Selected applications of superfluid extension of TDDFT



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<u>GOAL:</u>

Description of superfluid dynamics <u>far from equilibrium</u> within the framework of Time Dependent Density Functional Theory (TDDFT).

We would like to describe the time evolution of (externally perturbed) spatially inhomogeneous, superfluid Fermi system and in particular such phenomena as:

- Vortex dynamics in ultracold Fermi gases and neutron matter.
- Vortex impurity interaction, vortex reconnections.
- Quantum turbulence.
- Atomic cloud collisions.
- Nuclear dynamics: large amplitude collective motion, induced nuclear fission, reactions, fusion, excitation of nuclei with gamma rays and neutrons.

Outline

- Basics of superfluid TDDFT in the local density approximation.
- Vortex dynamics in ultracold atomic gases.
- Vortex-impurity interaction in superfluid neutron matter.
- Nonlinear response of nuclear system: relativistic Coulomb excitation, induced fission.
- Effective mass of nuclear impurity in superfluid neutron matter.
- Solitonic excitations in nuclear reaction.

Runge Gross mapping

and consequently the functional exists:

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

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 approach

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

Interacting system

Noninteracting system

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

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

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

Hence the DFT approach is essentially exact.

However as always there is a price to pay:

- Kohn-Sham potential in principle depends on the past (memory).
 Very little is known about the memory term and usually it is disregarded.
- Only one body observables can be reliably evaluated within standard DFT.

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).

and introducing anomalous density $\chi(\mathbf{r}\sigma,\mathbf{r}'\sigma')=\langle\hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}_{\sigma}(\mathbf{r})\rangle$

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

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

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

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

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

Formalism for Time Dependent Phenomena: TDSLDA

Local density approximation (no memory terms)

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

Density functional contains normal densities, anomalous density (pairing) and currents:

$$E(t) = \int d^3r \left[\varepsilon(n(\vec{r},t),\tau(\vec{r},t),\nu(\vec{r},t),\vec{j}(\vec{r},t)) + V_{ext}(\vec{r},t)n(\vec{r},t) + \dots \right]$$

- 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

Current capabilities of the code:

- volumes of the order of (L = 80³) capable of simulating time evolution of 42000 neutrons at saturation density (natural application: neutron stars)
- For nuclear systems: capable of simulating up to times of the order of 10⁻¹⁹ s (a few million time steps)
- <u>CPU vs GPU on Titan ≈ 15 speed-up</u> (likely an additional factor of 4 possible)
 Eg. for 137062 two component wave functions:
 CPU version (4096 nodes x 16 PEs) 27.90 sec for 10 time steps
 GPU version (4096 PEs + 4096GPU) 1.84 sec for 10 time step

Vortex generation in ultracold Fermi gases



Figure 2 | Vortices in a strongly practine permionic 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 (semagnetic fields were 740 G (a), 766 G (b), 792 G (c 843 G (f), 853 G (g) and 863 G (h). The field of view 880 μ m × 880 μ m.

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

Stirring the atomic cloud with stirring velocity lower than the critical velocity





Bulgac, Luo, Magierski, Roche, Yu, Science 332, 1288 (2011)

Stirring the atomic cloud with stirring velocity exceeding the critical velocity





Bulgac, Luo, Magierski, Roche, Yu, Science 332, 1288 (2011)

Vortex reconnections



Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b) after reconnection and vice versa.

Vortex reconnections are important for the energy dissipation mechanism in quantum turbulence.

TDSLDA can describe these processes as well as the energy transfer between collective and single particle degrees of freedom (which is a problem for simplified treatments based e.g. on Gross-Pitaevskii equation)

Bulgac, Luo, Magierski, Roche, Yu, Science 332, 1288 (2011)



Moreover with TDDFT we can reproduce the sequence of topological excitations observed experimentally (M.H.J. Ku et al. Phys. Rev. Lett. 113, 065301 (2014)).

