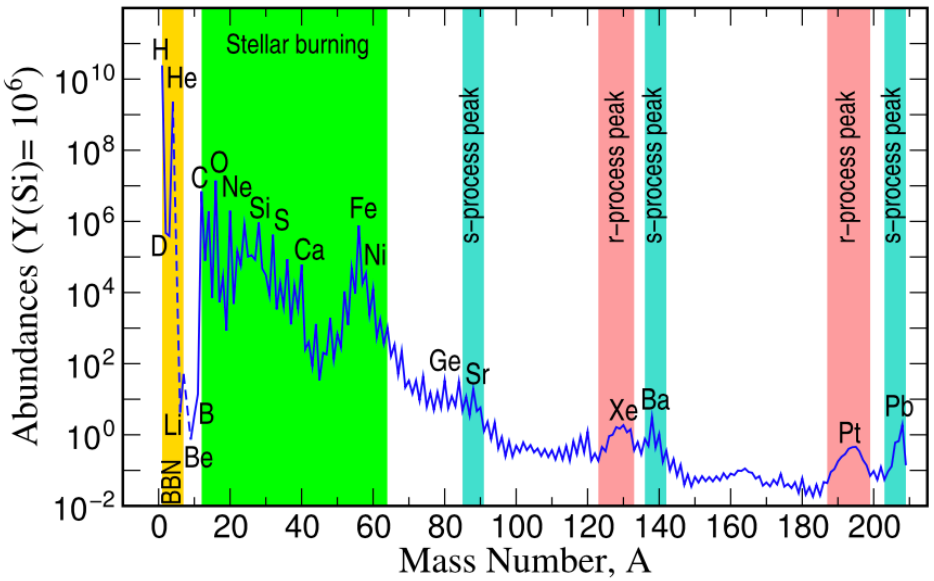
Statistical Properties of Nuclei: Beyond the Mean-Field Approximation

Paul Fanto

Yale University
Ph.D. Advisor: Prof. Yoram Alhassid
DOE NNSA SSGF Program Review
August 2021

Compound-nucleus reactions

- Compound nucleus (CN): equilibrated system of projectile and target nucleus. Bohr, Nature (1936)
- Theoretical models of CN reactions are needed for calculating reaction rates used in many applications.
- e.g., *r*-process nucleosynthesis, which produces the most neutron-rich nuclei.



Cowan *et al.*, Rev. Mod. Phys. (2021)

Nuclear data evaluation

- Nuclear data evaluation: provides databases of important nuclear reaction quantities for research, defense, and technological applications.
- Basis of evaluation process: large-scale reaction code fitted to data where available.

