Discussion during the ESNT workshop on "Nuclear many-body dynamics through barriers" - 13-14 April 2022

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We highlight some aspects discussed during the workshop and select a list of questions that were pointed out during the different talks and discussions.

I. GENERAL REMARKS

The scientific goal of the workshop was to discuss recent works on nuclear dynamics through barriers with a focus on the following areas:

1. Description of quantum tunneling using beyond real-time-dependent mean-field techniques;
2. Phenomenology of deep sub-barrier fusion and the ability of current models to predict experimental data;
3. Phenomenology of potential energy surfaces (PES) topology and the role of shell effects;
4. Production of improved PES for time-dependent generator-coordinate method (TDGCM) calculations;
5. Towards TDGCM calculations without the Gaussian Overlap Approximation (GOA).

Heavy-ion fusion and cluster decay were discussed as typical examples involving many-body tunneling. In addition, many applications were dedicated to nuclear fission, with a focus on generating state of the art PES, as well as on dynamical methods, including the real-time and imaginary-time-dependent Hartree-Fock theories (TDHF and ITDHF), the transition state method (TSM), and beyond mean-field approaches such as Phase-Space (PS) methods or TDGCM. Examples of topics that were discussed include:

- **Realistic PES to be used in TDGCM:** These calculations assume a small number of collective variables (typically quadrupole and octupole moments) to characterise the fission path and build PES at zero temperature with the adiabatic approximation. Recent improvements in the construction of PES avoiding discontinuities open interesting perspectives in applying TDGCM without the GOA. The investigation of the role of shell effects on PES topology also brings a deeper insight into the competition between various fission modes. Nevertheless, the use of EDF or density-dependent interactions in beyond mean-field calculations remains an open problem.
- **Quantum tunneling in many-body systems:** The Schrödinger equation cannot be solved exactly for many-particle systems and mean-field based approximations are often required. However, the price to pay for such a simplification is often to remove completely the possibility for quantum tunnelling of the many-body wave-function, resulting in classical trajectories of the composite systems where tunneling is forbidden. Approaches such as phase-space and ITDHF methods are expected to account for tunneling at some level. Alternatively, one can reduce the problem to a macroscopic dynamics with a microscopic description of the nucleus-nucleus potential (for applications to fusion) or of a PES (in the case of fission). Tunneling rates can then be computed with, e.g., WKB or a least action method.
- **Connecting states on each side of the barrier:** The structure of the compound nucleus being different to that of a dinuclear system (merging collision partners in fusion, or pre-fragments on their way to scission in fission), the question of a dynamical transition between these states is non-trivial. The TSM offers a framework based on level densities, that can be formulated microscopically with the GCM. Although in principle equivalent, there are pros and cons in formulating such dynamics in the time or energy domains.
- **Coherent extraction of observables that could be confronted with experimental observations:** With the progress of experimental techniques, new observables can be obtained especially related to the internal excitation or rotational properties of fragments before or after scission. However, due to the quantum entanglement between the fission fragments, specific quantum projection techniques are required to evaluate fragment properties such as particle number and angular momentum.

The complete program of the workshop including presentations are available in the ESNT website [1].

