Towards exascale simulations of quantum superfluids far from equilibrium

Piotr Magierski
(Warsaw University of Technology)
**HA-PACS(PACS-VIII) system**

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**Tightly Coupled Accelerators**

with cooperation of NVIDIA

Advanced Interdisciplinary Computational Science Collaboration Initiative (the MEXT of Japan)
GOAL: Unified description of superfluid dynamics of fermionic systems far from equilibrium based on microscopic theoretical framework.

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 hundred of thousands fermions.
TDDFT equations with local pairing field (TDSLDA):

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

The form of \( h(\mathbf{r}, t) \) and \( \Delta(\mathbf{r}, t) \) 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.

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.

<table>
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<th>N x N x N</th>
<th>Number of HFB equations</th>
<th># of CPUs</th>
<th>Time per step</th>
<th># of GPUs</th>
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<th>Speedup</th>
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<tr>
<td>48(^3)</td>
<td>110,592</td>
<td>110,592</td>
<td>3.9 sec</td>
<td>6,912</td>
<td>0.39 sec</td>
<td>10</td>
</tr>
<tr>
<td>64(^3)</td>
<td>262,144</td>
<td>262,144</td>
<td>20 sec</td>
<td>16,384</td>
<td>0.80 sec</td>
<td>25</td>
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Lattice=60*3, nwf=2*226,102

[Graphs and pie charts]
Areas of applications

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


Nuclear physics. Induced nuclear fission, fusion, collisions.

\[ \frac{\Delta}{\varepsilon_F} \leq 0.5 \]

\[ \frac{\Delta}{\varepsilon_F} \leq 0.1 - 0.2 \]

\[ \frac{\Delta}{\varepsilon_F} \leq 0.03 \]


Pairing as an energy gap

Quasiparticle energy:

$$E_{qp} = \sqrt{(\epsilon - \mu)^2 + |\Delta|^2}$$

Pairing as a field

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

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

Example of a nontrivial spatial dependence: quantum vortex

Vortex structure: section through the vortex core

Example of a topological excitation: magnitude of the pairing gap vanishes in the vortex core.
Examples of applications:

- Nuclear induced fission
- Solitonic cascades in ultracold atomic gases
- Collisions of medium or heavy superfluid nuclei
- Spin-polarized impurity stabilized by pairing field
- Quantum turbulence in fermionic atomic gases
- From microscopic dynamics to large scale models of neutron stars.
Time-scales of nuclear fission process


Low energy fission of nuclear systems investigated up to about 2016.

From N. Schunck’s lecture (Beijing 2018)
Fission dynamics of $^{240}$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.

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

Excitation energies are not shared proportionally to mass numbers of the fragments!

Nuclear data evaluation, Madland (2006)

Calculated TKEs slightly reproduce experimental data with accuracy < 2%

J. Grineviciute, et al. (in preparation)

see also:

Ultracold atomic gas:

Very cold (T of the order of (1-100)nK), very dilute (interparticle distance: ≈1000 Bohr radii) gas of atoms (fermionic or bosonic) confined in an external potential. System is metastable: lifetime is of the order of minutes.

Important dates:

✓ In 1999 DeMarco and Jin created a degenerate atomic Fermi gas.

✓ In 2005 Zwierlein/Ketterle group observed quantum vortices which survived when passing from BEC to unitarity - evidence for superfluidity!

System of fermionic $^6$Li atoms for various interatomic interaction strengths (various values of ext. magnetic field)

BEC side: $a>0$

BCS side: $a<0$

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 magnetic field was ramped to 725 G for imaging (see text for details). The 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.

In dilute atomic systems experimenters can control nowadays almost anything:

• The number of atoms in the trap: typically about $10^5$-$10^6$ atoms
• Shape of confining potential, dimensionality
• The density of atoms
• Mixtures of various atoms
• The temperature of the atomic cloud
• The strength of this interaction is fully tunable!

Solitonic cascades

Merging of two superfluid atomic clouds with different phases of pairing fields:

Creation of a "heavy soliton" after merging two superfluid atomic clouds.

Later it turned out that the cascade of solitons has been observed.
We can reproduce all stages of the experimentally observed solitonic cascade within time dependent SLDA.
Nuclear collisions

Collisions of superfluid nuclei having different phases of the pairing fields

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

\[ \Delta_1(r) = |\Delta_1(r)| e^{i\varphi_1(r)} \]
\[ \Delta_2(r) = |\Delta_2(r)| e^{i\varphi_2(r)} \]
\[ \Delta\varphi = \varphi_1 - \varphi_2 \]
 Modification of the capture cross section!