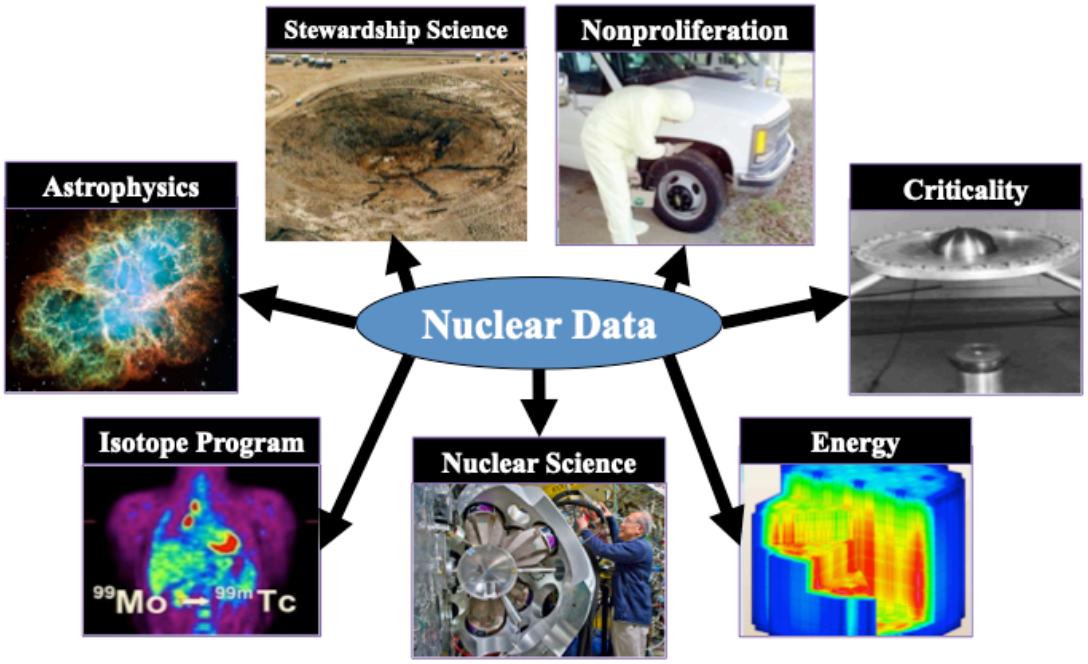


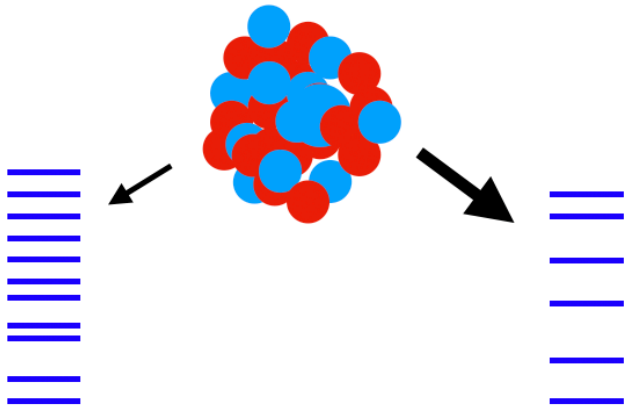
image from talk of Prof. Lee Bernstein, U.C. Berkeley, head of Bay Area Nuclear Data group

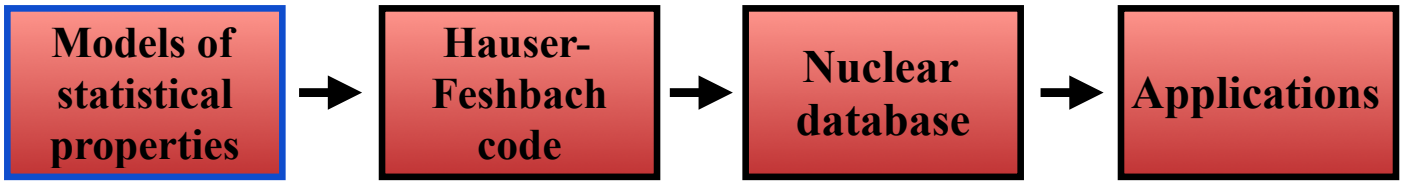
Statistical nuclear reaction model

- Statistical (Hauser-Feshbach) model: cross sections depend on relative probabilities of competing reaction channels.

  Hauser and Feshbach, Phys. Rev. (1952)

- Channel probabilities depend on statistical properties of nuclei:
  - ✶ Number of nuclear levels per unit energy: level density.
  - ✶ Average probability of decaying to a given level: strength functions.





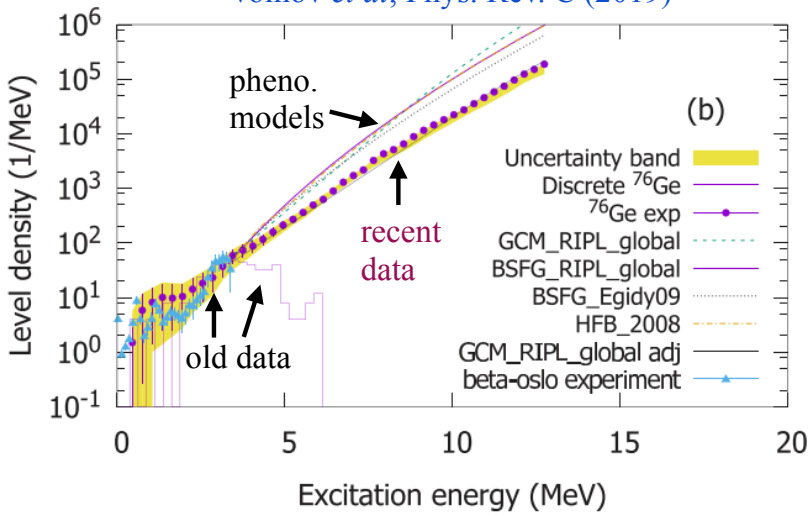
How can we improve the level densities used in statistical reaction codes?

