Open problems in nuclear dynamics



Piotr Magierski (Warsaw University of Technology) Nuclear fission and reactions involving medium mass or heavy nuclei are unquestionably the most challenging examples of nuclear dynamics.

The fundamental equation describing nuclear dynamics is known:

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi$$

However even if we knew nuclear Hamiltonian precisely, the problem of motion of more than 200 strongly interacting nucleons, described in terms of true many-body wave function is computationally intractable.

The wave function of ²⁴⁰Pu depends on 720 coordinates!!! It has 1.76×10⁷² spin components!!! <u>Typical framework for the theoretical description of nuclear dynamics</u> <u>at low energies</u>



Reversible energy flow is determined by: mass parameters, potential energy surface.

Irreversible energy flow is determined by <u>friction coefficients</u> and leads to collective energy dissipation.

Consequently, questions associated with nuclear dynamics are directly related to the treatment of various components of this framework:

- Determination of the set of collective variables and their eq. of motion
- Treatment of other degrees of freedom
- Assumptions concerning energy flows

Physics of nuclear superfluid dynamics



Quasiparticle energy: $E_{qp} = \sqrt{(\mathcal{E} - \mu)^2 + |\Delta|^2}$

Potential energy surface

 ϵ_{sp} $v(\xi)$ $v(\xi)$ Barrance Bertsch Breglia and Vigezzi ξ

From Barranco, Bertsch, Broglia, and Vigezzi Nucl. Phys. A512, 253 (1990) As a consequence of pairing correlations large amplitude nuclear motion becomes more adiabatic.

While a nucleus elongates its Fermi surface becomes oblate and its sphericity must be restored Hill and Wheeler, PRC, 89, 1102 (1953) Bertsch, PLB, 95, 157 (1980)



Low energy fission (less than about 10MeV excitation above the fission barrier) of nuclear systems investigated up to about 2016.

From K.-H. Schmidt, B. Jurado, Rep. Prog. Phys. 81 106301 (2018)

Theoretical description of nuclear dynamics at low energies

Potential energy surface (PES) + Langevin dynamics

- We set few collective variables (typically not more than 5)
- We calculate potential energy surface using either microscopicmacroscopic (eg. Woods-Saxon + Strutinsky shell correction), or Density Functional Theory (with Skyrme-like or Gogny functionals).



Figure 1. (color online) Potential energy surfaces obtained with the SkM^{*} (left) and D1S (right) EDF in axial symmetry. The red line separates configurations with $Q_N > 4$ from the others. The curvilinear abscissa ξ starts at the symmetric scission points and runs along the frontier (red line). Values of ξ are indicated along the scission line.

D. Regnier, N. Dubray, N. Schunck, M. Verriere, PRC93, 054611 (2016)

- We determine mass parameters (within a certain approximation: eg. cranking formula)
- Classical equation of motion for collective variables are set + Langevin type stochastic force simulating interaction with other degrees of freedom.
- Relation between stochastic force and dissipation is set based on dissipation-fluctuation theorem (classical version).

$$\dot{q}_{i} = \sum_{j} M_{ij}^{-1}(\vec{q}) p_{j}$$
friction
stochastic force
$$\dot{p}_{i} = -\frac{\partial V}{\partial q_{i}} - \frac{1}{2} \sum_{j,k} \frac{\partial M^{-1}{}_{jk}}{\partial q_{i}} p_{j} p_{k} - \sum_{j} \gamma_{ij} M^{-1}{}_{jk}(\vec{q}) p_{k} + \sum g_{ij}(\vec{q}) \xi_{j}(t)$$

$$\sum_{j} g_{ik} g_{jk} = \gamma_{ij} T$$
Fluctuation-dissipation theorem (classical)

P. Frobrich, I.I. Gontchar, Phys. Rep. 292 (1998) 131

- In the case of spontaneous fission the tunneling motion through the barrier is obtained in semiclassical WKB approximation:

k

$$S(L) = \int_{s_{\rm in}}^{s_{\rm out}} \sqrt{\frac{2\mathcal{M}_{\rm eff}(s)}{\hbar^2} \left(V(s) - E_0\right)} \, ds,$$

Spontaneous fission





J. Sadhukhan, W. Nazarewicz and N. Schunck, PRC 93, 011304(2016),

Induced fission



FIG. 1: Calculated and measured charge yields for fission of ²⁴⁰Pu and ^{236,234}U. The data in (a–c) are for (n_{th},f) reactions leading to $E^* \approx 6.5$ MeV [27], while the data in (d) is for (γ ,f) reactions leading to $E^* \approx 8 - 14$ MeV; they include contamination from fission of ²³³U ($\approx 15\%$) and ²³²U ($\approx 5\%$) [28]; the corresponding calculation was made for $E^* = 11$ MeV.

