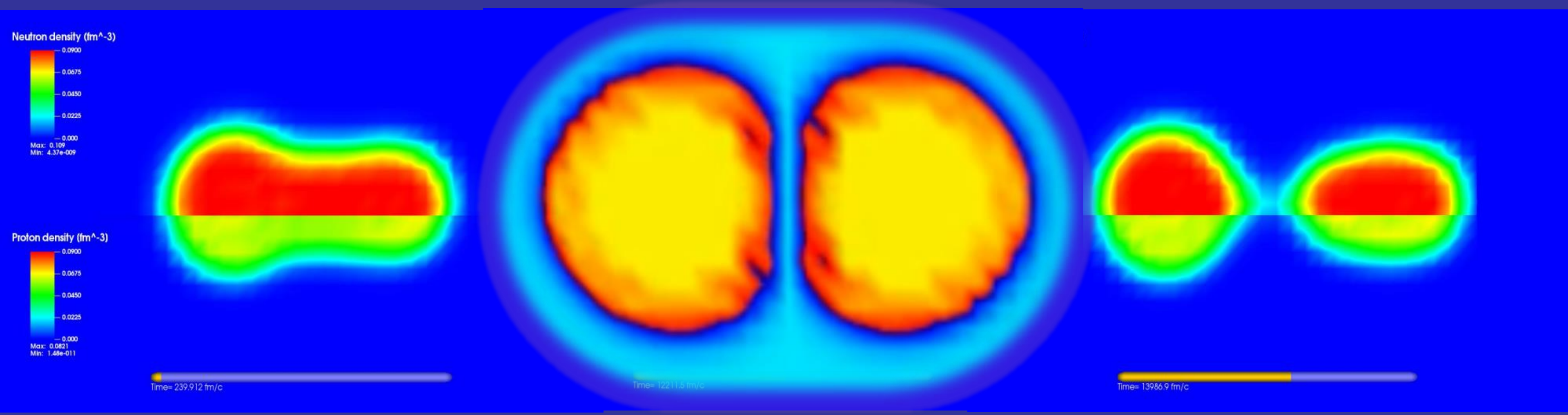
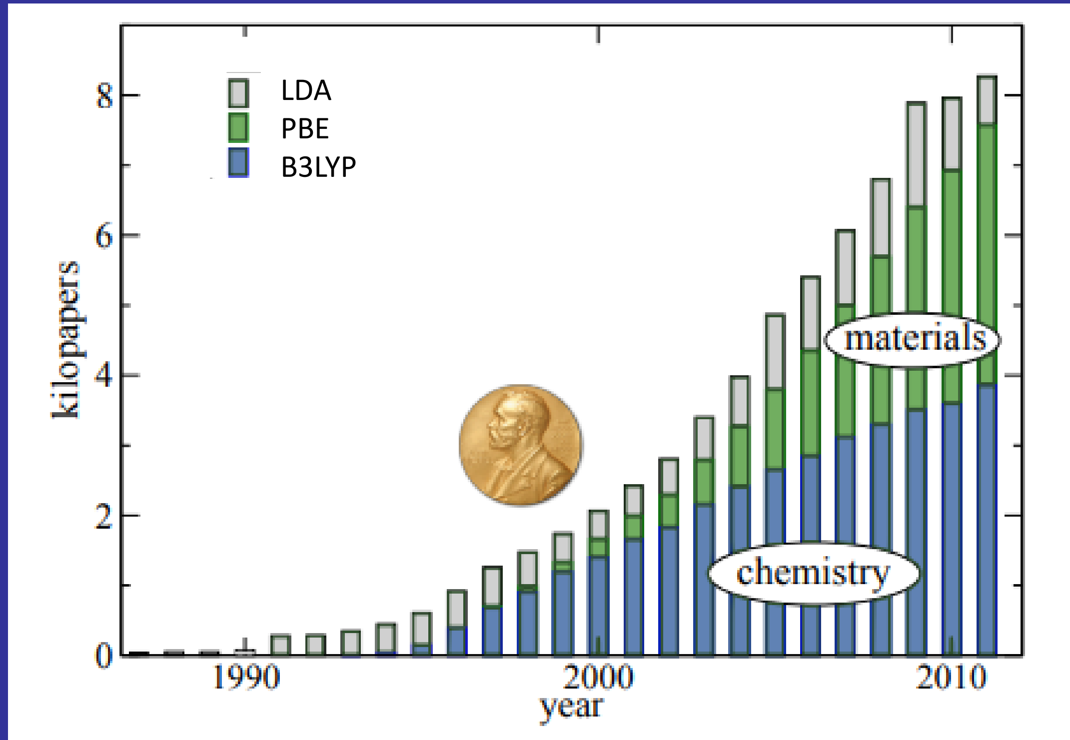
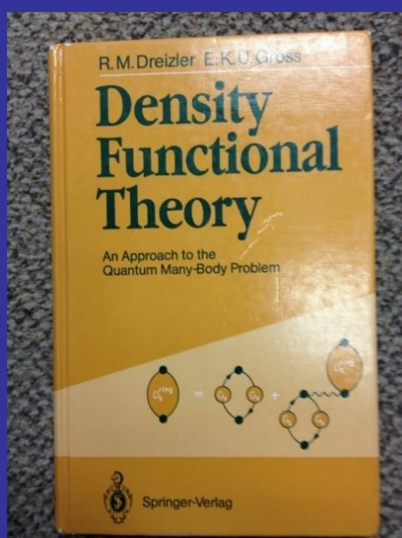
Reakcje nadciekłych jąder atomowych w świetle teorii funkcjonału gęstości.



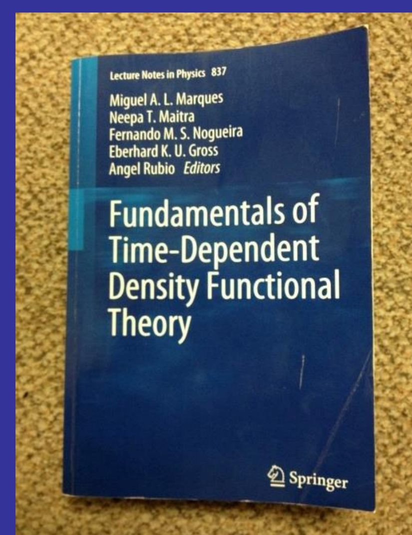
Piotr Magierski
(Warsaw University of Technology)



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

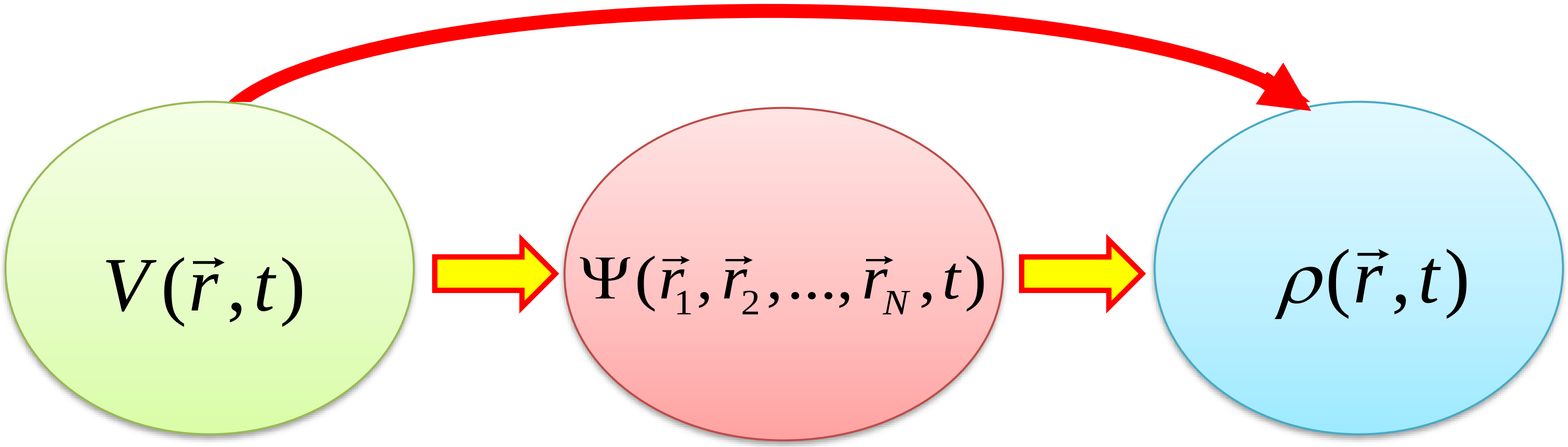


1990



2012

Time dependent selfconsistent mean-field
(time dependent density functional theory)



Runge-Gross mapping(1984):

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle, \quad |\psi_0\rangle = |\psi(t_0)\rangle$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0$$

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

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

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

Noninteracting system

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

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

Hence the DFT approach is essentially exact.

