Fermionic turbulence within the framework of time dependent density functional theory

Piotr Magierski Warsaw University of Technology



Collaborators:

Warsaw Univ. of Technology

Gabriel Wlazłowski

Konrad Kobuszewski (PhD student) Marek Tylutki Aurel Bulgac (Univ. of Washington) Michael M. Forbes (Washington State U.) Kazuyuki Sekizawa (Niigata University)

OUTLINE

• Vortex structure in spin imbalanced systems

 Time dependent density functional theory for superfluid Fermi gas

• Solitonic cascades: theory vs experiment

Preliminary studies of vortex tangles

Anatomy of the vortex core

BOSONS:

Vortex structure: Bose gas \rightarrow Gross-Pitaevskii eq. (GPE)



FERMIONS:

Vortex structure: Fermi gas \rightarrow BdG eq.



Andreev states affect the density distribution inside the core.

Vortex solution: Fermi gas \rightarrow BdG eq. with ansatz for the pairing field



$$\begin{array}{c} \Delta \\ -h_{\downarrow}^{*} \end{array} \begin{pmatrix} u_{n,\uparrow} \\ v_{n,\downarrow} \end{pmatrix} = \varepsilon_n \begin{pmatrix} u_{n,\uparrow} \\ v_{n,\downarrow} \end{pmatrix}$$

Form of the vortex-like solutions:

$$u_{\eta}(\mathbf{r}) = u_{nmk_z}(\rho)e^{im\varphi}e^{ik_z z}$$
$$v_{\eta}(\mathbf{r}) = v_{nmk_z}(\rho)e^{i(m+1)\varphi}e^{ik_z z}$$





Vortex in spin imbalanced Fermi gas: $N_{\uparrow} \neq N_{\downarrow}$



Due to increased spin-polarization the core expands see eg. Hu,Liu,Drummond, PRL98,060406(2007)

Spin-polarization effects: does the structure of the core affect vortex dynamics?

Density Functional Theory (DFT):

>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





Consequences:

Zenergy density functional E[n] exists and observables can be determined from densities

Kohn-Sham method (1965) provides practical way of extracting some of observables (energy and one-body observables)





Runge-Gross mapping(1984):

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

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

TDDFT variational principle also exists but it is more tricky:

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

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)

Energy density functional (EDF) for Unitary Fermi Gas (UFG): Superfluid Local Density Approximation (SLDA)

EDF for UFG: Superfluid Local Density Approximation (SLDA)

Local Density
Approximation (LDA)
$$E = \int dr \mathcal{H}(n(r))$$
Stationarity condition:
 $\frac{\delta E}{\delta n} = 0$ Generalized Gradient
Approximation (GGA) $E = \int dr \mathcal{H}(n(r), \nabla n(r))$ $\frac{\delta E}{\delta n} = 0$

EDF for UFG: Superfluid Local Density Approximation (SLDA)

Local Density
Approximation (LDA) $E = \int dr \mathcal{H}(n(r))$ Stationarity condition:
 $\frac{\delta E}{\delta n} = 0$ Generalized Gradient
Approximation (GGA) $E = \int dr \mathcal{H}(n(r), \nabla n(r))$ $\frac{\delta E}{\delta n} = 0$

Meta - GGA

. . .

Increasing quality and computing cost

$$E = \int d\mathbf{r} \,\mathcal{H}(n(\mathbf{r}), \boldsymbol{\nabla} n(\mathbf{r}), \tau(\mathbf{r}), \dots)$$

where: $n(\mathbf{r}) = \sum_{i} |\phi_{i}(\mathbf{r})|^{2} \quad \tau(\mathbf{r}) = \sum_{i} |\nabla \phi_{i}(\mathbf{r})|^{2}$
Stationarity condition:

$$\frac{\delta E}{\delta \phi_i} = 0$$

EDF for UFG: Superfluid Local Density Approximation (SLDA)



$$\phi_n \longrightarrow (u_{n,\uparrow}, u_{n,\downarrow}, v_{n,\uparrow}, v_{n,\downarrow})$$

