Real Time Dynamics of theUnitary Fermi Gas

arXiv:1011:5999 (in press)

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Goal:

Describe *accurately* the time-dependent evolution of an externally perturbed Fermi superfluid at T=0

Outline:

- **DFT extension to superfluid systems and time-dependent phenomena**
- **Real-time dynamics of vortices in a unitary Fermi gas vortex reconnection and onset of quantum turbulence**
- **Real-time collision of two unitary Fermi gas clouds**

How to treat inhomogeneous systems!

- Monte Carlo (feasible for small particle numbers only)

- Density Functional Theory (large particle numbers)

One needs:

1) to find an Energy Density Functional (EDF)
2) to extend DFT to superfluid phenomena (SLDA)
3) to extend SLDA to time-dependent phenomena

Kohn-Sham theorem (1965)

$$H = \sum_{i}^{N} T(i) + \sum_{i<j}^{N} U(ij) + \sum_{i<j<k}^{N} U(ijk) + \ldots + \sum_{i}^{N} V_{ext}(i)$$

$$H\Psi_0(1,2,\ldots N) = E_0 \Psi_0(1,2,\ldots N)$$

$$n(\vec{r}) = \left\langle \Psi_0 \left| \sum_{i}^{N} \delta(\vec{r} - \vec{r}_i) \right| \Psi_0 \right\rangle$$

Injective map (one-to-one)

$$\Psi_0(1,2,\ldots N) \;\Leftrightarrow\; V_{ext}(\vec{r}) \;\Leftrightarrow\; n(\vec{r})$$

$$E_0 = \min_{n(\vec{r})} \int d^3r \left\{ \frac{\hbar^2}{2m^*(\vec{r})} \tau(\vec{r}) + \varepsilon\left[n(\vec{r})\right] + V_{ext}(\vec{r}) n(\vec{r}) \right\}$$

$$n(\vec{r}) = \sum_{i}^{N} \left|\varphi_i(\vec{r})\right|^2, \qquad \tau(\vec{r}) = \sum_{i}^{N} \left|\vec{\nabla}\varphi_i(\vec{r})\right|^2$$

Universal functional of particle density alone

Independent of external potential

Normal Fermi systems only!

The SLDA (DFT) energy density functional at unitarity for equal numbers of spin-up and spin-down fermions

Dimensional arguments, renormalizability, and Galilean invariance determine the functional

$$\varepsilon(\vec{r}) = \left[\alpha \frac{\tau_c(\vec{r})}{2} - \Delta(\vec{r})\nu_c(\vec{r}) \right] + \beta \frac{3(3\pi^2)^{2/3} n^{5/3}(\vec{r})}{5}$$

$$n(\vec{r}) = 2 \sum_{0<E_k<E_c} \left| \mathrm{v}_k(\vec{r}) \right|^2, \quad \tau_c(\vec{r}) = 2 \sum_{0<E_k<E_c} \left| \vec{\nabla} \mathrm{v}_k(\vec{r}) \right|^2,$$

$$\nu_c(\vec{r}) = \sum_{0<E<E_c} \mathrm{u}_k(\vec{r}) \mathrm{v}_k^*(\vec{r})$$

Three dimensionless constants α, β, and γ determining the functional are extracted from QMC for homogeneous systems by fixing the total energy, the pairing gap and the effective mass

Formalism for Time-Dependent Phenomena

"The time-dependent density functional theory is viewed in general as a reformulation of the exact quantum mechanical time evolution of a many-body system when only one-body properties are considered."