A new local extension of DFT to superfluid systems (SLDA) and time-dependent phenomena (TDSLDA) has been 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*, *Frontiers in Nuclear and Particle Physics* vol. 2, 57 (2019)

Pairing correlations in time-dependent DFT (with local pairing field)

$$S = \int_{t_0}^{t_1} \left(\left\langle 0(t) \left| i \frac{d}{dt} \right| 0(t) \right\rangle - E[\rho(t), \chi(t)] \right) dt$$

Stationarity requirement produces the set of equations (TDHFB eq.):

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} U_\mu(\mathbf{r},t) \\ V_\mu(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h(\mathbf{r},t) & \Delta(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & -h^*(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} U_\mu(\mathbf{r},t) \\ V_\mu(\mathbf{r},t) \end{pmatrix},$$

$$B(t) = \begin{pmatrix} U(t) & V^*(t) \\ V(t) & U^*(t) \end{pmatrix} = \exp[iG(t)] \qquad G(t) = \begin{pmatrix} h(t) & \Delta(t) \\ \Delta^\dagger(t) & -h^*(t) \end{pmatrix}$$

Orthogonality and completeness has to be fulfilled: $B^\dagger(t)B(t) = B(t)B^\dagger(t) = I,$

In order to fulfill the completenes relation of Bogoliubov transform all states need to be evolved!
Otherwise Pauli principle is violated, i.e. the evolved densities do not describe a fermionic system (spurious bosonic effects are introduced).

Consequence: the computational cost increases considerably.

Advantages of TDDFT for nuclear reactions

- The same framework describes various limits: eg. linear and highly nonlinear regimes, adiabatic and nonadiabatic (dynamics far from equilibrium).
- Interaction with basically any external probe (weak or strong) easy to implement.
- TDDFT does not require introduction of hard-to-define collective degrees of freedom and there are no ambiguities arising from defining potential energy surfaces and inertias.
- One-body dissipation, the window and wall dissipation mechanisms 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 the nuclear system naturally and smoothly evolves into separated fission fragments.
- There is no need to introduce such unnatural quantum mechanical concepts as "rupture" and there is no worry about how to define the scission configuration.

Sometimes simplified assumptions are made eg. replacing
TDHFB (TDSLDA) 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 the quasiparticle scattering 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 complex field which has its own modes of excitations, 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.

TDSLDA - time dependent superfluid local density approximation

The well known effects in superconductors where the simplified BCS approach fails

1) Quantum vortices, solitonic excitations related to pairing field (e.g. domain walls)

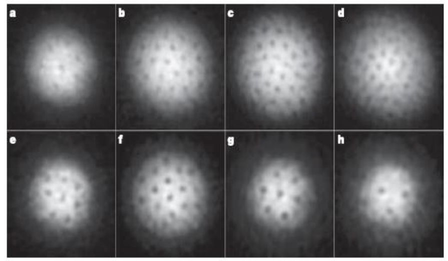
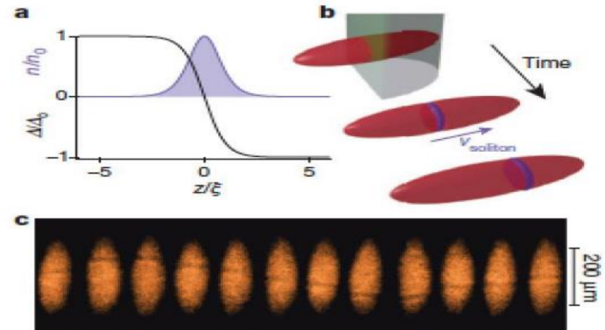
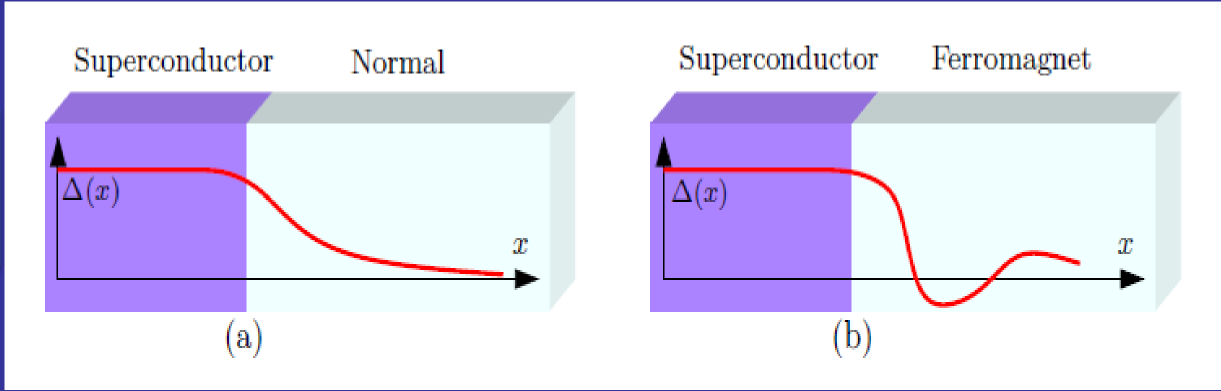


Figure 2 | Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (**a**) or 500 ms (**b–h**) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were 740 G (**a**), 766 G (**b**), 792 G (**c**), 812 G (**d**), 833 G (**e**), 843 G (**f**), 853 G (**g**) and 863 G (**h**). The field of view of each image is 880 μm × 880 μm.

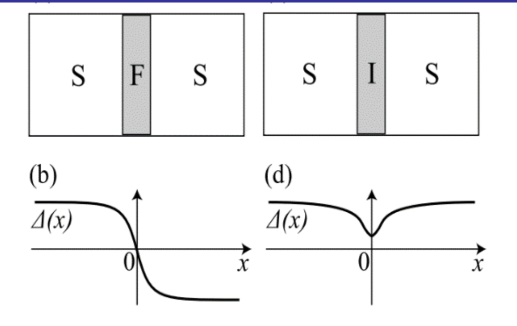


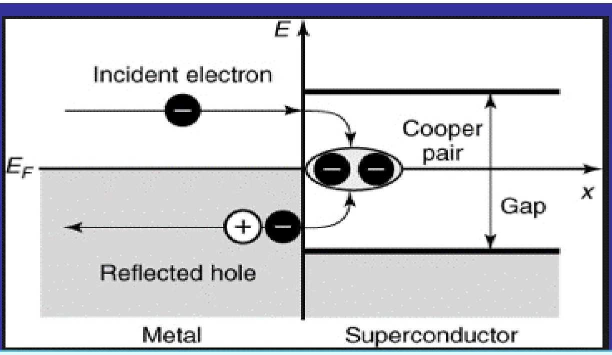
2) Bogoliubov – Anderson phonons

3) proximity effects: variations of the pairing field on the length scale of the coherence length.



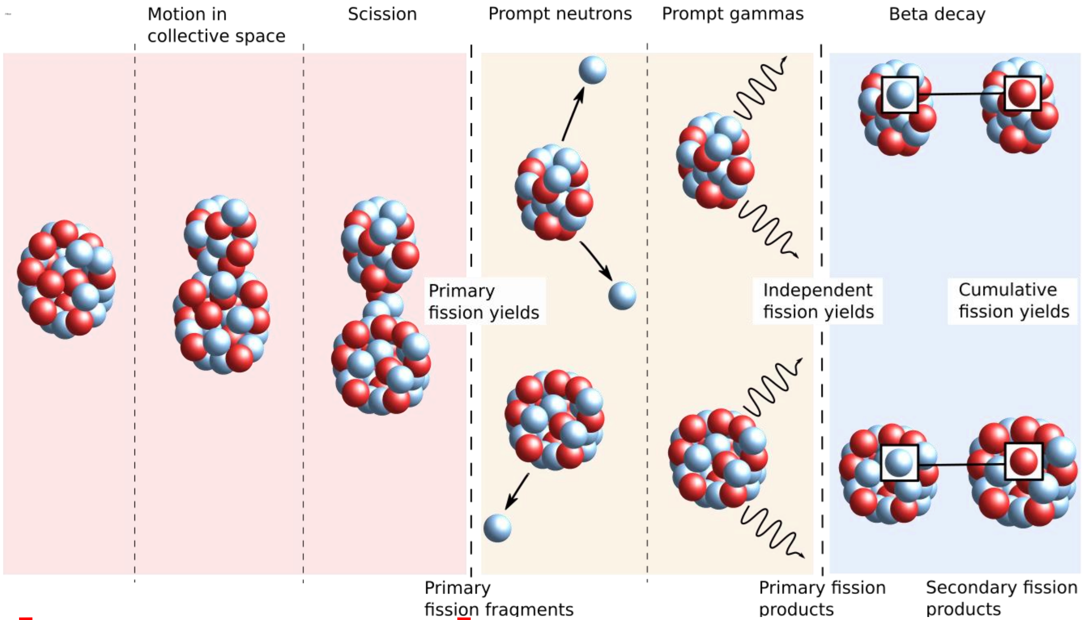
4) physics of Josephson junction (superfluid - normal metal), pi-Josephson junction (superfluid - ferromagnet)





