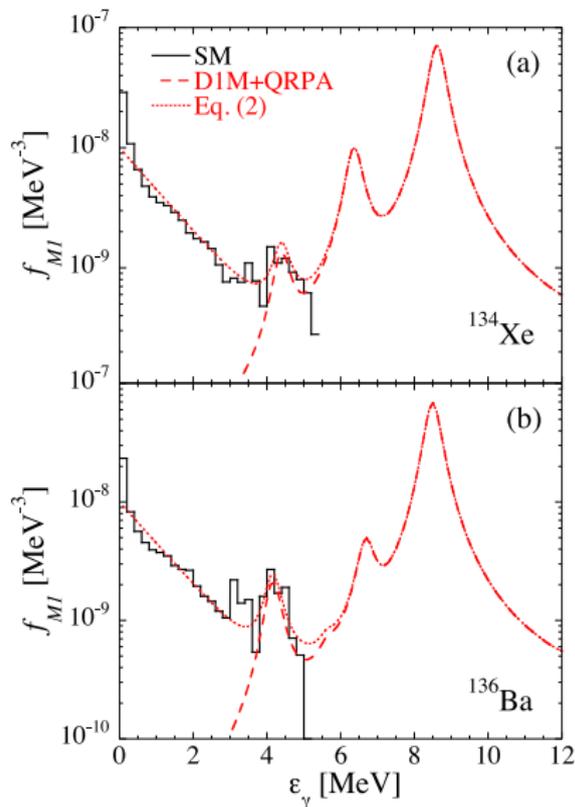


*K. Sieja, PRL119 (2017) 052502*

Qualitative agreement with data:

- the upbend is due to  $M1$  transitions
- the  $E1$  pattern is flat with the non-zero  $E_\gamma \rightarrow 0$  limit
- consistent with EGLO model

# Application of the low-energy limit to the QRPA results



*S. Goriely, S. Hilaire, S. Péru and K. Sieja, PRC98 (2018) 014327*

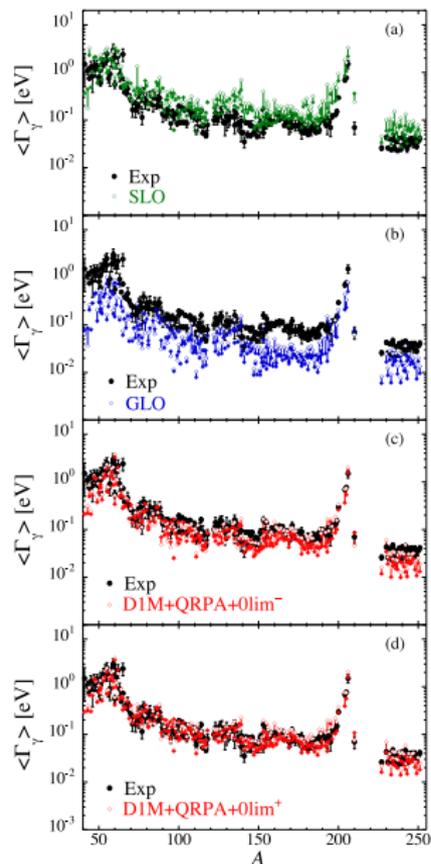
To describe radiative decay, phenomenological low-energy corrections fitted to reproduce SM trends and data are added to microscopic QRPA-Gogny  $M1$  and  $E1$  PSF:

$$f_{E1}(\varepsilon_\gamma) = f_{E1}^{QRPA}(\varepsilon_\gamma) + f_0 U / [1 + e^{(\varepsilon_\gamma - \varepsilon_0)}] \chi(1)$$