Wlazłowski, et al., Phys. Rev. A91, 031602 (2015)

Vortex dynamics and vortex-impurity interaction

The effective equations of motion for the vortex dynamics (per unit length of the vortex):

$$M_{vor} \frac{d^2 \vec{r}}{dt^2} = \vec{F}_M + \vec{F}_D + \vec{F}_{vor-impurity}$$

$$\vec{F}_{M} = \rho_{s}\vec{\Gamma} \times \left(\frac{d\vec{r}}{dt} - \vec{v}_{s}\right) - \text{Magnus force; } \vec{\Gamma} - \text{local vorticity;}$$
$$d\vec{r}$$

 $\frac{dt}{dt}$ - local vortex velocity, ρ_s – superfluid density, \vec{v}_s – superfluid velocity

 \vec{F}_D – frictional force (negligible at small T)

 $\vec{F}_{vor-impurity}$ - vortex-impurity force

To date the impurity-vortex interaction has been extracted from static calculations (Ginzburg-Landau, local density, HFB) with several severe approximations:

- Vortex is always straight
- Nucleus is spherical
- Only very symmetric configurations are considered: nucleus on vortex vortex inbetween two nuclei (intersitial configuration) nucleus at infinity

M.A. Alpar et al. Astrophys.J.213,527(1977);276,325(1984) R.I. Epstein, G.Baym, Astrophys.J.328,680(1988) R.K.Link,R.I.Epstein,Astrophys.J.373,592(1991) P.Pizzochero et al. PRL 79,3347(1997) R.Broglia et al.PRD50,4781(1994) M.Baldo et al. Nucl.Phys.515,409(1990) P.Donati,P.Pizzochero, PRL90,211101(2003); PLB640,74(2006);Nucl.Phys.A742,363(2004) P.Avogadro et al. PRC75,012805(2007);NPA811,378(2008)

From these assumptions the average force can be deduced and the energetically favorable configuration may be determined.

We use approach based on TDDFT which allow to extract the force from dynamics.

It has the following advantages:

- We can extract the force at various nonsymmetric configurations
- All degrees of freedom are treated on the same footing and in particular those associated with the vortex (bending) and nucleus (deformations) are taken into account
- One can get a better insight into the dynamics of the vortex-impurity system at various energy scales.

The procedure consists of dragging protons through the neutron medium with the vortex.

Such an approach has been shown to give the same force as extracted from static configurations (Bulgac, Forbes, Sharma, PRL 110, 241102 (2013)).

It is numerically much cheaper than searching for stationary solutions at various vortex-impurity configurations.





FIG. 5: (Color online) Example of initial unpinned configuration for n = 0.014 fm⁻³. The upper part of the box shows the total density distributions, while the lower part presents the absolute value of the neutron paring potential Δ . The vanishing pairing field and the depletion of the density along the tube symmetry axis are due to the presence of a quantum vortex. Arrows in the bottom part of the figure show the circular flow of neutrons.

<u>Vortex – impurity interaction</u>

The extrenal potential: $V_{EXT}(\vec{r}) = -\vec{F} \cdot \vec{r}$ keeps the nucleus moving along the straight line with a constant velocity below the critical velocity.



One can extract the total force and also the force exerted on each part of the vortex. Assuming that the force behaves asymptotically as $1/r^3$ (superfluid hydrodynamic estimate) one can extract the force per unit length by fitting the expression : $\sum_{n=1}^{n} a r^n$

$$f(r) = \frac{\sum_{k=0}^{k=0} a_n r^n}{\sum_{k=0}^{n+3} b_n r^n}; \ f(r) \sim \frac{1}{r^3}; \ b_0 = 1$$

G. Wlazłowski, K. Sekizawa, P. Magierski (in preparation)



FIG. 3: (Color online) Extracted force per unit length f(r) for different densities. Negative values means repulsive nature of the force. In inset (a) sketch explaining meaning of Eq. (4) is shown. Inset (b) shows the measured total force F(R) as shown in Fig. 1 for different densities. The force has been decomposed into tangential and centripetal components with respect of temporal vortex position.

Vortex tension (upper limit): how much energy one needs to deform the vortex



Vortex-impurity repulsive force



FIG. 8: (Color online) Excitation energy E(t) - E(0) of the system as a function of time. By dashed line work performed by external force computed by formula $W(t) = \int_0^t \mathbf{F}_{\text{ext}}(t') \cdot v(t') dt'$ is presented. In inset change of vortex length L(t) - L(0) is shown as function of time.

$$T = 1.4 MeV / fm$$
 for n=0.014 fm⁻³
 $T = 7.3 MeV / fm$ for n=0.031 fm⁻³

Effective mass of a nucleus in superfluid neutron environment

Suppose we would like to evaluate an effective mass of a heavy particle immersed in a uniform Fermi bath.

Can one come up with the effective (classical) equation of motion of the type:

$$M_{eff} \frac{d^2 q}{dt^2} - F_D\left(\frac{dq}{dt},\dots\right) = 0$$
?

In general it is a complicated task as the first and the second term may not be unambiguously separated.

However for the superfluid system it can be done as for sufficiently slow motion (below the critical velocity) the second term may be neglected due to the presence of the pairing gap.