5) Andreev reflection
(particle-into-hole and hole-into-particle scattering)
Andreev states cannot be obtained within BCS

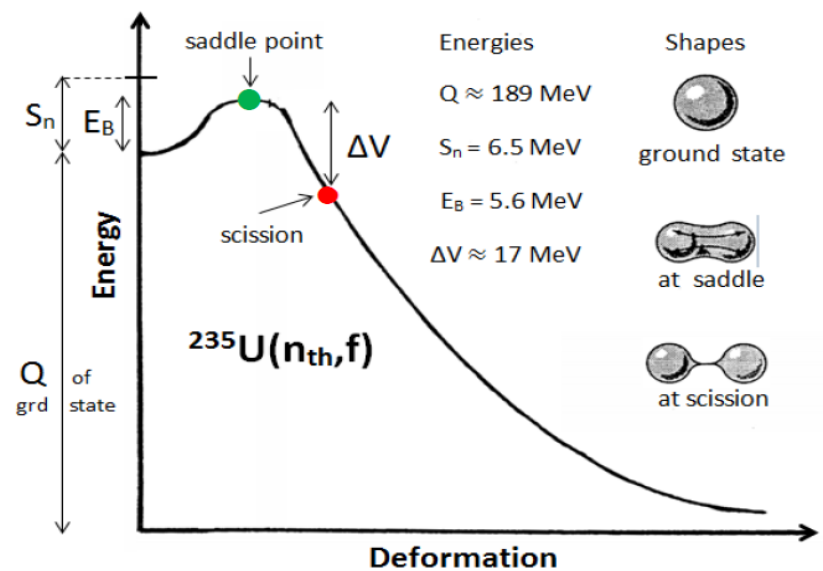
Theoretical description of nuclear induced fission



From LLNL-PRES-758023

Nuclear dynamics of interest

Potential energy versus deformation

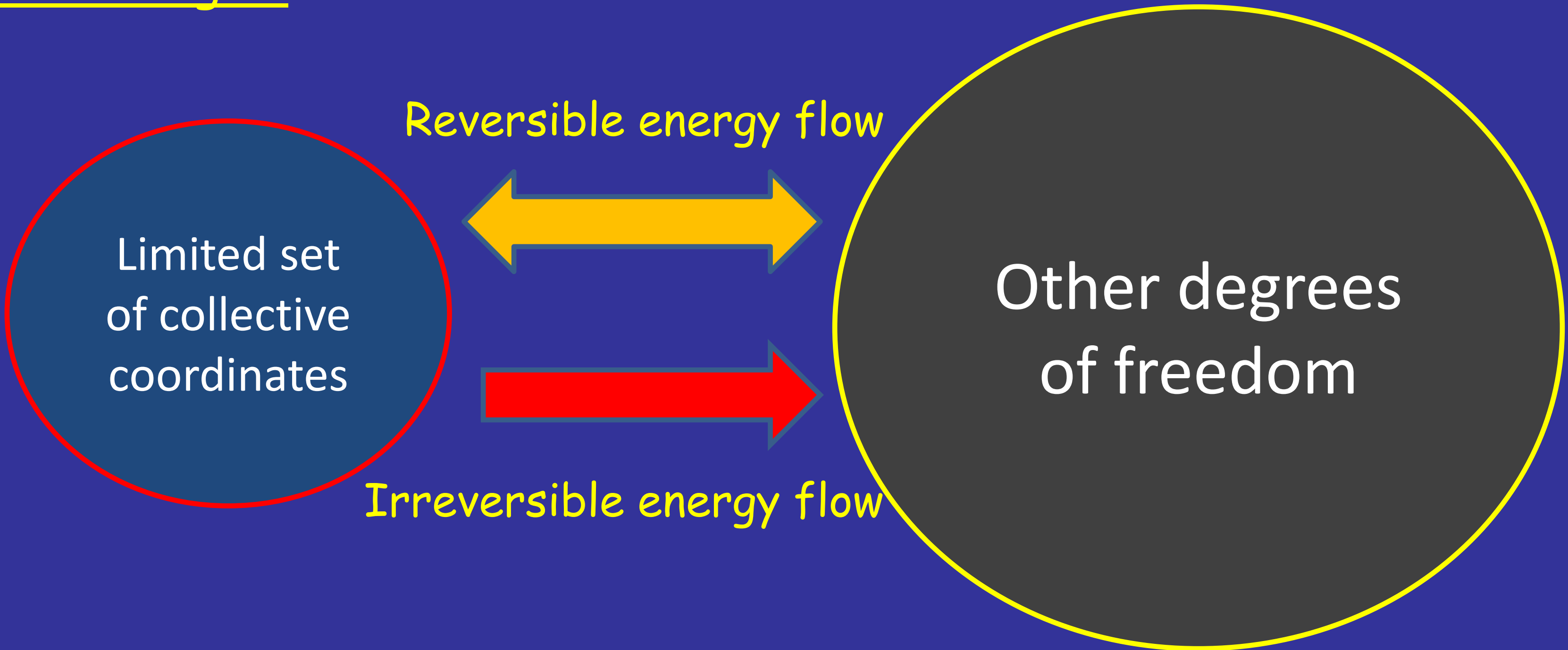


From F. Gonnenwein FIESTA2014

Estimation of characteristic time scales for low energy fission (<10MeV):

Ground state to saddle	-	1 000 000 zs
Saddle to scission	-	10-100 zs
Acceleration of fission fragments to 90% of their final velocity	-	10 zs
Neutron evaporation	-	1 000 zs

Typical framework for the theoretical description of nuclear dynamics at low energies



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

Irreversible energy flow is determined by friction coefficients 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

Induced fission – theoretical approaches

Potential energy surface (PES) + Langevin dynamics

Dissipative classical motion within the space spanned by chosen collective coordinates (not more than 5).

Features:

- Easy to use scheme, especially if for PES a micro-macro model is used.
- 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.

$$\dot{q}_i = \sum_j M_{ij}^{-1}(\vec{q})\, p_j$$

$$\dot{p}_i = -\frac{\partial V}{\partial q_i} - \frac{1}{2}\sum_{j,k}\frac{\partial M^{-1}{}_{jk}}{\partial q_i} p_j p_k \underbrace{-\sum_j \gamma_{ij} M^{-1}{}_{jk}(\vec{q})\, p_k}_{\text{friction}} + \underbrace{\sum g_{ij}(\vec{q})\,\xi_j(t)}_{\text{stochastic force}}$$

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

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

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 consistent way.

Time dependent generator coordinate method (TDGCM)

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.

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

$$\langle\Phi(\vec{q})|\Phi(\vec{q}\,')\rangle \sim exp(-\sum_k |\sigma_k(\vec{q})-\sigma_k(\vec{q}\,')|^2/2)$$ - 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

$B(\vec{q})$ - Mass tensor

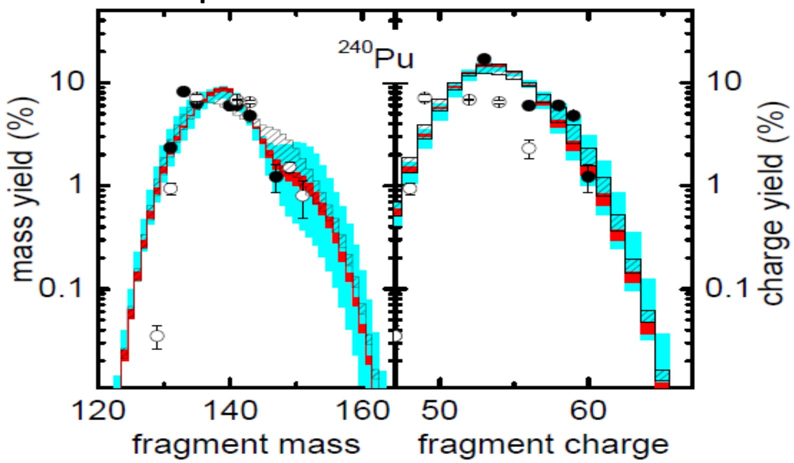
$g(\vec{q},t)$ - Probability amplitude for the system to be at point **q**

see eg.: D. Regnier et al. CPC 200, 350 (2016)