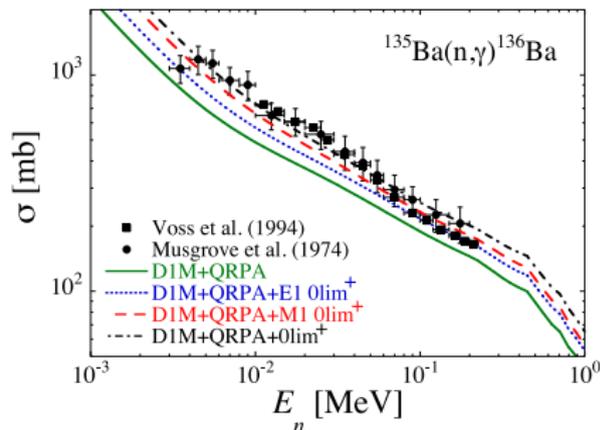
$$f_{M1}(\varepsilon_\gamma) = f_{M1}^{QRPA}(\varepsilon_\gamma) + C e^{-\eta \varepsilon_\gamma} \quad (2)$$

- upper limit ( $0\text{lim}^+$ )  
 $f_0 = 5 \cdot 10^{-10} \text{MeV}^{-4}$ ,  $\varepsilon_0 = 5 \text{MeV}$ ,  
 $C = 3 \cdot 10^{-8} \text{MeV}^{-3}$ ,  $\eta = 0.8 \text{MeV}^{-1}$
- lower limit ( $0\text{lim}^-$ )  
 $f_0 = 10^{-10} \text{MeV}^{-4}$ ,  $\varepsilon_0 = 3 \text{MeV}$ ,  
 $C = 10^{-8} \text{MeV}^{-3}$ ,  $\eta = 0.8 \text{MeV}^{-1}$

# Impact on radiative neutron capture

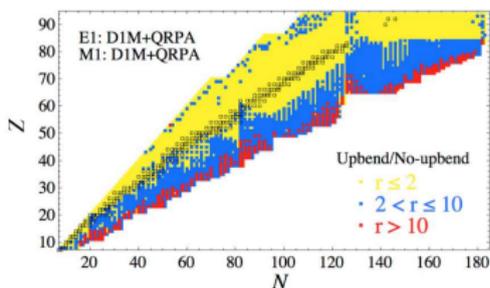
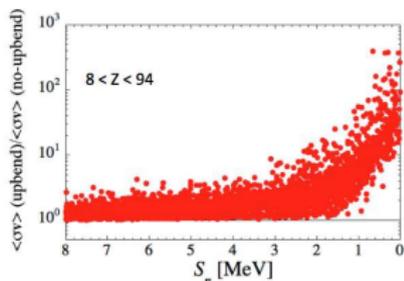
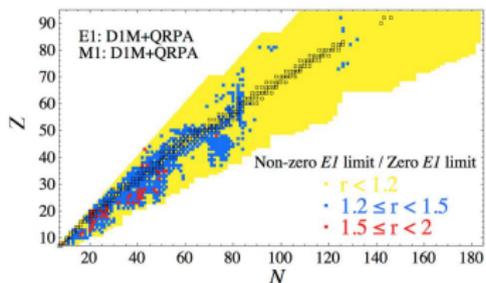
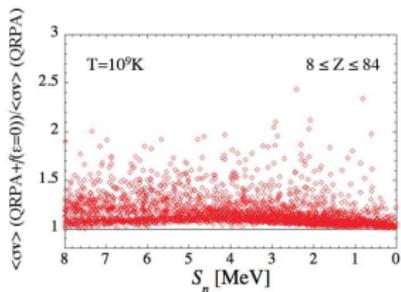


	rms/datum	
	$\langle \Gamma_\gamma \rangle$	$\langle \sigma \rangle$
0lim <sup>-</sup> (Comb)	0.88	1.07
0lim <sup>-</sup> (CT)	0.74	0.95
0lim <sup>+</sup> (Comb)	1.02	1.30
0lim <sup>+</sup> (CT)	0.90	1.15
GLO(Comb)	0.48	0.61
GLO(CT)	0.38	0.53



