

# Towards accurate description of non-equilibrium dynamics in superfluid neutron matter

### Gabriel Wlazłowski

Warsaw University of Technology University of Washington



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CENTRE



#### Our motivation: Glitch (a sudden increase of the rotational frequency)

Hierarchy of theories:





Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)





Normal component <->
<br/>
- rigid body rotation

Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)



Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)



#### Normal component

- rigid body rotation
- slows down due to energy radiation

Rotation frequency

time



time



Rotation frequency



Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)





В

Figure tak

time

Normal component - rigid body rotation - slows down due to energy radiation

Tension between N and SF component is generated!

Rotation frequency

component - can rotate only in form of vortices - in order to decrease the angular momentum number of vortices must SF change Ν C **Neutron Superfluid** 

> Neutron Vortex Proton Superfluid + Neutron Vortex Proton Superconductor Neutron Vortex 1 Nuclei in a lattice Magnetic Flux Tube

Normal component

- rigid body rotation
- slows down due to energy radiation

Tension between N and SF component is generated!

time

Rotation frequency



Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)

#### Superfluid component - can rotate only in form of vortices - in order to decrease the angular momentum number of vortices must change

 when vortices are ejected they transfer its angular momentum to N component

# GLITCH! PHYSICS.WUT

A lot of open problems:

- origin of pinning mechanism?
- vortex avalanche trigger mechanism?
- regular lattice of vortices or tangle of vortices?









Method: TDDFT DoF: fermionic (neutrons, protons...)



Method: Vortex filament model DoF: impurities and vortices





Method: Hydrodynamics DoF: fluid elements Matching theories is hard..





http://www.pharos.ice.csic.es/ (cost action CA16214)



Result is weakly sensitive to various assumptions of hydro model...

- P. Pizzochero, M. Antonelli, B. Haskell, S. Seveso, Nature Astronomy 1, 0134 (2017)
- M. Antonelli, P. Pizzochero, Journal of Physics: Conf. Series 861 (2017) 012024
- M. Antonelli, A. Montoli, P. M. Pizzochero, MNRAS 475, 5403 (2018)



# Challenge for MBT:

# Unified description of static and dynamic properties of large Fermi systems

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

We know what Eq. should be solved... The only problem: *How to do it in practice?* 

### Methods:

- QMC (static)
- <u>DFT</u> (static and <u>dynamic</u>)



Input: energy density functional





# Alternative frameworks



# Alternative frameworks





Accuracy of superfluid TDDFT was extensively tested over last years...

#### Example: fission of heavy nucleus

[Phys. Rev. Lett. 116, 122504 (2016)]











column). The last column demonstrate present

accuracy. Relative accuracy is at level 2% or better.

From P. Magierski talk "*Time-dependent density functional theory for nuclear reactions - advantages and disadvantages*", ECT\* Workshop: Spontaneous and induced fission of very heavy and super-heavy nuclei, 2018, Trento, Italy

Accuracy of superfluid TDDFT was extensively tested over last years...

#### Example: fission of heavy nucleus

[Phys. Rev. Lett. 116, 122504 (2016)]









Dilute neutron matter very well constrained by QMC calculations.



# unitary Fermi gas (superfluid properties demonstrate here

in form of topological defects)







To execute superfluid TDDFT we need supercomputers...



Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	<b>Sunway TaihuLight</b> - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway , NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
2	<b>Tianhe-2 (MilkyWay-2)</b> - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P , NUDT National Super Computer Center in Guangzhou China	3,120,000	33,862.7	54,902.4	17,808
3	<b>Piz Daint</b> - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect, NVIDIA Tesla P100, <b>Cray Inc.</b> Swiss National Supercomputing Centre (CSCS) <b>Switzerland</b>	361,760	19,590.0	25,326.3	2,272
4	<b>Gyoukou</b> - ZettaScaler-2.2 HPC system, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 700Mhz , <b>ExaScaler</b> Japan Agency for Marine-Earth Science and Technology Japan	19,860,000	19,135.8	28,192.0	1,350
5	<b>Titan</b> - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x <b>, Cray Inc.</b> DOE/SC/Oak Ridge National Laboratory <b>United States</b>	560,640	17,590.0	27,112.5	8,209
6	<b>Sequoia</b> - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom , IBM DOE/NNSA/LLNL United States	1,572,864	17,173.2	20,132.7	7,890

To execute superfluid TDDFT we need supercomputers...





