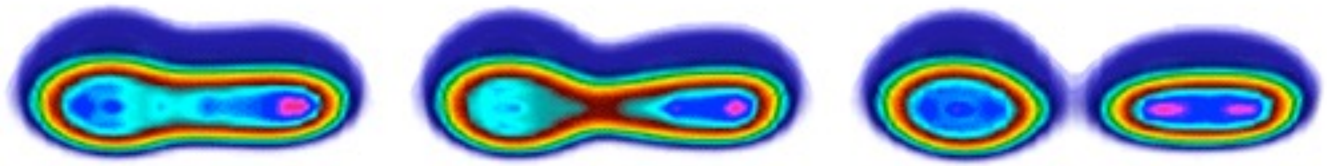
LA-UR-22-32055

Fission in microscopic framework: past and current successes and future needs



Ionel Stetcu

November 14-16, 2022

NSAC Long Range Plan Town Hall Meeting: Nuclear Structure, Reactions and Astrophysics

Nuclear fission: the most complex and least understood process

Relevant for applications to energy production, national security, space exploration, origin of elements.

Key ingredients (7 parameters):

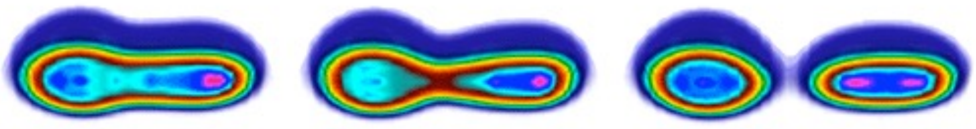
- ✓ Surface tension/surface energy and Coulomb energy
- ✓ Pairing interaction
- ✓ Spin-orbit interaction
- ✓ Symmetry energy
- ✓ Saturation energy and saturation density

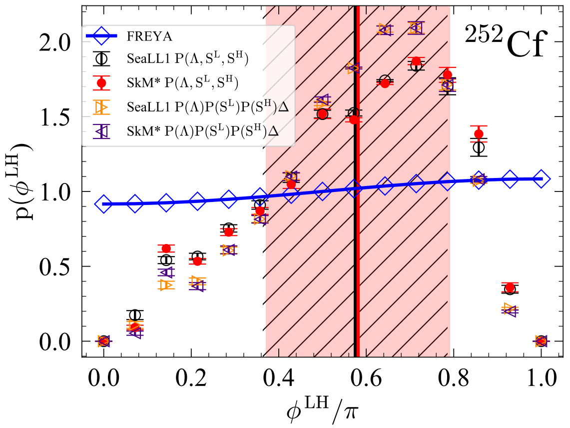
Theory:

- Many-body Schrödinger equations mathematically equivalent to DFT
- Formulation of a local extension of the Density Functional Theory (DFT), in the spirit of the Local Density Approximation (LDA) formulation of DFT due to Kohn and Sham, to superfluid time-dependent phenomena, the Superfluid Local Density Approximation (SLDA).
- Validation and verification of (TD)SLDA against a large set of theoretical and experimental data for various systems of strongly interacting fermions.
- Numerical implementation on leading edge supercomputers since 2007: Jaguar, Titan, Summit (all at ORNL), Sierra, Lassen (both at LLNL), Piz Daint (CSCS, Lugano), Polaris (ANL) …
- SLDA and TDSLDA are problems of extreme computational complexity, requiring the solution of 5M+ coupled complex 3D+1 PDEs