# Impact on the radiative capture

MACS ratio at  $T = 10^9\text{K}$

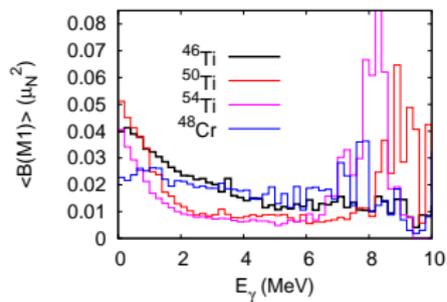
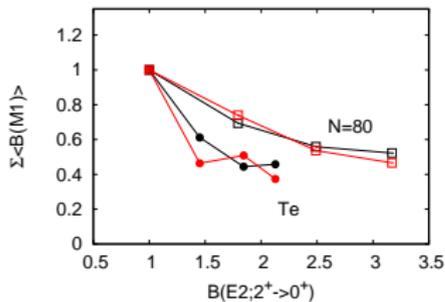
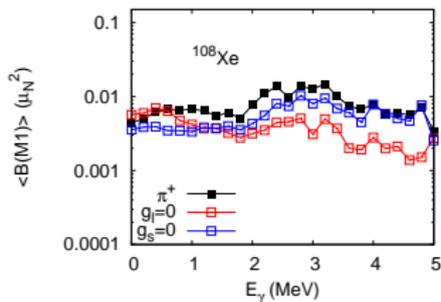
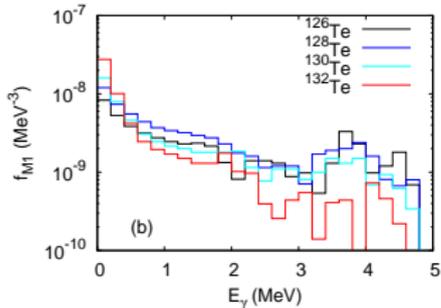


- Non-zero limit of the  $E1$  strength from SM impacts neutron capture on 20 – 50%
- $M1$  upbend can alternate the cross-section by a factor  $>10$  in exotic nuclei

*S. Goriely, S. Hilaire, S. Péru and K. Sieja, PRC98 (2018) 014327*

# M1 upbend: general trends from shell model

*K. Sieja, Phys. Rev. C98 (2018) 064312; Eur. Phys. J. Web of Conf.146 (2017) 05004 ND2016*



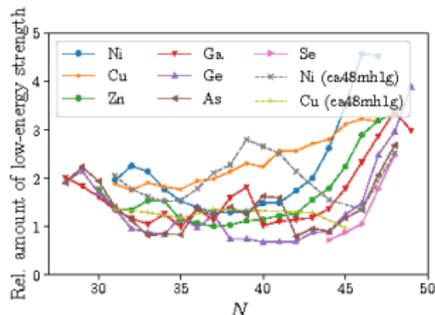
- ☞ The strength at  $E_\gamma = 0$  peaks around shell closures
- ☞ The strength is shifted towards higher  $\gamma$  in deformed nuclei

# M1 upbend: shell structure in quasi-continuum

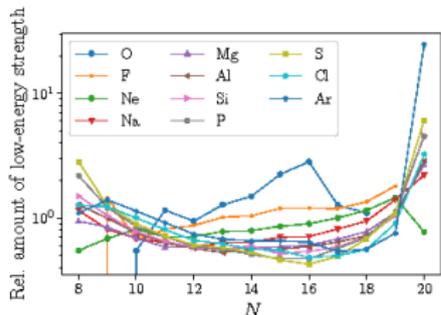
Ratio of  $B(M1)$  strength:

$$\frac{\langle B(M1) \rangle(0-2\text{MeV})}{\langle B(M1) \rangle(2-6\text{MeV})}$$

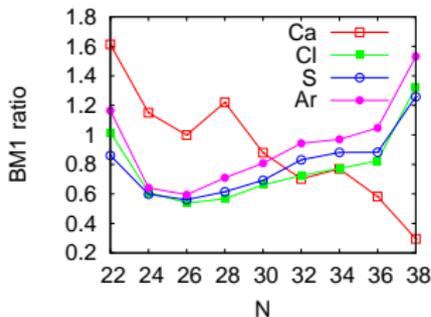
mid-mass nuclei:



$sd$ -shell nuclei:



$sd - pf$  nuclei:



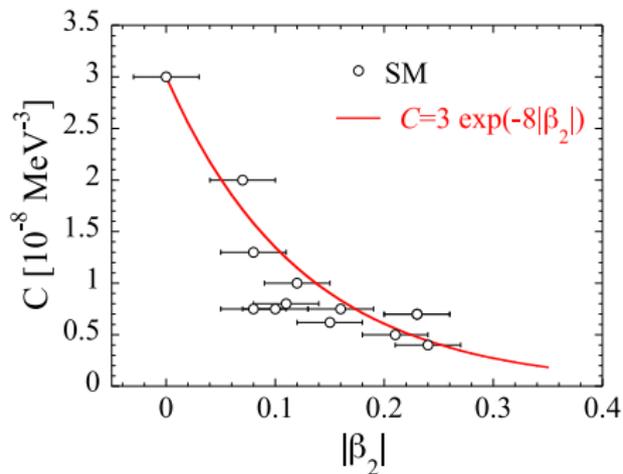
- Peaks towards the edges of the model spaces at  $N = 8, 20, 40, 50$ .
- Extra shell effects are present in the Ni chain.
- In  $sd$ - $pf$  nuclei the ratio peaks at  $N = 28$  for Ca only.

*J. Midtbo et al., Phys. Rev. C98 (2018) 064321*

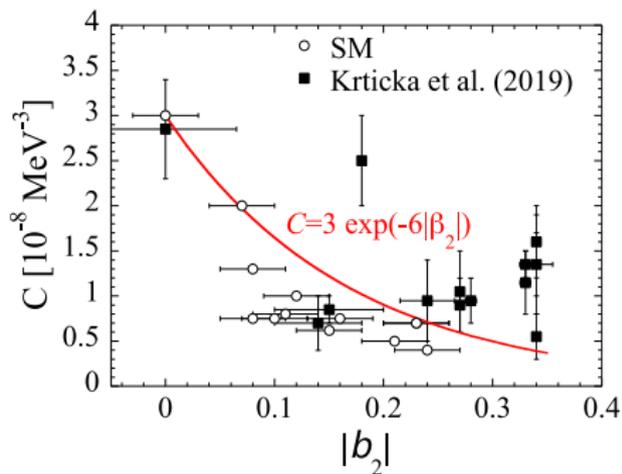
*K. Sieja and S. Goriely, Acta. Phys. Pol. B (2020) 535*

# Deformation dependence of the low-energy limit

$$f_{M1}(\varepsilon_\gamma) = f_{M1}^{QRPA}(\varepsilon_\gamma) + Ce^{-\eta\varepsilon_\gamma}$$



