Time Dependent Density Functional Theory for nuclear reactions – advantages and disadvantages.







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GOAL:

Microscopic framework = explicit treatment of fermionic degrees of freedom.

# Why Time Dependent Density Functional Theory (TDDFT)?

We need to describe the time evolution of (externally perturbed) spatially inhomogeneous, superfluid Fermi system.

Within current computational capabilities TDDFT allows to describe real time dynamics of strongly interacting, superfluid systems of <u>hundred of thousands</u> fermions.



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





2012



the ground state density:  $\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = \Psi[\rho](\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)$ 



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 scheme

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 <u>local extension</u> of DFT to superfluid systems (SLDA) and time-dependent 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)

## **Pairing correlations in DFT**

One may extend DFT to superfluid systems by defining the pairing field:

$$\Delta(\mathbf{r}\sigma,\mathbf{r}'\sigma') = -\frac{\delta E(\rho,\chi)}{\delta\chi^*(\mathbf{r}\sigma,\mathbf{r}'\sigma')}.$$

L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett. 60 2430 (1988).
O.-J. Wacker, R. Kümmel, E.K.U. Gross, Phys. Rev. Lett. 73, 2915 (1994).
Triggered by discovery of high-Tc superconductors

and introducing anomalous density 
$$~\chi({f r}\sigma,{f r}'\sigma')=\langle\hat\psi_{\sigma'}({f r}')\hat\psi_{\sigma}({f r})
angle$$

However in the limit of the local field these quantities diverge unless one renormalizes the coupling constant:

$$\begin{split} \Delta(\mathbf{r}) &= g_{eff}(\mathbf{r})\chi_c(\mathbf{r}) \\ \frac{1}{g_{eff}(\mathbf{r})} &= \frac{1}{g(\mathbf{r})} - \frac{mk_c(\mathbf{r})}{2\pi^2\hbar^2} \left(1 - \frac{k_F(\mathbf{r})}{2k_c(\mathbf{r})}\ln\frac{k_c(\mathbf{r}) + k_F(\mathbf{r})}{k_c(\mathbf{r}) - k_F(\mathbf{r})}\right) \end{split}$$

which ensures that the term involving the kinetic and the pairing energy density is finite:

$$\frac{\tau_c(r)}{2m} - \Delta(r)\chi_c(r), \quad \tau_c(r) = \nabla \cdot \nabla' \rho_c(r, r')|_{r=r'}$$

A. Bulgac, Y. Yu, Phys. Rev. Lett. 88 (2002) 042504A. Bulgac, Phys. Rev. C65 (2002) 051305

It allows to reduce the size of the problem for static calculations by introducing the energy cutoff

Pairing correlations in time-dependent DFT

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

Stationarity requirement produces the set of equations:

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} U_{\mu}(\mathbf{r},t) \\ V_{\mu}(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h(\mathbf{r},t) & \Delta(\mathbf{r},t) \\ \Delta^{*}(\mathbf{r},t) & -h^{*}(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} U_{\mu}(\mathbf{r},t) \\ V_{\mu}(\mathbf{r},t) \end{pmatrix};$$
$$B(t) = \begin{pmatrix} U(t) & V^{*}(t) \\ V(t) & U^{*}(t) \end{pmatrix} = \exp[iG(t)] \qquad G(t) = \begin{pmatrix} h(t) & \Delta(t) \\ \Delta^{\dagger}(t) & -h^{*}(t) \end{pmatrix}$$

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.

## <u>Pairing as an energy gap</u>

Quasiparticle energy:



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)



Deformation



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

Both magnitude and phase may have a nontrivial spatial and time dependence.

Example of a nontrivial spatial dependence: *quantum vortex* 



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

Experiments with ultracold Li6 atoms: pictures of the vortex lattice.

M.W. Zwierlein et al.. Nature, 435, 1047 (2005)

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.

Sometimes simplified assumptions are made eg. replacing TDHFB by TDBCS (see Guillaume Scamps talk):

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

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.

#### 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 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

## **TDDFT equations with local pairing field (TDSLDA):**

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}u_{k\uparrow}(\mathbf{r},t)\\u_{k\downarrow}(\mathbf{r},t)\\v_{k\uparrow}(\mathbf{r},t)\\v_{k\downarrow}(\mathbf{r},t)\end{pmatrix} = \begin{pmatrix}h_{\uparrow,\uparrow}(\mathbf{r},t)&h_{\uparrow,\downarrow}(\mathbf{r},t)&0&\Delta(\mathbf{r},t)\\h_{\downarrow,\uparrow}(\mathbf{r},t)&h_{\downarrow,\downarrow}(\mathbf{r},t)&-\Delta(\mathbf{r},t)&0\\0&-\Delta^{*}(\mathbf{r},t)&-h_{\uparrow,\uparrow}^{*}(\mathbf{r},t)&-h_{\uparrow,\downarrow}^{*}(\mathbf{r},t)\\\Delta^{*}(\mathbf{r},t)&0&-h_{\uparrow,\downarrow}^{*}(\mathbf{r},t)&-h_{\downarrow,\downarrow}^{*}(\mathbf{r},t)\end{pmatrix} \begin{pmatrix}u_{k\uparrow}(\mathbf{r},t)\\u_{k\downarrow}(\mathbf{r},t)\\v_{k\uparrow}(\mathbf{r},t)\\v_{k\downarrow}(\mathbf{r},t)\end{pmatrix}$$

The form of h(r,t) and  $\Delta(r,t)$  is determined by EDF (Energy Density Functional)

- The system is placed on a large 3D spatial lattice.
- No symmetry restrictions.
- Number of PDEs is of the order of the number of spatial lattice points.
- The limit for the time evolution for nuclear systems: 10^(-19) sec.

