Dynamics of superfluid <u>quantum</u> atomic gases and atomic nuclei within the framework of **Density Functional Theory** 

## Piotr Magierski (Warsaw Unversity of Technology)

# Collaborators:

A. Bulgac - Seattle Y-L. (Alan) Luo - Seattle K.J. Roche - PNNL - LANL I. Stetcu

Y. Yu

- - Wuhan



## **Cold atomic gas in the unitary regime**

$$n r_0^3 << 1 |n|a|^3 >> 1$$

- n particle density
- a scattering length
- r<sub>0</sub> effective range

Universality: 
$$E = \xi_0 E_{FG}$$
 for  $T = 0$   
 $\xi_0 = 0.376(5)$  - Bertsch parameter (Exp.estimate)  
 $E_{FG}$  - Energy of noninteracting Fermi gas

## UNITARY REGIME



Cold atomic gases and high Tc superconductors



From Fischer et al., Rev. Mod. Phys. 79, 353 (2007) &

P. Magierski, G. Wlazłowski, A. Bulgac, Phys. Rev. Lett. 107, 145304 (2011)

## Gap in the single particle fermionic spectrum - theory



<u>Pairing pseudogap</u>: suppression of low-energy spectral weight function due to incoherent pairing in the normal state  $(T > T_c)$ 

Magierski, Wlazłowski, Bulgac, Phys. Rev. Lett.107,145304(2011) Magierski, Wlazłowski, Bulgac, Drut, Phys. Rev. Lett.103,210403(2009)

## Shear viscosity to entropy ratio of a unitary Fermi gas



#### SLDA - Extension of Kohn-Sham approach to superfluid Fermi systems

#### SLDA – Superfluid Local Density Approximation



GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007) FN-DMC - von Stecher, Greene and Blume, PRL <u>99</u>, 233201 (2007) PRA <u>76</u>, 053613 (2007)

Bulgac, PRA 76, 040502(R) (2007)

#### Formalism for Time Dependent Phenomena: TDSLDA

A.K. Rajagopal and J. Callaway, Phys. Rev. B <u>7</u>, 1912 (1973) V. Peuckert, J. Phys. C <u>11</u>, 4945 (1978) E. Runge and E.K.U. Gross, Phys. Rev. Lett. <u>52</u>, 997 (1984)

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

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

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

Density functional for unitary Fermi gas

Nuclear energy functional: SLy4, SkP, SkM\*,...

Both codes: SLDA and TDSLDA are formulated on the 3D lattice without any symmetry restrictions. SLDA generates initial conditions for TDSLDA.

# **Selected capabilities of the SLDA/TDSLDA codes:**

- ✓ full 3D simulations with no symmetry restrictions
- number of evolved quasiparticle wave functions is of the order of the lattice size:
  O(10<sup>4</sup>)- O(10<sup>6</sup>)
- ✓ high numerical accuracy for spatial derivatives using FFTW
- for TD high-accuracy and numerically stable Adams–Bashforth–Milne 5<sup>th</sup> order predictor-corrector-modifier algorithm with only 2 evaluations of the rhs per time step and with no matrix operations
- ✓ excellent weak and strong scaling
- ✓ very fast I/O capabilities
- volumes (so far) of the order of (L = 50 to 100)<sup>3</sup>, larger volumes possible (E.g.in such volumes one can describe about 50,000 neutrons at saturation density)
- ✓ capable of simulating up to times of the order of 10<sup>-19</sup> s (a few million time steps)
  ✓ TDSLDA is about 1000 times complex than existing TDHF codes.
- Presented calculations for unitary Fermi gas required over 200,000 cores of JaguarPF

## **Excitation of vortices through stirring**



## dynamics of vortex rings

Heavy spherical object moving through the superfluid unitary Fermi gas



# Road to quantum turbulence

**Classical turbulence:** energy is transferred from large scales to small scales where it eventually dissipates.

Kolmogorov spectrum:  $E(k)=C \epsilon^{2/3} k^{-5/3}$ 

- E kinetic energy per unit mass associated with the scale 1/k
- $\epsilon$  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.

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 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.

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

Nuclear dynamics from time dependent density functional theory

$$S(E) = \sum_{\nu} |\langle \nu | \hat{F} | 0 \rangle|^2 \delta(E - E_{\nu})$$
  
$$S(\omega) = \operatorname{Im} \{ \delta F(\omega) / [\pi f(\omega)] \}$$

Photoabsorption cross section for heavy, deformed nuclei.

(gamma,n) reaction through the excitation of GDR



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

#### **Evolution of occupation probabilities**



FIG. 1. (Color online) The time-dependent proton and neutron occupation probabilities of a a number of quasiparticle states around the Fermi level for  $^{238}$ U calculated as described in the main text with SLy4.

## **TDSLDA applications:**

- 1) Nuclear physics:
- **Electromagnetic response**
- Pairing vibrations
- Heavy ion collisions
- Induced fission
- Neutron scattering/capture
- 2) Neutron stars:
  - **Dynamics of vortices**
  - Vortex pinning mechanism in the neutron star crust (glitches)
- 3) Various applications in cold atom physics.

## Limitations:

- Only one body observables can be described accurately (possibly can be overcome by Balian-Veneroni method)
- Requires large computer resources
- The results depend on the quality of the density functional