United States

To execute superfluid TDDFT we need supercomputers...





Negele&Vautherin,Nucl.Phys.A207,298(1973)

# Example of initial configuration...

Self-consistent solution of static problem with constraints:

- fixed center of mass of protons
- nonzero total angular momentum of neutrons

J. Negele and D. Vautherin, Nucl. Phys. A 207, 298 (1973)

Zone	Element	Ζ	Ν	$R_{WS}$ [fm]	$\rho_b \; [\mathrm{g} \cdot \mathrm{cm}^{-3}]$	$k_{F,n}  [{\rm fm}^{-1}]$
11	$^{180}\mathrm{Zr}$	40	140	53.6	$4.67\cdot10^{11}$	0.12
10	$^{200}\mathrm{Zr}$	40	160	49.2	$6.69 \cdot 10^{11}$	0.15
9	$^{250}\mathrm{Zr}$	40	210	46.4	$1.00 \cdot 10^{12}$	0.19
8	$^{320}\mathrm{Zr}$	40	280	44.4	$1.47 \cdot 10^{12}$	0.23
7	$^{500}\mathrm{Zr}$	40	460	42.2	$2.66 \cdot 10^{12}$	0.31
6	$^{950}\mathrm{Sn}$	50	900	39.3	$6.24 \cdot 10^{12}$	0.43
5	$^{1100}\mathrm{Sn}$	50	1050	35.7	$9.65\cdot10^{12}$	0.51
4	$^{1350}\mathrm{Sn}$	50	1300	33.0	$1.49\cdot 10^{13}$	0.60
3	$^{1800}\mathrm{Sn}$	50	1750	27.6	$3.41 \cdot 10^{13}$	0.80
2	$^{1500}\mathrm{Zr}$	40	1460	19.6	$7.94 \cdot 10^{13}$	1.08
1	$^{982}\mathrm{Ge}$	32	950	14.4	$1.32\cdot 10^{14}$	1.33



Lowest energy state (constrained) for Z=50 and N=2,530 confined in tube of radius R=30fm

# PHYSICS.WUT

G. Wlazłowski, K. Sekizawa, P. Magierski, A. Bulgac, M.M. Forbes, Phys. Rev. Lett. 117, 232701 (2016)

# **Vortex Filament Model**

- Each filament of the vortex line generates rotational flow around it,
- The total flow at arbitrary position can be calculated by means of Biot-Savart,



# Vortex Filament Model

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- The total flow at arbitrary position can be calculated by means of Biot-Savart,

#### <u>Equation of motion for the vortex line:</u>

Balance of forces (mass of vortex negligible):



vortex

line

dl

# Vortex Filament Model (VFM)

- Each filament of the vortex line generates rotational flow around it,
- The total flow at arbitrary position can be calculated by means of Biot-Savart,

#### Equation of motion for the vortex line:

Balance of forces (mass of vortex negligible):

$$\kappa \rho_s \hat{t} \times (\dot{s} - v_{ind} - v_{ext}) + f^{VN} + f^D = 0$$



#### Our aim:

Construct such VFM that reproduces dynamics seen in microscopic simulations



#### Vortex Filament Model should reproduce it (at qualitative and quantitative level)

time= 8921 fm/c  $F_m$  ( 9.9)= 0.59 MeV/fm Q= 9 fm<sup>2</sup>







#### "Fluid element"



Two-fluid hydrodynamics





We use Newton's 3<sup>rd</sup> law and extract the force from motion of the nucleus..... Consider Eq. of motion for impurity:

![](_page_34_Figure_1.jpeg)

We use Newton's 3<sup>rd</sup> law and extract the force from motion of the nucleus..... Consider Eq. of motion for impurity:

![](_page_35_Figure_1.jpeg)

![](_page_36_Figure_0.jpeg)

![](_page_37_Figure_0.jpeg)

![](_page_38_Figure_0.jpeg)

![](_page_39_Figure_0.jpeg)

IMINARY RESULTS

![](_page_40_Picture_0.jpeg)

Put all elements together...