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

http://www.tddft.org

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

$$\begin{cases} [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathrm{u}_i(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)] \mathrm{v}_i(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{u}_i(\vec{r},t)}{\partial t} \\ [\Delta^*(\vec{r},t) + \Delta^*_{ext}(\vec{r},t)] \mathrm{u}_i(\vec{r},t) - [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathrm{v}_i(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{v}_i(\vec{r},t)}{\partial t} \end{cases}$$

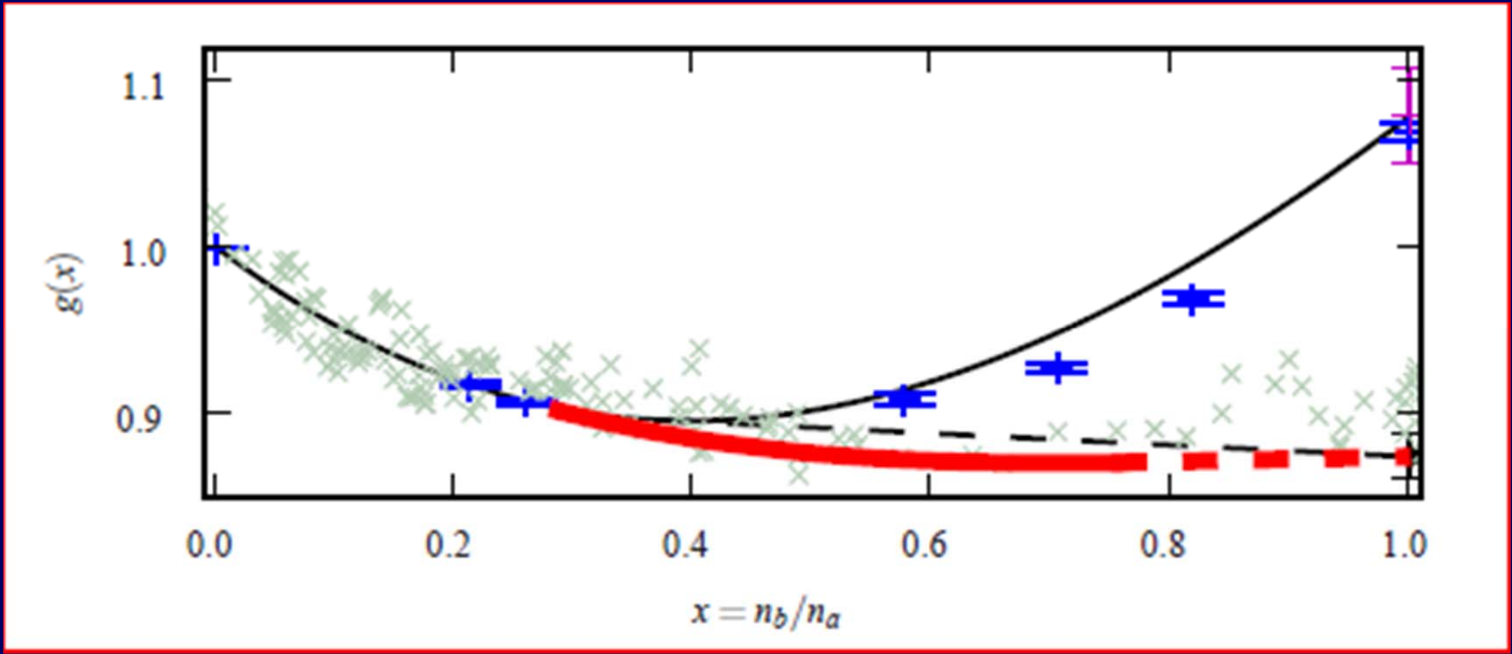
For time-dependent phenomena one has to add currents.
Galilean invariance determines the dependence on currents.

Normal State			
(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)
(3,1)	6.6 ± 0.01	6.687	1.3%
(4,1)	8.93 ± 0.01	8.962	0.36%
(5,1)	12.1 ± 0.1	12.22	0.97%
(5,2)	13.3 ± 0.1	13.54	1.8%
(6,1)	15.8 ± 0.1	15.65	0.93%
(7,2)	19.9 ± 0.1	20.11	1.1%
(7,3)	20.8 ± 0.1	21.23	2.1%
(7,4)	21.9 ± 0.1	22.42	2.4%
(8,1)	22.5 ± 0.1	22.53	0.14%
(9,1)	25.9 ± 0.1	25.97	0.27%
(9,2)	26.6 ± 0.1	26.73	0.5%
(9,3)	27.2 ± 0.1	27.55	1.3%
(9,5)	30 ± 0.1	30.77	2.6%
(10,1)	29.4 ± 0.1	29.41	0.034%
(10,2)	29.9 ± 0.1	30.05	0.52%
(10,6)	35 ± 0.1	35.93	2.7%
(20,1)	73.78 ± 0.01	73.83	0.061%
(20,4)	73.79 ± 0.01	74.01	0.3%
(20,10)	81.7 ± 0.1	82.57	1.1%
(20,20)	109.7 ± 0.1	113.8	3.7%
(35,4)	154 ± 0.1	154.1	0.078%
(35,10)	158.2 ± 0.1	158.6	0.27%
(35,20)	178.6 ± 0.1	180.4	1%