Limitations of phenomenological level densities

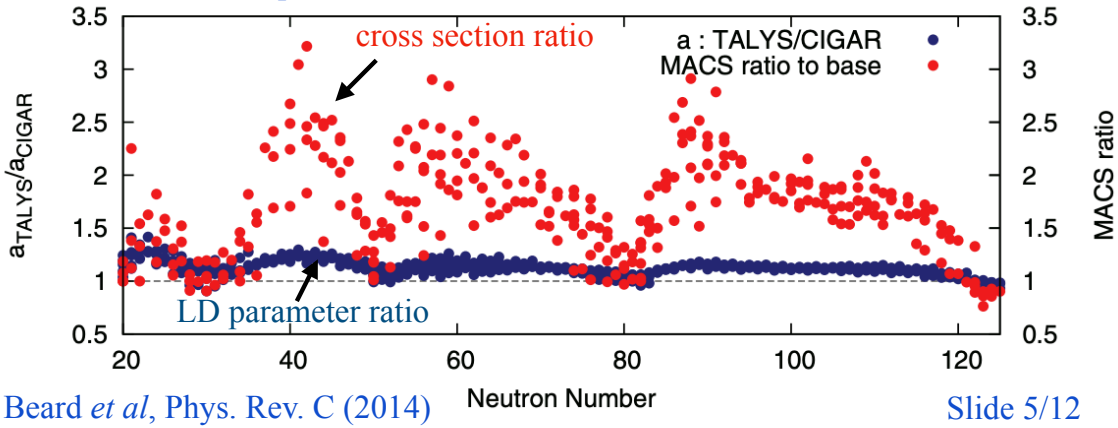
- Reaction codes rely on phenomenological level densities: parameterized functions fitted to data.
- Phenomenological models become unreliable when extrapolated away from data.
- Level densities are challenging to measure, and data are typically available in restricted energy ranges.
- Reaction rates are sensitive to level density variations.

Goal: replace phenomenological level densities with a microscopic method

Voinov *et al*, Phys. Rev. C (2019)



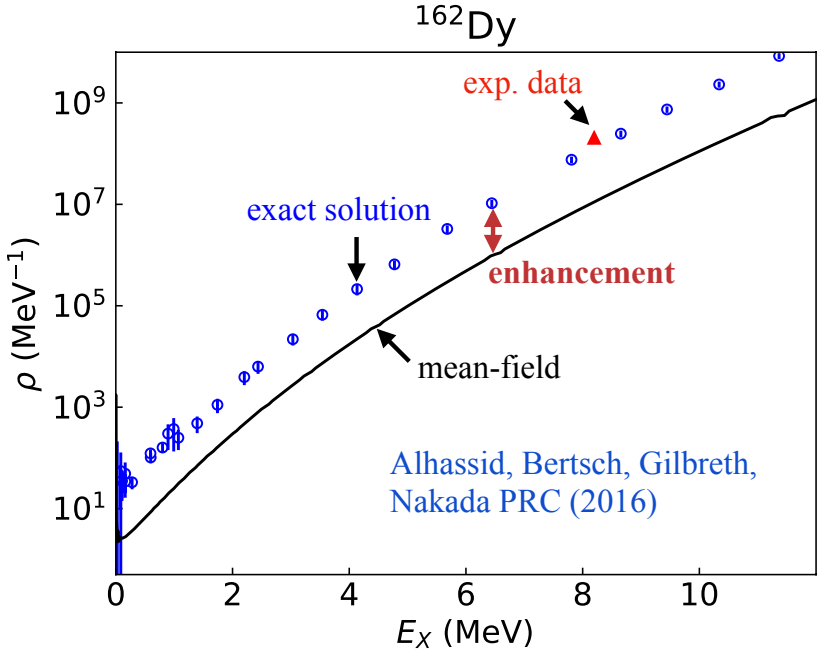
Comparison of LDs/cross sections in two reaction codes