![](_page_41_Picture_1.jpeg)

$$V_{ext} < V_{crit}$$

From diploma thesis of Konrad Kobuszewski, WUT 2018

#### Put all elements together...

![](_page_42_Picture_1.jpeg)

**PHYSICS.WUT** 

 $V_{ext} > v_{crit}$ 

From diploma thesis of Konrad Kobuszewski, WUT 2018

Put all elements together...

![](_page_43_Picture_1.jpeg)

→ 
$$V_{ext} \approx V_{crit}$$

From diploma thesis of Konrad Kobuszewski, WUT 2018

![](_page_44_Figure_0.jpeg)

From K. Kobuszewski talk, POLNS18, 26-28 March 2018, Warsaw

# Magnetic field and the vortex core structure

Fig. From: Stein et.al., Phys. Rev. C 93, 015802 (2016)

![](_page_45_Figure_2.jpeg)

$$\alpha = \frac{\rho_{\uparrow} - \rho_{\downarrow}}{\rho_{\uparrow} + \rho_{\downarrow}}$$

FIG. 15: (Color online) Magnetic field required to create a specified spin polarization as a function of the density for two polarization values  $\alpha = 0.1$  (a) and 0.2 (b) and temperatures T = 0.25 (solid line), 0.5 (dashed line), and 0.75 (dash-dotted line).

# Magnetic field and the vortex core structure

#### Expectation:

 $P = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}}$ 

 $\rightarrow \dots$ 

 $\rightarrow \dots$ 

→ short range physics – affected by the magnetic filed

![](_page_46_Figure_6.jpeg)

FIG. 15: (Color online) Magnetic field required to create a specified spin polarization as a function of the density for two polarization values  $\alpha = 0.1$  (a) and 0.2 (b) and temperatures T = 0.25 (solid line), 0.5 (dashed line), and 0.75 (dash-dotted line).

$$N_{\uparrow} = 304, \ N_{\downarrow} = 202, \ P = 20\%$$

![](_page_46_Figure_9.jpeg)

 $\alpha = \frac{\rho_{\uparrow} - \rho_{\downarrow}}{\rho_{\uparrow} + \rho_{\downarrow}}$ 

Examples

 $\rightarrow$  Vortex tension (T= $\Delta E_v/\Delta L$ )

 $\rightarrow$  Short distance vortex-nucleus interaction

 $\rightarrow$  Short distance vortex-vortex interaction

![](_page_47_Picture_4.jpeg)

![](_page_47_Picture_5.jpeg)

![](_page_47_Picture_6.jpeg)

![](_page_47_Picture_7.jpeg)

# CONCLUSIONS

- DFT route for unified description of static and dynamic properties of large Fermi systems
- **TDDFT** can be used as a source of microscopic input for pulsar glitch models
  - We have defined information propagation scheme: TDDFT → VFM → Hydro
  - Target: indentify dominant source of pinning (crust or core)
- We plan to execute campaign of systematic simulations in 2019-2020 (scan over densities with modern BSk functional).
- TDDFT has also been applied to other systems
  - Dynamics in ultracold atoms (vortex dynamics, quantum turbulence, shock waves...)
  - Dynamics of nuclear systems (fission, nuclear reactions, relativistic coulomb excitation...)