Superfluid State			
(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)
(1,1)	2.002 ± 0	2.302	15%
(2,2)	5.051 ± 0.009	5.405	7%
(3,3)	8.639 ± 0.03	8.939	3.5%
(4,4)	12.573 ± 0.03	12.63	0.48%
(5,5)	16.806 ± 0.04	16.19	3.7%
(6,6)	21.278 ± 0.05	21.13	0.69%
(7,7)	25.923 ± 0.05	25.31	2.4%
(8,8)	30.876 ± 0.06	30.49	1.2%
(9,9)	35.971 ± 0.07	34.87	3.1%
(10,10)	41.302 ± 0.08	40.54	1.8%
(11,11)	46.889 ± 0.09	45	4%
(12,12)	52.624 ± 0.2	51.23	2.7%
(13,13)	58.545 ± 0.18	56.25	3.9%
(14,14)	64.388 ± 0.31	62.52	2.9%
(15,15)	70.927 ± 0.3	68.72	3.1%
(1,0)	1.5 ± 0.0	1.5	0%
(2,1)	4.281 ± 0.004	4.417	3.2%
(3,2)	7.61 ± 0.01	7.602	0.1%
(4,3)	11.362 ± 0.02	11.31	0.49%
(7,6)	24.787 ± 0.09	24.04	3%
(11,10)	45.474 ± 0.15	43.98	3.3%
(15,14)	69.126 ± 0.31	62.55	9.5%

Bulgac, Forbes, and Magierski, arXiv:1008:3933

EOS for spin polarized systems



Red line: Larkin-Ovchinnikov phase (unitary Fermi supersolid)

Black line: normal part of the energy density

Blue points: DMC calculations for normal state, Lobo et al, PRL 97, 200403 (2006)

Gray crosses: experimental EOS due to Shin, Phys. Rev. A 77, 041603(R) (2008)

$$E(n_a,n_b)=\frac{3}{5}\frac{(6\pi^2)^{2/3}\hbar^2}{2m}\left[n_a g\left(\frac{n_b}{n_a}\right)\right]^{5/3}$$

Bulgac and Forbes,
Phys. Rev. Lett. 101, 215301 (2008)

Full 3D implementation of TD-SLDA is a petaflop problem and it has been completed.

Bulgac and Roche, J. Phys. Conf. Series 125, 012064 (2008)

Recently Run Jobs at NCCS

Processors	Project
217,800	FY2010 DOE/ASCR Joule Metric on Computational Effectiveness
10,000	Predictive and Accurate Monte Carlo-based Simulations for Mott Insulators, Cuprate Superconductors, and Nanoscale Systems
4,096	Intermittency and Star Formation in Turbulent Molecular Clouds
2,292	Climate-Science Computational End Station Development and Grand Challenge Team
2,160	CHIMES: Coupled High-Resolution Modeling of the Earth System

