Building a predictive theory of photoabsorption/deexcitation

Needs and opportunities

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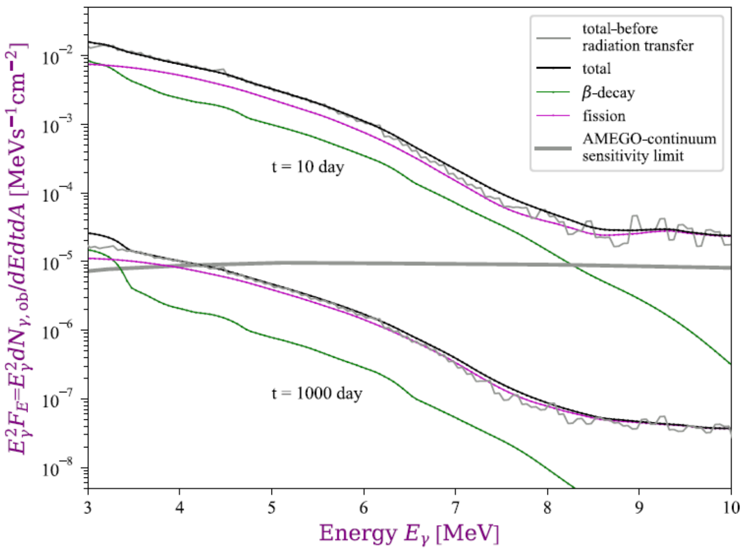
Electromagnetic processes

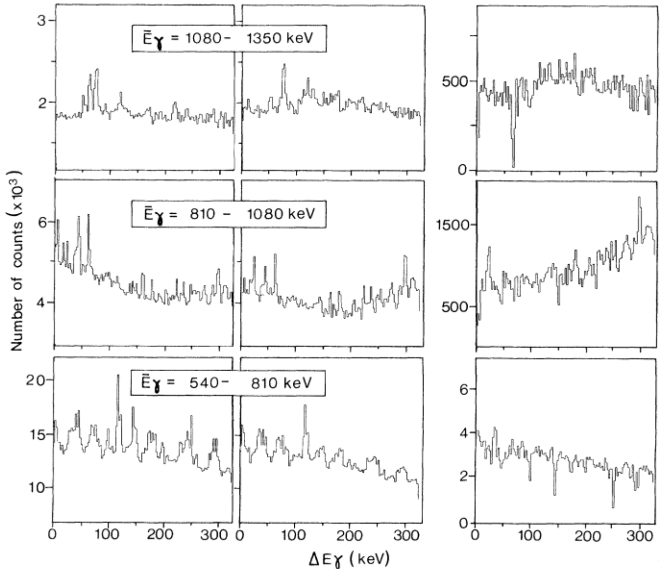
Photon data – photo-induced reactions, γ decay or electron capture – play a critical role in understanding the formation of elements, in probing nuclear structure and in validating fission theories

ApJL **903,** L3 (2020)



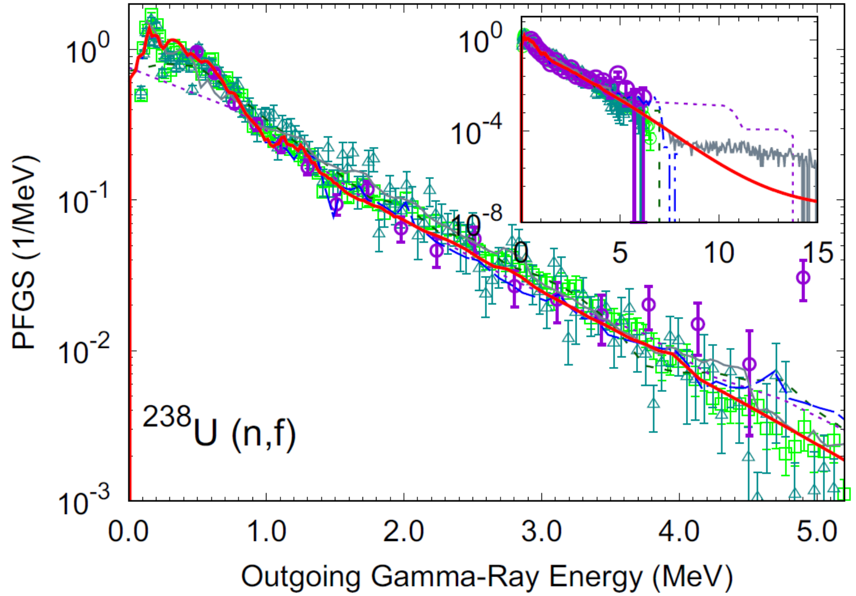
High-energy γ rays from neutron-rich fission products may signal actinide production in neutron star mergers

