Low-Energy Nuclear Dynamics, Reactions, and Fission with TDDFT

Nuclear superfluidity/pairing is a hallmark of nuclear structure and reactions, playing a crucial role in determining the nuclear shapes, transition probabilities, nucleon transfer rates, fission and fusion dynamics.

Time-Dependent Density Functional Theory (TDSLDA - incarnation of TDDFT with pairing correlations) bridges in a natural way for the first time the divide between structure and low-energy nuclear reactions, including fission and fusion processes.

Evaluated nuclear reaction data, based heavily on experiment and often on very simple assumptions, are used in transport simulations for various applications: nuclear astrophysics, energy generation, nuclear forensics, and stockpile stewardship. A microscopic description of a large body of missing experimental information is thus highly desirable.

In fission reactions and FRIB a large number of far from stability nuclei are created. Their properties cannot always be measured. However, a large range of fission observables can be measured with high precision: the average number of prompt neutrons and γ-rays emitted before β decays toward stability, their energy spectra, and even correlations between the emitted particles. TDSLDA is <u>the</u> ideal microscopic tool for calculating input necessary for fission simulations (mass, kinetic and excitation energy, spin, parity, and angular fission fragment distributions, etc.), input that can only indirectly be extracted from experiment.

Current Status

We developed the TDSLDA framework, implemented it on leadership-class computers, and verified and validated it thoroughly during the last decade in the cold atom systems. Cold atoms share many similarities with nuclear systems. Many QMC calculations for cold atoms are available, and a large variety of experiments have been performed and confronted with <u>fully</u> microscopic theoretical QMC and TDSLDA pre-dictions and post-dictions.

TDSLDA has been applied to calculate the photo-absorption and relativistic Coulomb excitation, neutron scattering of nuclei and induced nuclear fission. TDSLDA provided so far the only microscopic treatment of the excitation of triaxial open shell nuclei with correct description of pairing correlations.

The great advantage of GPUs vs CPUs on Titan

$N_xN_yN_z$	N_{wf}	memory	CPU comp. + comm.	CPU comp.	GPU comp. + comm.	GPU comp.	# of GPUs	speedup
48^3	110592	10 TB	3.9s	2.4s	0.39s	0.023s	6912	10
64^3	262144	56 TB	20s	9.1s	0.80s	0.48s	16384	25

Over 1 million time-dependent 3D nonlinear complex coupled PDEs.
One of the largest Direct Numerical Simulations ever attempted.

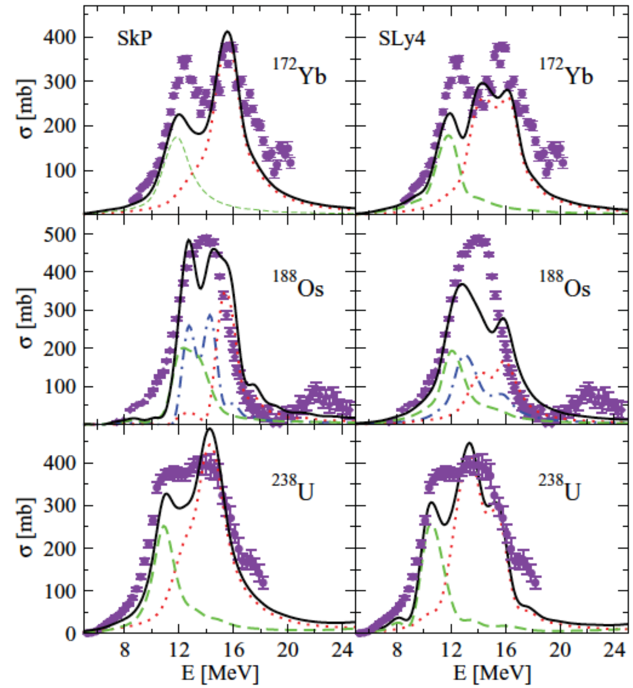
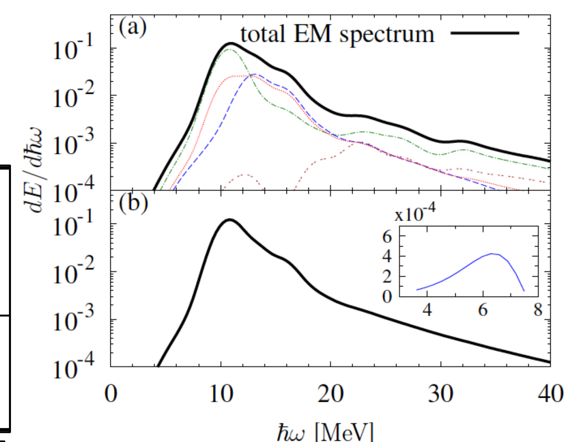


Photo-absorption cross section of select superfluid, arbitrarily deformed nuclei

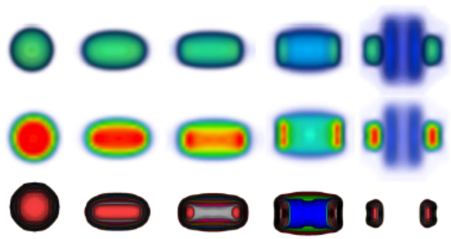


EM power emitted in relativistic Coulomb excitation of ^{238}U

Future

Study of spontaneous fission dynamics from the saddle point, induced fission and fusion, and other low-energy nuclear reactions:

- Investigate of neutrons emitted at the neck rupture
- Calculate of initial mass, charge, total kinetic energy, and angular momentum distributions of fission fragments
- Use the calculated input in Hauser-Feshbach statistical codes to calculate prompt neutron and γ-ray observables
- Benchmark against measured fission quantities (post neutron-emission kinetic energies, prompt neutron and γ-spectra, angular and energy correlations)
- Detail the role of pairing correlations in large amplitude collective motion



FUTURE NEEDS:

- Computing: 120-150M core hours/year
- People: 2-3 grad students, 1-2 postdocs, 2 international collaborators, 3 senior people