SM: Ti & Cr chains

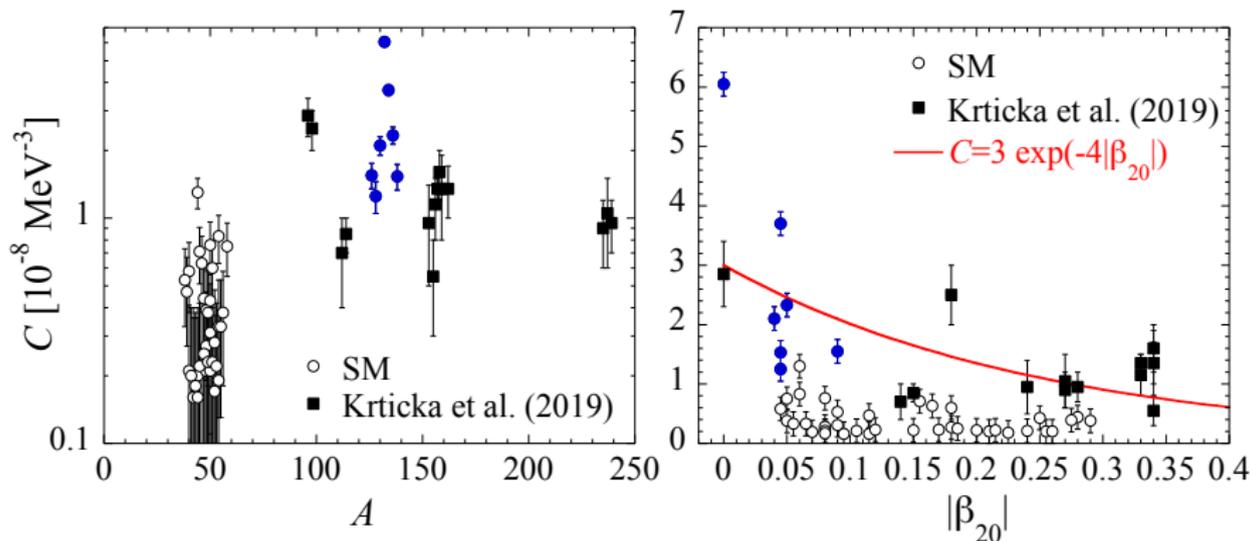


EXP: Selected nuclei from Mo-U

*M. Krticka et al., Phys. Rev. C99 (2019) 044308*

# Deformation dependence of the low-energy limit

K. Sieja and S. Goriely, *Acta. Phys. Pol. B* (2020) 535



- no simple deformation dependence with all nuclei included
- need of a complete, fully microscopic description (QRPA) of  $\gamma$  decay
- Benchmark study QRPA/SM with the same Hamiltonian now in progress

# Direct capture studies using SM input

$$\sigma^{DC}(E) = \sum_{f=0}^x S_f \sigma_{J_f^{\pi}}(E)$$

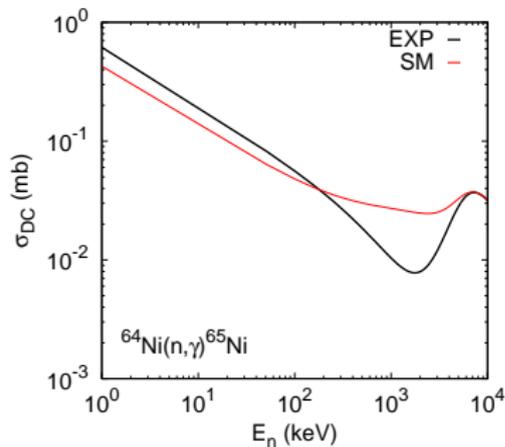
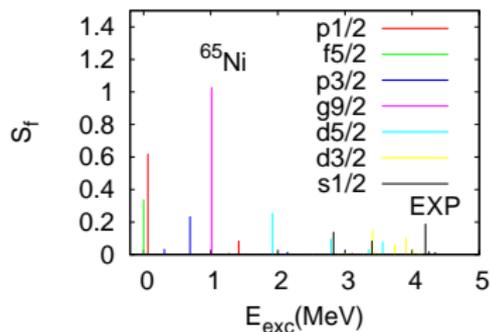
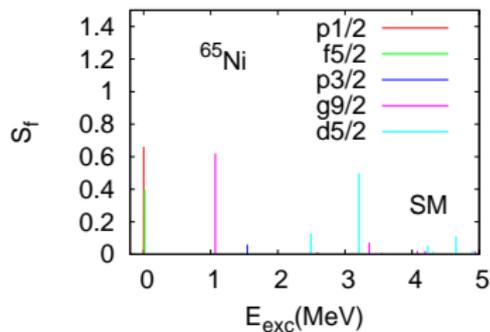
- **crucial observables: low energy levels and their spectroscopic factors**
  - E1, M1, E2 transitions
  - optical potential
- ➡ Compare global theoretical approximations for spectra and  $S_f$  to SM results in exotic nuclei