![](_page_48_Picture_9.jpeg)

60

50

Warsaw University of Technology (Poland): P. Magierski, G. Wlazłowski, B. Tuzemen, J. Olenicz, K. Kobuszewski

![](_page_49_Picture_1.jpeg)

University of Washington (USA): A. Bulgac, S. Jin

Washington State University (USA): M. Forbes, R. Corbin

![](_page_49_Picture_4.jpeg)

Niigata University (Japan): K. Sekizawa

PRAL

![](_page_49_Picture_6.jpeg)

![](_page_49_Picture_7.jpeg)

Los Alamos National Lab (USA): I. Stetcu

PHAROS

![](_page_49_Picture_9.jpeg)

Pacific Northwest National Lab (USA): K. Roche (HPC)

Nicolaus Copernicus Astronomical Center (Poland): B. Haskell, M. Antonelli, V. Khomenko

![](_page_49_Picture_12.jpeg)

![](_page_49_Picture_13.jpeg)

ICM (Poland): M. Marchwiany (HPC)

Lawrence Livermore National Lab (USA): N. Schunck

![](_page_49_Picture_16.jpeg)

![](_page_49_Picture_17.jpeg)

![](_page_50_Figure_0.jpeg)

# Thank you

Contact: gabrielw@if.pw.edu.pl

![](_page_51_Figure_0.jpeg)

HF equations  
What about superfluids?  

$$\begin{bmatrix} [-\nabla^2/2m + v_{KS}(\mathbf{x})]\phi_i(\mathbf{x}) = \varepsilon_i\phi_i(\mathbf{x}) \\ v_{KS} = \frac{\delta E_{int}}{\delta\rho} + U_{ext} \\ pairing (anomalous) \\ density \end{bmatrix}$$

$$\begin{bmatrix} [h(\mathbf{r}) - \mu]u_k(\mathbf{r}) + \Delta(\mathbf{r})v_k(\mathbf{r}) = E_k u_k(\mathbf{r}), \\ \Delta^*(\mathbf{r})u_k(\mathbf{r}) - [h(\mathbf{r}) - \mu]v_k(\mathbf{r}) = E_k v_k(\mathbf{r}), \\ h(\mathbf{r}) = -\nabla^2/2m + v_{KS}(\mathbf{x}) \\ \Delta = -\frac{\delta E_{int}}{\delta\nu^*} \end{bmatrix}$$
HFB equations  

$$\begin{bmatrix} h(\mathbf{r}) - \nu^2/2m + v_{KS}(\mathbf{x}) \\ Density - Functional Theory for Time-Dependent Systems \\ Erich Runge and E. K. U. Gross \\$$

Phys. Rev. Lett. 52, 997 – Published 19 March 1984

#### Solving time-dependent problem for superfluids...

The real-time dynamics is given by equations, which are formally equivalent to the Time-Dependent HFB (TDHFB) or Time-Dependent Bogolubov-de Gennes (TDBdG) equations

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

where h and  $\Delta$  depends on "densities":

We explicitly track fermionic degrees of freedom!

$$n_{\sigma}(\boldsymbol{r},t) = \sum_{E_n < E_c} |v_{n,\sigma}(\boldsymbol{r},t)|^2, \qquad \tau_{\sigma}(\boldsymbol{r},t) = \sum_{E_n < E_c} |\nabla v_{n,\sigma}(\boldsymbol{r},t)|^2,$$

$$v(\boldsymbol{r},t) = \sum_{E_n < E_c} u_{n,\uparrow}(\boldsymbol{r},t) v_{n,\downarrow}^*(\boldsymbol{r},t), \qquad \boldsymbol{j}_{\sigma}(\boldsymbol{r},t) = \sum_{E_n < E_c} \operatorname{Im}[v_{n,\sigma}^*(\boldsymbol{r},t) \nabla v_{n,\sigma}(\boldsymbol{r},t)],$$

a lot of nonlinear coupled 3D Partial Differential Equations (in practice 10<sup>5</sup> - 10<sup>6</sup>)

disturbance of velocity field by impurity  $\rightarrow$  origin of effective vortex-nucleus interaction

![](_page_54_Figure_1.jpeg)

![](_page_54_Figure_2.jpeg)

Neutrons velocity field [c]

#### We performed 3D, dynamical simulations by TDDFT with superfluidity

**TDSLDA** equations (similar to TDHFB, TD-BdG)

$$i\hbar\frac{\partial}{\partial t}\left(\begin{array}{c}u_k\\v_k\end{array}\right) = \left(\begin{array}{c}h&\Delta\\\Delta^*&-h\end{array}\right)\left(\begin{array}{c}u_k\\v_k\end{array}\right)$$