J. Randrup and P. Möller, PRL **106**, 132503 (2011) Strongly damped nuclear dynamics

P. Nadtochy and G. Adeev, PRC 72, 054608 (2005); P. N. Nadtochy, A. Kelić, and K.-H. Schmidt, PRC 75, 064614 (2007); J. Randrup and P. Möller, PRL 106, 132503 (2011); J. Randrup, P. Möller, and A. J. Sierk, PRC 84, 034613 (2011); P. Möller, J. Randrup, and A. J. Sierk, PRC 85, 024306 (2012); J. Randrup and P. Möller, PRC 88, 064606 (2013); J. Sadhukhan, W. Nazarewicz and N. Schunck, PRC 93, 011304 (2016), J. Sadhukhan, W. Nazarewicz and N. Schunck, PRC 96, 061361 (2017).

Advantages:

- Easy to use scheme, especially if for PES a micro-macro model is used (can be done on a laptop).
- Allows for global systematic calculations.
- Mass/charge distribution is obtained.
- Total kinetic energies can be extracted once the scission point is defined.
- Both spontaneous and induced fission can be studied.
- Disadvantages:
- Set of collective coordinates is specified based on intuition (kept constant during evolution)
- Potential energy surface is taken from the mean-field potential (Woods-Saxon or DFT), but mass parameter are calculated usually within the cranking approximation (which is not precisely consistent with adiabatic expansion)
- Pairing is incorporated within the BCS approach (to produce a gap)
- Motion on PES comes from classical theory assuming coupling with a heat-bath at certain temperature.

(it implies the treatment within the canonical ensemble – however the microcanonical ensemble is more appropriate).

<u>Summarizing</u>: the main problem with this approach lies in the fact that it contains various components which are included inconsistently.

Once we face a problem (comparing results to exp. data) we do not know which component of the approach need to be corrected, and what is more important, how to do it in a <u>consistent way</u>.

Time dependent generator coordinate method (TDGCM)

PES is obtained using Density Functional Theory. Instead of Langevin dynamics the time dependent generator coordinate is used:

$$|\Psi(t)\rangle = \int f(\vec{q},t) |\Phi(\vec{q})\rangle d^N q$$
 - Ansatz for the wave function

$$\left\langle \Phi(\vec{q}) \left| \Phi(\vec{q}') \right\rangle \sim exp(-\sum_{k} \left| \sigma_{k}(\vec{q}) - \sigma_{k}(\vec{q}') \right|^{2}/2)$$
 - GOA approx.

Instead of Langevin equation the evolution on the PES is governed by:

$$i\hbar \frac{\partial}{\partial t} g(\vec{q}, t) = H_{coll}(\vec{q}) g(\vec{q}, t)$$
$$H_{coll}(\vec{q}) = -\frac{\hbar^2}{\gamma^{1/2}(\vec{q})} \sum_{i,j} \frac{\partial}{\partial q_i} \gamma^{1/2}(\vec{q}) B_{ij}(\vec{q}) \frac{\partial}{\partial q_j} + V(\vec{q})$$

- γ Metric tensor
- $B(ec{q})$ Mass tensor
- $g(ec{q},t)$ Probability amplitude for the system to be at point ${f q}$

In TDGCM we have a fully quantum motion on the PES instead of classical Langevin-like equation.

However there is no irreversible energy flow - i.e. the motion is fully adiabatic. The system remains cold during motion: no energy transfer from collective degrees of freedom to other degrees of freedom.

The TDGCM is best suited to account for mass/charge distribution of fragments: the scission line has to be determined and the probability flux through the scission line is calculated determining yields.