Densities: $n_{\sigma}(\mathbf{r}) = \sum_{E_n < E_c} |v_{n,\sigma}(\mathbf{r})|^2$, $\tau_{\sigma}(\mathbf{r}) = \sum_{E_n < E_c} |\nabla v_{n,\sigma}(\mathbf{r})|^2$,
 $\nu(\mathbf{r}) = \sum_{E_n < E_c} u_{n,\uparrow}(\mathbf{r}) v_{n,\downarrow}^*(\mathbf{r})$, $\mathbf{j}_{\sigma}(\mathbf{r}) = \sum_{E_n < E_c} \operatorname{Im}[v_{n,\sigma}^*(\mathbf{r}) \nabla v_{n,\sigma}(\mathbf{r})]$,

$$\phi_n \longrightarrow (u_{n,\uparrow}, u_{n,\downarrow}, v_{n,\uparrow}, v_{n,\downarrow})$$

Densities: $n_{\sigma}(\mathbf{r}) = \sum_{E_n < E_c} |v_{n,\sigma}(\mathbf{r})|^2$, $\tau_{\sigma}(\mathbf{r}) = \sum_{E_n < E_c} |\nabla v_{n,\sigma}(\mathbf{r})|^2$,
 $v(\mathbf{r}) = \sum_{E_n < E_c} u_{n,\uparrow}(\mathbf{r}) v_{n,\downarrow}^*(\mathbf{r})$, $\mathbf{j}_{\sigma}(\mathbf{r}) = \sum_{E_n < E_c} \operatorname{Im}[v_{n,\sigma}^*(\mathbf{r}) \nabla v_{n,\sigma}(\mathbf{r})]$,

EDF:

$$\frac{\text{EDF:}}{\mathcal{H}} = \alpha_{\uparrow}(p) \frac{\hbar^2 \tau_{\uparrow}}{2m_{\uparrow}} + \alpha_{\downarrow}(p) \frac{\hbar^2 \tau_{\downarrow}}{2m_{\downarrow}}$$

$$+D(n_{\uparrow},n_{\downarrow})$$

$$+g(n_{\uparrow},n_{\downarrow})\nu + [1-\alpha_{\uparrow}(p)]\frac{j_{\uparrow}^{2}}{2n_{\uparrow}} + [1-\alpha_{\downarrow}(p)]\frac{j_{\downarrow}^{2}}{2n_{\downarrow}}$$

$$\phi_n \longrightarrow (u_{n,\uparrow}, u_{n,\downarrow}, v_{n,\uparrow}, v_{n,\downarrow})$$

$$\underline{\text{Densities:}} \quad n_{\sigma}(\mathbf{r}) = \sum_{E_n < E_c} |v_{n,\sigma}(\mathbf{r})|^2, \qquad \tau_{\sigma}(\mathbf{r}) = \sum_{E_n < \mathbf{k}} |v_{n,\sigma}(\mathbf{r})|^2, \qquad \mathbf{k} = \sum_{E_n < E_c} |u_{n,\uparrow}(\mathbf{r})v_{n,\downarrow}^*(\mathbf{r}), \qquad \mathbf{j}_{\sigma}(\mathbf{r}) = \sum_{E_n < E_c} \mathbf{I}$$



$$+ g(n_{\uparrow}, n_{\downarrow})v^{\dagger}v$$

$$+ [1 - \alpha_{\uparrow}(p)] \frac{j_{\uparrow}^{2}}{2n_{\uparrow}} + [1 - \alpha_{\downarrow}(p)] \frac{1}{2n_{\downarrow}}$$

$$and guis is attained by the set of the s$$

Kinetic term:

Effective mass α_{σ} of the particle depends on local polarization

$$p(\mathbf{r}) = \frac{n_{\uparrow}(\mathbf{r}) - n_{\downarrow}(\mathbf{r})}{n_{\uparrow}(\mathbf{r}) + n_{\downarrow}(\mathbf{r})}$$

and guarantees that correct limit is attained for $n_1 >> n_1$, where the problem reduces to the *polaron* problem

$$\phi_{n} \longrightarrow (u_{n,\uparrow}, u_{n,\downarrow}, v_{n,\uparrow}, v_{n,\downarrow})$$

$$\underline{\text{Densities:}} \quad n_{\sigma}(\mathbf{r}) = \sum_{E_{n} < E_{c}} |v_{n,\sigma}(\mathbf{r})|^{2}, \qquad \tau_{\sigma}(\mathbf{r}) = \sum_{E_{n} < E_{c}} |\nabla v_{n,\sigma}(\mathbf{r})|^{2},$$

