Static and dynamic properties of exotic nuclei: the role of experiments in developing predictive theory

FRIB-TA Topical Program:

Theoretical Justifications and Motivations for Early High-Profile FRIB Experiments

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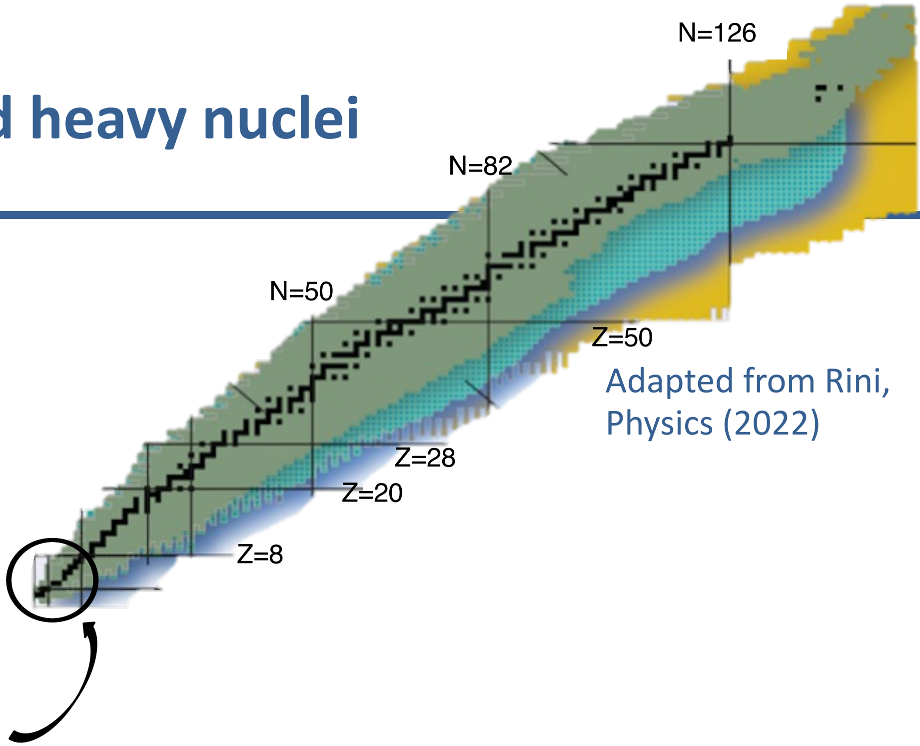
Questions

How does nuclear structure change as one approaches the drip line and how are those changes reflected in nuclear reactions?

How do collective excitations evolve/emerge with increasing neutron number? Examples include GDR, PDR, other multipolarities. What can we learn about the interplay of single-particle and collective excitations in nuclei from theory predictions? How can we test the predictions experimentally?

How do we get all the information we need to calculate cross sections needed for applications? Do we need to revise our reaction theory or can we get away with better inputs?

Integrated structure & reaction theory for medium-mass and heavy nuclei



Adapted from Rini, Physics (2022)

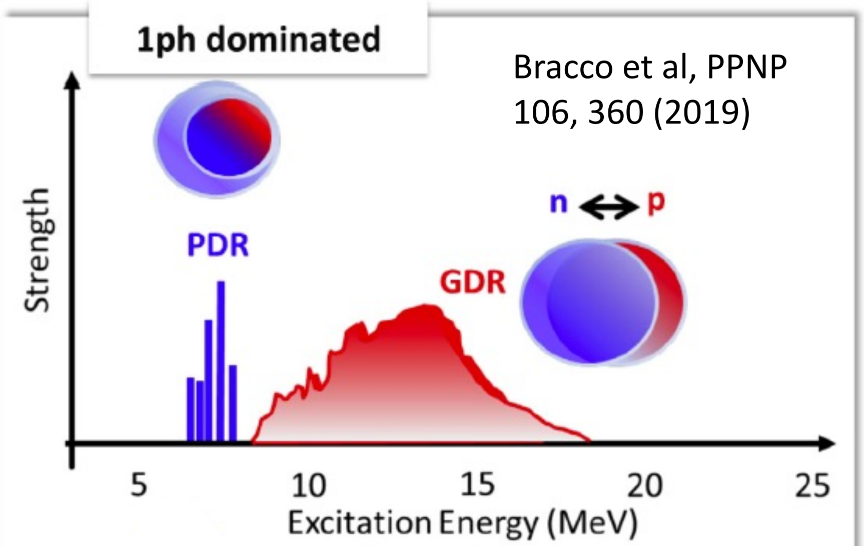
- We need to predict reactions involving nuclei across the isotopic chart
  - ➢ guide experiments, which in turn provide stringent tests for theory
  - ➢ study evolution of shell structure, deformation, collective excitation modes
  - ➢ generate inputs for astrophysical simulations, which in turn provide insights into stellar evolution, origin of elements
  - ➢ complement measurements to populate databases for applications
- For light nuclei we have seen substantial progress with RGM approaches
  - ➢ Treat structure and reactions simultaneously, account for correlations
  - ➢ Consistent use of interactions based on χEFT
  - ➢ Symmetry-adapted bases provide path forward to medium-mass nuclei
- For heavier nuclei we ignore the internal structure of the interacting nuclei
  - ➢ Focus on improving reaction mechanisms: transfer, inelastic scattering, breakup
  - ➢ Include higher-order reaction processes: multi-step, coupled-channels, breakup-fusion, etc.

We need to take advantage of state-of-the-art structure theories to improve reaction descriptions!

For both direct and statistical reactions!

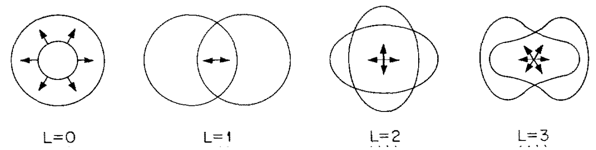
Direct reactions: Inelastic scattering is a valuable tool to study collective nuclear excitations

- Collective modes studied via direct inelastic scattering
- Dipole resonance important for photonuclear reactions and capture reactions
- Isoscalar monopole resonance related to nuclear matter compressibility, impact models of neutron stars
- Unresolved questions to be addressed for unstable isotopes and exotic modes of excitation.

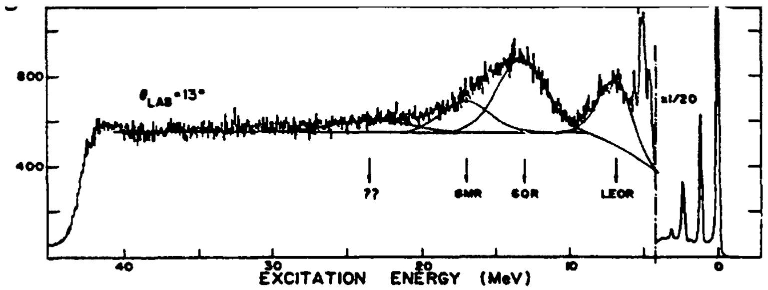


GIANT MULTIPOLE RESONANCES - PERSPECTIVES AFTER TEN YEARS

Fred E. BERTRAND



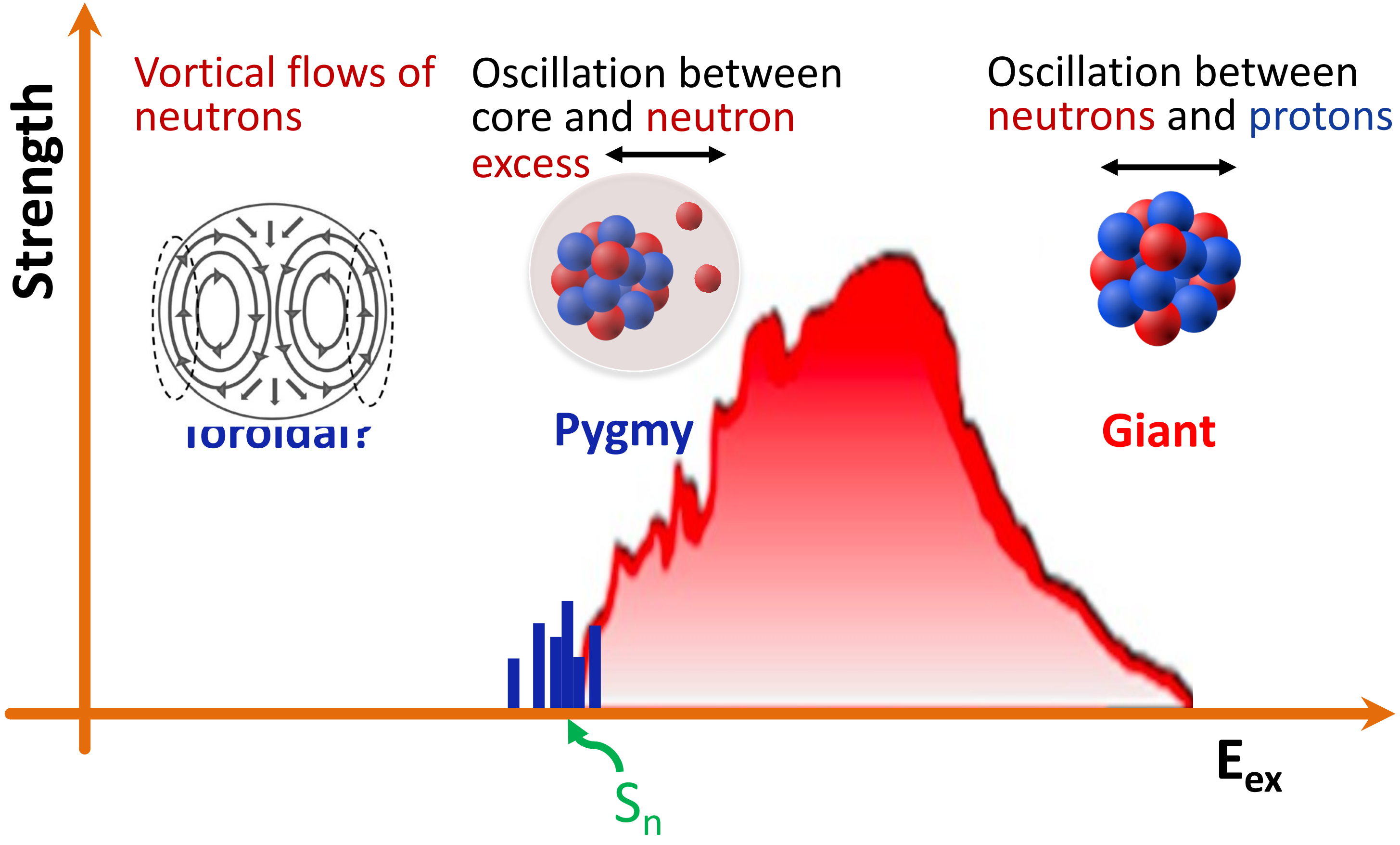
Modes of nuclear oscillations.



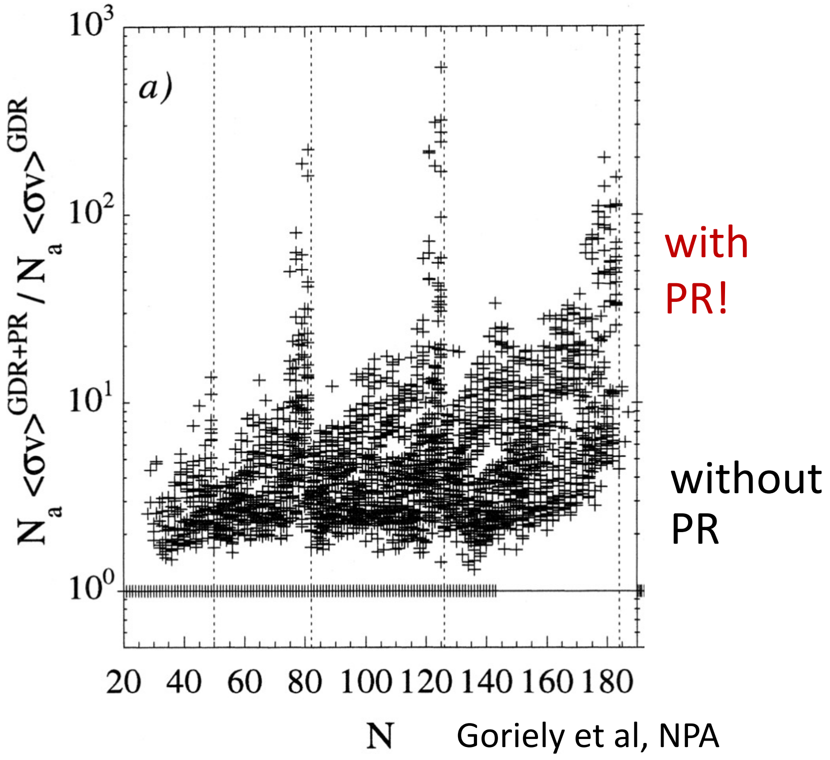
Energy dependence of cross section.

Nucl. Phys. A 354, 129 (1981)

How does collective motion emerge and manifest itself?
Even dipole excitations are poorly understood: GDR, Pygmy and toroidal resonances



Impact on neutron capture rates



Goriely et al, NPA 739, 331 (2004)

How does this picture change with increasing neutron excess?
How do the resonances affect our calculations of neutron capture rates for astrophysics simulations!