PRL **55,** 1380 (1985)



γ-ray spectroscopy has been used for decades to probe the energy spectrum of atomic nuclei

Nucl. Data Sheets **163**, 261 (2020)



Prompt fission γ spectrum is important metric for applications

Robust theoretical models of e.m. processes are indispensable to make reliable predictions and interpret/guide experimental programs

QRPA/Linear response theory

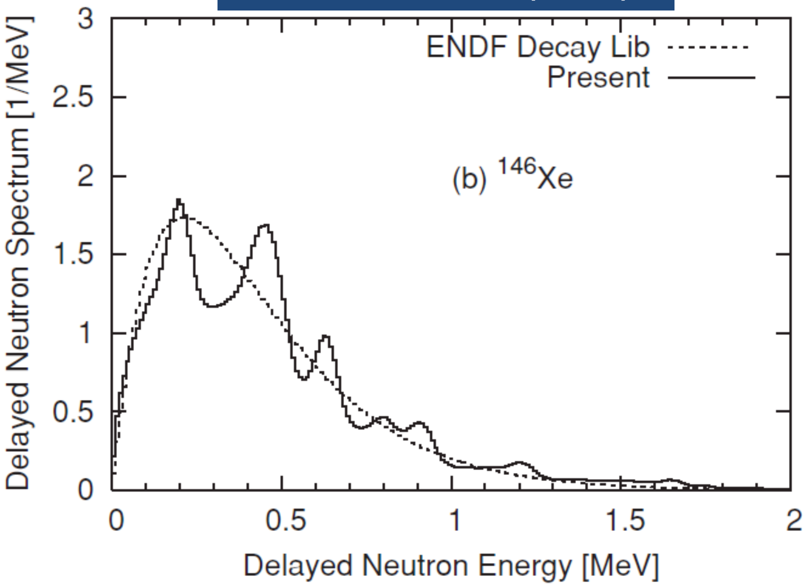
Linear response theory is currently the only approach that predicts electromagnetic observables at the scale of the entire nuclear chart

- QRPA / linear response theory:
  - Part of broader framework of nuclear density functional theory
  - Response of the nucleus to a small perturbation
- Perturbation operator characteristics of the physical process
  - E1 electric dipole operator for leading effect in radiative capture (=photoabsorption)
  - E1, E2, M1 operators for most relevant γ decay of excited nuclear states
  - Fermi, Gamow-Teller, first-forbidden for β decay (charge-changing operators)
- Two methods of solution:
  - Direct: Build a large, dense matrix and diagonalize
    - Get excited levels and wavefunctions and construct transition strengths out of them
    - Computational cost grows (significantly) with broken symmetries
  - Finite-amplitude method (FAM): Solve directly for the strength function (introduced in 2007)
    - Constant computational cost
    - No (direct) access to excited levels and wavefunctions

"Simplified" QRPA

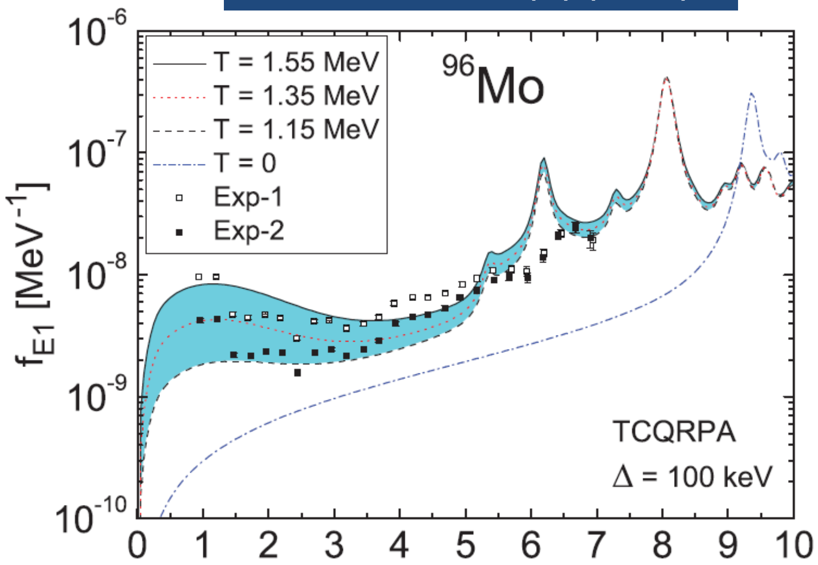
The residual interaction responsible for the response may be very different from the nuclear forces that determine the ground state of the nucleus, and some symmetries may be assumed