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

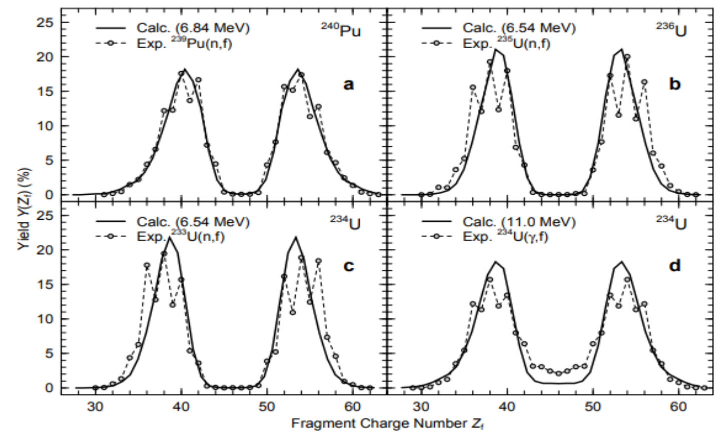
Mass/charge distribution in PES + Langevin approach

Spontaneous fission



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

Induced fission

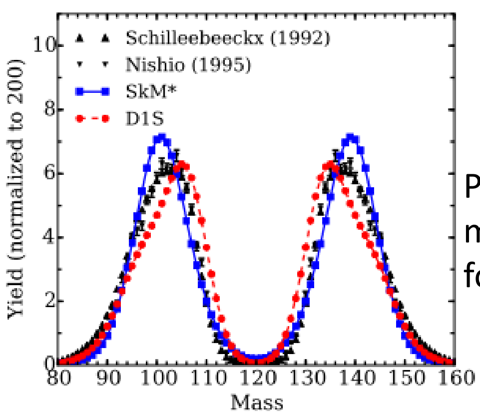


J. Randrup and P. Möller, PRL **106**, 132503 (2011)

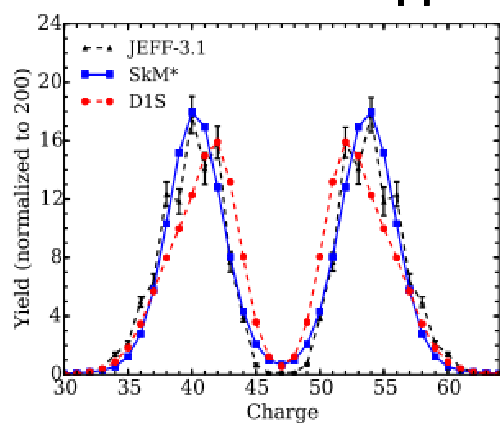
Strongly damped nuclear dynamics

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).

Mass/charge distribution in TDGCM approach



Pre-neutron mass yields for: 239Pu(n,f)



Charge yields for: 239Pu(n,f)

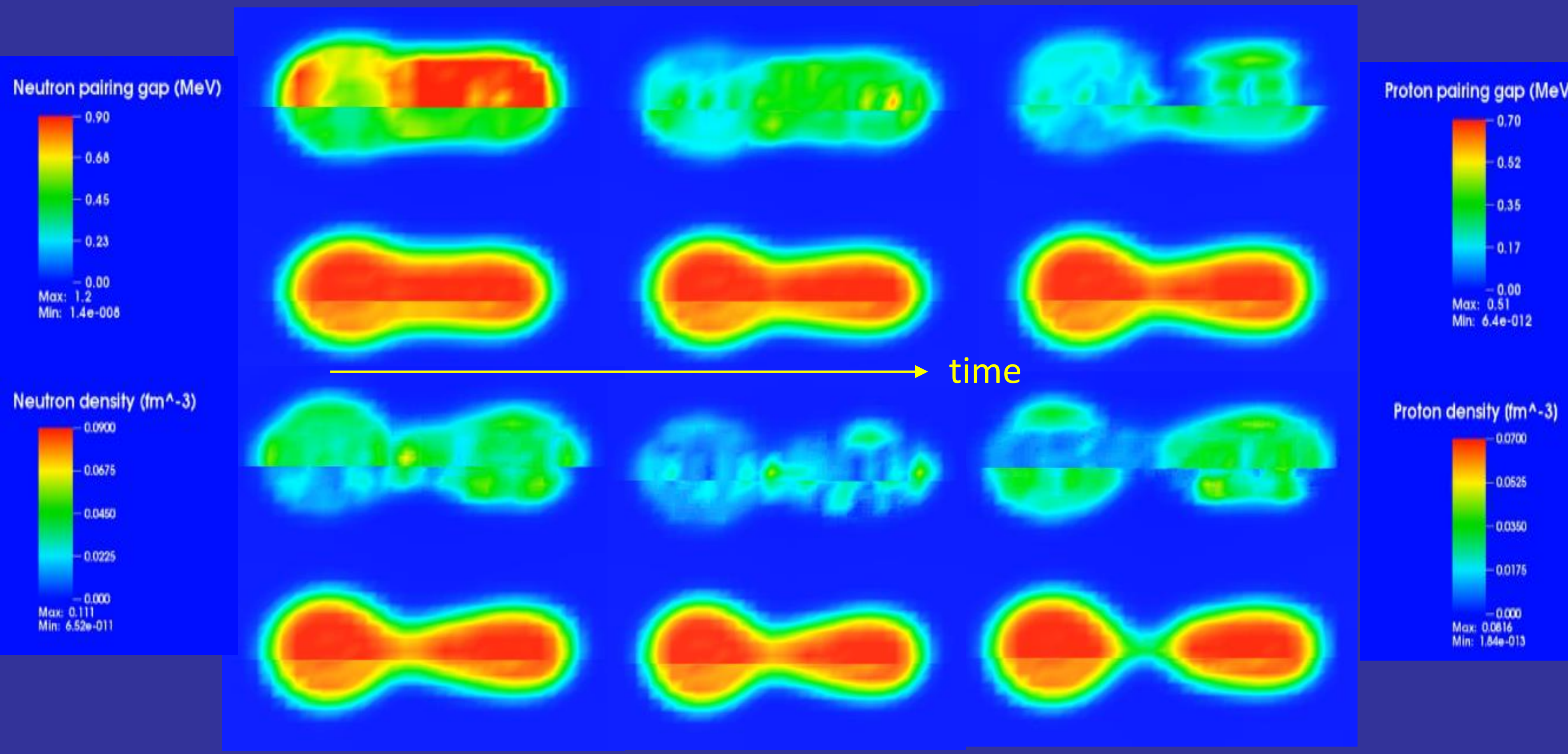
J.-F. Berger, M. Girod, D. Gogny, CPC **63**, 365 (1991); H. Goutte, J.-F. Berger, P. Casoli, D. Gogny, PRC **71** 024316 (2005); D. Regnier, N. Dubray, N. Schunck, and M. Verrière, PRC **93**, 054611 (2016); D. Regnier, M. Verriere, N. Dubray, and N. Schunck, CPC **200**, 350 (2016)

Mass and charge distributions are not sensitive to the character of nuclear motion prior to the scision point.

They depend predominantly on the structure of the collective energy surface

Fission dynamics of ^{240}*Pu within TDDFT*

No need to define collective variables
No need to assume the nature of energy transfer between collective variables and the rest of the system - all fermionic degrees of freedom are evolved.