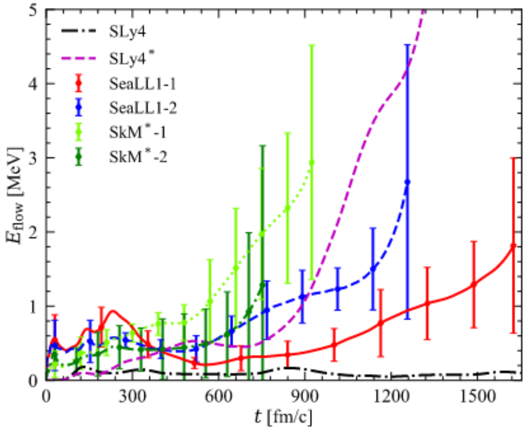
Key Successes

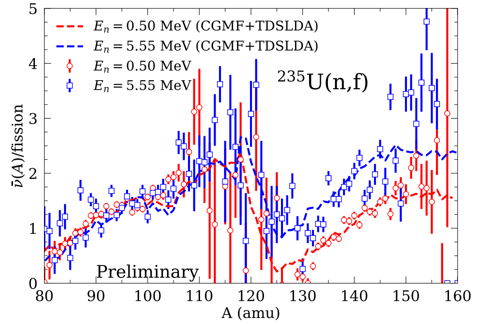
- Achieved scission and full separation of fission fragments in a pure microscopic framework, starting near the outer fission barrier, without any assumptions or unchecked approximations.
- Established the strong damped character of the nuclear large amplitude collective motion beyond the outer saddle-point.
- Fission fragments excitation energies and their sharing mechanism before and after separation (TXE); excitation energy sharing and neutron multiplicities. Guide phenomenological models (CGMF, FREYA, FIFRELIN)
- Intrinsic fission fragment spins and their correlations.
- Evaluated the intrinsic fission fragments spins and their correlations.
- Total kinetic energy of fission fragments (TKE).
- Evolution of these properties with the initial excitation energy of the compound nucleus.
- Established the time-dependence of the orbital entanglement entropy in fission, which is related to the complexity of the many-body wave function

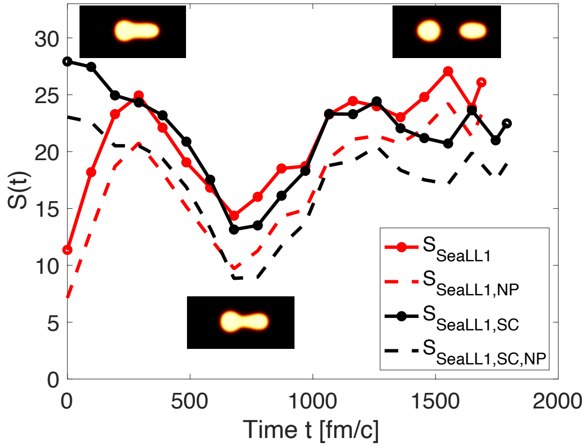


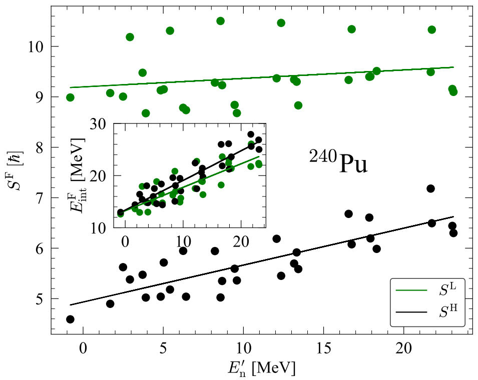


This result inspired several new experimental proposals.









Future: to boldly go where no man has gone before

- Extend the theoretical framework to odd and odd-odd nuclei.
- Scission neutrons (require large computational resources)
- Include proton-neutron short range correlations in order to correctly describe evolution of nucleon momentum distribution and thus combine in the same framework long- and short-range correlations in a fully quantum approach (a fully quantum BUU equation).
- Extend projection on many/all quantum numbers
- Improve the accuracy, execution time, portability of the codes.
- Use of machine learning tools to study dynamics of complex nuclear systems.
- Study the role of angular momentum of the compound nucleus in fission.
- Study fission of nuclei relevant to nuclear astrophysics, which is not possible in the lab.
- Seek a better understanding of experimental data (all measurements are made after neutron emission) to make an informed comparison