Systematic SM calculations (50 neutron-rich targets from mass 38 to 88) using well-established and newly developed interactions:

- SDPF-U for *sdpf* nuclei  
*F. Nowacki and A. Poves, Phys. Rev. C79 (2009) 014310*
- LNPS for *fpgd* nuclei  
*S.M. Lenzi et al., Phys. Rev. C82 (2010) 054301*
- LNPS+gds for nuclei towards  $^{78}\text{Ni}$   
*K. Sieja, unpublished*
- Ni78-II for nuclei above  $^{78}\text{Ni}$   
*K. Sieja et al., Phys. Rev. C88 (2013) 034327*

# Direct capture rates using SM results

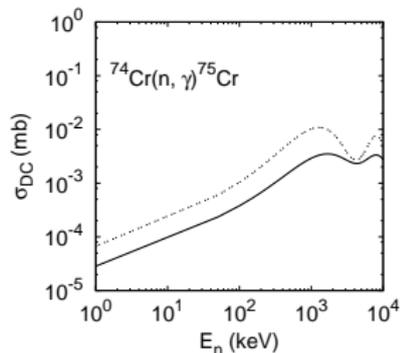
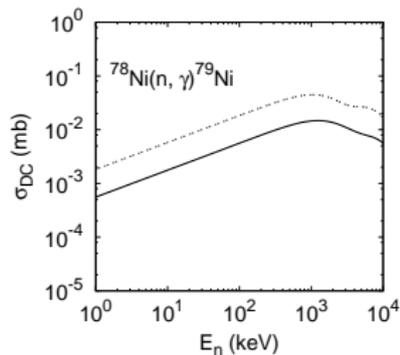
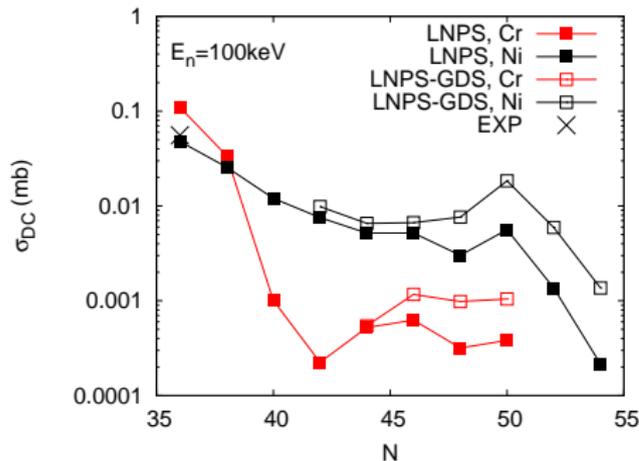
$^{64}\text{Ni}(n, \gamma)^{65}\text{Ni}$



# Direct capture: influence of the model space

LNPS:  $fp$  for protons,  $fp g_{9/2} d_{5/2}$  for neutrons

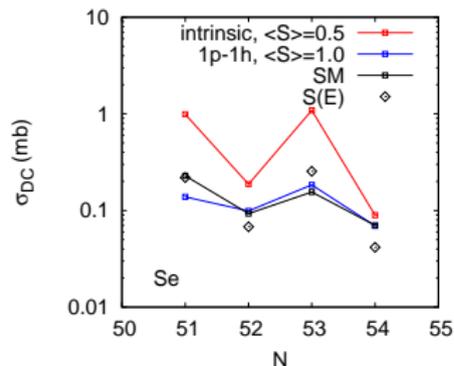
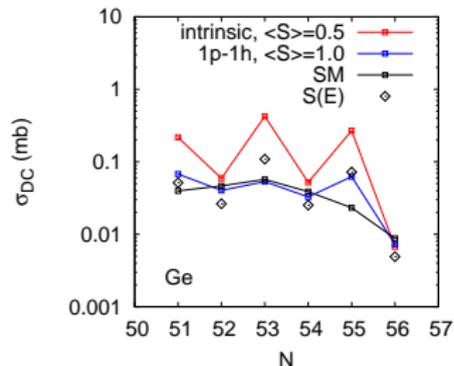
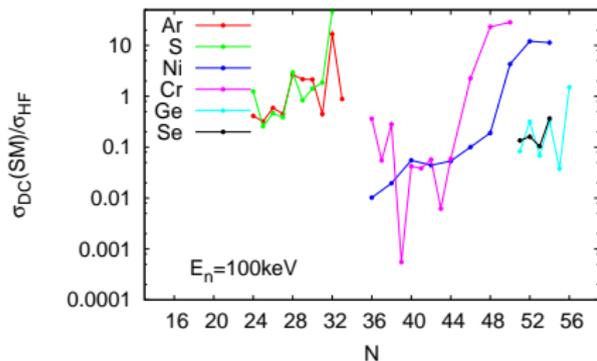
LNPS+gds:  $fp$  for protons,  $gds$  for neutrons