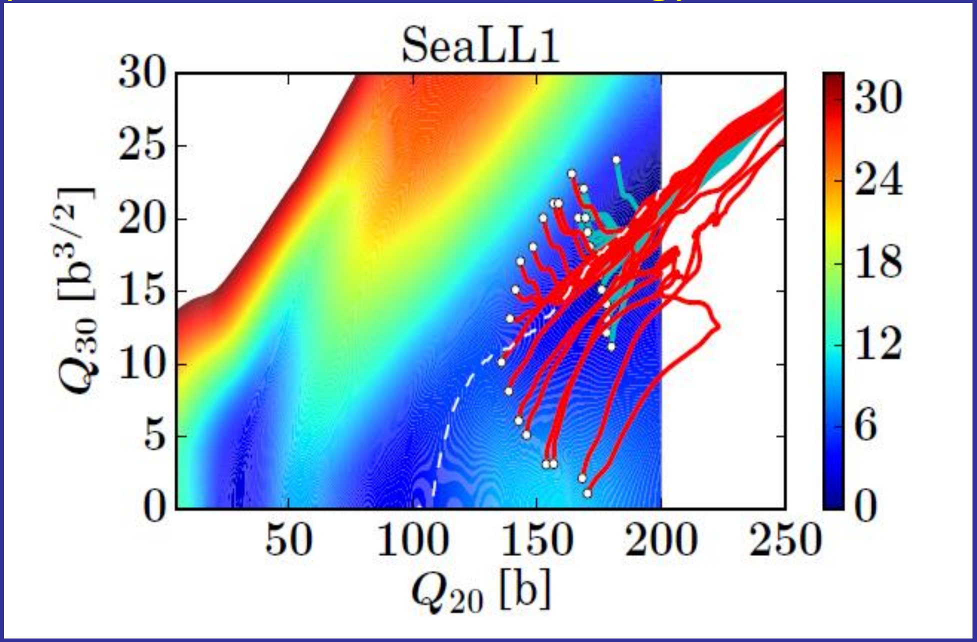
Note that the pairing fields (upper panels) vary considerably during nuclear motion – **many pairing modes are excited!**

<u>The saddle-scission time is considerably longer (4000 – 10000 fm/c)</u> than in simplified approaches.

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

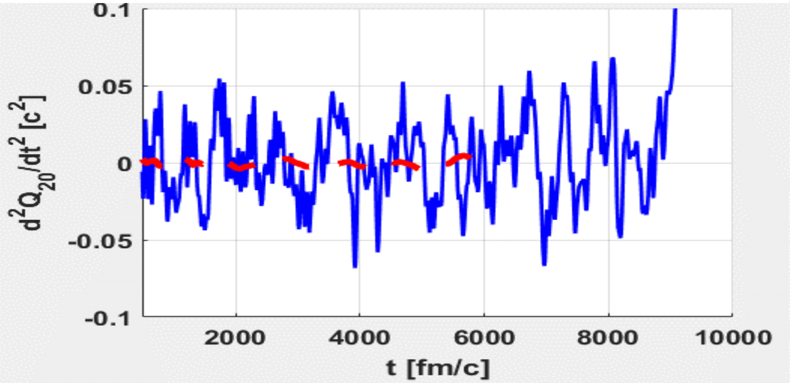
Fission dynamics of ^{240}Pu

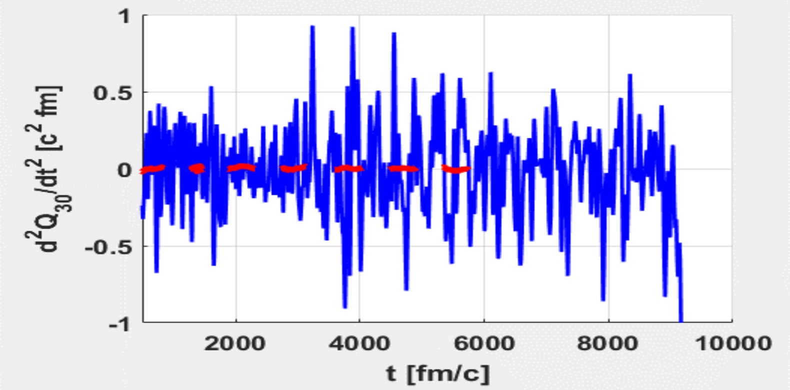
Trajectories of fissioning ^{240}Pu in the collective space at excitation excitation energy of *E=8-9 MeV*:



A. Bulgac, et al. Phys. Rev. C 100, 034615 (2019)

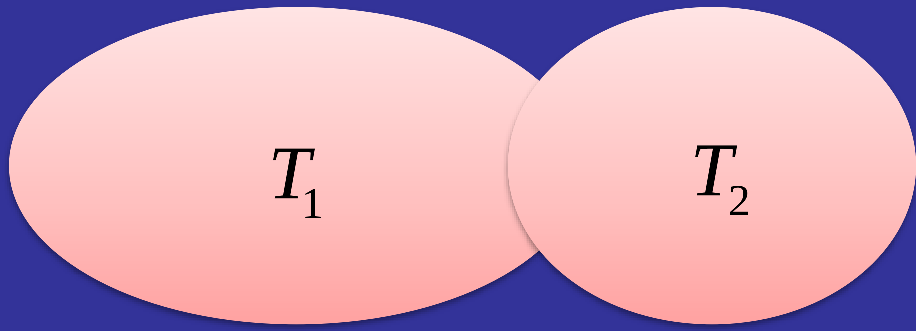
Accelerations in quadrupole and octupole moments along the fission path

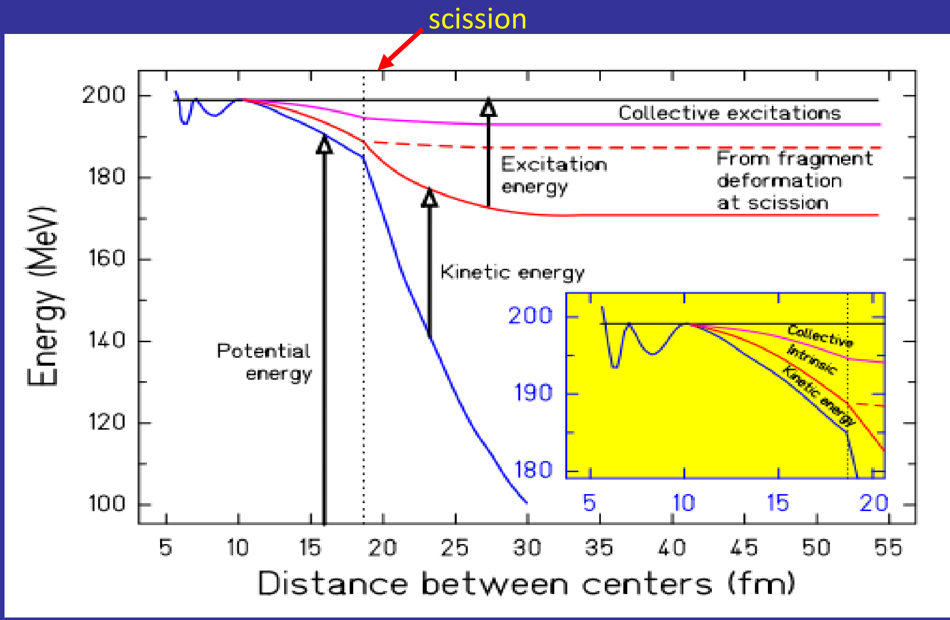




Note that despite the fact that nucleus is already beyond the saddle point the collective motion on the time scale of 1000 fm/c and larger is characterized by the constant velocity (*see red dashed line for an average acceleration*) till the very last moment before splitting. On times scales, of the 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

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





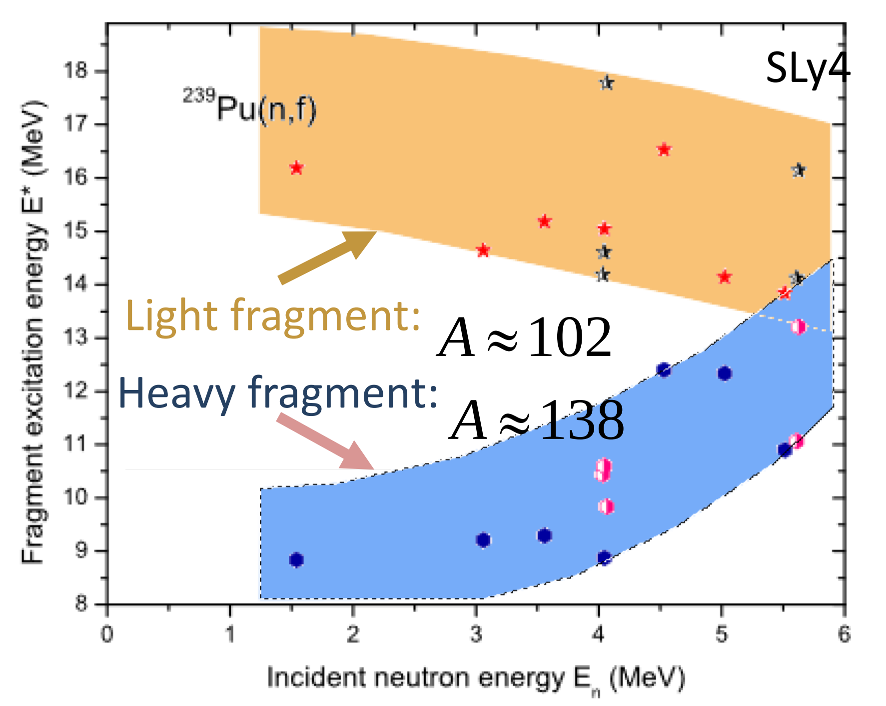
Schmidt&Jurado:Phys.Rev.C83:061601,2011

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 dynamically (no sufficient time for equilibration).



