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:
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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,
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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