Coupled-channels framework provides approach to integrate structure and reaction theory

$$\left\{\frac{d^2}{dr^2} - \frac{l_c(l_c+1)}{r^2} - \frac{2\mu_c}{\hbar^2}V^{\mathfrak{J}}_{cc}(r) + k_c^2\right\} u_c(r) = \sum_{c'\neq c} \frac{2\mu_c}{\hbar^2} V^{\mathfrak{J}}_{cc'}(r)\, u_{c'}(r),$$

Input to reaction code

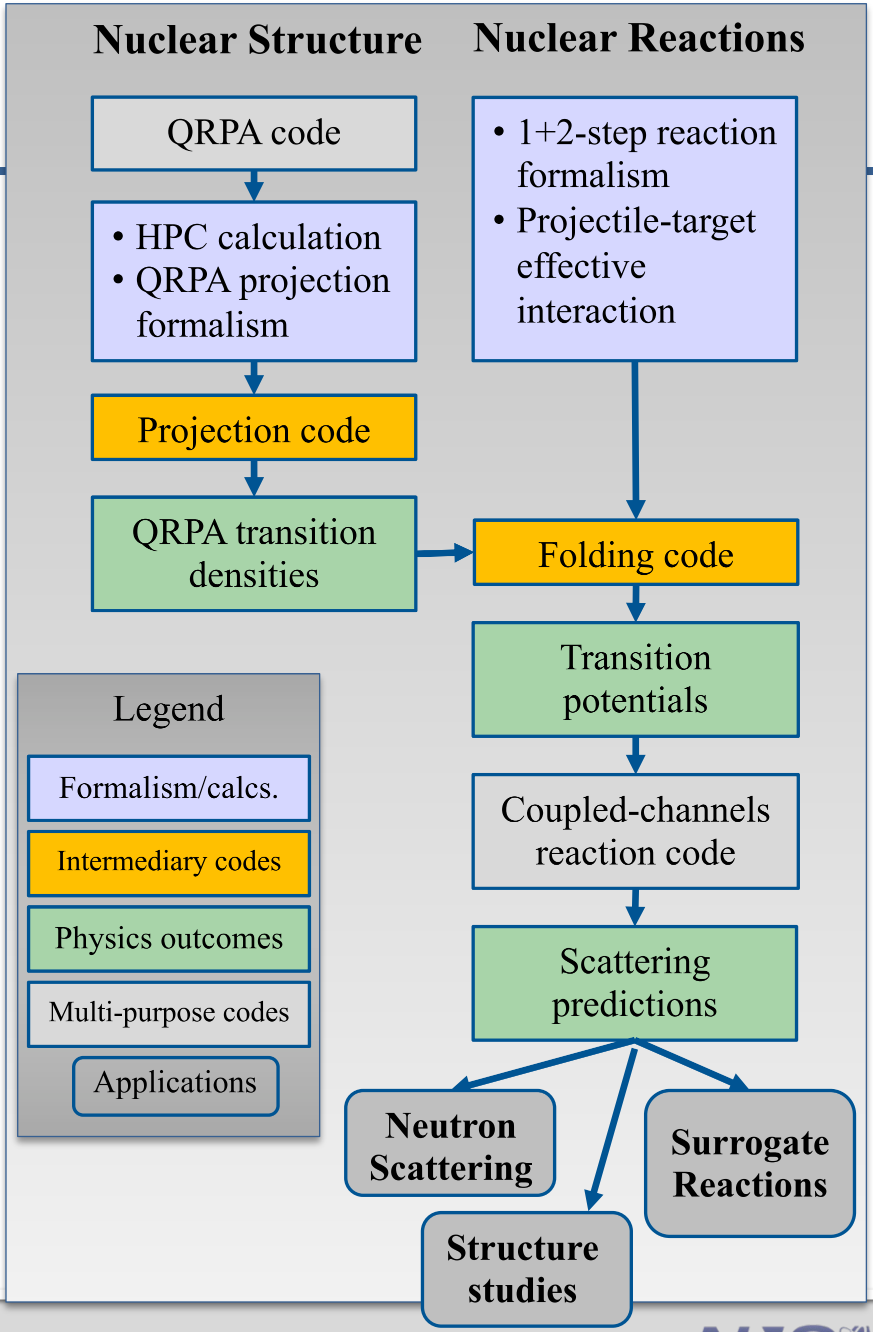
$$V_{cc'}^{\mathfrak{J}}(r) = \sum_{LSJTq} (-1)^{j_{c'}+I_c+\mathfrak{J}} \begin{Bmatrix} \mathfrak{J} & I_c & j_c \\ J & j_{c'} & I_{c'} \end{Bmatrix} (-1)^{L+S-J}$$

$$\times \left(\beta_c(l_c s_c)j_c; t_c \| [Y_L(\hat{\mathbf{r}}) \times \mathcal{S}_S]_J\, \mathcal{T}^\dagger_{Tq} \| \beta_{c'}(l_{c'}s_{c'})j_{c'}; t_{c'}\right)$$

$$\times \left(\alpha_c I_c \| \sum_n v_L^{ST}(r,r_n)[Y_L(\hat{\mathbf{r}}_n)\times \mathcal{S}^n_S]_J\, \mathcal{T}^n_{Tq} \| \alpha_{c'} I_{c'}\right),$$

$$4\pi\sqrt{2I_c+1}\int_0^\infty dr_t\, r_t^2\, v_L^{ST}(r,r_t)\,\rho^{Tq,cc'}_{LSJ}(r_t),$$

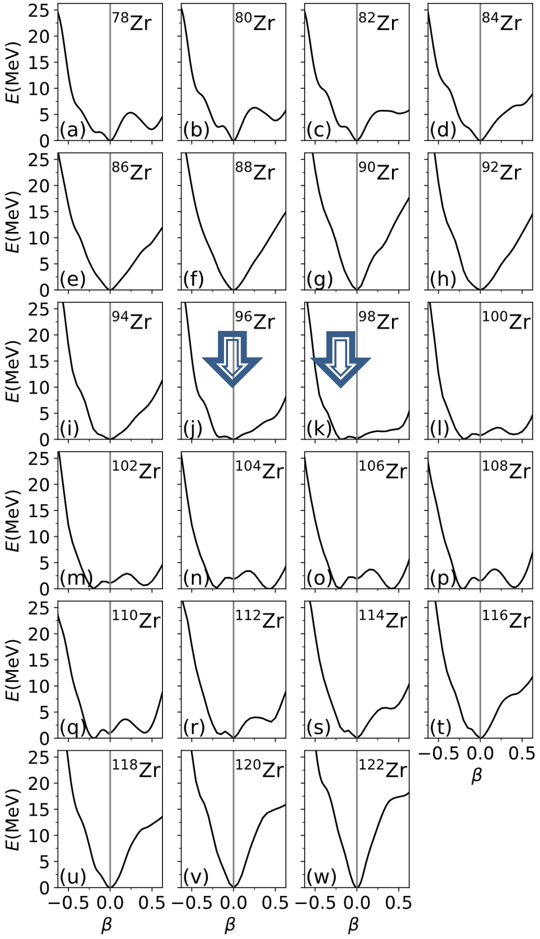
From QRPA



Structure predictions from HFB: ground state properties of the Zr isotopes

Chimanski, In, Escher, Peru, Younes (to be submitted)

Energy as function of β

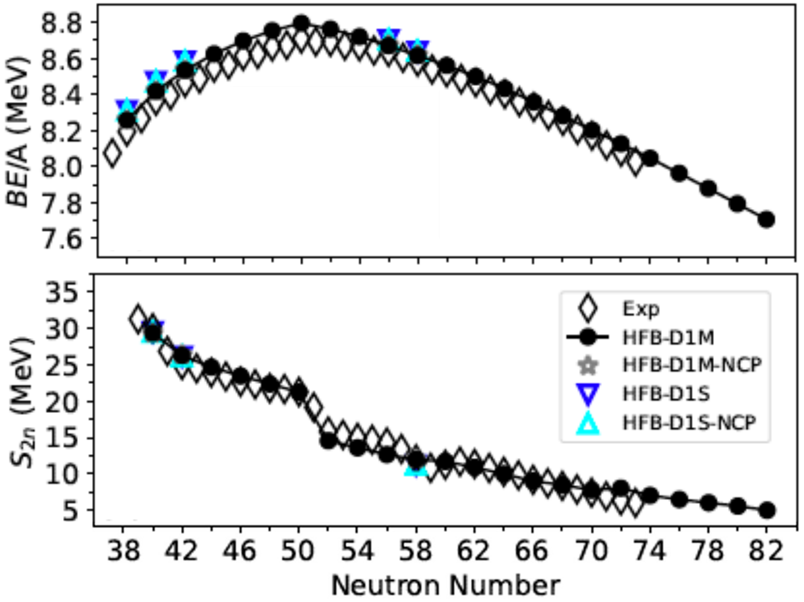


Gogny D1M interaction

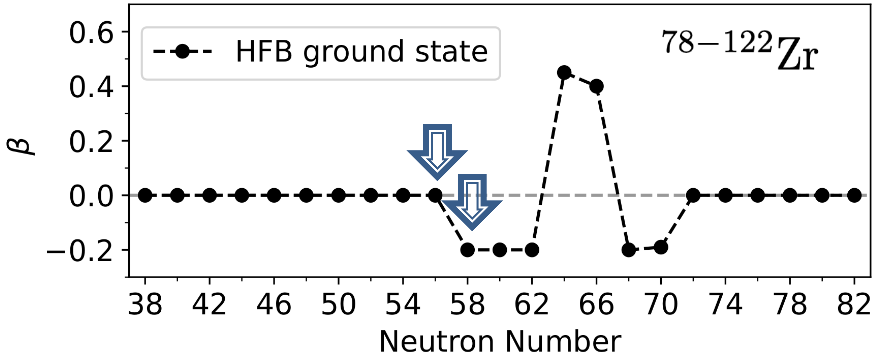
Axially-symmetric deformed basis

11 oscillator shells

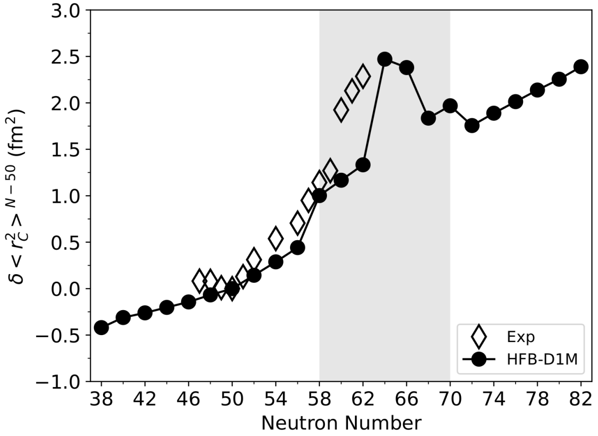
Binding energies/two-neutron separation energies



Shape Evolution of ground state Zr isotopes:



HFB isotopic charge radius shifts



Predicted systematics agree well with experiment - with some exceptions

Structure predictions from HFB: ground state properties of the Zr isotopes

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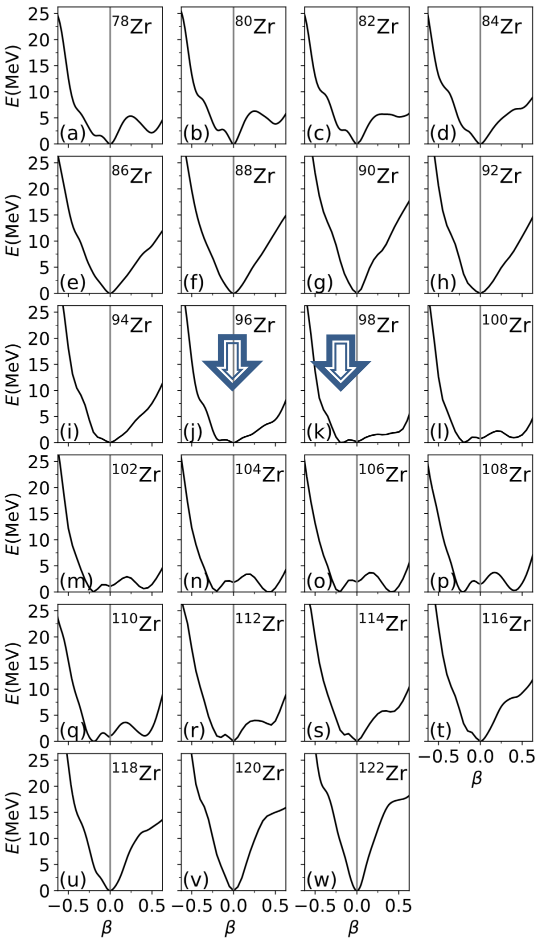
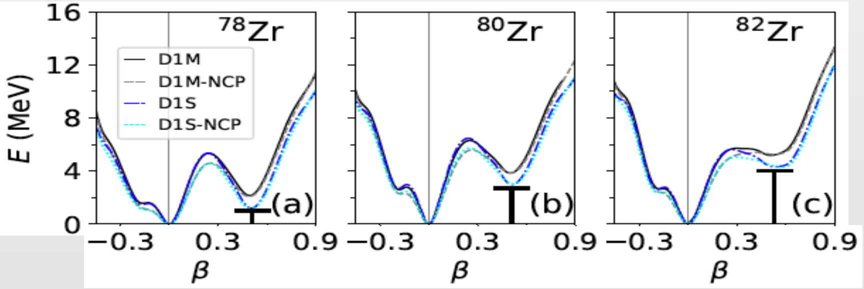
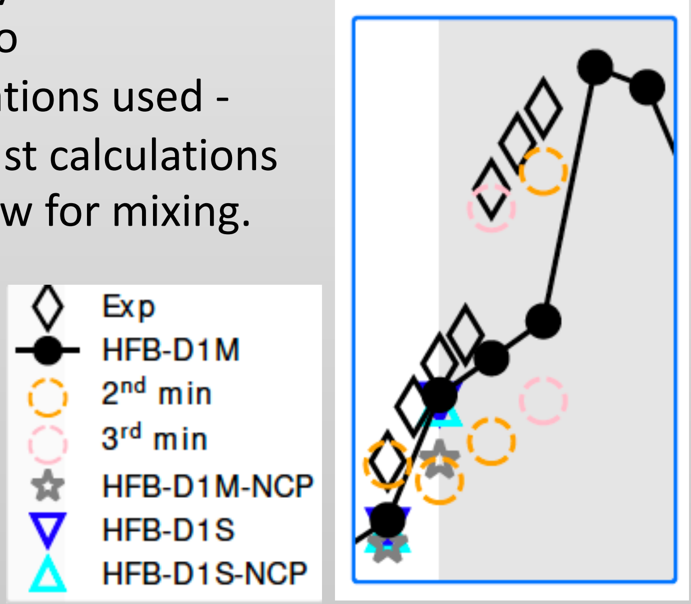
Energy as function of β

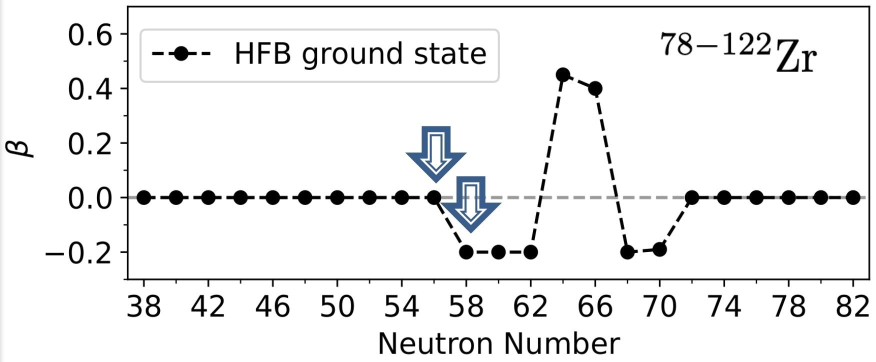




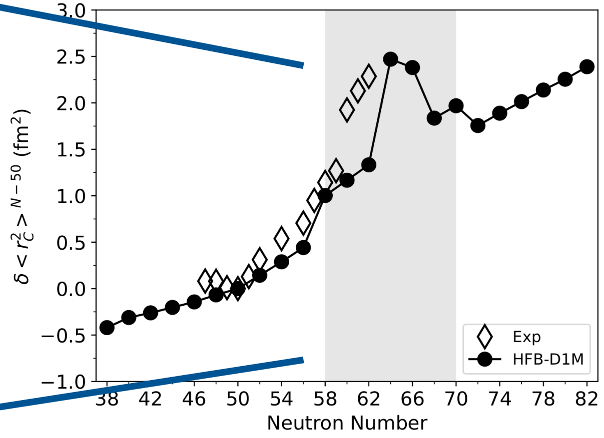
The energy surface is sensitive to approximations used - more robust calculations would allow for mixing.