Effective mass of a nucleus immersed in superfluid neutron matter:

We apply the external potential for protons (50) of the form: $V_{EXT}(\vec{r}) = -\vec{F} \cdot \vec{r}$ and measure the C.M. velocity of the system



At low velocities: $v(t) \sim t$

The deviations for higher velocities indicate excitations of other modes

Dragging 50 protons the effective mass corresponds to dragging about 207 nucleons for lower density and about 228 nucleons for higher density.

K. Sekizawa, G. Wlazłowski, P. Magierski (preliminary results)

Linear response regime

Photoabsorption cross section for heavy, deformed nuclei.

$$\begin{split} h_{\tau,\sigma\sigma}(\mathbf{r},t) &\Rightarrow h_{\tau,\sigma\sigma}(\mathbf{r},t) + F_{\tau}(\mathbf{r})f(t) \quad F_{\tau}(\mathbf{r}) = N_{\tau}\sin(\mathbf{k}\cdot\mathbf{r}_{\tau})/|\mathbf{k}| \\ S(E) &= \sum_{\nu} |\langle \nu | \hat{F} | 0 \rangle|^2 \delta(E - E_{\nu}) \\ S(\omega) &= \operatorname{Im}\{\delta F(\omega) / [\pi f(\omega)]\} \end{split}$$

(gamma,n) reaction through the excitation of GDR

I.Stetcu, A.Bulgac, P. Magierski, K.J. Roche, Phys. Rev. C84 051309 (2011)



Beyond linear regime: Relativistic Coulomb excitation

 $^{238}U + ^{238}U \rightarrow ^{238}U * +...$ at about 700 MeV/n



The coordinate transformation has been applied to keep CM in the center of the box at all times.

Coupling to e.m. field:

$$\vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$
$$\vec{B} = \vec{\nabla} \times \vec{A}$$

$$\vec{\nabla}\psi \to \vec{\nabla}_A \psi = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right)\psi$$
$$\vec{\nabla}\psi^* \to \vec{\nabla}_{-A}\psi^* = \left(\vec{\nabla} + i\frac{e}{\hbar c}\vec{A}\right)\psi^*$$
$$i\hbar\frac{\partial}{\partial t}\psi \to \left(i\hbar\frac{\partial}{\partial t} - e\phi\right)\psi$$

which implies that $\vec{\nabla}\psi\psi^* \to \vec{\nabla}\psi\psi^*$.

Consequently the densities change according to:

- density: $\rho_A(\mathbf{r}) = \rho_A(\mathbf{r})$
- spin density: $\vec{s}_A(\mathbf{r}) = \vec{s}(\mathbf{r})$
- current: $\vec{j}_A(\mathbf{r}) = \vec{j}(\mathbf{r}) \frac{e}{\hbar c} \vec{A} \rho(\mathbf{r})$
- spin current (2nd rank tensor): $\mathbf{J}_A(\mathbf{r}) = \mathbf{J}(\mathbf{r}) \frac{e}{\hbar c} \vec{A} \otimes \vec{s}(\mathbf{r})$
- spin current (vector): $\vec{J}_A(\mathbf{r}) = \vec{J}(\mathbf{r}) \frac{e}{\hbar c} \vec{A} \times \vec{s}(\mathbf{r})$

• kinetic energy density:
$$\tau_A(\mathbf{r}) = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right) \cdot \left(\vec{\nabla}' + i\frac{e}{\hbar c}\vec{A}\right) \rho(\mathbf{r},\mathbf{r}')|_{r=r'}$$

= $\tau(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}\cdot\vec{j}(\mathbf{r}) + \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\rho(\mathbf{r}) = \tau(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}\cdot\vec{j}_A(\mathbf{r}) - \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\rho(\mathbf{r})$

• spin kinetic energy density: $\vec{T}_A(\mathbf{r}) = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right) \cdot \left(\vec{\nabla}' + i\frac{e}{\hbar c}\vec{A}\right)\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$ = $\vec{T}(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}^T \cdot \mathbf{J}(\mathbf{r}) + \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\vec{s}(\mathbf{r}) = \vec{T}(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}^T \cdot \mathbf{J}_A(\mathbf{r}) - \frac{e^2}{\hbar^2 c^2}|\vec{A}|^2\vec{s}(\mathbf{r})$

Energy deposited for two nuclear orientations (y – perpendicular, z – parallel)