*Table 1: Comparison of profit gained by using GPUs instead of CPUs for two example lattices. The timing was obtained on Titan supercomputer. Note, Titan has 16x more CPUs than GPUs.* 

		<b>CPU</b> impleme	ntation	<b>GPU</b> impleme	ntation	
	Number of HFB					
N <sub>x</sub> N <sub>y</sub> N <sub>z</sub>	equations	# of CPUs	time per step	# of GPUs	time per step	SPEEDUP
48 <sup>3</sup>	110,592	110,592	3.9 sec	6,912	0.39 sec	10
64 <sup>3</sup>	262,144	262,144	20 sec	16,384	0.80 sec	25

Note that in TDHF the number of equations is of the order of the number of particles evolved i.e. in the case of atomic nuclei: <u>couple hundred eqs</u>.

Using the most powerful supercomputers we can currently evolve up to 100 000 particles

## **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>.
- Simulations follow closely the way how experiments are conducted.
- 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</u> <u>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>.

# **Challenges 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 (important for scattering):

$$S_{fi} = \lim_{t \to \infty} \left\langle \Phi_f \left| \Phi(t) \right\rangle; \quad \lim_{t \to -\infty} \left| \Phi(t) \right\rangle = \left| \Phi_i \right\rangle$$

- momentum distributions
- transitional densities (defined in linear response regime)
- various conditional probabilities
- mass distributions (needs an extension to stochastic TDDFT or combining with TDGCM)
- 3) Memory effects.

In general the evolution of the system in TDDFT will depend on the past. Very little is known about the memory terms, but in principle it can be long ranged (see eg. Dobson, Brunner, Gross, Phys. Rev. Lett. 79 (1997) 1905)

Memory effects are usually neglected . Result: dissipation effects are not correctly taken into account except for one-body dissipation



## **Areas of applications**



Ultracold atomic (fermionic) gases. Unitary regime. Dynamics of quantum vortices, solitonic excitations, quantum turbulence.





Science **332**, 1288 (2011). Phys. Rev. Lett. **112**, 025301 (2014)



Astrophysical applications. Modelling of neutron star interior (glitches): vortex dynamics, dynamics of inhomogeneous nuclear matter (in strong magnetic fields).





Phys. Rev. Lett. **117**, 232701 (2016) Phys. Rev. Lett. 110, 241102 (2013) Nuclear physics. Induced nuclear fission, fusion, collisions.





Phys. Rev. Lett. **119**, 042501 (2017) Phys. Rev. Lett. **116**, 122504 (2016) Phys. Rev. Lett. **114**, 012701 (2015) **Examples of applications:** 

- Nuclear induced fission
- Collisions of medium or heavy superfluid nuclei

# Fission dynamics of <sup>240</sup>Pu

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 <sup>240</sup>Pu



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



Induced fission of 240Pu

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

Energies are not shared proportionally to mass numbers of the fragments!

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

#### Remarks on the fragment 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 <u>to the total entropy maximization</u> of two nascent fragments (i.e. according to temperatures, level densities) and the <u>fission dynamics does not matter.</u>

In TDDFT such a decomposition can be performed as well (in progress). Note that both deformation energy and collective energy may depend on the functional. The intrinsic energy in TDDFT will be partitioned <u>dynamically</u> (no sufficient time for equilibration).

## **Nuclear collisions**

## Collisions of superfluid nuclei having <u>different phases</u> of the <u>pairing fields</u>

Motivated by experiments on ultracold atomic gases: merging two 6Li clouds





Creation of a "<u>heavy soliton</u>" after merging two superfluid atomic clouds. T. Yefsah et al., Nature 499, 426 (2013).

Sequence of decays of topological excitations is reproduced by TDSLDA: Wlazłowski, et al., Phys. Rev. A91, 031602 (2015)

<u>In the context of nuclear systems the main questions are:</u> -how a possible solitonic structure can be manifested in nuclear system? -what observable effect it may have on heavy ion reaction: kinetic energies of fragments, capture cross section, etc.?

Clearly, we cannot control phases of the pairing field in nuclear experiments and the possible signal need to be extracted after averaging over the phase difference.

# 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):

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

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

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



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



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)

# Summarizing

- TDDFT extended to superfluid systems and based on the local densities offers a flexible tool to study quantum superfluids far from equilibrium.
- TDDFT offers an unprecedented opportunity to test the nuclear energy density functional for large amplitude collective motion, non-equilibrium phenomena.
- For nuclear fission of 240Pu TKEs are reproduced with <2% accuracy for the range of the neutron incident energies: 1.5 - 5.5 MeV.
   TDDFT offers an easy way to extract excitation energy sharing between fragments (experimental data needed!).
- In the context of nuclear reaction extension of TDDFT is needed in order to be able to address the mass and TKE distributions.

# Future plans:

- Ultracold atoms: investigation of <u>quantum turbulence</u> in Fermi systems; topological excitations in <u>spin-polarized</u> atomic gases in the presence of <u>LOFF phase</u>.
- Neutron star: Provide a link between <u>large scale models</u> of neutron stars and microscopic studies; towards the first simulation of the glitch phenomenon based on microscopic input.
- Nuclear physics: The dependence of <u>quasifission</u> process on pairing.

#### Selected supercomputers (CPU+GPU) currently in use:



#### Piz Daint: 7.787 PFlops (Swiss National Supercomputing Centre)

HA-PACS: 0.802 PFlops (University of Tsukuba)





Tsubame: 5.7 PFlops (Tokyo Institute of Technology)

**TSUBAME** 

#### Titan: 27 PFlops (ORNL Oak Ridge)



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