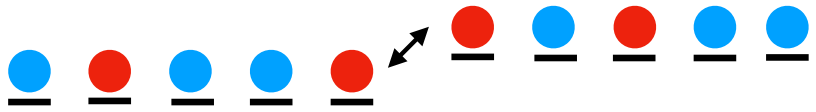
Beard *et al*, Phys. Rev. C (2014)

Limitations of current methods

- **Mean-field approximation**
  - ✳ Main microscopic method for calculating level densities for Hauser-Feshbach codes.
  - ✳ Replaces nuclear interaction with a self-consistent one-body potential.
  - ✳ Mean-field methods cannot reproduce important correlation effects, e.g., collective enhancement.
  - ✳ Empirical models of collective enhancement are used in mean-field calculations. Hilaire, Girod, Goriely, and Koning Phys. Rev. C (2012)

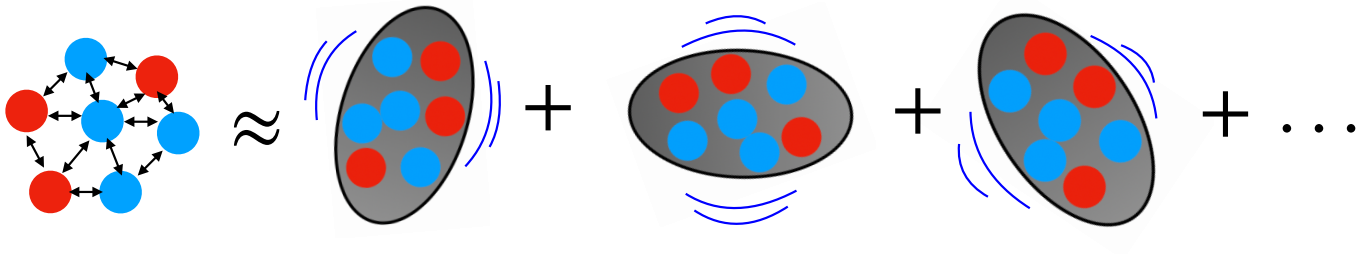


- **Configuration-interaction (CI) shell model**
  - ✳ Nucleons fill sets of orbitals (configurations), and the interaction mixes configurations.
  - ✳ Computational cost becomes prohibitively large for heavy nuclei.



Static-path plus random-phase approximation (SPA+RPA)

- Calculate level densities of heavy nuclei from finite-temperature observables in the CI framework.
- SPA+RPA: integrates over an ensemble of non-interacting nuclear systems in external potentials.
  - ✴ Integration variables: static auxiliary fields that define the external potentials.
  - ✴ Accounts for small-amplitude time-dependent quantal fluctuations: random-phase approximation.



- SPA+RPA found to be accurate in solvable models above a low breakdown temperature. Puddu, Bortignon, Broglia, Ann. Phys. (1991) Attias and Alhassid, Nucl. Phys. A (1997)
- We evaluate SPA+RPA finite-temperature observables using a Monte Carlo method.
- Shell model Monte Carlo (SMMC): includes all correlations beyond the mean field, can calculate (most) finite-temperature observables exactly. Alhassid, in *Emergent Phenomena in Atomic Nuclei from Large-Scale Modeling: a Symmetry-Guided Perspective*, ed. Launey (2017)