Critical velocity in a unitary gas

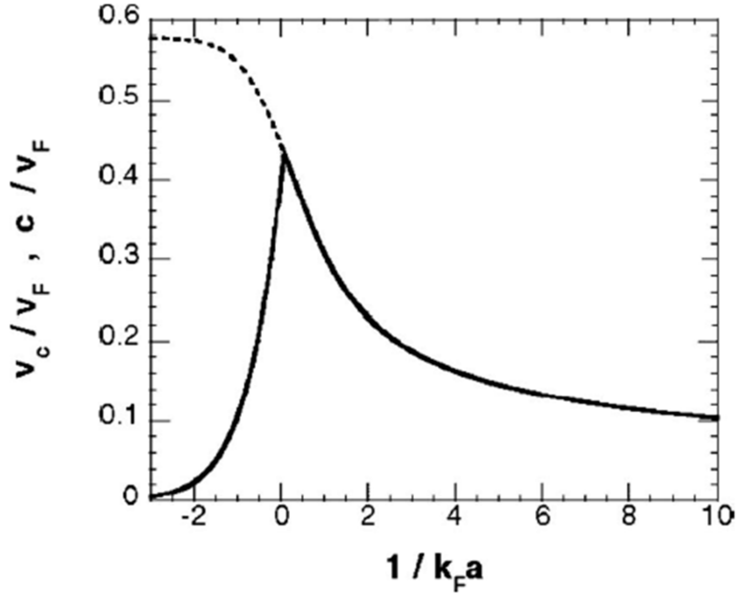


FIG. 20. Landau's critical velocity (in units of the Fermi velocity) calculated along the crossover using BCS mean-field theory. The critical velocity is largest near unitarity. The dashed line is the sound velocity. From Combescot, Kagan, and Stringari, 2006.