Shape Evolution of ground state Zr isotopes:



HFB isotopic charge radius shifts

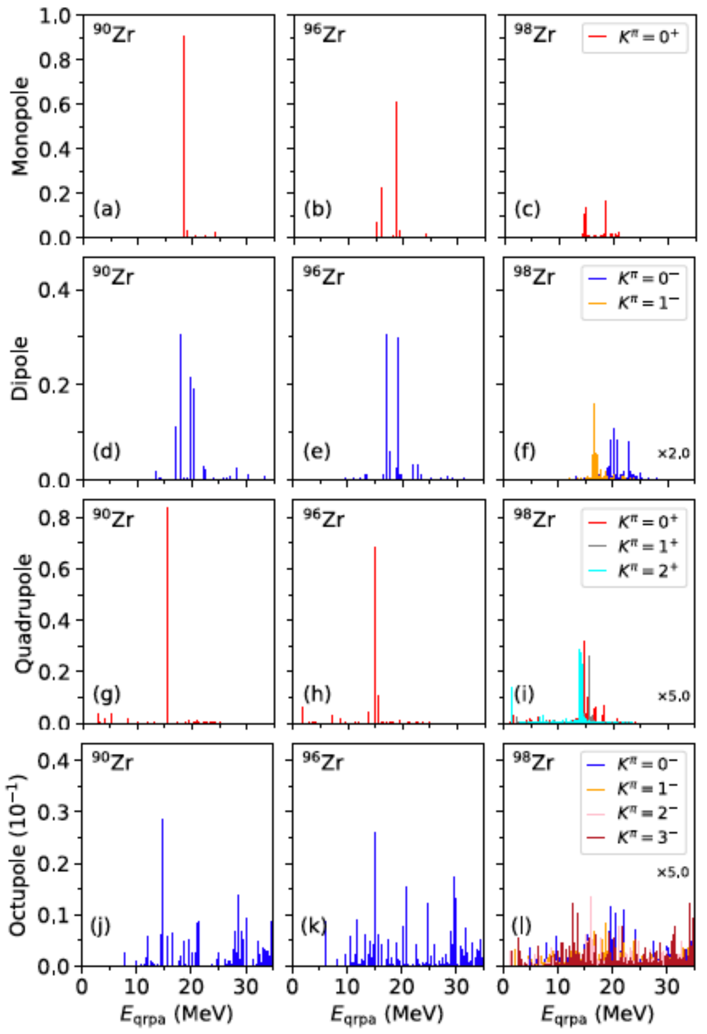


Discrepancies reveal shortcomings in method or implementation: approximations, interaction,…

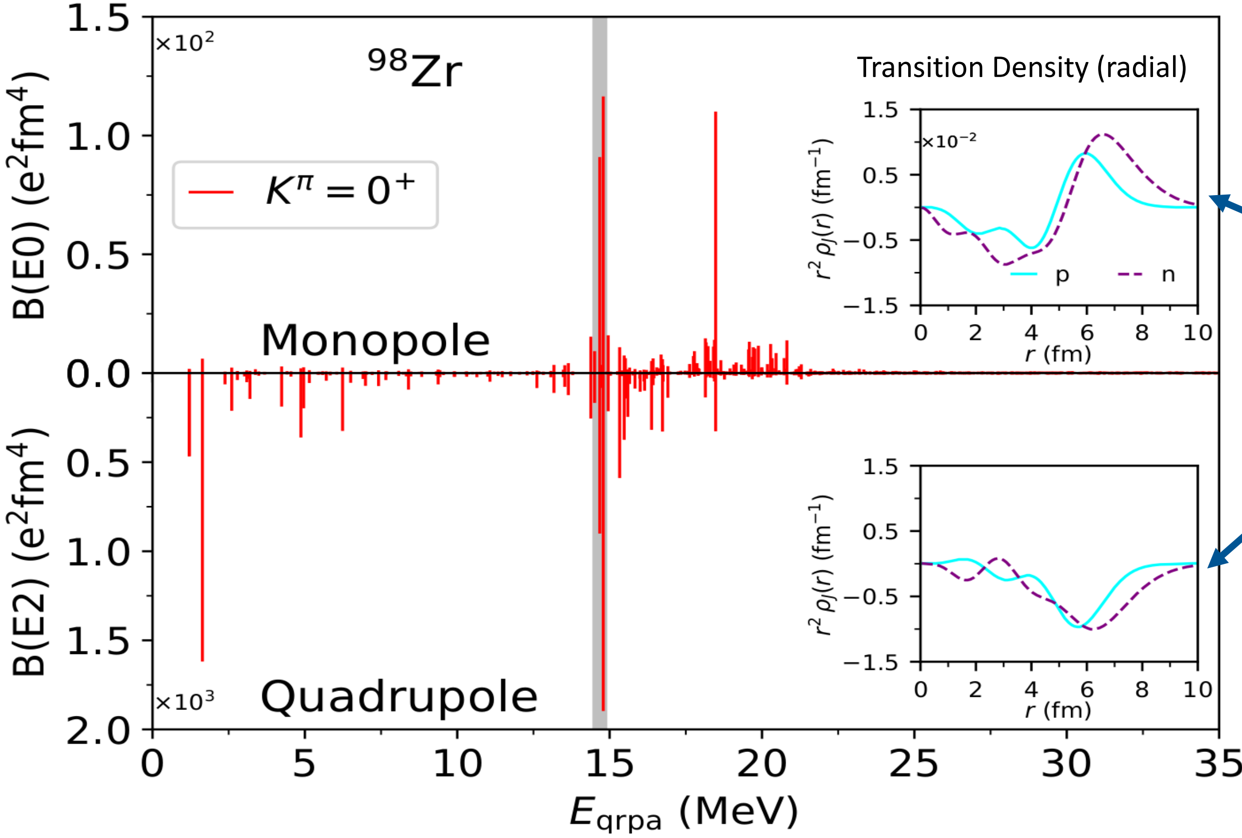
Structure predictions from HFB+QRPA for highly-excited states in Zr isotopes: electromagnetic response and transition densities for ^{98}Zr

Chimanski, In, Escher, Peru, Younes

Responses for multipoles λ=0-4



Electric monopole & quadrupole in detail



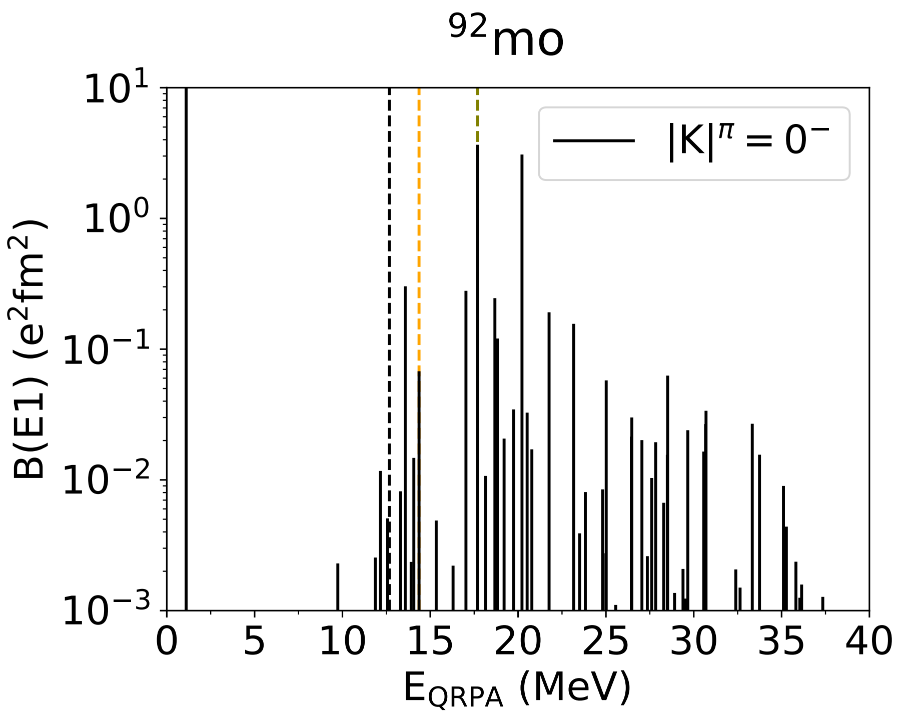
Radial transition densities for scattering calculations

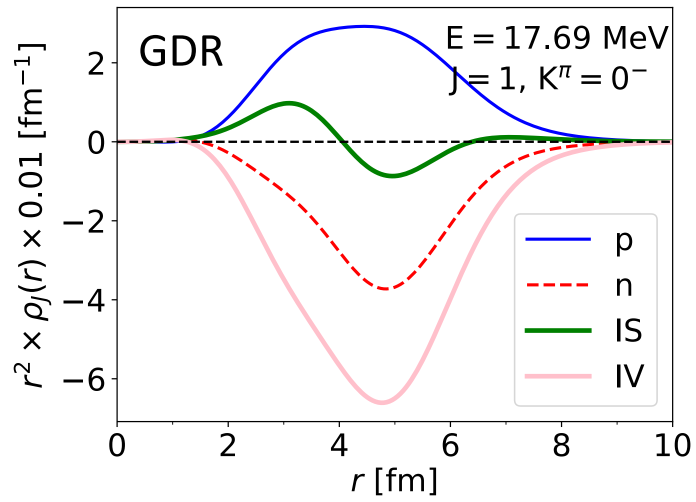
Calculated transition densities determine the potential couplings for coupled-channels calculations

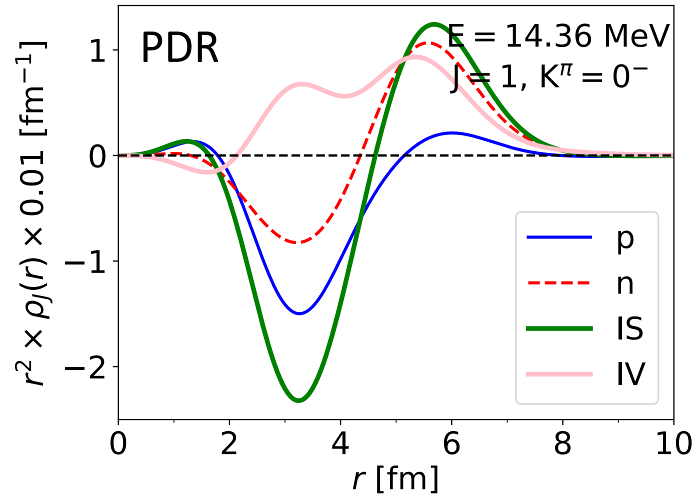
Structure predictions from HFB+QRPA for Mo isotopes: Can we understand the nature of the various resonances?

In, Chimanski, Escher, Peru, Younes (wip)

Excitations spectrum alone does not provide information on the nature of the excitation…





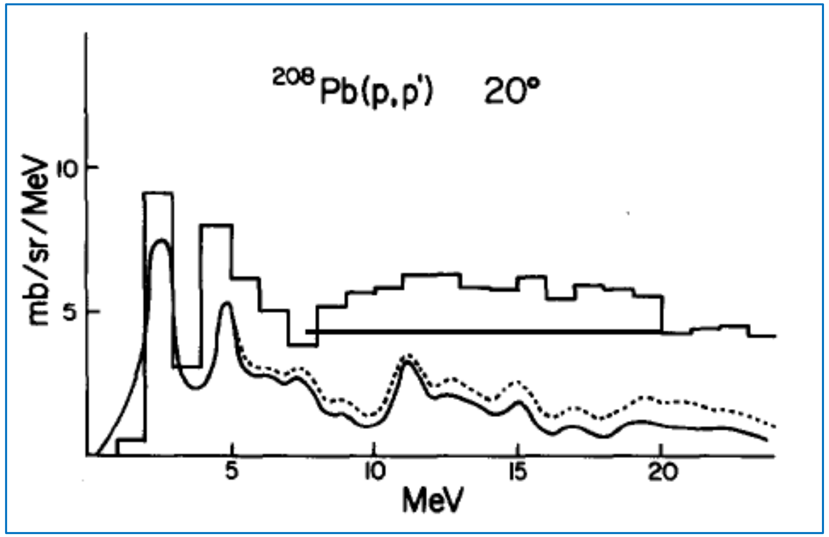


… but the transition densities reveal differences in the underlying structure!