II. SOME QUESTIONS LISTED DURING AND AFTER THE WORKSHOP

- **Potential Energy Surfaces**
  - What is the minimal set of collective coordinates for realistic calculations (Q_{20}, Q_{30}, Q_{40}, Q_{neck}...) of fission?
  - When considering a state $|\Psi(q)\rangle$ that is not fully local in q, what is the meaning of $V(q)$? Does the meaning change depending on the approach (GCM+GOA, adiabatic TDHF, etc)? Does the question even make sense considering the fact that the potential is not an observable?
  - As physics can only be continuous, what happens in the adiabatic landscape when we observe a discontinuity. How to best identify these discontinuities (overlaps, density distances...)? What is the most efficient approach to smooth them (linear interpolation, adding a new coordinate locally, Dynamic Programming Method, Generative Machine Learning...)?
  - Is the use of "cold" PES justified and how to account for the role of finite excitation energy in the HFB states (constraining temperature, adding another degree of freedom associated with the number of quasiparticle excitations...)?
  - How to best identify the role of Compound nucleus and fragments shell effects on fission paths (level density near Fermi energy, Strutinski shell energy correction...) and how to interpret "Standard" Brossa modes (including in the sub-lead region)? What is the role of the tensor force on these shell effects and how to constrain it from physical observables?
  - When does the adiabatic approximation breaks down and how to couple "static" HFB states with time-dependent HFB solution near scission?
- **Theoretical methods, their interpretation, and practical aspects**
  - How to determine a realistic initial state before any type of further evolution (account for zero-point motion, excitation energy, fake trapping potential versus boost...)?
  - What is the quantitative effect of considering GCM states like $|\Phi(q)\rangle$ instead of $|\Phi(q,p)\rangle$ where (p,q) are conjugated variables?
  - What EDF, or interaction, should be used in full TDGCM or more generally beyond mean-field calculations to avoid divergences? Could the ab-initio approaches provide effective Hamiltonians that we could use to perform beyond mean field calculations?
  - What is the theoretical justification for using collective Schrödinger equations (e.g. cross sections from WKB, or half-life of spontaneous decay) directly on adiabatic potentials coming from constrained HFB approaches? TDGCM+GOA gives one framework to do it but the metric, the inertia and the local potential contains things like zero point energies. Are these corrections necessary, and how to implement them, in the case of fusion or alpha/cluster decay?
  - Does a GOA like approximation hold when using HFB states projected on good quantum numbers ?
  - Could we apply density-constrained TDHF(B) (DCTDHFB) to generate a relevant path of HFB states for alpha/cluster emission ?
  - Are there realistic nuclear physics circonstances where dynamical models lead to a statistical distributions of the nuclear state ?
  - How should we couple the few transistion states close to the fission saddle points to the statistical ensemble of states representing on one side the compound nucleus and on the other side all the possible output channels. Can we use here a random Hamiltonian matrix approach ?
- **Specific questions on the tunneling problem**
  - What are the pros and cons of using a representation in the time domain or in the energy domain? Do they depend on the time-scale of the mechanism (e.g., spontaneous fission)? Do energy based methods like transition/doorway states approach provide convenient alternatives to time-dependent calculations?
  - How to account for the energy dependence of the repulsion between nuclei due to the Pauli exclusion principle (Pauli repulsion) which is expected to disappear at high energy?
  - How to account for capture into a resonance state of the compound nucleus in a microscopic way?

- Is the near-barrier dynamics used in DCTDHF(B) (or similar techniques) to determine nucleus-nucleus potentials still relevant far below the barrier?
- How to go beyond toy-model applications of ITDHF calculations while avoiding numerical instabilities inherent to non unitary evolutions? Does the normalisation if the single particle states need to be enforced in some way? Would removing the single-particle energy from the mean field Hamiltonian $h[\rho] - \epsilon_i$ help?
- Could we compute spontaneous fission half-lives by applying the Green's function method on the TDGCM+GOA collective Schrödinger equation augmented with an absorption potential beyond the saddle point ?

- **Interpretation and connection with observations**
  - How to connect (beyond) mean-field calculations with experimental observables other than fragment mass distributions ($N - Z$ asymmetry, TKE, neutron multiplicity, angular momentum...)?
  - How to account for fluctuations of particle number and angular momentum in the fragments (projection techniques, TDRPA, phase-space...)?
  - When are the fission fragment properties decided? Can we evaluate these properties from the pre-scission configurations, as in adiabatic approaches, or do we need an approach that follows the system beyond scission?
  - What is the meaning of trajectory in collective space when we use quasiparticle many-body states eventually coupled with each others? In particular, these states have significant zero-point fluctuations hat prevents from a simple classical interpretation of observables.
  - What is the appropriate methodology to extract observables from different theories that could be confronted to experiments?

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[1] `https://esnt.cea.fr/Phocea/Page/index.php?id=106`