$$c_s = 0.370(5)\mathrm{v_F}$$

$$\min\left(\frac{\varepsilon_{qp}}{k}\right) = 0.385(3)$$

$$\Rightarrow \quad \mathrm{v}_c = 0.370(5)\mathrm{v_F}$$

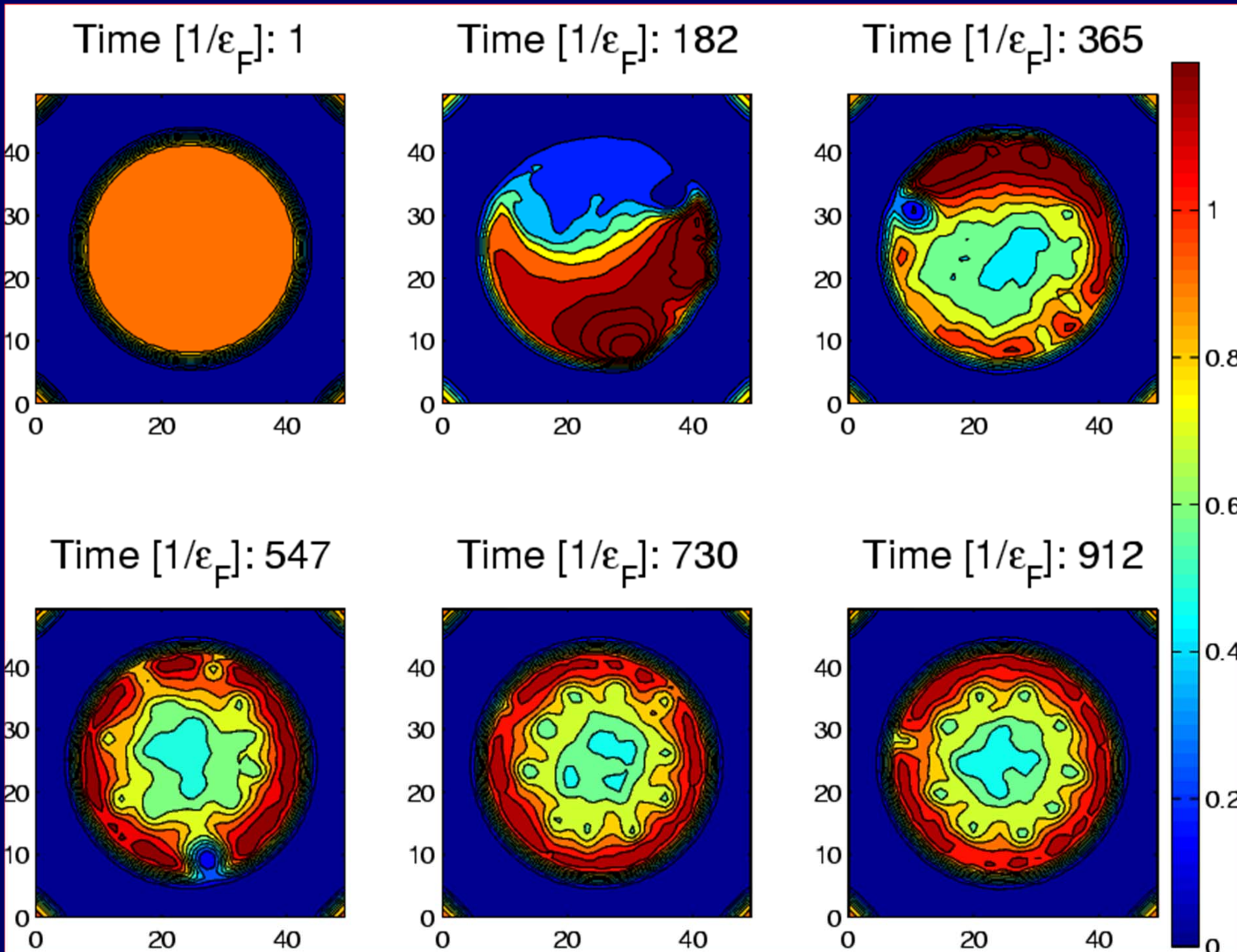
Values obtained using QMC data

$$\mathrm{v}_c \approx 0.25(3)\mathrm{v}_F$$

Miller et al. (MIT, 2007)

From Giorgini, Pitaevskii and Stringari, Rev. Mod. Phys., 80, 1215 (2008)

Study based on BCS/Leggett approximation

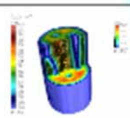
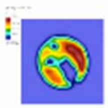
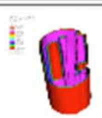


Density cut through a stirred unitary Fermi gas at various times.