PRC **78**, 054601 (2008)



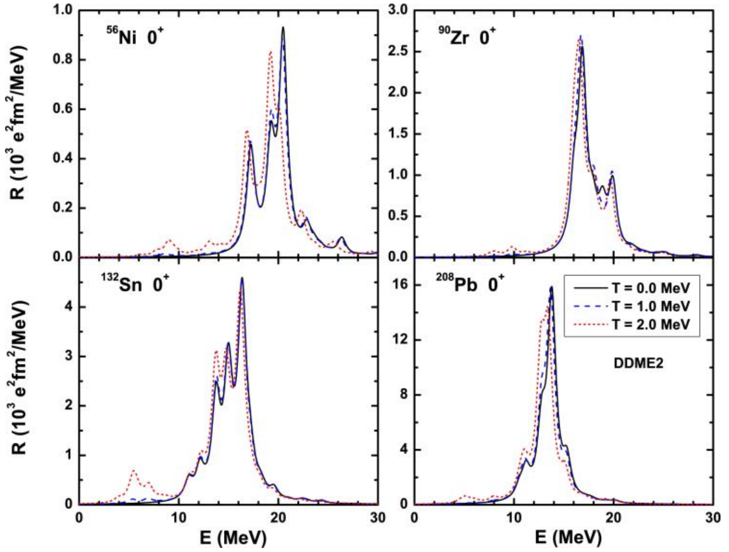
- Deformed Nilsson potential
- QRPA with simplified residual interaction

PRC **88**, 031302(R) (2013)



- Spherical Woods-Saxon
- Continuum, temperature-dependent QRPA with simplified interaction

PLB **681**, 315 (2019)



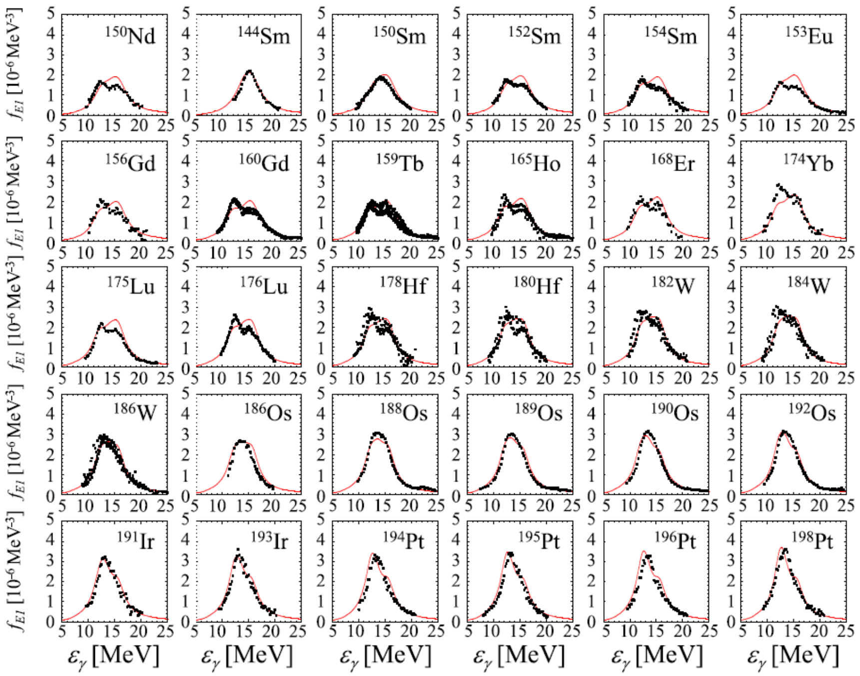
- Spherical RHB
- Continuum, temperature-dependent QRPA with consistent interaction

Besides empirical fits, flavors of simplified QRPA have been the cornerstone of evaluations for photon data (and β-decay related observables) for the last 15 years