E^* (MeV)	E_n (MeV)	TKE_{TDSLDA} (MeV)	TKE_{syst} (MeV)	err (%)	Z_L	N_L
8.08	1.542	173	177.26	1.95	40.825	62.246
9.60	3.063	174	176.73	1.13	40.500	61.536
10.10	3.560	179	176.56	1.43	41.625	62.783
10.57	4.032	173	176.39	1.55	40.092	61.256
10.58	4.043	173	176.39	1.70	40.146	61.388
10.58	4.047	175	176.39	0.72	40.313	61.475
10.60	4.065	174	176.38	0.92	40.904	62.611
11.07	4.534	176	176.22	0.14	41.495	63.134
11.56	5.024	175	176.05	0.51	40.565	61.894
12.05	5.515	176	175.88	0.49	40.412	61.809
12.15	5.610	176	175.84	0.29	40.355	61.695
12.16	5.626	176	175.84	0.15	41.386	62.764

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!

$$\mathrm{TKE} = 177.80 - 0.3489 E_n \quad [\text{in MeV}],$$

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)

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.

Usefulness of various fission observables

Mass/charge distribution – does not provide us 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 – 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 - this quantity 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 - <u>depending on dynamics</u> and density of states at scission. <u>**Very severe test for TDDFT: theoretical predictions already exist.**</u>

Primary gamma emission - may give some information on ang. momentum distribution of fragments, but as far as I know, not directly comparable to theories presented here.

DFT and broken symmetry framework

DFT works within the symmetry broken framework using the concept of „deformation".

„Deformation" means that the many-body system does not conserve certain quantum number, but instead in its description one introduces „deformation variables"

Examples:
1) Nuclear deformation - violation of total angular momentum conservation
2) Pairing gap (field) - violation of particle number conservation
etc.

The reason for such description is simplicity: we get a better insight into physics of certain effects, which otherwise are difficult to grasp using fully quantum mechanical description.

As a consequence, instead of eigenstates of Hamiltonian with well defined quantum numbers, we deal with description in terms of variables, which are canonically conjugate to conserved quantities:

1) **Nuclear deformation**: *angles defining orientation in space*
2) **Pairing**: *gauge angle defining phase of the Cooper pairs condensate.*

In the case when calculated observables are sensitive to the broken symmetries we need however to restore them.

Two ways of dealing with the problem:

1. Projection.

We pick the component of „wave function" with correct quantum numbers and use it for calculation of observables.

Strategy usually applied in the static calculations:

- projection on a good angular momentum value,
- projection on a good particle number,

etc.

Drawback:

It is in general ill-defined procedure in DFT.

2. Averaging over „deformation variables".

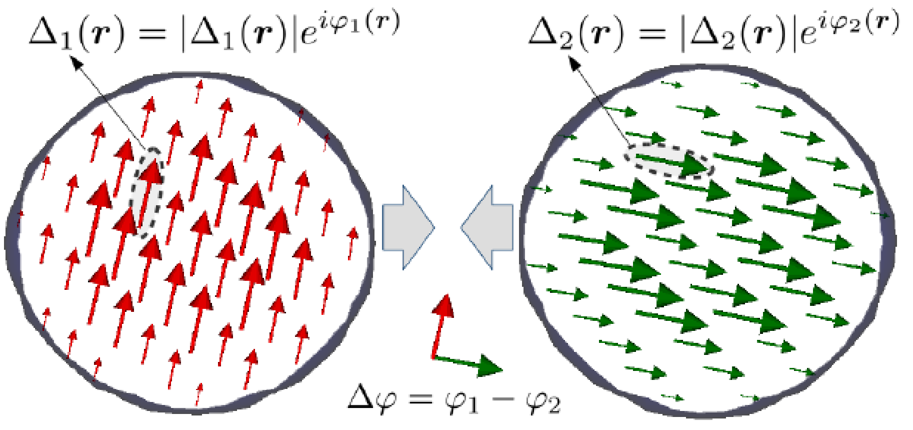
In the case of studies of time evolution there is a certain time scale associated with the process under consideration (eg. time scale related to nuclear collision).

If the time scale is much longer than the characteristic time related to the excitation associated with broken symmetries (Goldstone mode) then one may work within broken symmetry framework and average results over many orientations of „deformation parameters".

Example:

Suppose we want to investigate the role of the phase of pairing field in nuclear collision.

$$\Delta(\vec{r},t) = |\Delta(\vec{r},t)| e^{i\phi(\vec{r},t)}$$



The time scale of the Goldstone mode related to pairing field phase is governed by the chemical potential:

$$T = \hbar \frac{\pi}{\mu}$$

The proton/neutron pairing field „rotates" in time with frequency: $\omega = 2\mu / \hbar$

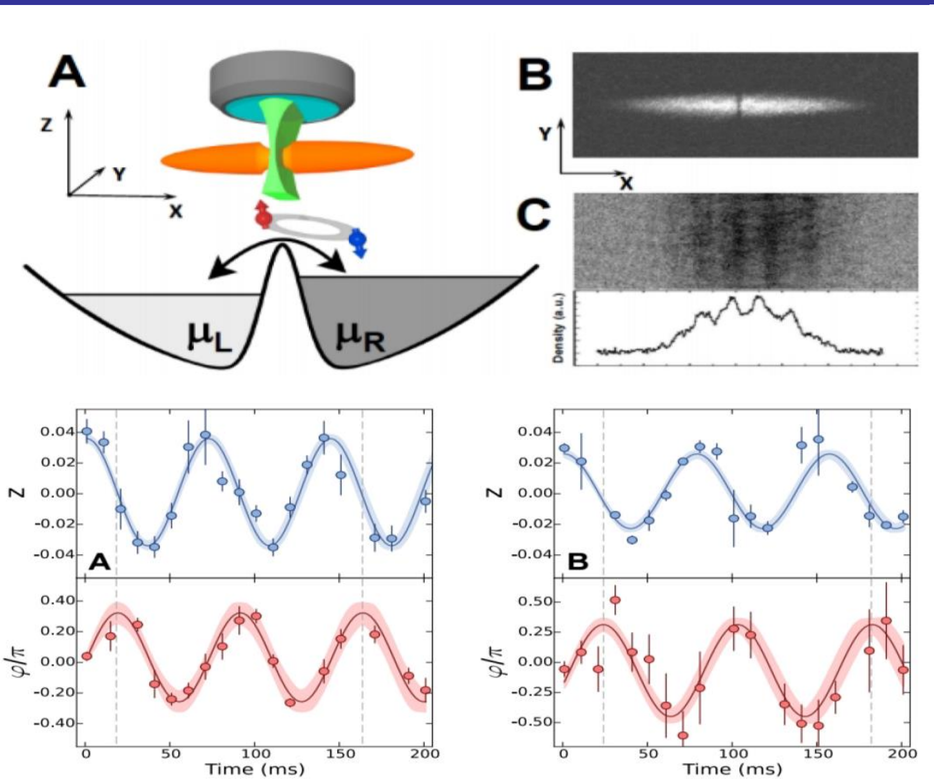
However what matters here is the difference in rotation between left and right nucleus.

$$\omega = 2\Delta\mu / \hbar$$

Therefore choosing two identical nuclei we may „freeze" their relative phase.