The Superfluid Local Density Approximation Applied to Unitary Fermi Gases -Supplementary Material

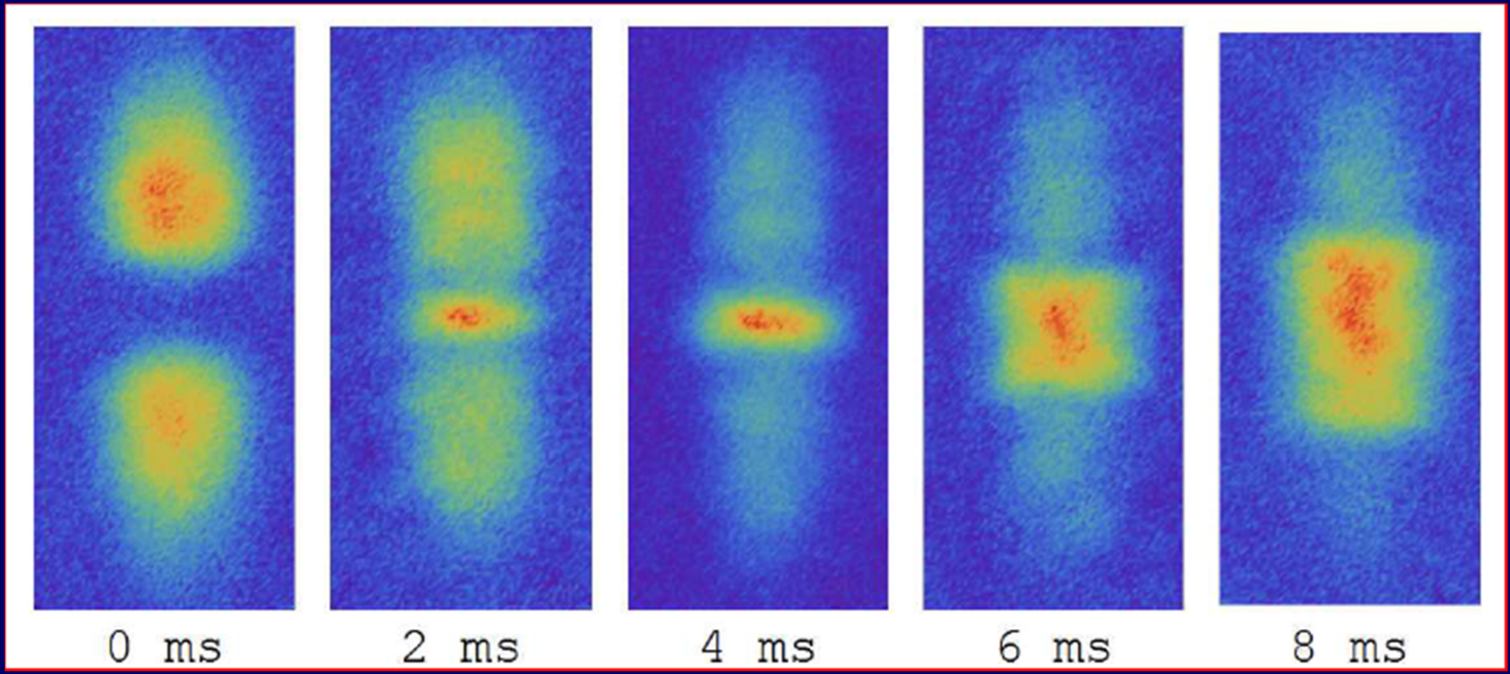
All simulations can be found here: http://www.phys.washington.edu/groups/qmbnt/UFG. The simulations can be categorized by the excitations: ball and rod, centered ball, centered small ball, centered big ball, centered supersonic ball, off-centered ball, and twisted stirrer. The following table matches simulations with numerical experiments. In several studies, we present multiple perspectives of the event as well as different plotting schemes to reveal different features of the dynamics.