Microscopic QRPA

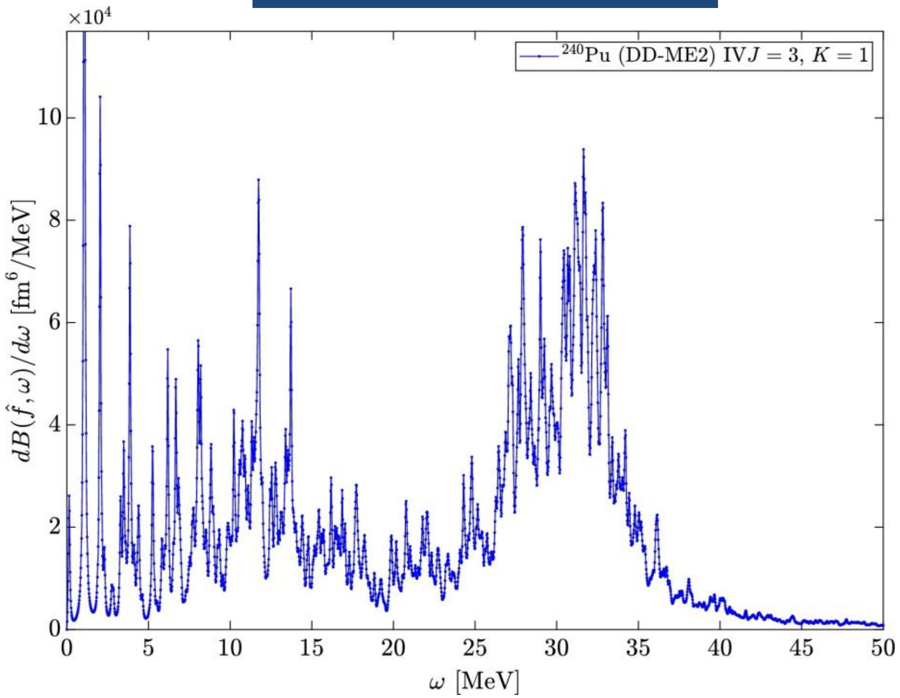
The residual interaction responsible for the response is the same as the nuclear forces that determine the ground state of the nucleus and, all relevant symmetries are broken

PRC **98,** 014327 (2021)



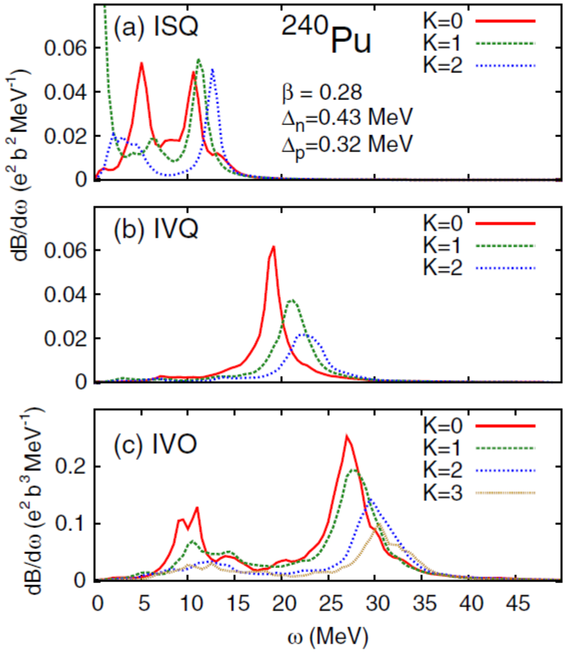
Axially-deformed QRPA with the Gogny force

CPC **287,** 108689 (2022)



Axially-deformed QRPA with the relativistic mean field + FAM

PRC **92**, 051302(R) (2015)



Axially-deformed QRPA with the Skyrme force + FAM

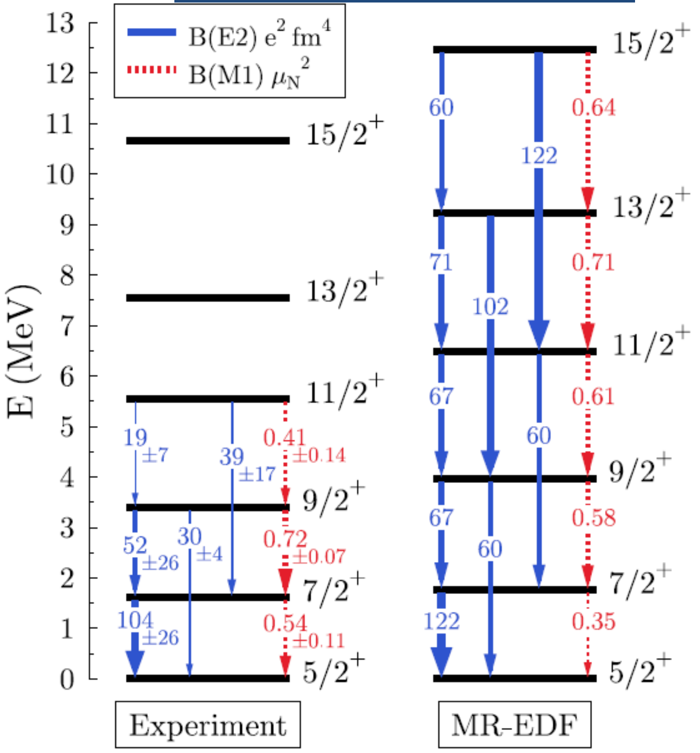
Current computational resources mean we can now compute the linear response fully self-consistently across the mass table – consistency will significantly improve UQ