$$v(\mathbf{r}) = \sum_{E_{n} < E_{c}} u_{n,\uparrow}(\mathbf{r}) v_{n,\downarrow}^{*}(\mathbf{r}), \qquad \mathbf{j}_{\sigma}(\mathbf{r}) = \sum_{E_{n} < E_{c}} \text{Im}[v_{n,\sigma}^{*}(\mathbf{r})\nabla v_{n,\sigma}(\mathbf{r})],$$

$$\underline{\text{EDF:}} \qquad \mathcal{H} = \alpha_{\uparrow}(p) \frac{\hbar^{2} \tau_{\uparrow}}{2m_{\uparrow}} + \alpha_{\downarrow}(p) \frac{\hbar^{2} \tau_{\downarrow}}{2m_{\downarrow}} \qquad \text{Normal interaction energy:} \\ + D(n_{\uparrow}, n_{\downarrow}) + \mathbf{r} \\ + g(n_{\uparrow}, n_{\downarrow}) v^{\dagger} v \qquad + [1 - \alpha_{\uparrow}(p)] \frac{j_{\uparrow}^{2}}{2n_{\downarrow}} + [1 - \alpha_{\downarrow}(p)] \frac{j_{\downarrow}^{2}}{2n_{\downarrow}}$$

$$\begin{split} \phi_{n} &\longrightarrow (u_{n,\uparrow}, u_{n,\downarrow}, v_{n,\uparrow}, v_{n,\downarrow}) \\ \underline{\text{Densities:}} \quad n_{\sigma}(\mathbf{r}) = \sum_{E_{n} < E_{c}} |v_{n,\sigma}(\mathbf{r})|^{2}, \qquad \tau_{\sigma}(\mathbf{r}) = \sum_{E_{n} < E_{c}} |\nabla v_{n,\sigma}(\mathbf{r})|^{2}, \\ v(\mathbf{r}) = \sum_{E_{n} < E_{c}} u_{n,\uparrow}(\mathbf{r})v_{n,\downarrow}^{*}(\mathbf{r}), \qquad \mathbf{j}_{\sigma}(\mathbf{r}) = \sum_{E_{n} < E_{c}} \text{Im}[v_{n,\sigma}^{*}(\mathbf{r})\nabla v_{n,\sigma}(\mathbf{r})], \\ \underline{\text{EDF:}} \\ \mathcal{H} = \alpha_{\uparrow}(p) \frac{\hbar^{2}\tau_{\uparrow}}{2m_{\uparrow}} + \alpha_{\downarrow}(p) \frac{\hbar^{2}\tau_{\downarrow}}{2m_{\downarrow}} \\ + D(n_{\uparrow}, n_{\downarrow}) \cdot \\ + g(n_{\uparrow}, n_{\downarrow})v^{\dagger}v \\ + [1 - \alpha_{\uparrow}(p)] \frac{j_{\uparrow}^{2}}{2n_{\uparrow}} + [1 - \alpha_{\downarrow}(p)] \frac{j_{\downarrow}^{2}}{2n_{\downarrow}} \\ \end{split}$$
More details:
A. Bulgac, M.M. Forbes, P. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Magierski,
The Unitary Fermi Gas: From Monte Carlor to Density Functionals,
B. Bullac, M.M. Forbes, B. Ballac, M. Sorbes, B. Ballac,
B. Bullac,
B. Bullac, M. Sorbes, B. Ballac,
B. Bullac, M. Sorbes, B. Ballac,
B. Bullac, M. Sorbes, B. Ballac,
B. Bullac,
B. Bullac, B. Bullac,
B. Bullac,
B. Bullac,
B. Bullac,
B. Bullac,
B. Bullac,
B.