Differences in transition densities are expected to be reflected in scattering cross sections >> WIP

Can we expect to get agreement between theory and experiment? An old problem appears to persist….

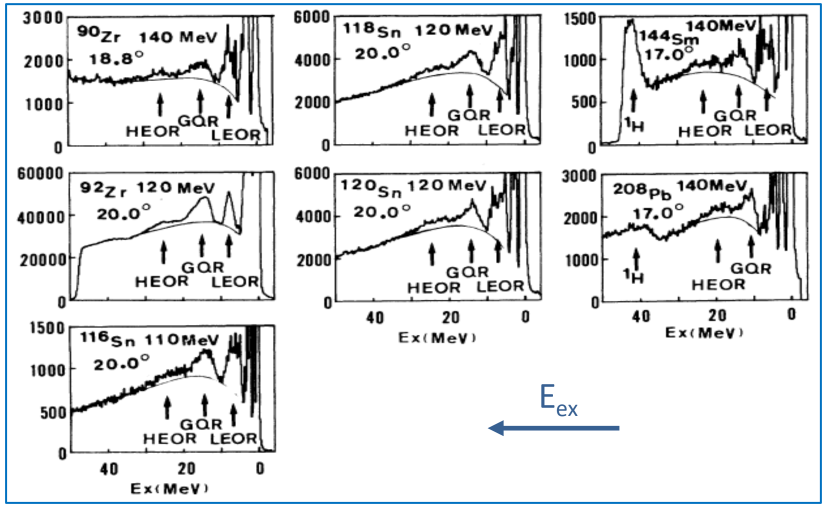
It has been long known that (Q)RPA + DWBA does not reproduce measured inelastic cross sections at higher E_{ex}



Bertsch & Tsai, Phys. Rep 2, 125 (1975)
RPA vs experiment

What is the challenge?

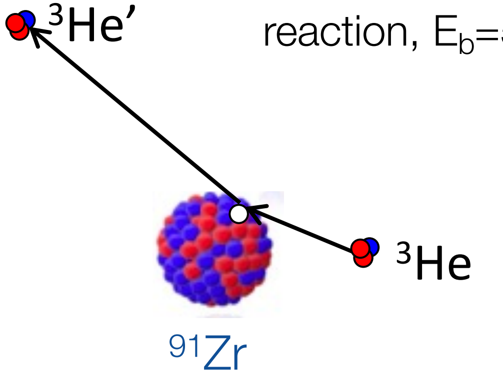
- Inelastic scattering calculations with microscopic structure input reproduce only a fraction of the observed cross section.
- Standard procedure is *ad hoc* removal of 'background'
- Is this 'experimental background' or missing physics?



Yamagata, PRC 23, 937 (1981)
^{3}He scattering

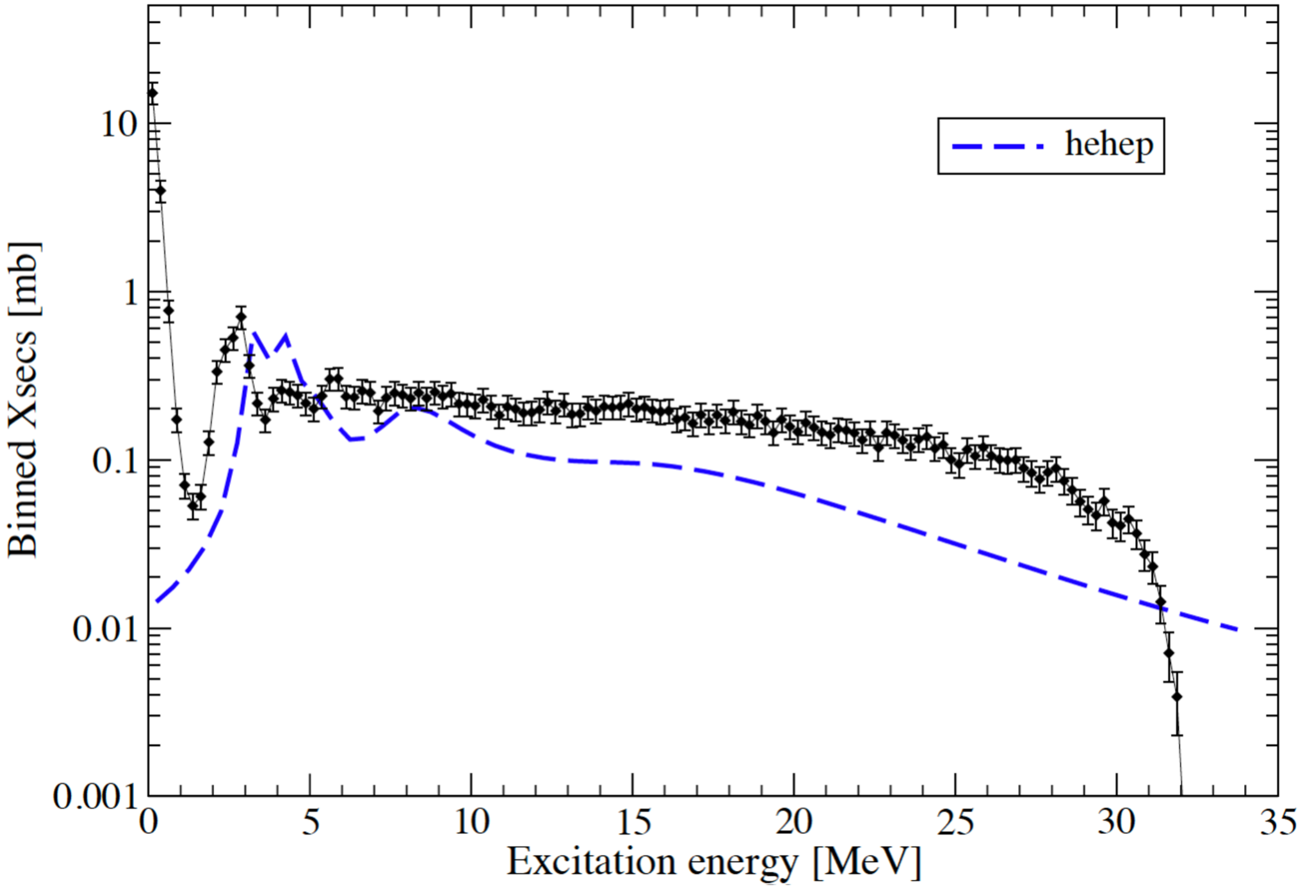
Inelastic scattering predictions using QRPA transition densities and folding

Escher, wip (2023)



Inelastic ^{3}He scatter reaction, E_b=50 MeV

Angle-integrated cross section

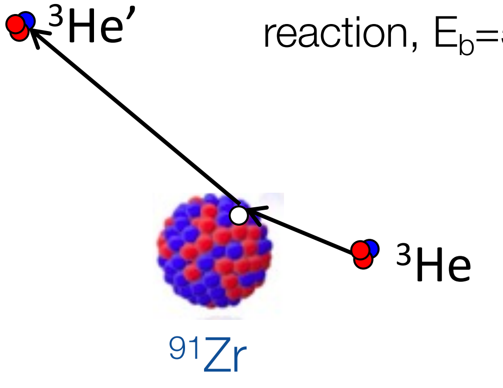


Skyrme transition densities from:
Nobre et al, PRL 105, 202502 (2010)
Nobre et al, PRC 84, 064609 (2011)
Updates with Gogny D1M in progress

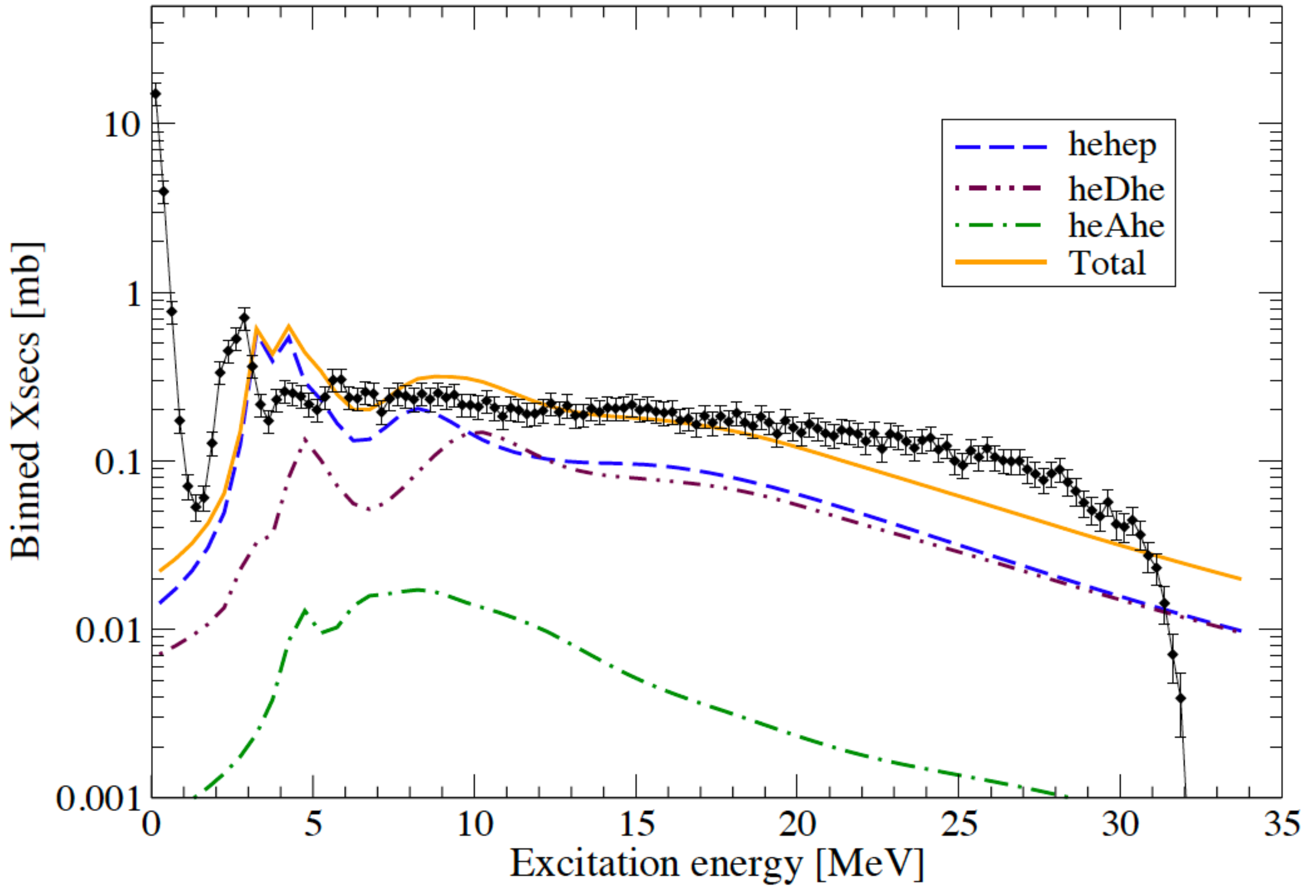
Inelastic scattering predictions using QRPA transition densities and folding - supplemented by two-step reaction contributions

Escher, wip (2023)

Inelastic ^{3}He scatter reaction, E_b=50 MeV



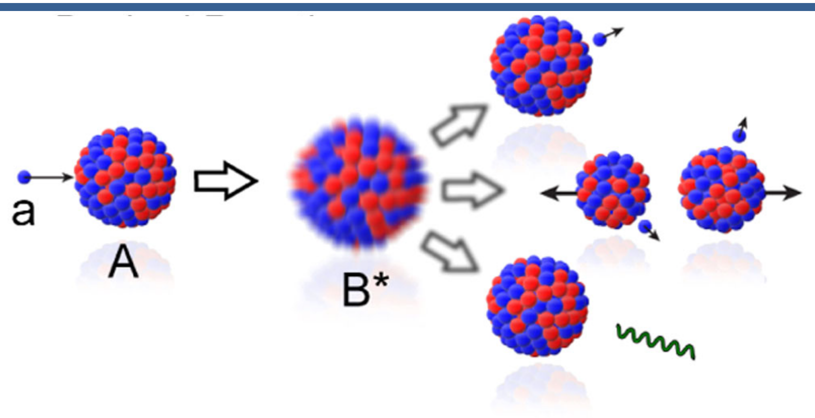
Angle-integrated cross section



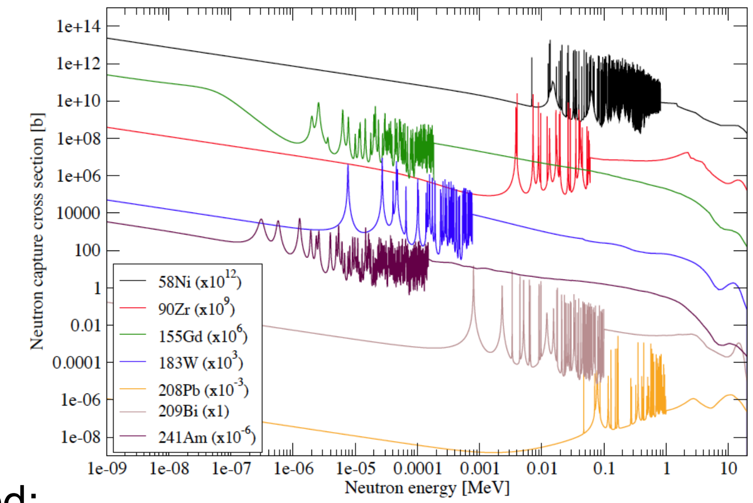
It appears that the longstanding problem of underpredicting inelastic cross sections is (mostly) solved by including two-step contributions!