See also for light nuclei: Y. Hashimoto, G. Scamps, Phys. Rev. C94, 014610 2016)
Effective barrier height for fusion as a function of the phase difference

What is an average extra energy needed for the capture?

\[ E_{\text{extra}} = \frac{1}{\pi} \int_{0}^{\pi} \left( B(\Delta \varphi) - V_{\text{Bass}} \right) d(\Delta \varphi) \approx 10\text{MeV} \]

The phase difference of the pairing fields of colliding medium or heavy nuclei produces a similar solitonic structure 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 30 MeV for medium nuclei and occur for energies up to 20-30% of the barrier height.


G. Scamps, Phys. Rev. C 97, 044611 (2018): the effect may be weaker than predicted by TDDFT
Stable polarized droplets in the unitary Fermi gas

Can the pairing field stabilize the spin-polarized impurity?

Let’s induce locally the spin-polarized region in the unitary Fermi gas: (unitary Fermi gas: $k_F \rightarrow 0, \; k_F a \rightarrow \pm \infty$)

Why the spin-polarized region does not vanish?!

Even though the spin current is suppressed due to the pairing field the „impurity” should eventually dissolve

P. Magierski, B. Tuzemen, G. Wlazłowski, in preparation
**Phase difference is** $\pi$

**Maximum polarization occurs within a shell where the pairing field vanishes.**

**Pairing structure of the impurity**

Due to the difference in chemical potentials of spin-up and spin-down particles the pairing field starts to oscillate giving rise to the pairing phase inversion in the center of the impurity. (similar to the „pi” Josephson junction)

The impurity cannot collapse because it would require to destroy the nonzero pairing field inside, which has an inverted phase.

As a result one obtains the collective excitation stabilized by the pairing field.
Impurity tends to be spherical irrespective of initial deformation.

Central collision of two impurities

Potential: $A = 2\varepsilon_F$, $\sigma_x = 4.71\xi$, $\sigma_y = 6.28\xi$, $\sigma_z = 7.85\xi$

Potential is **ON**
Suggestion for experimental detection

Two crossing laser beams, each polarizing the atomic cloud with the strength of approx. Fermi energy should be applied. Separately these two beams are too weak to produce the long-lasting, spin-polarized region.

However at the crossing region the strength of beams will be sufficient to generate a localized spin-polarized impurity.

For a typical experimental setup the time interval for applying laser beams has to be about 2ms and the predicted lifetime of the impurity: > 12ms.
Quantum turbulence in fermionic ultracold gases

Superfluid turbulence (quantum turbulence): disordered set of quantized vortices. The friction between the superfluid and normal part of the fluid serves as a source of energy dissipation.

**Problem:** how the energy is dissipated in the superfluid system at small scales at $T=0$? - „pure” quantum turbulence

**Possibility:** vortex reconnections $\rightarrow$ Kelvin waves $\rightarrow$ phonon radiation

Vortex dynamics is crucial to understand the rate of energy dissipation and the energy distribution stored at various length scales during the turbulent motion (classically the energy distribution obeys the Kolmogorov formula:

$$E(k) = C \varepsilon^{2/3} k^{-5/3}$$

$\varepsilon$ - energy rate (per unit mass) transferred to the system at large scales.

$k$ - wave number (from Fourier transformation of the velocity field).

$C$ – dimensionless constant.

Two regimes of the turbulent state decay (preliminary)

Vortex reconnections

Vortex interactions

Wlazłowski, Sekizawa, Magierski – in preparation
Building the model of turbulent motion in neutron stars

Neutron star is a huge superfluid

glitch phenomenon = a sudden speed up of rotation.
To date more than 300 glitches have been detected in more than 100 pulsars

Hierarchy of theoretical models of neutron star dynamics

Method: TDDFT
DoF: neutrons and protons.
Scale: \( \sim 10^{-13} \) m

Method: Vortex Filament Model
DoF: impurities and vortices
Scale: \( \sim 10^{-9} \) m

Method: Hydrodynamics
DoF: fluid elements
Scale: \( \sim \) size of star

In collaboration with astrophysical group at CAMK (Warsaw): B. Haskell, M. Antonelli, V. Khomenko
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.

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