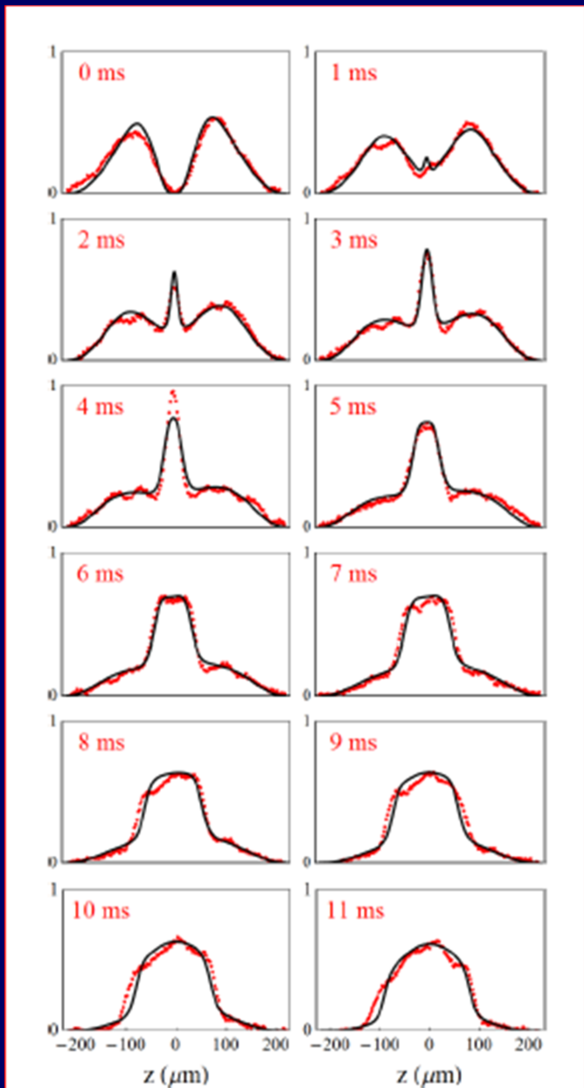
3D Simulations

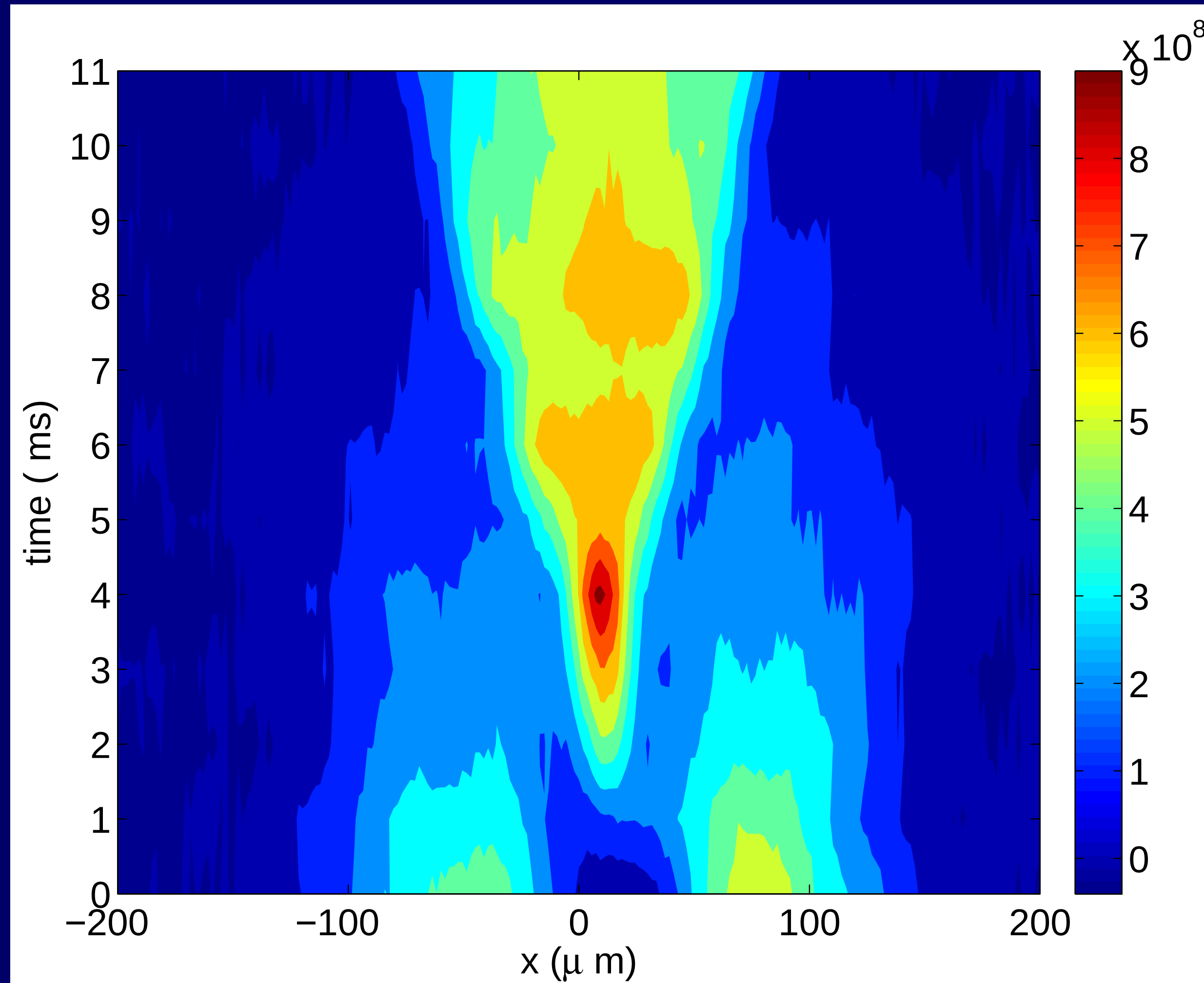
Excitation	Link	Description
Ball and Rod		
	nt-ball-rod-dns.m4v	density volume plot of magnitude of pairing field; front facing with quarter segment slice; 5m28s duration (20.9 MB)
	nt-ball-rod-dns-pln.m4v	density volume plot of magnitude of pairing field; 2D slice; 5m28s duration (9.8MB)
	nt-ball-rod-thin-angl.m4v	density contour plot of magnitude of pairing field focused on vortices ; angled front-facing with quarter segment slice; 5m28s duration (12.8MB)
Centered Ball		
	nt-ball-c.m4v	density contour plot of magnitude of pairing field focused on vortices; full geometry ; 3m29s