Ultracold atomic gases: two regimes for realization of dynamics induced by relative phase of pairing fields

Weak coupling (weak link)



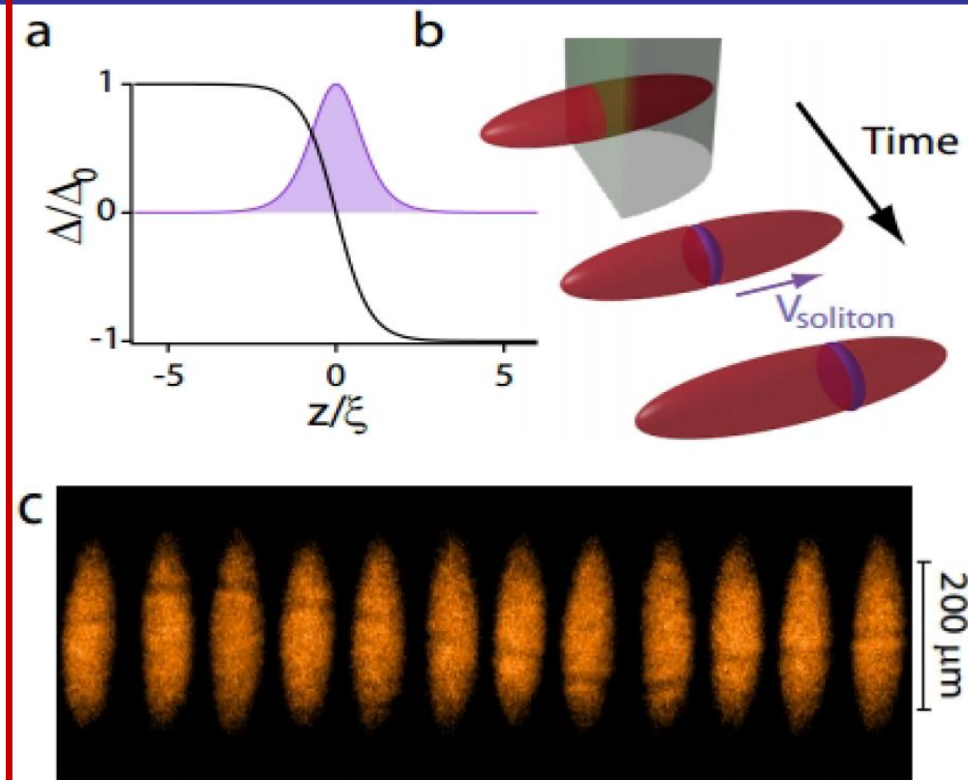
Observation of ***AC Josephson effect*** between two 6Li atomic clouds.

$$J(t) = J_c \sin\left(\Delta\varphi(t)\right)$$

$$\frac{d\left(\Delta\varphi\right)}{dt} = \frac{2eU}{\hbar}$$

G. Valtolina et al., Science 350, 1505 (2015).

Strong coupling



Creation of a „heavy soliton" after merging two superfluid atomic clouds.

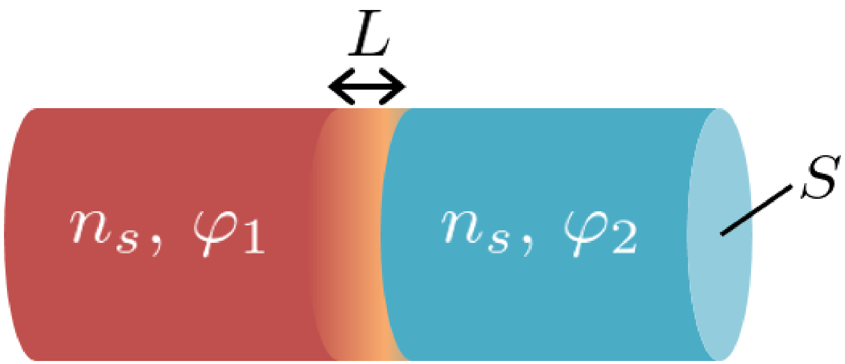
T. Yefsah et al., Nature 499, 426 (2013).

Estimates for the magnitude of the effect

At first one may think that the magnitude of the effect is determined by the nuclear pairing energy which is of the order of MeV's in atomic nuclei (according to the expression):

$$\frac{1}{2} g(\varepsilon_F) |\Delta|^2; \quad g(\varepsilon_F) \text{ - density of states}$$

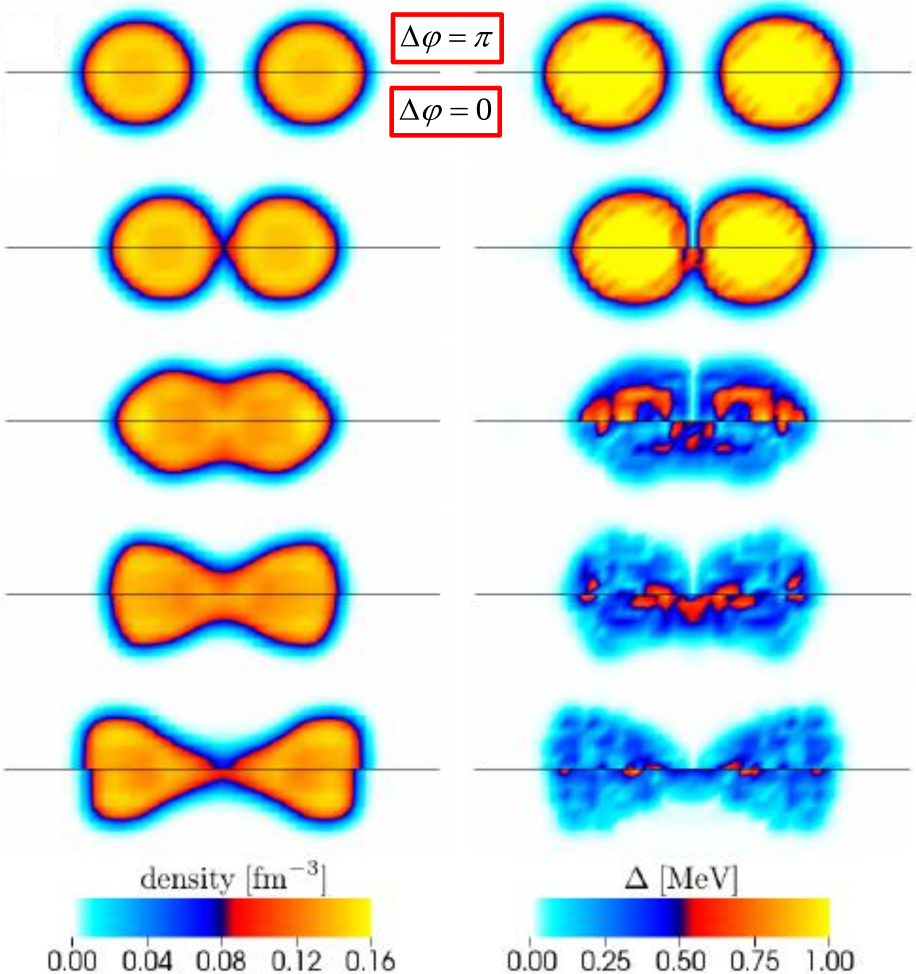
On the other hand the energy stored in the junction can be estimated from Ginzburg-Landau (G-L) approach:



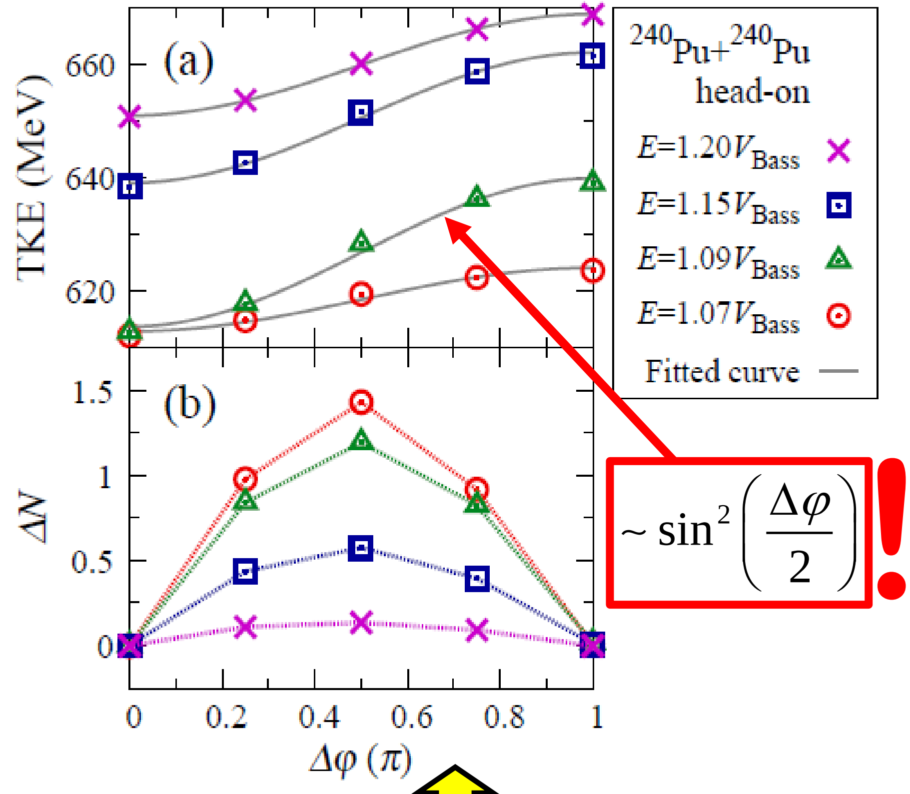
$\Delta\varphi \ (\equiv \varphi_1 - \varphi_2)$