Monte Carlo method

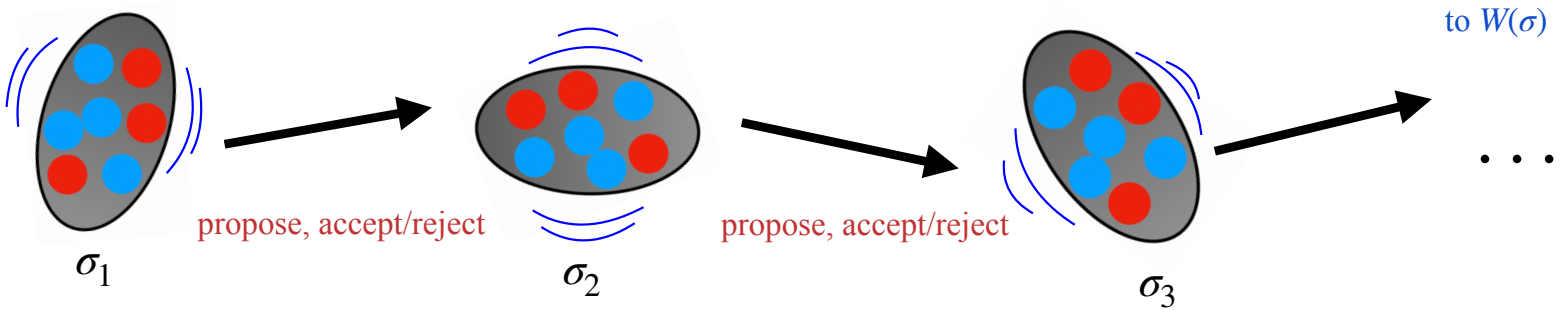
- Generate samples σ_k from weight function $W(\sigma)$ by executing a random walk in the space of static fields.
- Metropolis-Hastings algorithm: propose updates $\sigma \to \sigma'$ and accept with probability $A(\sigma' \,|\, \sigma) = \min\left(W(\sigma')/W(\sigma), 1\right)$.

weight function

$$\mathcal{O} \approx \frac{\int d\sigma W(\sigma)\mathcal{O}(\sigma)}{\int d\sigma W(\sigma)} \approx \frac{1}{n}\sum_k \mathcal{O}(\sigma_k)$$

observable

sampled according to $W(\sigma)$



- Averages over decorrelated samples estimate the expectation values, and the standard deviations quantify the statistical errors.
- Computational cost scales gently with the number of integration variables.

SPA+RPA state densities of samarium isotopes

- Isotopes $^{148\text{-}155}$Sm describe the crossover from vibrational to rotational collectivity. Özen and Alhassid, Phys. Rev. Lett. (2013)
- Nuclear state density: counts all 2J+1 degenerate states associated with a level of spin J.

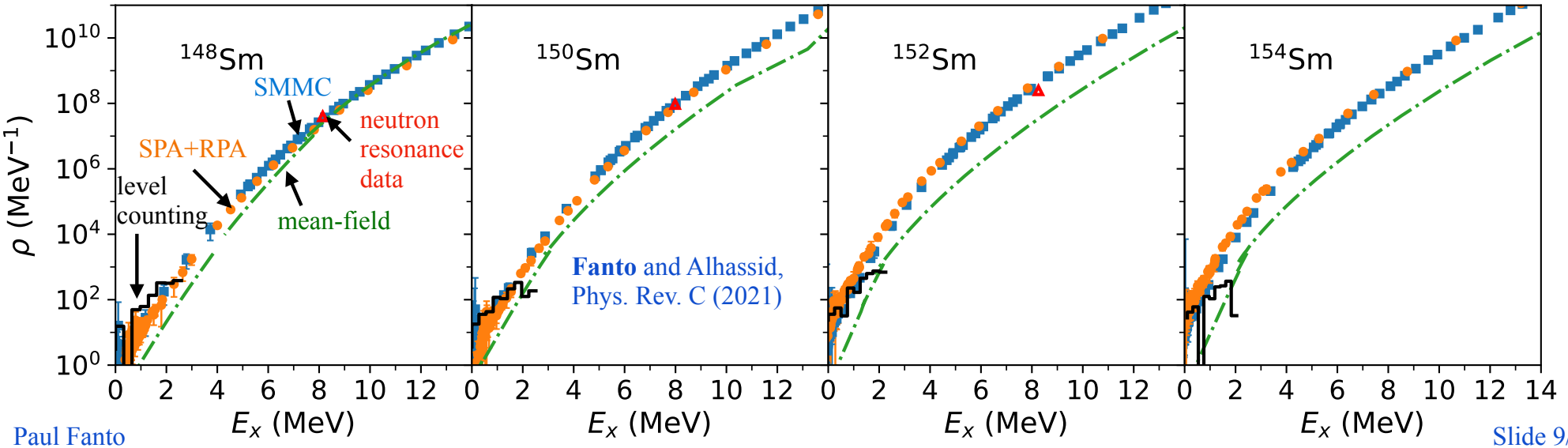
$$\rho(E) \approx \frac{e^{S}}{\sqrt{2\pi T^2 C}}$$