J.-F. Berger, M. Girod, D. Gogny, CPC 63, 365 (1991); H. Goutte, J.-F. Berger, P. Casoli, D. Gogny, PRC 71 024316 (2005); D. Regnier, N. Dubray, N. Schunck, and M. Verrière, PRC 93, 054611 (2016); D. Regnier, M. Verrière, N. Dubray, and N. Schunck, CPC 200, 350 (2016)

60



Runge-Gross mapping(1984):

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle, \quad |\psi_0\rangle = |\psi(t_0)\rangle \qquad \qquad \frac{\partial\rho}{\partial t} + \nabla \cdot \vec{j} = 0$$

$$\rho(\vec{r}) \leftrightarrow e^{i\alpha(t)} \Psi[\rho](\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)$$

TDDFT variational principle also exists but it is more tricky:

$$F[\psi_0,\rho] = \int_{t_0}^{t_1} \langle \psi[\rho] | \left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) | \psi[\rho] \rangle dt$$

E. Runge, E.K.U Gross, PRL 52, 997 (1984)
B.-X. Xu, A.K. Rajagopal, PRA 31, 2682 (1985)
G. Vignale, PRA77, 062511 (2008)

Kohn-Sham procedure

Suppose we are given the density of an interacting system. There exists a unique noninteracting system with the same density.

Interacting system

Noninteracting system

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = (\hat{T} + \hat{V}(t) + \hat{W}) |\psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} \left| \varphi(t) \right\rangle = (\hat{T} + \hat{V}_{KS}(t)) \left| \varphi(t) \right\rangle$$

$$\rho(\vec{r},t) = \left\langle \psi(t) \left| \hat{\rho}(\vec{r}) \right| \psi(t) \right\rangle = \left\langle \varphi(t) \left| \hat{\rho}(\vec{r}) \right| \varphi(t) \right\rangle$$

Hence the DFT approach is essentially exact.

A new local extension of DFT to superfluid systems (SLDA) and timedependent phenomena (TDSLDA) was developed. Reviews: A. Bulgac, Time-Dependent Density Functional Theory and Real-Time

Dynamics of Fermi Superfluids, Ann. Rev. Nucl. Part. Sci. 63, 97 (2013);

P. Magierski, Nuclear Reactions and Superfluid Time Dependent Density Functional Theory,

in "Progress of time-dependent nuclear reaction theory" (Betham Science Publishers 2016)



Number of papers using variants of DFT from K.Burke, J.Chem. Phys. 136, 150901 (2012)





2012

Advantages of TDDFT for nuclear reactions

- The same framework describes various limits: eg. <u>linear and highly nonlinear</u> regimes, <u>adiabatic and nonadiabatic (dynamics far from equilibrium)</u>.
- Interaction with basically any external probe (weak or strong) easy to implement.
- TDDFT <u>does not require</u> introduction of hard-to-define <u>collective degrees of</u> <u>freedom</u> and there are no ambiguities arising from defining <u>potential energy</u> <u>surfaces and inertias</u>.
- <u>One-body dissipation, the window and wall dissipation mechanisms</u> are automatically incorporated into the theoretical framework.
- All shapes are allowed and the nucleus chooses dynamically the path in the shape space, the forces acting on nucleons are determined by the nucleon distributions and velocities, and <u>the nuclear system naturally and smoothly evolves into separated fission fragments</u>.
- There is no need to introduce such unnatural quantum mechanical concepts as "rupture" and there is <u>no worry about how to define the scission configuration</u>.

Sometimes simplified assumptions are made eg. replacing TDHFB by TDBCS :

 $\Delta(\vec{r},t) \rightarrow \Delta(\rho(\vec{r},t))$ - severe limitation in pairing degrees of freedom.

e.g. G.Scamps. D. Lacroix, G.F. Bertsch, K. Washiyama, PRC85, 034328 (2012).

More precisely: BCS as compared to HFB approach neglects <u>the quasiparticle scattering</u> and consequently all effects originated from this effect are missed.

The main advantage of TDSLDA over TDHF (+BCS) is related to the fact that in TDSLDA the pairing correlations are described as a true <u>complex field which has its own modes of excitations</u>, which include spatial variations of both amplitude and phase. Therefore in TDSLDA description the evolution of nucleon Cooper pairs is treated consistently with other one-body degrees of freedom.

Fission dynamics of ²⁴⁰Pu

Initial configuration of ${}^{240}Pu$ is prepared at the barrier (saddle point) at quadrupole Deformation Q=165b and excitation energy E=8.08 MeV:



During the process shown, the exchange of about 2 neutrons and 3 protons occur between fragments before the actual fission occurs.

Interestingly the fragment masses seem to be relatively stiff with respect to changes of the initial conditions.

The saddle-scission time is considerably longer than in simplified approaches.

