Toward a Predictive Theory of Fission

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Fission, a fundamental nuclear decay of great relevance to society, has eluded a microscopic theoretical understanding. Phenomenological models have offered substantial insights into the fission process, but their capabilities, while successfully descriptive, lack predictive power. A predictive theory of fission is expected to yield a significant impact on our ability to computationally model components and materials for stockpile stewardship, as well as the next generation of nuclear reactor design. The pursuit of a predictive theory of fission is a challenging problem for basic research which would also impact our understanding of the synthesis of superheavy nuclei, and the astrophysical production of elements heavier than lead.

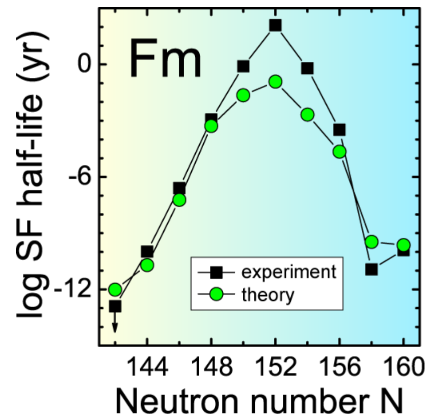

Figure 1

Using the nuclear density functional theory (DFT) and the larger supercomputing platforms currently available, we are developing a microscopic model for fission that will be predictive and extendable. We study fundamental properties of fission: half-lives and the distribution of mass, kinetic energy, and excitation energy between the fission fragments. Figure 1 shows the calculated fission half lives of even-even fermium isotopes, with 242 ≤ A ≤ 260, compared with experimental data [Staszczak et al. Phys. Rev. C **80**, 014309 (2009)].

We are studying the fission of actinides such as thorium-232 as a test of theoretical predictions against experimental data. For example, as some actinide nuclei deform towards fission, they exhibit three local minima in the energy surface. Furthermore, the mass distribution of daughter products tends to be asymmetric. As seen in Figure 2, our DFT calculations successfully reproduce the three minima of thorium-232, finding the third minimum to be reflection asymmetric - indicating that the division of mass between the fragments will be asymmetric, just as the data indicate.

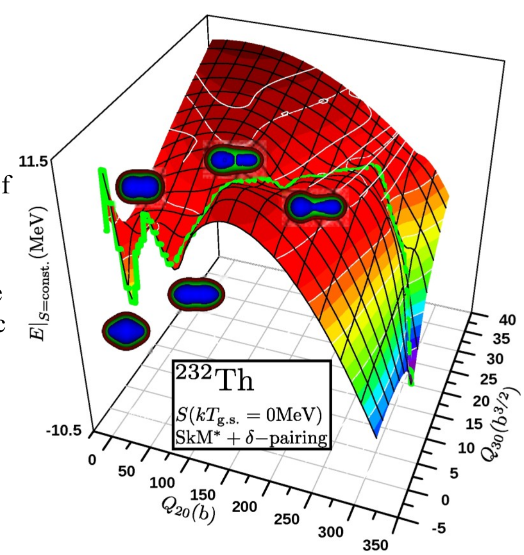

Figure 2

We have extended our study to excited nuclei. We find that the third, reflection-asymmetric minimum dissolves so that the nucleus divides symmetrically (see Figure 3). Experimental data support this prediction: excited nuclei fission with a symmetric mass yield.

Extreme-scale computing affords us the opportunity to relax assumptions, so that we can calculate fission properties with increasing fidelity, and therefore enables validation with experiments. We see this trend continuing during the next 5–10 years as supercomputing reaches toward the exascale.

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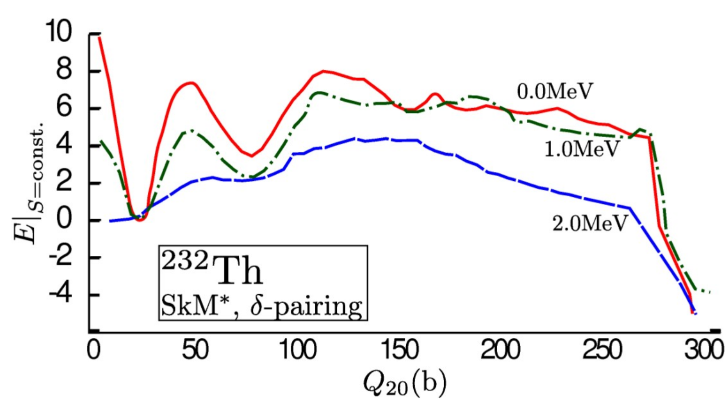

Figure 3