Statistical reactions and Hauser-Feshbach calculations

- Hauser-Feshbach (HF) theory describes compound-nuclear reactions that can be statistically averaged
- HF calculations are essential component of nuclear data evaluations
- Astrophysics simulations rely on neutron capture rates calculated with HF



(n,γ) cross sections
for select stable isotopes (ENDF/B-VII)

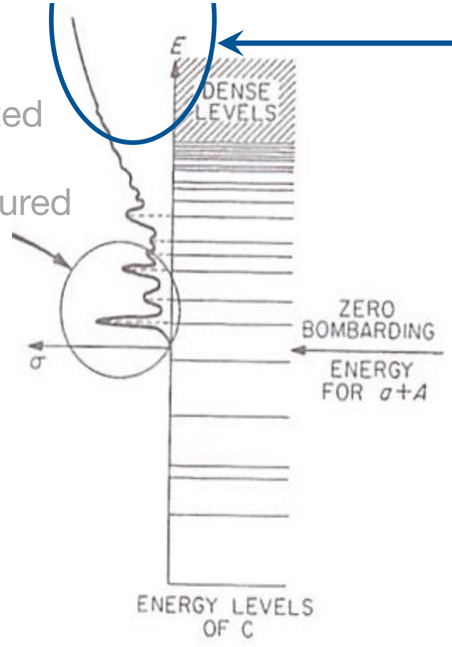


Inputs needed:

- Optical-model potentials
- Level densities (LDs) and γ-ray strength functions (γSF)
- Constraints: D_0, $<\Gamma_\gamma>$, cross section data

R-matrix regime

- Assumes isolated resonances
- Requires measured data or fully microscopic calculation



Hauser-Feshbach regime

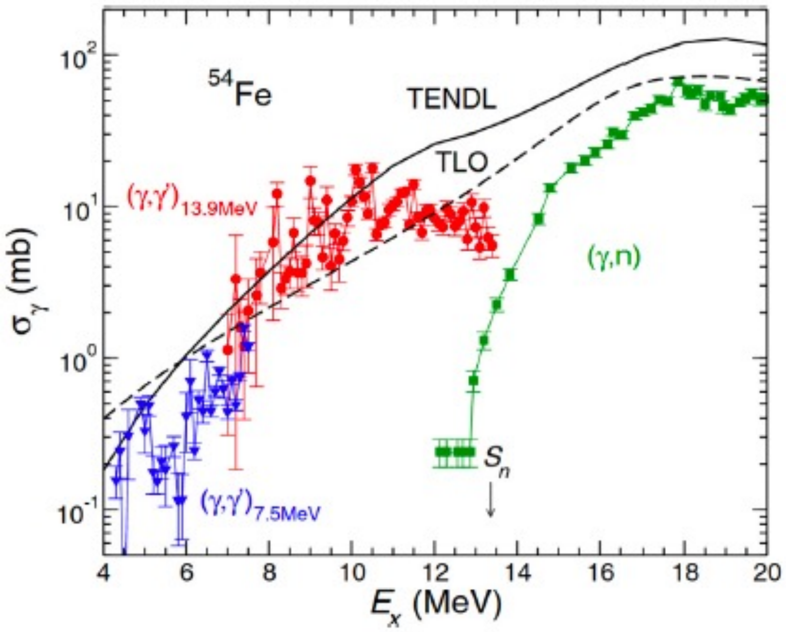
- Assumes strongly overlapping resonances
- Requires structure models and parameters

$$\sigma_{\alpha\chi} = \Sigma_{J,\pi}\, \sigma_\alpha^{CN}(E,J,\pi) \cdot G^{CN}_\chi(E,J,\pi)$$

*WFC omitted here to simplify notation.

Getting sufficient experimental constraints for all isotopes is a daunting task

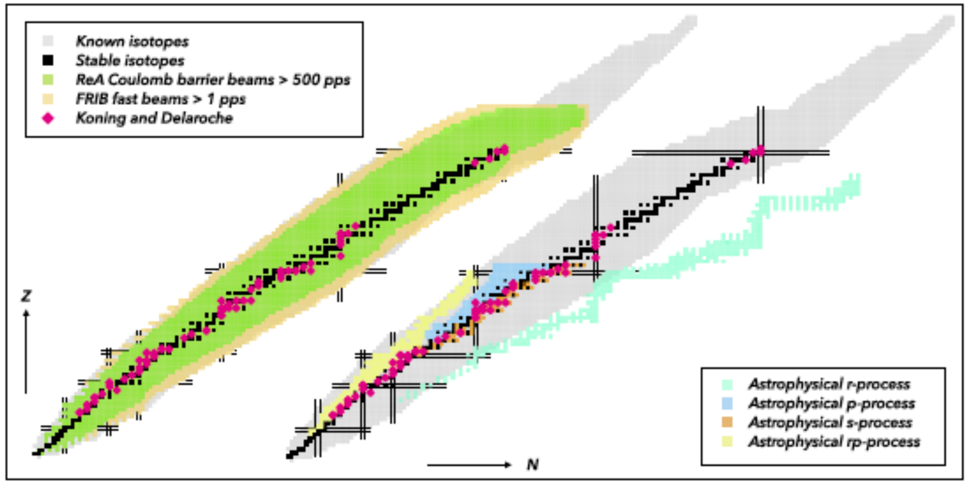
- Measuring D_0 and $<\Gamma_\gamma>$ requires stable targets
- Convolution of LDs and γSF causes ambiguities when extracting components
- Partial level densities are often needed or measured
- Brink-Axel hypothesis is liberally used for γSF
- Conflicting results from different methods
- Can we extrapolate OMPs away from stability?
- Too many nuclei to measure them all!



Zilges *et al*, PPNP 122 (2022) 103903

Optical-Model Potentials

- Expected influx of data for reactions on unstable isotopes from FRIB requires developing new OMPs for neutron-rich isotopes, including fission fragments.
- The status of OMPs was reviewed at a Topical Program at FRIB and findings were published in a review paper:
  C. Hebborn *et al*, "Optical potentials for the rare-isotope beam area," J. Phys. G. 50, 060501 (2023).
  https://arxiv.org/abs/2210.07293
- The publication discusses state-of-the-art potentials, identifies shortcomings, and charts a path for future theoretical and experimental work.



Estimates of the reach of FRIB (left) and paths of astrophysical processes (right). Nuclei whose properties were used to constrain the widely-used Koning-Delaroche OMP (in pink) highlight the dramatic extrapolations made. Fission fragments lie between r-process isotopes (teal) and stable isotopes (black).

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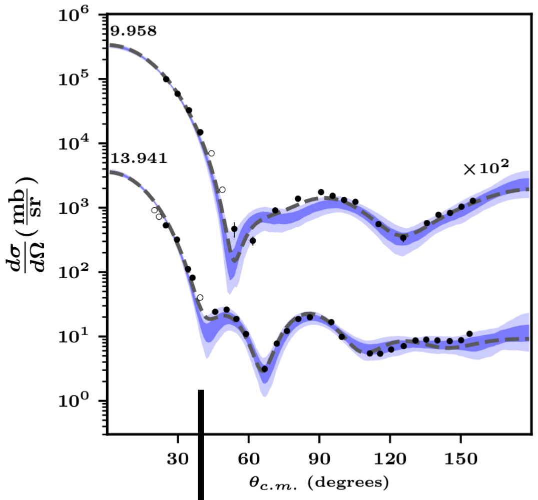
- The publication discusses state-of-the-art potentials, identifies shortcomings, and charts a path for future theoretical and experimental work.

	Mass	Energy	D.	Mic.	UQ
KD	$24 \leq A \leq 209$	1 keV $\leq E \leq 200$ MeV	✗	✗	✗
KDUQ	$24 \leq A \leq 209$	1 keV $\leq E \leq 200$ MeV	✗	✗	✓
DOM (STL)	C, O, Ca, Ni, Sn, Pb isotopes	$-\infty < E < 200$ MeV	✓	✗	✓
MR	$12 < Z < 83$	$E < 200$ MeV	✓	✗	✗
MBR	$12 < Z < 83$	$E < 200$ MeV	✓	✗	✗
NSM	^{40}Ca, ^{48}Ca, ^{208}Pb	$E < 40$ MeV	✓	✓	✗
SCGF	O, Ca, Ni isotopes	$E < 100$ MeV	✓	✓	✗
MST-B	$A \leq 20$	$E \gtrsim 70$ MeV	✗	✓	✗
MST-V	$4 \leq A \leq 16$	$E \gtrsim 60$ MeV	✗	✓	✗
WLH	$12 \leq A \leq 242$	$0 \leq E \leq 150$ MeV	✗	✓	✓
JLMB	$A > 30$	1 keV $< E < 340$ MeV	✗	✓	✗

Uncertainty-Quantified (UQ) Optical Potentials: KDUQ and CHUQ

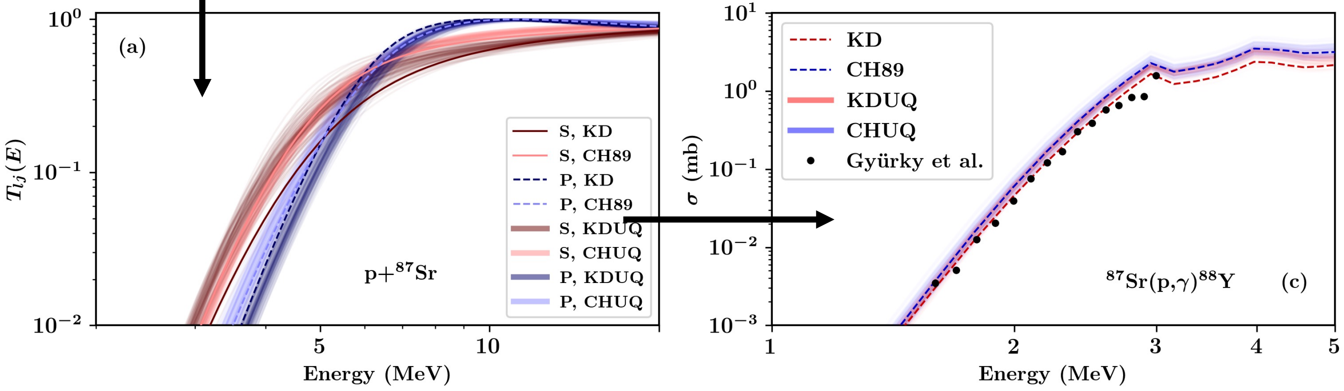
Pruitt, Escher, Rahman, PRC 107, 014602 (2023)

- We developed *well-calibrated uncertainties* for two widely used optical potentials
- Advances include *outlier identification*, assessment of *unaccounted-for uncertainty*
- We can now pinpoint how optical-potential uncertainties impact compound (low-energy) and direct (higher energy) reactions within a self-consistent framework
- Parameters provided with uncertainty ranges and as posterior collection - see PRC supplement.



After training (left), the UQ optical potential, shown as blue bands, spans its training data and performs well against test data not used in training (not shown).

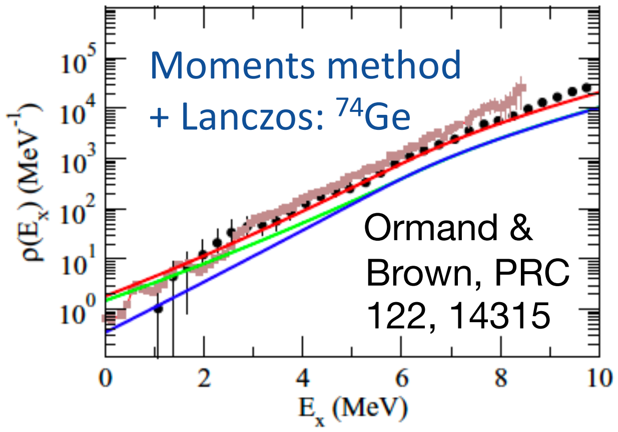
Uncertainties can then be propagated forward to transmission coefficients (below left) and capture cross sections (below right), here for ^{87}Sr(p,γ)^{88}Y.



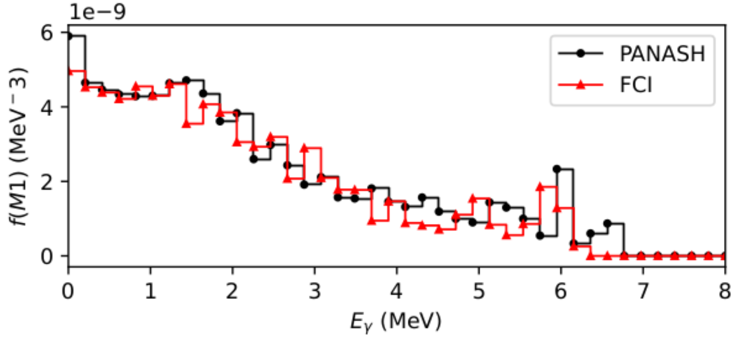
A global phenomenological dispersive OMP is under development.
Dispersive OMPs connect to bound-state properties - which helps address the lack of data for exotic nuclei.