Normal State				Superfluid State			
$(N_a, N_b) E_{FNDMC}$	E_{ASLDA}	(error)	$(N_a,$	$N_b) E_{FNDMC}$	E _{ASLDA}	(error)	
$(3,1)$ 6.6 ± 0.01	6.687	1.3%	(1	$1,1) 2.002 \pm 0$	2.302	15%	
(4,1) 8.93 ± 0.01	8.962	0.36%	(2	$(2,2)$ 5.051 \pm 0.009	5.405	7%	
$(5,1)$ 12.1 \pm 0.1	12.22	0.97%	(3	$(3,3)$ (8.639 ± 0.03)	8.939	3.5%	
$(5,2)$ 13.3 \pm 0.1	13.54	1.8%	(4	$(4,4)$ 12.573 ± 0.03	12.63	0.48%	
$(6,1)$ 15.8 \pm 0.1	15.65	0.93%	(:	$(5,5)$ 16.806 \pm 0.04	16.19	3.7%	
$(7,2)$ 19.9 \pm 0.1	20.11	1.1%	($(6,6)$ 21.278 \pm 0.05	21.13	0.69%	
(7,3) 20.8 ± 0.1	21.23	2.1%	($(7,7)$ 25.923 ± 0.05	25.31	2.4%	
$(7,4)$ 21.9 \pm 0.1	22.42	2.4%	()	$(8,8)$ 30.876 \pm 0.06	30.49	1.2%	
(8,1) 22.5 ± 0.1	22.53	0.14%	()	$(9,9)$ 35.971 ± 0.07	34.87	3.1%	
(9,1) 25.9 ± 0.1	25.97	0.27%	(10,	(10) 41.302 ± 0.08	40.54	1.8%	
(9,2) 26.6±0.1	26.73	0.5%	(11,	(11) 46.889 ± 0.09	45	4%	
(9,3) 27.2 ± 0.1	27.55	1.3%	(12,	(12) 52.624 \pm 0.2	51.23	2.7%	
(9,5) 30±0.1	30.77	2.6%	(13,	(13) 58.545 ± 0.18	56.25	3.9%	
$(10,1)$ 29.4 \pm 0.1	29.41	0.034%	(14,	$(14) 64.388 \pm 0.31$	62.52	2.9%	
$(10,2)$ 29.9 \pm 0.1	30.05	0.52%	(15,	(15) 70.927 \pm 0.3	68.72	3.1%	
(10,6) 35 ± 0.1	35.93	2.7%) ($1,0) 1.5\pm0.0$	1.5	0%	
$(20,1)$ 73.78 \pm 0.01	73.83	0.061%	(2	(2,1) 4.281 ± 0.004	4.417	3.2%	
(20,4) 73.79 ± 0.01	74.01	0.3%	($(3,2)$ 7.61 \pm 0.01	7.602	0.1%	
(20, 10) 81.7 ± 0.1	82.57	1.1%	(4	$(4,3)$ 11.362 ± 0.02	11.31	0.49%	
(20, 20) 109.7 ± 0.1	113.8	3.7%	Č	$(7,6)$ 24.787 ± 0.09	24.04	3%	
$(35,4)$ 154 \pm 0.1	154.1	0.078%	(11,	(10) 45.474 ± 0.15	43.98	3.3%	
$(35,10)$ 158.2 \pm 0.1	158.6	0.27%	(15,	$(14) 69.126 \pm 0.31$	62.55	9.5%	
(35,20) 178.6±0.1	180.4	1%		· •			

Table 9.2 Comparison between the ASLDA density functional as described in this section and the FN-DMC calculations 136 137 for a harmonically trapped unitary gas at zero temperature. The normal state energies are obtained by fixing $\Delta = 0$ in the functional: In the FN-DMC calculations, this is obtained by choosing a nodal ansatz without any pairing. In the case of small asymmetry, the resulting "normal states" may be a somewhat artificial construct as there is no clear way of preparing a physical system in this "normal state" when the ground state is superfluid.