A. Bulgac, P.Magierski, K.J. Roche, and I. Stetcu, Phys. Rev. Lett. 116, 122504 (2016)

Fission dynamics of ²⁴⁰Pu



Note that despite the fact that nucleus is already <u>beyond the saddle point</u> the collective motion on the time scale of 1000 fm/c and larger is characterized by <u>the constant velocity</u> (*see red dashed line for an average acceleration*) till the very last moment before splitting. On times scales, of the order of 300 fm/c and shorter, the collective motion is a subject to random-like kicks indicating strong coupling to internal d.o.f

Nuclear induced fission dynamics:

It is important to realize that these results indicate that the motion is not adiabatic, although it is slow.

Although the average collective velocity is constant till the very last moment before scission, the system heats up as the energy flows irreversibly from collective to intrinsic degrees of freedom.

This may create problems for approaches based on ATDHF(B) or TDGCM as no irreversible energy transfer between collective and Intrinsic is possible there.

Remarks on the fragment kinetic and excitation energy sharing within the TDDFT



Schmidt&Jurado:Phys.Rev.C83:061601,2011

In the to-date approaches it is usually assumed that the excitation energy has 3 components (Schmidt&Jurado:Phys.Rev.C83:061601,2011 Phys.Rev.C83:014607,2011):

- deformation energy
- collective energy (energy stored in collective modes)
- intrinsic energy (specified by the temperature)

It is also assumed that the intrinsic part of the energy is sorted according to the total entropy maximization of two nascent fragments (i.e. according to temperatures, level densities) and the fission dynamics does not matter.

In TDDFT such a decomposition can be performed as well. The intrinsic energy in TDDFT will be partitioned <u>dynamically</u> (no sufficient time for equilibration).



Induced fission of 240Pu

The lighter fragment is more excited (and strongly deformed) than the heavier one.

Excitation energies are not shared proportionally to mass numbers of the fragments!

 $TKE = 177.80 - 0.3489E_n$ [in MeV],

Nuclear data evaluation, Madland (2006)

Calculated TKEs slightly reproduce experimental data with accuracy < 2%

J. Grineviciute, et al. (in preparation) see also:

A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu, Phys. Rev. Lett. 116, 122504 (2016)

Decomposition of the excitation energy into collective and noncollective part

Intrinsic excitation energy of the fragments:



J. Grineviciute, et al. (in preparation)

Energy stored in collective modes: < 2MeV

The intrinsic energy is not shared proportionally to fragment masses at low excitation energy!

Open problems of TDDFT

- There are easy and difficult observables in DFT. In general: easy observables are one-body observables. They are easily extracted and reliable.
- 2) But there are also important observables which are difficult to extract. For example:
 - S matrix
 - momentum distributions
 - transitional densities (defined in linear response regime)
 - various conditional probabilities
 - mass distributions (needs an extension to stochastic TDDFT or combining with TDGCM)
 - Stochastic extensions are under investigation:

D. Lacroix, A. Ayik, Ph. Chomaz, Prog.Part.Nucl.Phys.52(2004)497 S.Ayik, Phys.Lett. B658 (2008) 174 A. Bulgac, S.Jin, I. Stetcu, arxiv:1806.00694

- 3) Dissipation: transition between one-body dissipation regime and two-body dissipation regime.
- 4) Incorporation of odd-particle system dynamics consistently within TDDFT

Experimental observables vs theory

Mass/charge distribution – important, but do not give us deep insight into nuclear dynamics e.g. it is relatively well reproduced both by PES+Langevin and TDGCM theories, despite of the fact that completely different character of nuclear motion is assumed.

Odd-even mass effect – very interesting, but so far it is difficult to compare it to any theory without making uncontrollable asumptions. All theories that were presented are unable to incorporate consistently odd-particle system in the dynamics.

Total kinetic energy

- distributions useful quantity, but as far as we know TKE is determined practically at the scission point. So similarly to mass/charge distributions it is not very sensitive to nuclear dynamics prior to the scission point.
- Scission neutrons extremely useful quantity as it can be easily extracted in TDDFT, without further assumptions.

Measurement of scission neutrons can provide stringent test for the applicability of TDDFT theory to describe neutron emission in real-time.

Excitation energy sharing

Primary gamma emission

- extremely important quantity, depending on dynamics and density of states at scission. Very severe test for TDDFT: theoretical predictions already exist.
- may give some information on ang. momentum distribution of fragments, but as far as I know, not directly comparable to theories presented here.