Predicting level densities and γ strength functions: Advances in shell-model theory allow us to address these challenges

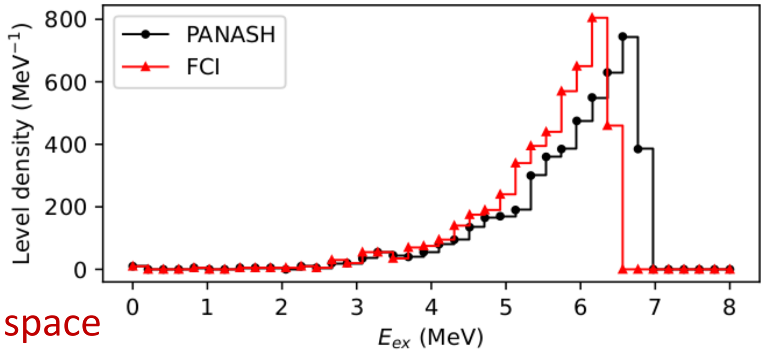
- The shell model provides a microscopic predictions for LDs and γSFs
- Smart truncations and modern computers increase reach of shell model
- Innovative combination of moments method with Lanczos algorithm enable new LD calculations
- Shell-model advantages:
  - Includes important correlations
  - Yields total and partial level densities
  - Gives low-energy γSF
  - Provides insights into structure
- Challenges:
  - Model space sizes for very heavy nuclei
  - Interactions needed



Gamma-ray strength function (γSF, M1) well-reproduced in truncated basis: ^{70}Ge

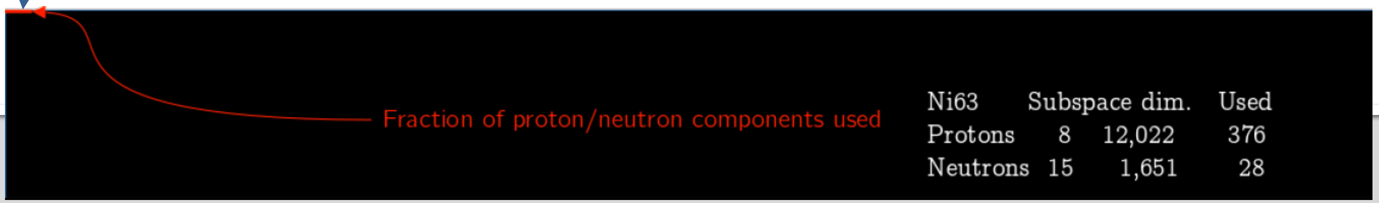


Level density (LD) is approximated in same truncated basis : ^{70}Ge



Smart truncation to small fraction of FCI model space

Gorton *et al*, arxiv:2210.05904



Surrogate reactions provide a viable method to extract information on neutron capture rates from indirect measurements

Determining capture rates for unstable nuclei directly is hard

- Short-lived target make measurements difficult/impossible
- Statistical Hauser-Feshbach (HF) calculations lack predictive power away from stability

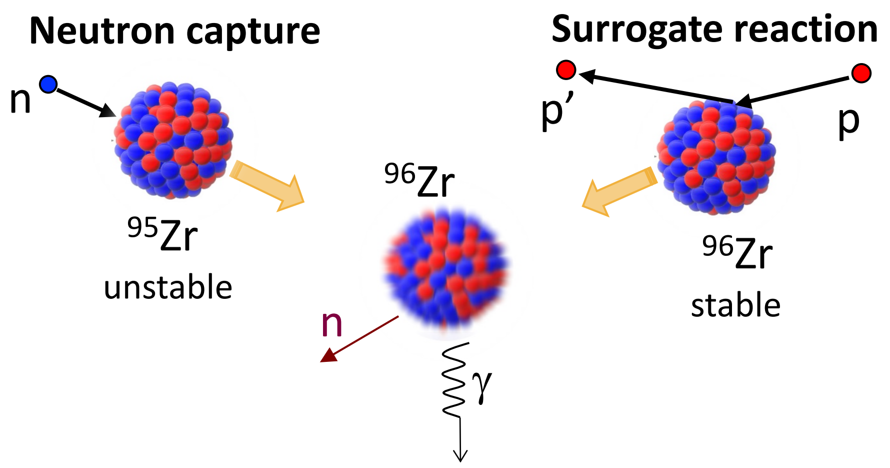
Surrogate reactions provide a solution

- A transfer or inelastic scattering experiment produces the compound nucleus and the decay is measured
- Advanced reaction theory turns this data into constraints for calculations of the desired neutron capture rate

Outcomes:

- Capture cross sections have been obtained from surrogate reactions using (p,d) and (d,p) transfers and inelastic scattering.
- Cross sections for capture involving isomers have been obtained.
- Level densities and γ strength functions can be obtained.
- Work is underway to apply the approach to inverse-kinematics experiments.
- Applications to fission are planned.

Neutron capture on s-process branch point ^{95}Zr from inelastic scattering



– (p,d)

PHYSICAL REVIEW LETTERS 121, 052501 (2018)

Constraining Neutron Capture Cross Sections for Unstable Nuclei with Surrogate Reaction Data and Theory

J. E. Escher,[1,*] J. T. Burke,[1] R. O. Hughes,[1] N. D. Scielzo,[1] R. J. Casperson,[1] S. Ota,[2] H. I. Park,[2] A. Saastamoinen,[2] and T. J. Ross[3]

– (α,α')

PHYSICAL REVIEW LETTERS 125, 122502 (2020)

Simultaneous Determination of Neutron-Induced Fission and Radiative Capture Cross Sections from Decay Probabilities Obtained with a Surrogate Reaction

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– (d,p)

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Towards Neutron Capture on Exotic Nuclei: Demonstrating $(d,p\gamma)$ as a Surrogate Reaction for (n,γ)

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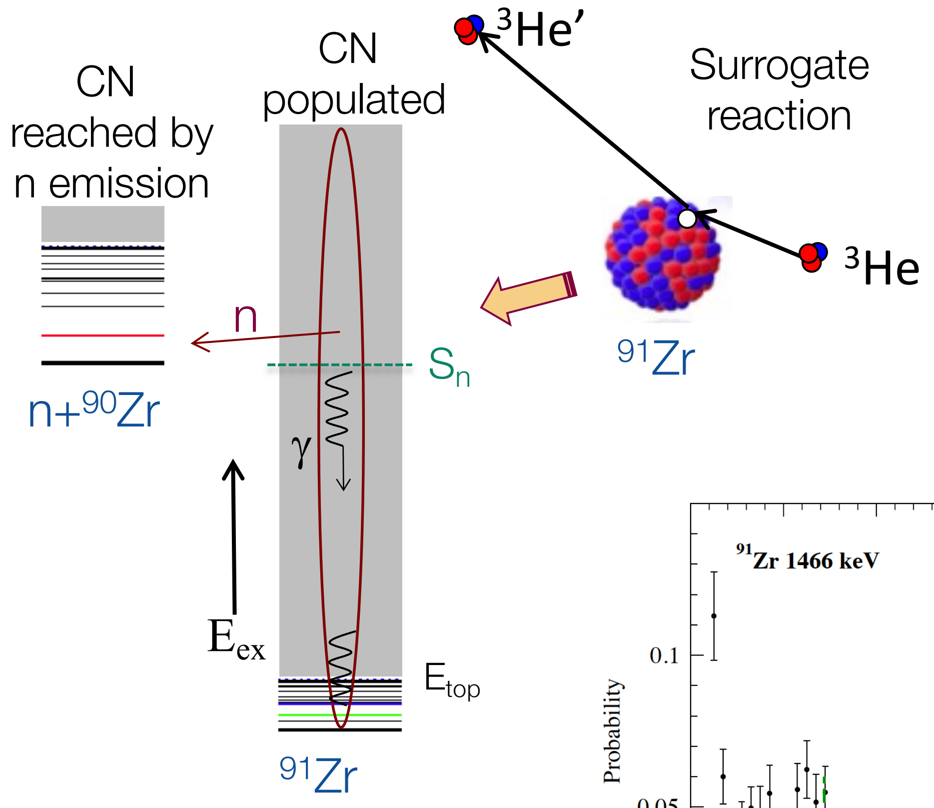
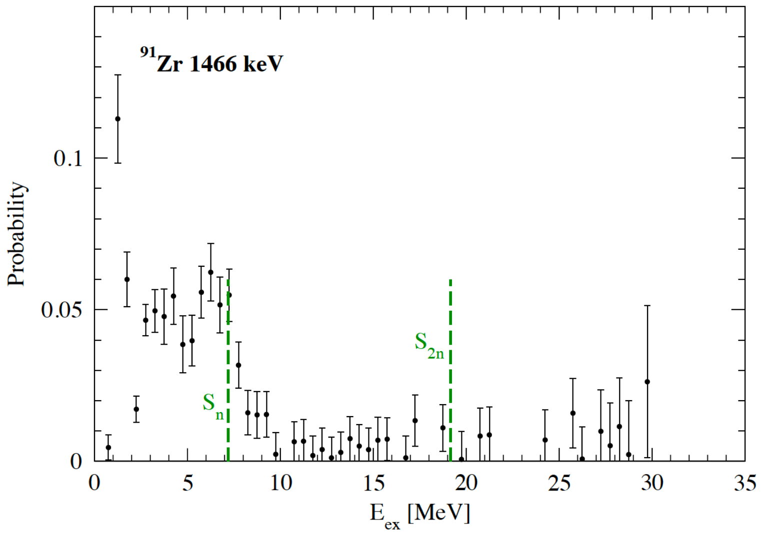
Surrogate reactions method for neutron capture



From experiment



From theory

To be determined

A Surrogate experiment gives

$$P_{(3He,3He'\gamma)}(E) = \sum_{J,\pi} F_{(3He,3He')}^{CN}(E,J,\pi) \cdot G^{CN}_{\gamma}(E,J,\pi)$$

^{90}Zr(n,γ) cross section:

$$\sigma_{(n,\gamma)} = \sum_{J,\pi} \sigma_{n+target}^{CN}(E,J,\pi) \cdot G^{CN}_{\gamma}(E,J,\pi)$$

The new cross section we want

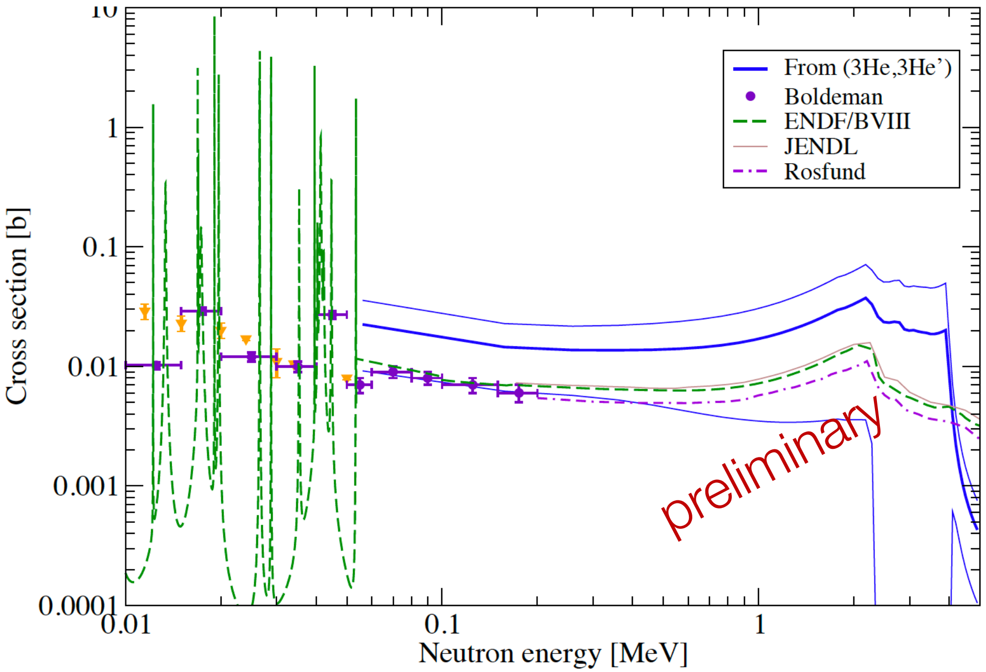
Well modelled from nuclear theory

Concept: Escher *et al*, RMP 84 (2012) 353; EPJConf 122 (2016) 12001

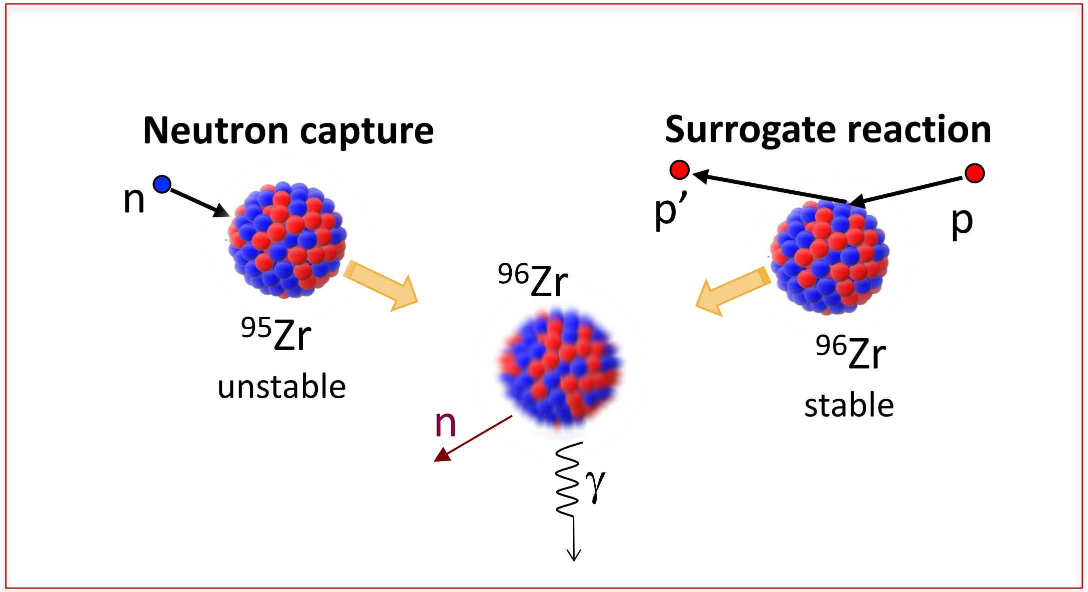
*Width fluctuation corrections are omitted here, but accounted for in applications.