Longer Term Perspectives

Extended QRPA theories and/or multi-reference energy density functional methods have shown potential to describe phenomena such as strength fragmentation or low-lying e.m. transitions

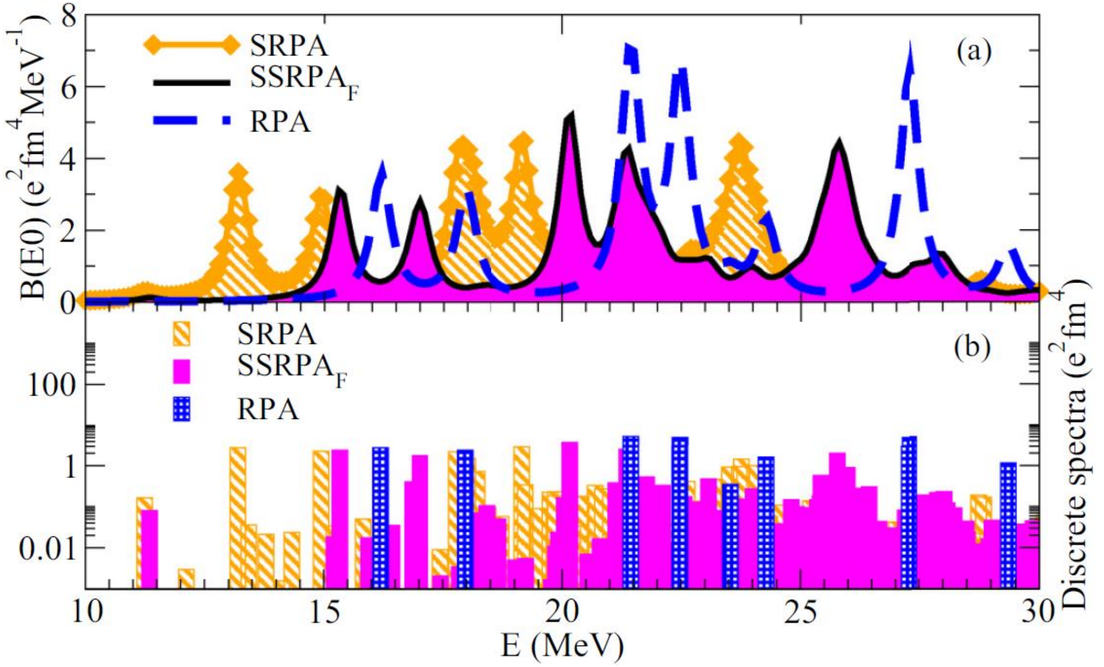
- Linear response theory is 2nd order approximation in small amplitude collective motion: go beyond 2nd order
- Large-amplitude collective motion captured by (response to) deformation: use configuration mixing

PRL **113**, 162501 (2014)



Multi-reference energy density functional method (= projected GCM) in ^{25}Mg

PRC **92**, 034303 (2015)



Giant monopole resonance
Second RPA (subtraction method)

Outlook

Theoretical models of photoexcitations have significantly improved over the past 15 years – some of the new models can and should be put to systematic tests against available experimental data

- Short term
  - Systematic, self-consistent calculations of γ-strength functions are possible with the FAM – including, e.g., odd-mass and odd-odd nuclei (LLNL contribution to NA22-funded “Evaluation of γ-ray production”
  - Combine UQ and modular reaction codes to disentangle γ-strength functions from level densities, transmission coefficients, etc., to obtain constraints on γ-strength functions
  - Photon data provides experimental constraints on the time-odd channel of energy functionals (Skyrme, Gogny, relativistic, etc.) $\Rightarrow$ paves the way for more predictive DFT
- Longer term
  - Extended (Q)RPA models must be tested in more realistic calculations (=deformed nuclei)
  - Quality of predictions of photon processes largely contingent on good nuclear structure models
    - Nuclear shell model provides coherent framework for both low-lying levels, discrete transitions and γ-strength functions
    - Multi-reference EDF methods (aka: beyond mean field) are a potentially good, global alternative applicable in every nucleus
- More microscopic theories with fewer (and more correlated) parameters are key ingredients for uncertainty quantification and propagation

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