(e^S ← entropy; $\sqrt{2\pi T^2 C}$ ← heat capacity)

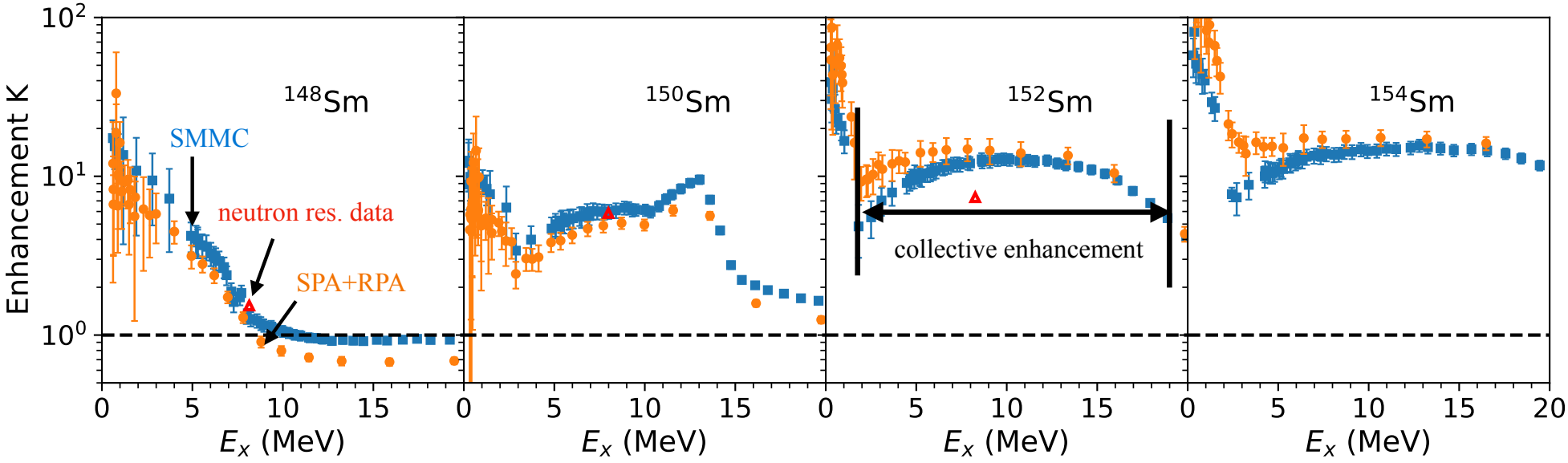
$$E = E(T)$$

(E: thermal energy)

- We find good quantitative agreement with exact SMMC state densities and experimental data.
- The SPA+RPA improves over mean-field state densities calculated with the finite-temperature Hartree-Fock-Bogoliubov (HFB) approximation. Ryssens and Alhassid, Eur. Phys. J. A (2021)