$$E_j = \frac{S}{L} \frac{\hbar^2}{2m} n_s \sin^2 \frac{\Delta\varphi}{2}$$

For typical values characteristic for two medium nuclei: $E_j \approx 30 MeV$



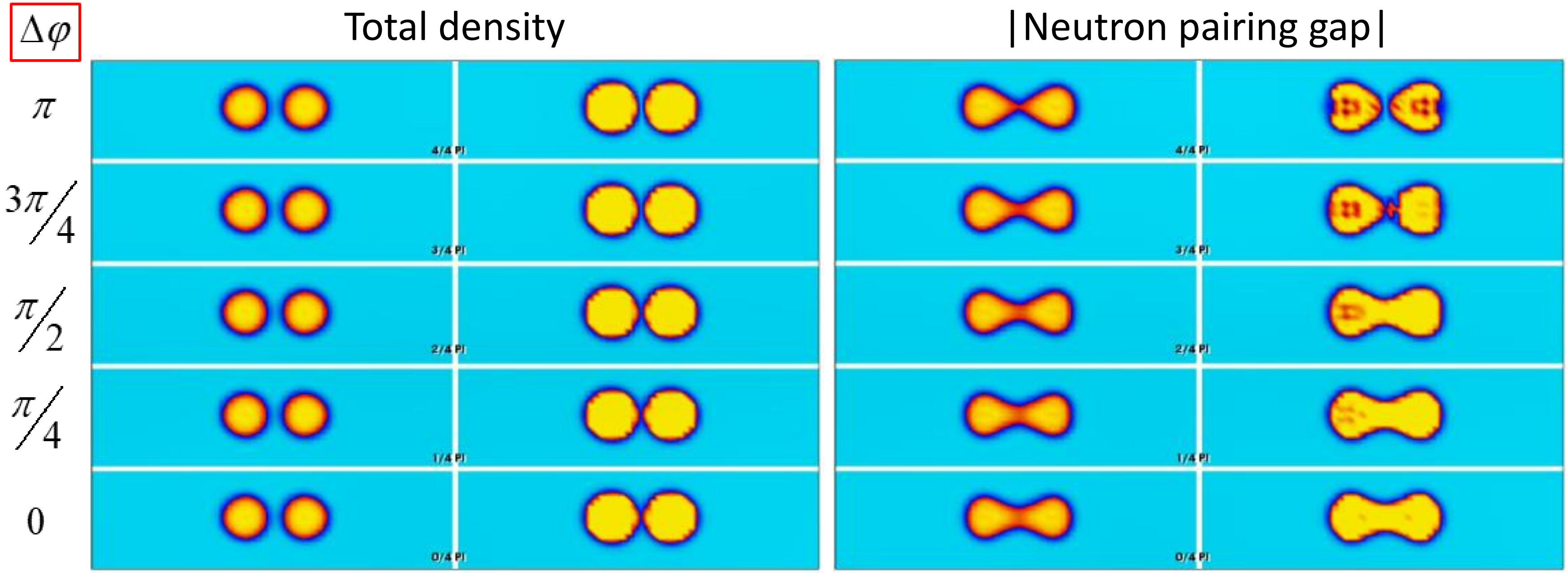
Total kinetic energy of the fragments (TKE)

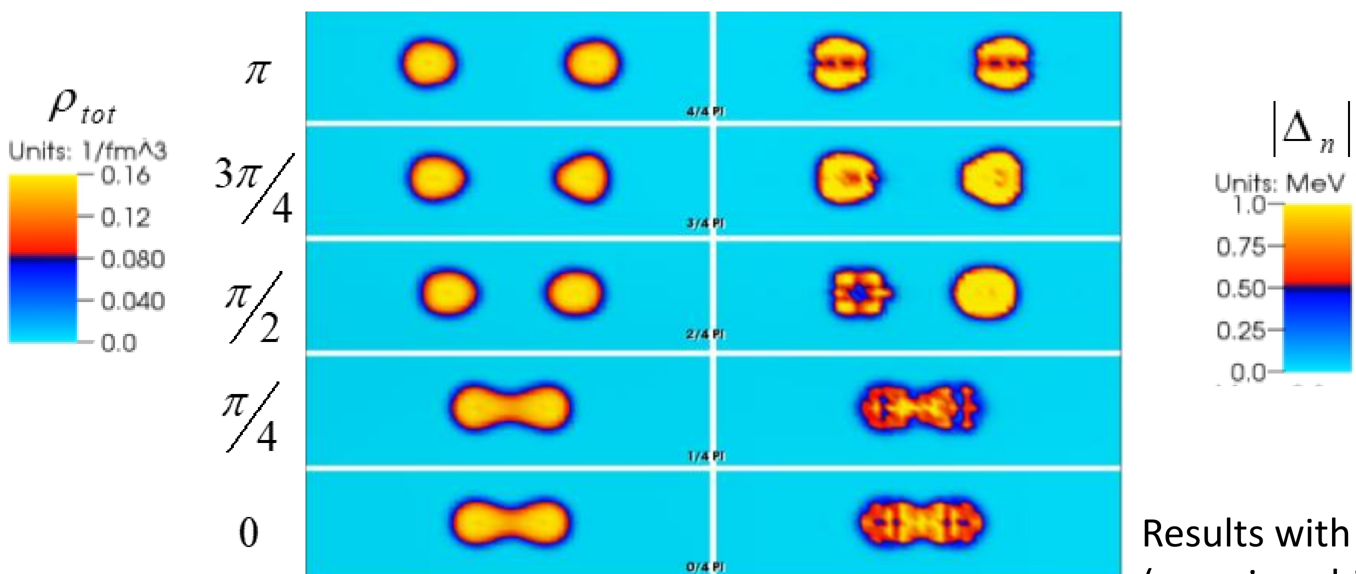


Average particle transfer between fragments.

Creation of the solitonic structure between colliding nuclei prevents energy transfer to internal degrees of freedom and consequently enhances the kinetic energy of outgoing fragments.
Surprisingly, the gauge angle dependence from the G-L approach is perfectly well reproduced in the kinetic energies of outgoing fragments!

$^{90}Zr + {}^{90}\mathrm{Zr}$ at energy $E \simeq V_{Bass}$

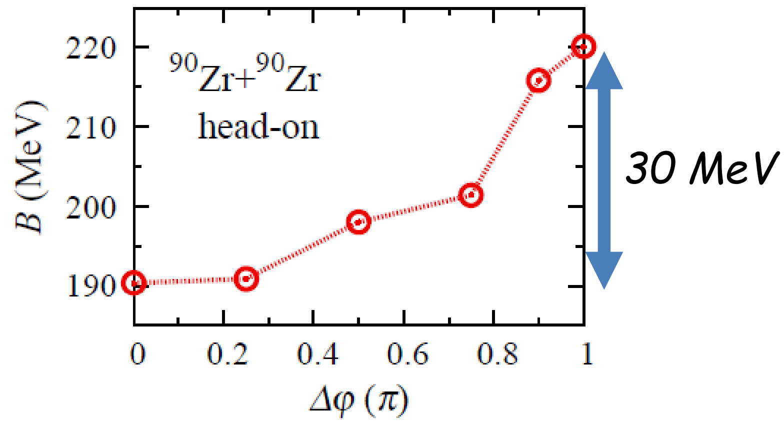




Results with Fayans functional
(no spin-orbit term)

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

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



Results with Fayans functional (no spin-orbit term)

What is an average extra energy needed for the capture?

$$E_{extra} = \frac{1}{\pi}\int_0^{\pi}\left(B(\Delta\varphi) - V_{Bass}\right) d(\Delta\varphi) \approx 10MeV$$

The effect is found (within TDDFT) 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): barrier fluctuations extracted from experimental data indicate that the effect exists although is weaker than predicted by TDDFT

	^{90}Zr	^{96}Zr	
	$\Delta_n = 0.0MeV$	$\Delta_n = 0.73MeV$	$\Delta_n = 1.98MeV$
	$\Delta_p = 0.09MeV$	$\Delta_p = 0.93MeV$	$\Delta_p = 0.32MeV$
$E_{min}(0)$ (MeV)	184	180	179
$E_{min}(\pi)$ (MeV)	184	186	185

Recent results with SLy4 functional: Minimum energy needed for capture. M. Barton et al.

Open problems of TDDFT

1) 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

   Stochastic extensions of TDDFT 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, Phys. Rev. C 100, 014615 (2019)

3) Dissipation: transition between one-body dissipation regime and two-body dissipation regime.

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