Inelastic scattering theory will enable indirect measurements for neutron capture and other reactions on unstable isotopes

Benchmark: ^{90}Zr(n,γ) from ^{91}Zr(^{3}He,^{3}He')

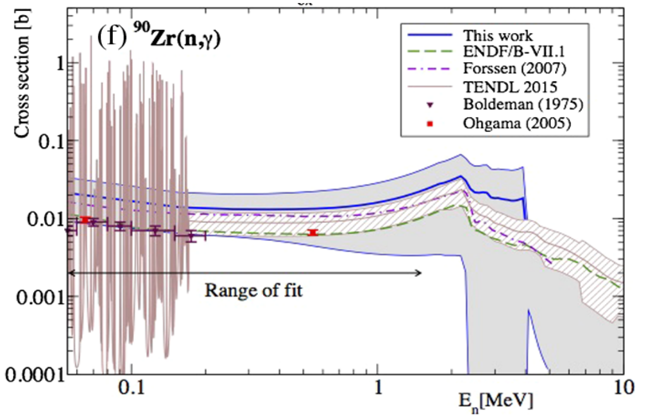


WIP: ^{95}Zr(n,γ) from ^{96}Zr(p,p')

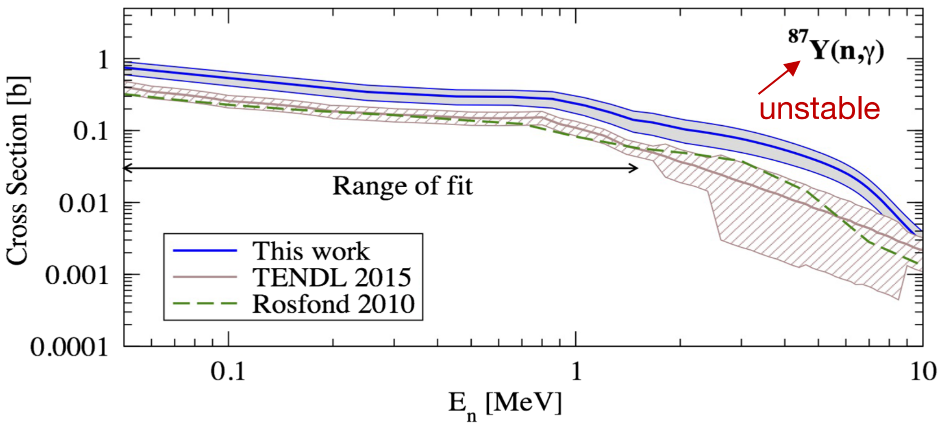


Surrogate reaction method gives LDs, γSF, capture cross sections, isomer cross sections, (n,n’) and (n,2n) cross sections

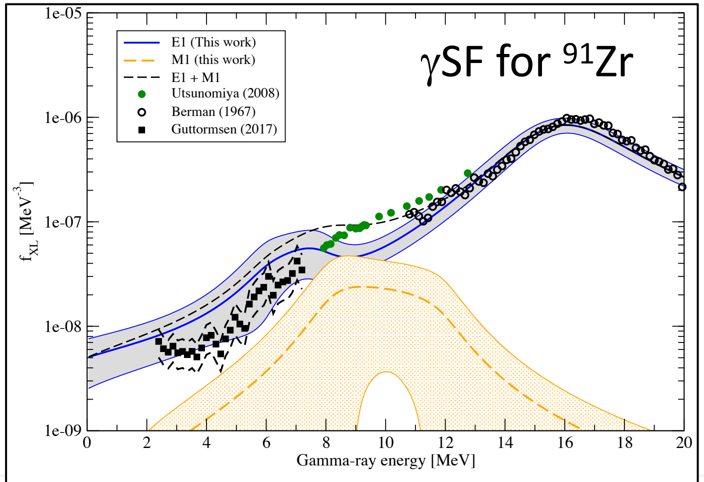
Escher et al. PHYSICAL REVIEW LETTERS **121**, 052501 (2018)



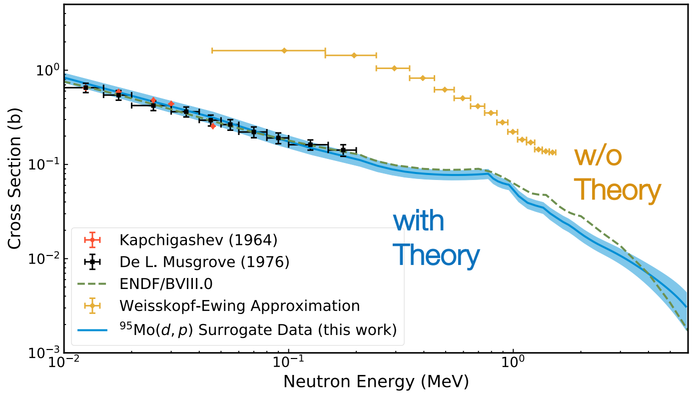
✓ Benchmark: ^{90}Zr(n,γ) from ^{92}Zr(p,dγ)



Application: ^{87}Y(n,γ) cross section from ^{89}Y(p,dγ)



PHYSICAL REVIEW LETTERS Ratkiewicz, Cizewski, Escher et al. (2019)



✓ Benchmark: ^{95}Mo(n,γ) cross section from ^{95}Mo(d,pγ)

Key features:

- Advanced theoretical description of surrogate reaction mechanism.
- Uses experimental observable indicating decay into channel of interest.
- Bayesian parameter determination for decay model → UQ is built-in!
- The Surrogate method does not use auxiliary quantities which are unavailable for unstable isotopes.

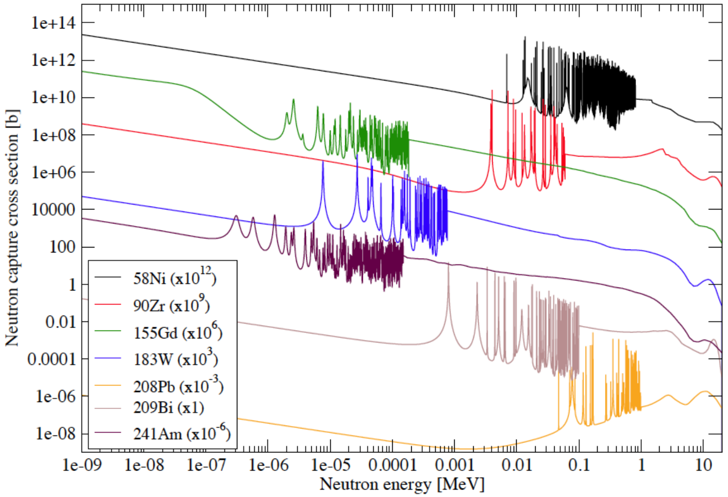
We need to address the limitations of Hauser-Feshbach calculations

Problem 1: HF calculations make an averaging assumption, but problems occur for low energies, closed shells, light nuclei, far from stability

We need:

- Criteria for estimating the limits of validity for HF
- Usable prescriptions for treating compound reactions proceeding through isolated or weakly-overlapping resonances, bridge to HF
- Structure information for calculating direct-reaction contributions
- An assessment of uncertainties and experimental information

(n,γ) cross sections
for select stable isotopes (ENDF/B-VII)



Problem 2: Some reactions fail to produce a compound nucleus. Pre-equilibrium neutron reactions are known to have limitations. Indirect measurements may be affected.

Consider:

- When do doorway states proceed to damp?
- Transfers, inelastic scattering have been studied for surrogate reactions
- β-decay may be of concern

Hauser-Feshbach regime

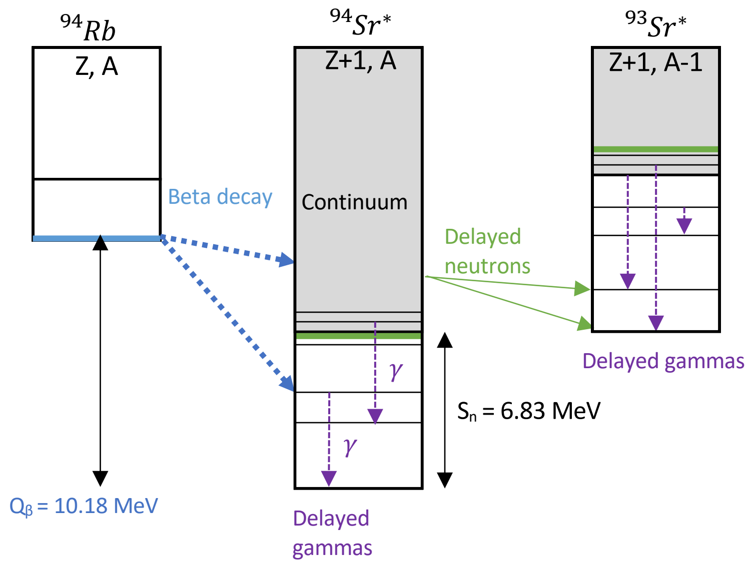
- Assumes strongly overlapping resonances
- Requires structure models and parameters

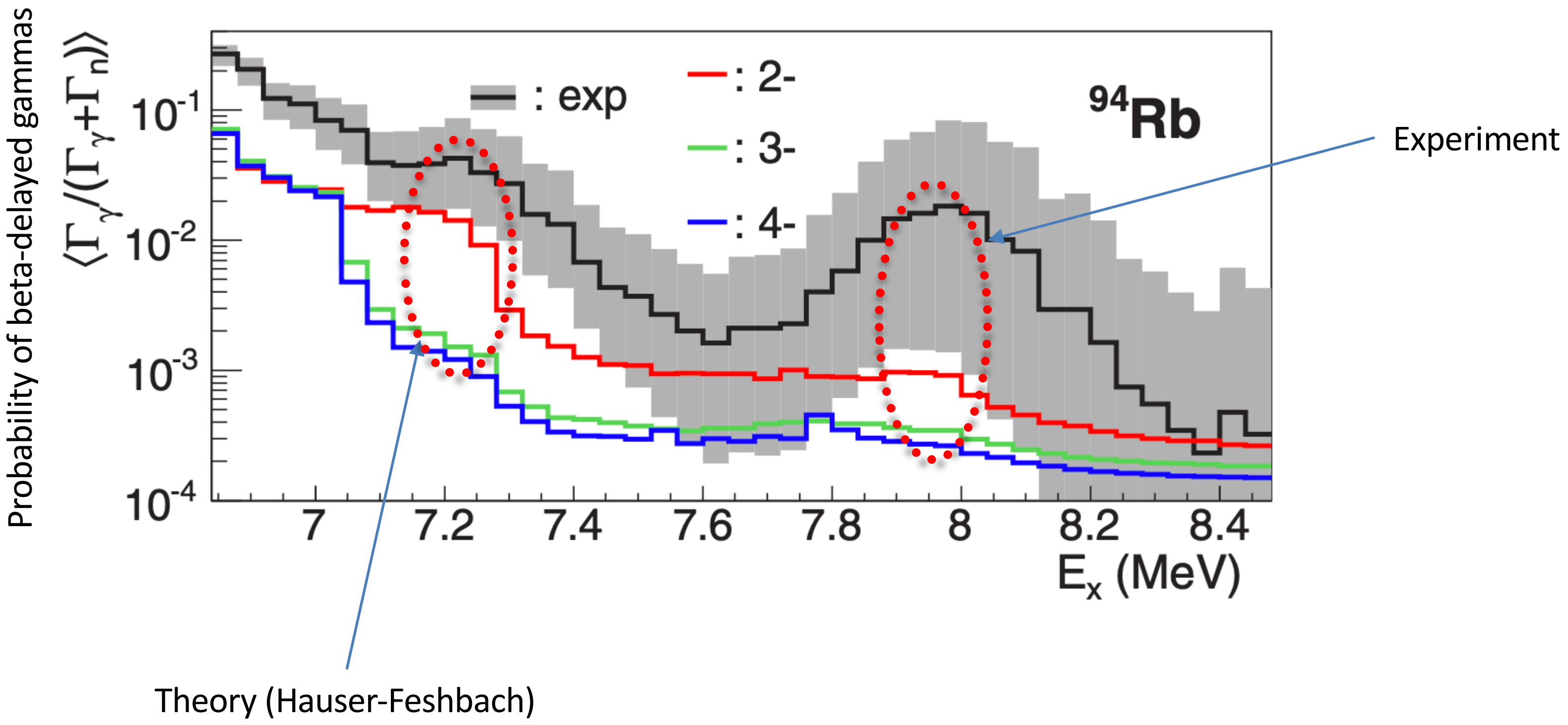
$$\sigma_{\alpha\chi} = \sum_{J,\pi} \sigma_\alpha^{CN}(E,J,\pi) \cdot G^{CN}_\chi(E,J,\pi)$$

*WFC omitted here to simplify notation.