PHYSICAL REVIEW C 92, 034606 (2015)

Characterization of the scission point from fission-fragment velocities

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FIG. 5. (Color online) (a) Total kinetic energy of fission fragments at scission of 240 Pu (blue dots) and 250 Cf (red squares). The blue dashed line show data from thermal-neutron induced fission of 239 Pu [27]. (b) Ratio between the distance between fragments at scission and that as spherical touching nuclei for fission of 240 Pu (blue dots) and 250 Cf (red squares).



FIG. 7. (Color online) Minimum energy released in neutron evaporation and excitation energy shared according with the mass ratio of the fragments for ²⁴⁰Pu (blue dots and dashed line) and ²⁵⁰Cf (red squares and long-dashed line).

The calculation of a lower limit of excitation energy released by neutron evaporation as a function of Z suggests that the partition of TXE^* between the fragments according to their masses is not valid for these systems with $E_{FS}^* \sim 9$ and ~ 42 MeV; being more suitable the description with unbalanced temperatures and continuous flow of energy from the light to the heavy fragment [32].

Isotopic fission-fragment distributions of ²³⁸U, ²³⁹Np, ²⁴⁰Pu, ²⁴⁴Cm, and ²⁵⁰Cf produced through inelastic scattering, transfer, and fusion reactions in inverse kinematics

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FIG. 11. Isotopic fission-fragment yields of 238 U ($\langle E_x \rangle = 7.4$ MeV). Present data (in black) are compared with data from Coulomb-induced fission [13] (in red).



FIG. 16. Elemental fission-fragment yields. Each color represents one fissioning system, with an average excitation energy indicated in parentheses.



FIG. 17. Elemental fission-fragment yields of different U isotopes. Present data (in black) are compared with previous measurements at different E_x , obtained from Coulomb-induced fission [1,13] (dashed lines) and *n*-induced fission [41] (squares). The corresponding E_x are indicated in parentheses.

Interesting aspect of pairing influence on nuclear dynamics



See also for light nuclei: Y. Hashimoto, G. Scamps, Phys. Rev. C94, 014610 2016)

Effective barrier height for fusion as a function of the phase difference



What is an average extra energy needed for the capture?

$$E_{extra} = \frac{1}{\pi} \int_{0}^{\pi} \left(B\left(\Delta\varphi\right) - V_{Bass} \right) d\left(\Delta\varphi\right) \approx 10 MeV$$

The phase difference of the pairing fields of colliding medium or heavy nuclei produces a similar <u>solitonic structure</u> as the system of two merging atomic clouds. The energy stored in the created junction is subsequently released giving rise to an increased kinetic energy of the fragments. The effect is found to be of the order of <u>30MeV</u> for medium nuclei and occur for <u>energies up to 20-30% of the barrier height</u>.

P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)

G. Scamps, Phys. Rev. C 97, 044611 (2018): the effect may be weaker than predicted by TDDFT

Dynamics of nuclear colission and de-excitation

Entrance channel (HIPSE)



B

Fission dynamics (Langevin equations)



Understanding pre-equilibrium processes in function of excitation energy, asymmetry of entrance channel ... Dependence on the centrality of the reaction.

Study the GDR emitted in the way to fission/evaporation via PARIS and/or FAZIA or others.

K. Mazurek, M. Ciemała, M. Kmiecik, A. Maj, APPB Conf Proc. 11,108 (2018)

Jacobi/Poincare shape transition



Critical new developments for nuclear dynamics

• In <u>THEORY</u>:

Formulation of a local extension of the <u>Density Functional Theory (DFT</u>) to superfluid time-dependent phenomena, the <u>Superfluid Local Density</u> <u>Approximation (SLDA)</u>.

It offers a qualitative leap in studying nuclear fission and reaction processes involving medium or heavy nuclei. It hopefully will allow to make a shift <u>from more phenomenology and adjusted</u> <u>parameters to more fundamental theory and increased predictive power</u>

In <u>HIGH PERFOMANCE COMPUTING</u>:

Emergence of very powerful computational resources, non-trivial numerical implementation of TDSLDA, advanced capabilities of leadership class computers due to hybrid architecture integrating CPUs with <u>Graphics Processing Units</u> (<u>GPU</u>).

SLDA and TDSLDA are problems of extreme computational complexity, requiring the solution of <u>10,000s</u> ... <u>1,000,000s</u> coupled complex non-linear timedependent <u>3D</u> partial differential equations. Thanks to:

M. Caamaňo

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