I. Stetcu, C. Bertulani, A. Bulgac, P. Magierski, K.J. Roche Impact parameter b=12.2fm Phys. Rev. Lett. 114, 012701 (2015) Excitation energy (CM motion subtracted) 50 ∑⁰ ₩ 30 C20 Euergy 10 10 ſ 1000 2000 3000 4000 0 time [fm/c] **Energy transferred to the target nucleus** in the form of internal excitations 40 35 ergy (MeV) 52 **TDSLDA** – perpendicular orientation Deposited Er **TDSLDA** – parallel orientation

10

12

14

impact parameter (fm)

16

18

20

22

Goldhaber-Teller like model: proton and neutron density distributions oscillating against each other

One body dissipation

Let us assume that the collective energy of dipole oscillation is proportional the square of the amplitude of electric dipole moment:

$$E_{coll}(t) \propto \left[D_{\max}(t)\right]^2$$



I. Stetcu, C. Bertulani, A. Bulgac, P. Magierski, K.J. Roche Phys. Rev. Lett. 114, 012701 (2015) Induced nuclear fission by neutron capture: pairing dynamics

Fission of ²⁴⁰Pu at excitation energy $E_x = 8.08$ MeV



Bulgac, Magierski, Roche, Stetcu, PRL 116, 122504 (2016)

Induced nuclear fission by neutron capture

Fission of ²⁴⁰Pu at excitation energy $E_x = 8.05$; 7.91; 8.08 MeV



Time= 0.000000 fm/c

Bulgac, Magierski, Roche, Stetcu, PRL 116, 122504 (2016)

TABLE I: The simulation number, the pairing parameter η , see Eq. (1), the excitation energy (E^*) of the mother ${}^{240}_{94}$ Pu₁₃₆ and of the daughter nuclei $(E^*_{H,L})$, the equivalent neutron incident energy (E_n) , the starting initial quadrupole moment, the "saddle-to-scission" time, the total kinetic energy (TKE), atomic $(A_{H,L})$, neutron $(N_{H,L})$ and proton $(Z_{H,L})$ numbers of the heavy and light fragments, and the number of neutrons (ν) , estimated using a Hauser-Feshbach approach and experimental neutron separation energies [8, 68, 69]. Units are MeV, fm² and fm/c where appropriate.

S#	η	E^*	E_n	Qzz	S-S time	TKE	A_H	A_L	N_H	N_L	Z_H	Z_L	E_H^*	E_L^*	ν_H	ν_L
S 1	0.75	8.05	1.52	16,500	14,419	182	136.0	104.0	83.2	62.8	52.8	41.2	5.26	17.78	0	1.9
S2	0.5	7.91	1.38	16,500	4,360	183	133.7	106.3	82.0	64.0	51.7	42.3	9.94	11.57	1	1
S3	0	8.08	1.55	16,500	14,010	180	134.5	105.5	82.4	63.6	52.1	41.9	3.35	29.73	0	2.9
S 4	0	6.17	-0.36	19,000	12,751	181	136.1	103.9	83.4	62.6	52.7	41.3	7.85	9.59	1	1

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

Nuclear data evaluation, Madland (2006)

estimated TKEs slightly overestimate the observed values by no more than 3 - 6 MeV.

This is indicative of the fact that in our simulations the system scissions a bit too early.

The evaluated average number of emitted neutrons in this case is close to 3, which is higher than the values we estimate.

Solitonic excitations in nuclear reactions

From the talk of K. Sekizawa

$$E_{\rm kin}(E,\Delta\varphi) = A(E) - B(E)\cos(\Delta\varphi)$$

From the talk of K. Sekizawa

Energy of the junction between two superfluids of different phase:

$$E \propto \left|\Delta\right|^2 \sin^2\left(\frac{\Delta\varphi}{2}\right)$$

K. Sekizawa, G. Wlazłowski, P. Magierski (preliminary results)

Summary:

- TDSLDA offers insights into nuclear processes which are either not easy or impossible to obtain in the laboratory.
- We were able to describe nucleus-vortex interaction from the dynamics without any symmetry constraints, taking into account internal degrees freedom of the nucleus and the vortex.
- We extracted the force per unit of the vortex length, which can be used as an input for simplified large scale calculations for the neutron star crust (eg. based on filament model).
- For neutron matter we were able to extract the effective mass of impurity (nucleus) immersed in the neutron environment.
- The quality of the agreement with experimental observations for fission is surprisingly good, taking into account we made no effort to reproduce any measured data.
- TDSLDA predicts <u>much longer time-scales for fission</u>, even though it takes into account one-body dissipation only (both window and wall mechanisms are present). The nuclear system superficially behaves like an extremely viscous system, but the collective motion at the same time is not overdamped.

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