Statistical models underpredict β-delayed γ spectrum

Gorton, Johnson, Escher (wip)



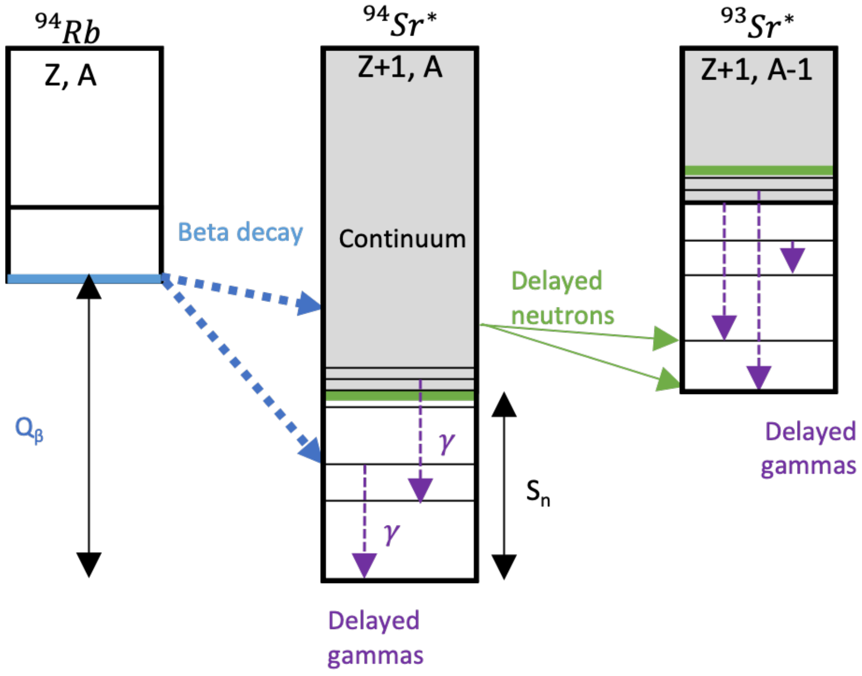


Valencia, et al., 2017 https://link.aps.org/doi/10.1103/PhysRevC.95.024320

See also: Robert Grzywacz *et al*. nonstatistical nature of neutron emission near ^{134}Sn

Why are we getting this so wrong?
BDNE is a powerful test for nuclear structure and reactions

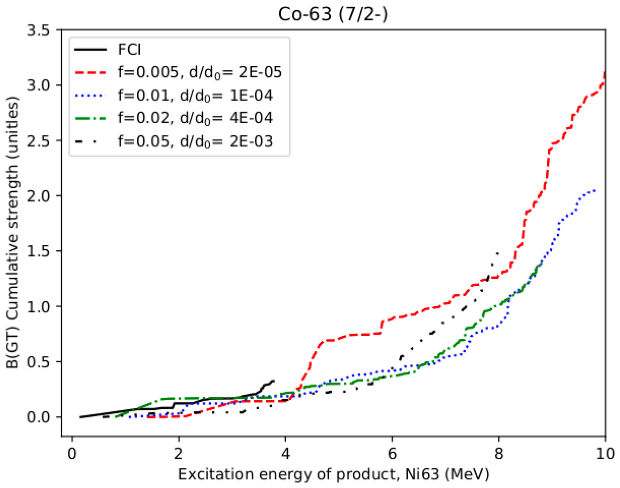
Gorton, Johnson, Escher (wip)

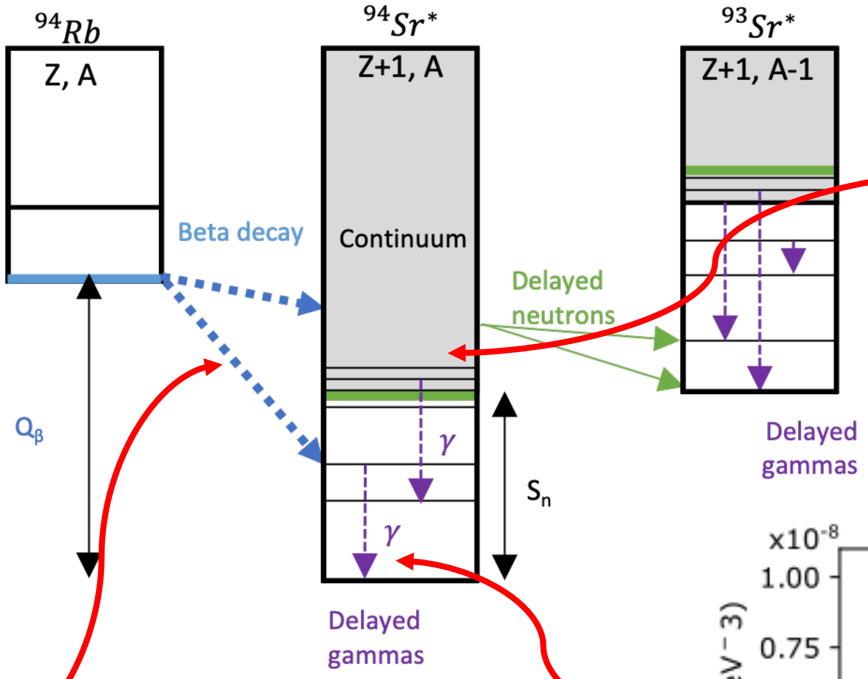


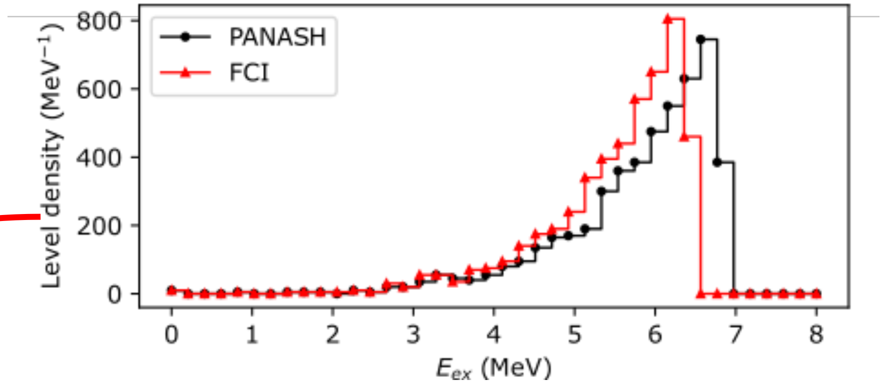
- Does β-decay fail to create a well-equilibrated (statistical) nucleus?
- Does an unexpectantly large "forbidden" β-decay block neutron emission?
- Is the γ-ray decay strength greatly enhanced?

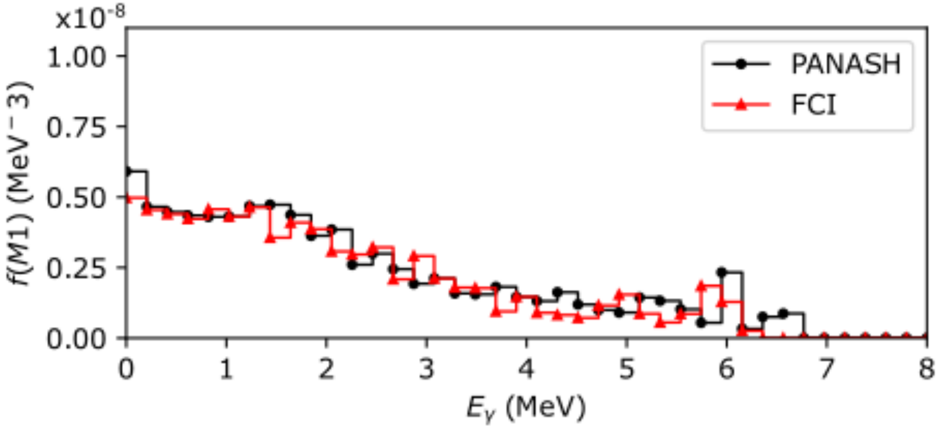
To model nuclei beyond the standard shell model, approximate truncation methods are being developed

Gorton, Johnson, Escher (wip)









But we will need new interactions!

Items on my wish list

Generally:
Systematic trends (single-particle properties, collective properties,…)

Inelastic scattering:
- Charged-particle scattering off a chain of isotopes, angular distributions
- Protons, deuterons, ^{3}He, ^{4}He
- Careful assessment (elimination?) of background
- Coincident measurements of decays (γ, particle emission) for surrogate applications

Surrogate reaction development:
- Multiple measurements producing the same compound nucleus
- Information on low-lying states and their decays

Optical potential development:
- Elastic scattering angular distributions
- Single-particle energies

Shell-model development:
- data to build new interactions

Challenging:
- Tests of equilibration of nucleus in β-decay and reactions
- Brilliant ideas for dealing with the limits of statistical averaging

Thank you!

A thank you to my collaborators:

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Rutgers U.: J. Cizewski
SDSU: O. Gorton, C. Johnson
UTK/ORNL: S. Pain, R. Grzywacz, J. Heideman
CEA/France: M. Dupuis, S. Peru

Hauser-Feshbach (statistical reaction) formalism for compound reactions

$$\sigma_{\alpha\chi}(E) = \sum_{J\pi} \sigma_\alpha^{CN}(E,J,\pi)\, G_\chi^{CN}(E,J,\pi)$$

Formation of CN

$$\sigma_\alpha^{CN}(E,J,\pi) = \pi \lambda_\alpha \omega_\alpha^J \sum_{ls} T_{\alpha ls}^J$$

Probability for decay of CN

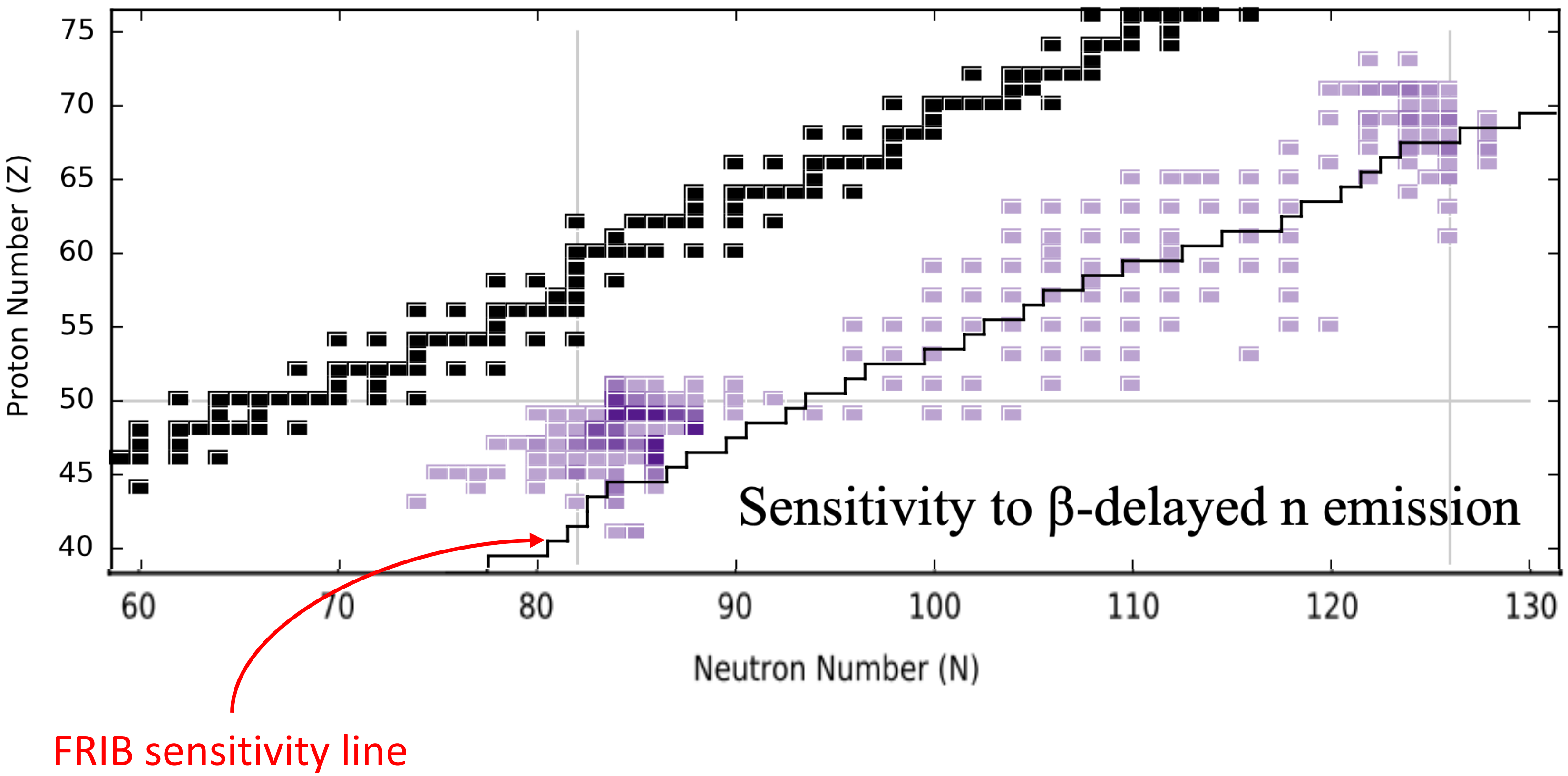
$$G_\chi^{CN}(E,J,\pi) = \frac{\sum_{l's'} T_{\chi l's'}^J \, \rho_{I'}(U')}{\sum_{\chi''l''s''} \int T_{\chi''l''s''}^J \, \rho_{I''}(U')\, dE_{\chi''}}$$

Need

- Transmission coefficients T_χ for all channels χ: neutron, proton, charged particles, γ, fission
- Level densities
- Discrete levels with J, π
- Width fluctuation correction WFC factors

*Width fluctuation corrections are omitted here, but accounted for in applications.

Beta-delayed neutron emission is important for astrophysical element synthesis – and FRIB reaches many high-impact nuclei



It's important to have a strong theoretical description of BDNE

Mumpower, et al., 2015 https://doi.org/10.1016/j.ppnp.2015.09.001

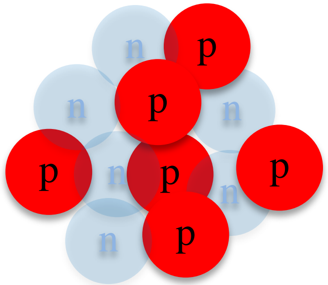
Proton and Neutron Approximate Shell Model (PANASH)

$$H = H_p + H_n + H_{pn}$$

- Wave functions factorize into PN-partition eigenstates
- Coefficients decay exponentially
- Proton neutron entanglement decreases when N>Z (arxiv 2210.14338)

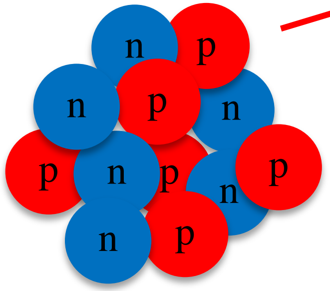
Bipartite Partitioning

(Orders of magnitude smaller!)



Proton Hamiltonian

$$H_p \left| j_p \right\rangle = E_p \left| j_p \right\rangle$$

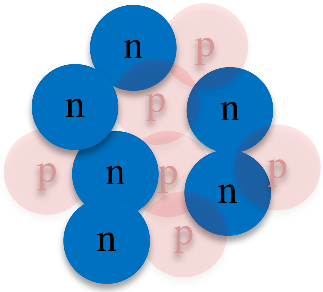


$$\hat{H}|\Psi\rangle = E|\Psi\rangle.$$

Full Configuration Hamiltonian

$$\left| j_p j_n \right| J\rangle = \left| j_p \right\rangle \otimes \left| j_n \right\rangle \Big|_J$$

j-j coupled basis



Neutron Hamiltonian

$$H_n \left| j_n \right\rangle = E_n \left| j_n \right\rangle$$

$$|\Psi\rangle \approx \sum_{ab}^{d \ll D} c_{ab} \left| j_p \right\rangle \left| j_n \right\rangle$$

(There is some freedom in the sum)