 $\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_{\text{pair}}$ 

 $\mathcal{E}_0$ : Fayans EDF (FaNDF<sup>0</sup>) w/o LS S.A. Fayans, JETP Letters 68, 169 (1998);

**FP81**: B. Friedman and V. R. Pandharipande, Nucl. Phys. A 361, 502 (1981)

**WFF88**: R. B. Wiringa, V. Fiks, and A. Fabrocini, Phys. Rev. C 38, 1010 (1988).

$$\square \text{ Potentials}$$

$$h = \frac{\delta \mathcal{E}}{\delta n}, \ \Delta = \frac{\delta \mathcal{E}}{\delta \nu^*}$$

$$n(\mathbf{r}) = \sum_{0 < E_k < E_c} |v_k(\mathbf{r})|^2$$

$$\nu(\mathbf{r}) = \sum_{0 < E_k < E_c} u_k(\mathbf{r}) v_k^*(\mathbf{r})$$

![](_page_55_Figure_9.jpeg)

#### We performed 3D, dynamical simulations by TDDFT with superfluidity

2

1.8

1.6 1.4

[ 1.2 1 ∇ 0.8

0.8

0.6

0.4

0.2

0

0

0.2

0.4

0.6

**TDSLDA** equations (similar to TDHFB, TD-BdG)

$$i\hbar\frac{\partial}{\partial t}\left(\begin{array}{c}u_k\\v_k\end{array}\right) = \left(\begin{array}{cc}h&\Delta\\\Delta^*&-h\end{array}\right)\left(\begin{array}{c}u_k\\v_k\end{array}\right)$$

• Energy density functional (EDF)

$$\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_{\mathrm{pair}}$$

$$\mathcal{E}_{\text{pair}}(\boldsymbol{r}) = g(n(\boldsymbol{r})) \left[ |\nu_n(\boldsymbol{r})|^2 + |\nu_p(\boldsymbol{r})|^2 \right]$$

The coupling constant g is chosen to reproduce the neutron pairing gap in pure neutron matter.

Potentials  

$$h = \frac{\delta \mathcal{E}}{\delta n}, \ \Delta = \frac{\delta \mathcal{E}}{\delta \nu^*}$$

$$n(\mathbf{r}) = \sum_{0 < E_k < E_c} |v_k(\mathbf{r})|^2$$

$$\nu(\mathbf{r}) = \sum_{0 < E_k < E_c} u_k(\mathbf{r})v_k^*(\mathbf{r})$$

n=0.014 fm<sup>-</sup>

0.8

 $k_{F}$  [fm<sup>-1</sup>]

1

1.2

1.4

1.6

#### **Vortex-impurity interaction – present status**

only calculations of pinning energy ...

![](_page_57_Figure_2.jpeg)

![](_page_58_Figure_0.jpeg)

Fig. from: P. Avogadro et al., Phys. Rev. C 75, 012805(R) (2007) Figs from: P. Donati et al., Nuclear Physics A 742 (2004) 363

![](_page_59_Figure_0.jpeg)

### **Dragging force**

external time-dependent potential couples only to protons and it is constant in space.

$$U_{\text{ext}}(\boldsymbol{r},t) = -\frac{1}{Z}\boldsymbol{F}_{\text{ext}}(t) \cdot \boldsymbol{r}$$
$$\frac{d\langle \hat{\boldsymbol{p}} \rangle}{dt} = -\langle \boldsymbol{\nabla} U_{\text{ext}}(\boldsymbol{r},t) \rangle = \boldsymbol{F}_{\text{ext}}(t)$$

Dragging speed: 
$$v_0=0.001c\ll v_{
m crit}$$

This force moves the center of mass of the protons together with those neutrons bound (entrained) in the nucleus without significantly modifying the internal structure of the nucleus and surrounding neutron medium

![](_page_60_Picture_5.jpeg)

### **Force decomposition**

![](_page_61_Figure_1.jpeg)

![](_page_62_Figure_0.jpeg)