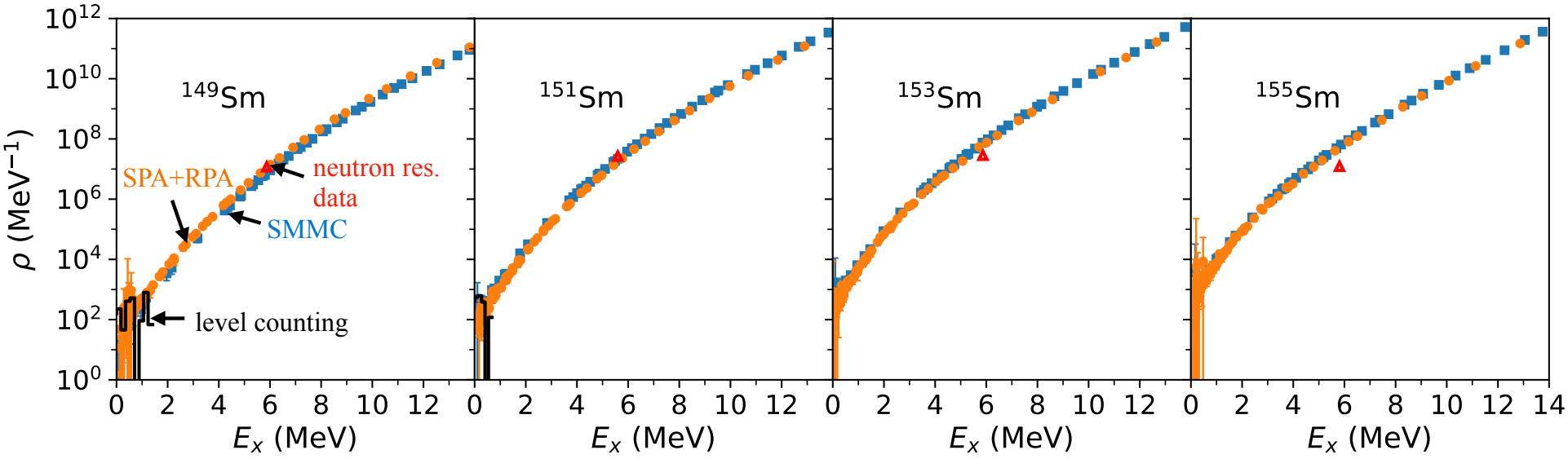
Collective enhancement over mean field



Fanto and Alhassid, Phys. Rev. C (2021)

- Collective enhancement factor $K = \rho/\rho_{\text{mean-field}}$.
- Origin of enhancement: rotational bands that are not described by the HFB approximation.
- SPA+RPA naturally describes the collective enhancement. **No need for empirical collective enhancement factors.**

State densities of odd-mass $^{149\text{-}155}$Sm



Fanto and Alhassid, Phys. Rev. C (2021)

- SPA+RPA results agree well with exact SMMC results and experimental data for odd-mass samarium isotopes.

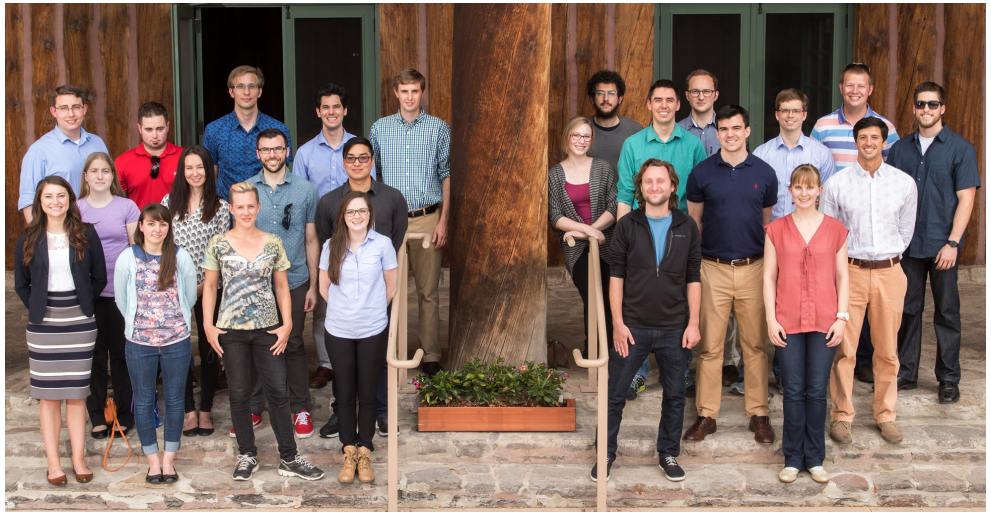
Conclusions

- The static-path plus random-phase approximation (SPA+RPA) can be applied to calculate state densities of heavy nuclei with a Monte Carlo method.
- SPA+RPA state densities of samarium isotopes are in excellent agreement with exact SMMC and experimental state densities.
- The SPA+RPA naturally reproduces the collective rotational enhancement of the state density in deformed nuclei.

Outlook

- Extend SPA+RPA calculations to actinide nuclei, e.g., uranium isotopes.
- Calculate γ-ray strength functions in heavy nuclei with the SPA+RPA (in progress).

Thank you, SSGF!



Dr. Toshihiko Kawano
Los Alamos National Laboratory

Next stop, D.C.!