*K. Sieja and S. Goriely, Eur. Phys. J*

*A57 (2021) 110*

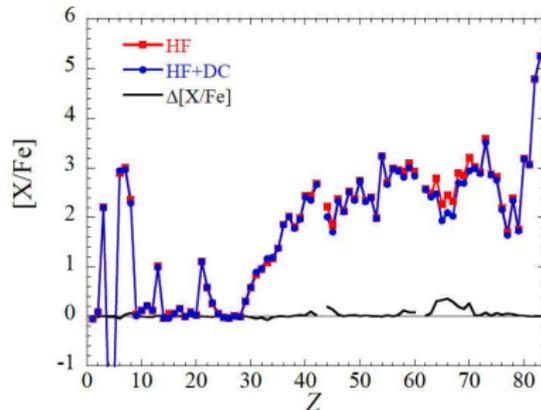
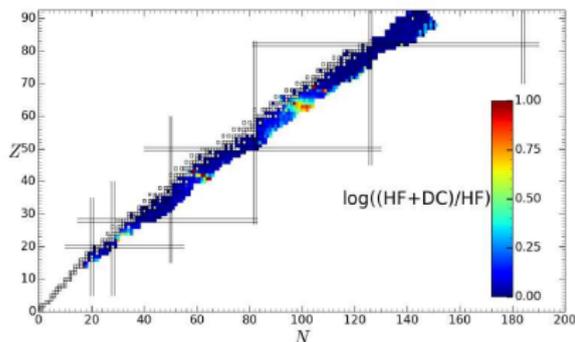
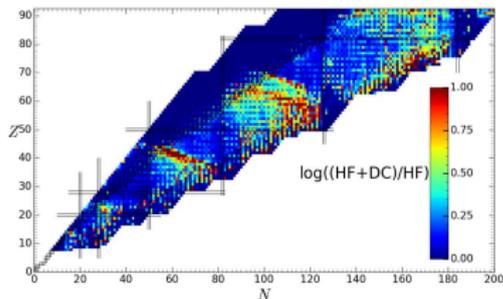
# Direct capture vs resonant capture



- factor 10 difference after passing  $N = 50$  shell closure
- largest discrepancies between models in triaxial nuclei
- different prescription for  $S(E)$  used to reduce inter-model differences

# Direct capture: influence on i-process

K. Sieja and S. Goriely, *Eur. Phys. J A57* (2021) 110



- DC appears important for i-process in low-metallicity AGB stars
- Dedicated SM calculations needed in  $10^2 - 10^4 M_{\odot}$  nuclei

S. Goriely et al., *Astronomy and Astrophysics*, 654, A129 (2022)

# Summary

- The Brink-Axel hypothesis holds for E1 sum rules, giant resonance and in PDR region
- Deviation from BA hypothesis for M1 transitions observed for sum rules and PSF
- Shell effects survive at high excitation energy and are visible in RSF
- SM necessary to constrain DC and HF capture contributions for i-process

SM studies are continued to benchmark QRPA models of decay strength functions and of combinatorial models of nuclear level densities

Thanks to:

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