Figure from: A. Bulgac, M.M. Forbes, P. Magierski, Lecture Notes in Physics, Vol. 836, Chap. 9, p.305-373 (2012)

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

$$h \sim f_{1}(n,\nu,...)\nabla^{2} + f_{2}(n,\nu,...) \cdot \nabla + f_{3}(n,\nu,...)$$

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

where h and Δ depends on "densities":

We explicitly track fermionic degrees of freedom!

$$n_{\sigma}(\boldsymbol{r},t) = \sum_{E_n < E_c} |v_{n,\sigma}(\boldsymbol{r},t)|^2, \qquad \tau_{\sigma}(\boldsymbol{r},t) = \sum_{E_n < E_c} |\nabla v_{n,\sigma}(\boldsymbol{r},t)|^2,$$
$$v(\boldsymbol{r},t) = \sum_{E_n < E_c} u_{n,\uparrow}(\boldsymbol{r},t) v_{n,\downarrow}^*(\boldsymbol{r},t), \qquad \boldsymbol{j}_{\sigma}(\boldsymbol{r},t) = \sum_{E_n < E_c} \operatorname{Im}[v_{n,\sigma}^*(\boldsymbol{r},t) \nabla v_{n,\sigma}(\boldsymbol{r},t)],$$

huge number of nonlinear coupled 3D Partial Differential Equations (in practice n=1,2,..., 10⁵ - 10⁶)

To execute superfluid TDDFT we need supercomputers...

Rpeak Rmax Power Rank System (TFlop/s) (TFlop/s) (kW) Cores Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, 2,397,824 143,500.0 200,794.9 9,783 NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States 2 Sierra - IBM Power Syst Present computing capabilities: NVIDIA Volta GV100. Dua NVIDIA / Mellanox DOE/NNSA/LLNL United States full 3D (unconstrained) All further results Sunway TaihuLight - Sur 3 shown here were superfluid dynamics Sunway, NRCPC generated on National Supercomputin Piz Daint (CSCS) China spatial mesh up to 100³ Tianhe-2A - TH-IVB-FEF 4 TH Express-2, Matrix-20 National Super Compute max. number of particles of the order of 10⁴ China Piz Daint - Cray XC50, Xe 5 interconnect, NVIDIA Te up to 10^6 time steps Swiss National Supercor (for cold atomic systems it gives Switzerland 6 Trinity - Cray XC40, Xeon a trajectory of length of a few ms) 68C 1.4GHz, Aries interc DOE/NNSA/LANL/SNL United States

7 Al Bridging Cloud Infrastructure (ABCI) - PRIMERGY CX2570 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR, Fujitsu National Institute of Advanced Industrial Science and Technology

391,680 19,880.0 32,576.6 1,649

https://www.topa500.org/



(superfluid properties manifest here in the form of topological defects)



G. Wlazłowski, K. Sekizawa, M. Marchwiany, P. Magierski, Phys. Rev. Lett. **120**, 253002 (2018)



Spin imbalanced UFG

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



The vortex core becomes polarized!

This may be understood noting that the most energetically favorable place to store excess of unpaired spins is at the core of the vortex where, $\Delta = 0$ - no Cooper pairs need to be broken.

New effects predicted for spin-polarized systems:

Impact on the solitonic cascade:

final product of the cascade depends on the spin imbalance in the system



Stability of topological defect depends on its internal structure...

→ For sufficiently large spin-imbalance dark solitons become stable (no snake instability) (see also: Reichl & Mueller, PRA 95, 053637; Lombardi, et. al., PRA 96, 033609)

G. Wlazłowski, K. Sekizawa, M. Marchwiany, P. Magierski, Phys. Rev. Lett. **120**, 253002 (2018)

Spin-imbalanced atomic gases may offer a new platform for studies of the quantum turbulence phenomenon in fermionic systems.

Both superfluid and normal component coexist even at zero temperature limit.

- ☑ Changes of rigidity of topological defects → Kelvin waves.
- ☑ Changes for vortex-vortex interaction → vortex reconnections

We observe that mutual dynamics of two vortices depend on its internal structure...

0

π

(a)

(b)

P=0%

P=20%

Towards quantum turbulence in fermionic gas

Problem 1: how to generate the turbulence?

→ Our suggestion: *imprint few dark solitons on existing vortex lattice* → *rotating turbulence* (nonzero total angular momentum)











time = $0 [\varepsilon_F^{-1}]$















CONCLUSIONS

 \blacksquare (TD)DFT – route for unified description of static and dynamic properties of large strongly correlated Fermi systems \rightarrow studies of the quantum turbulence in the reach

Spin-imbalanced system may provide new platform for studies of QT

- Coexistence of superfluid (paired) and normal (unpaired) components even at zero temperature limit
- Significant changes of internal structure of topological defects
- Changes of stability and rigidity of topological defects due to polarization effects





Thank you