Observation of shock waves in a strongly interacting Fermi gas

J. Joseph, J.E. Thomas, M. Kulkarni, and A.G. Abanov
Phys. Rev. Lett. 106, 150401 (2011)





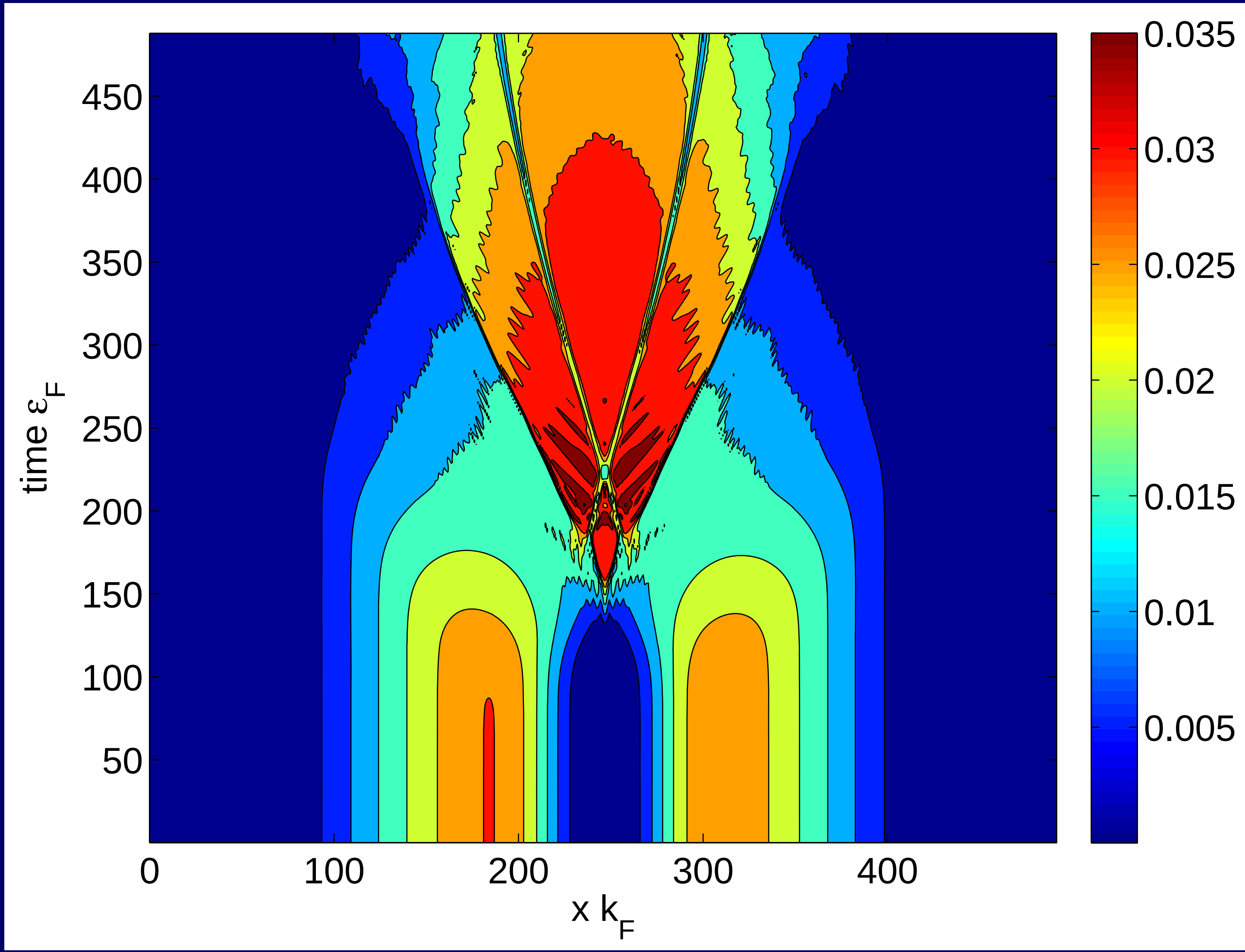


$$\partial_t n = -\partial_z (nv)$$

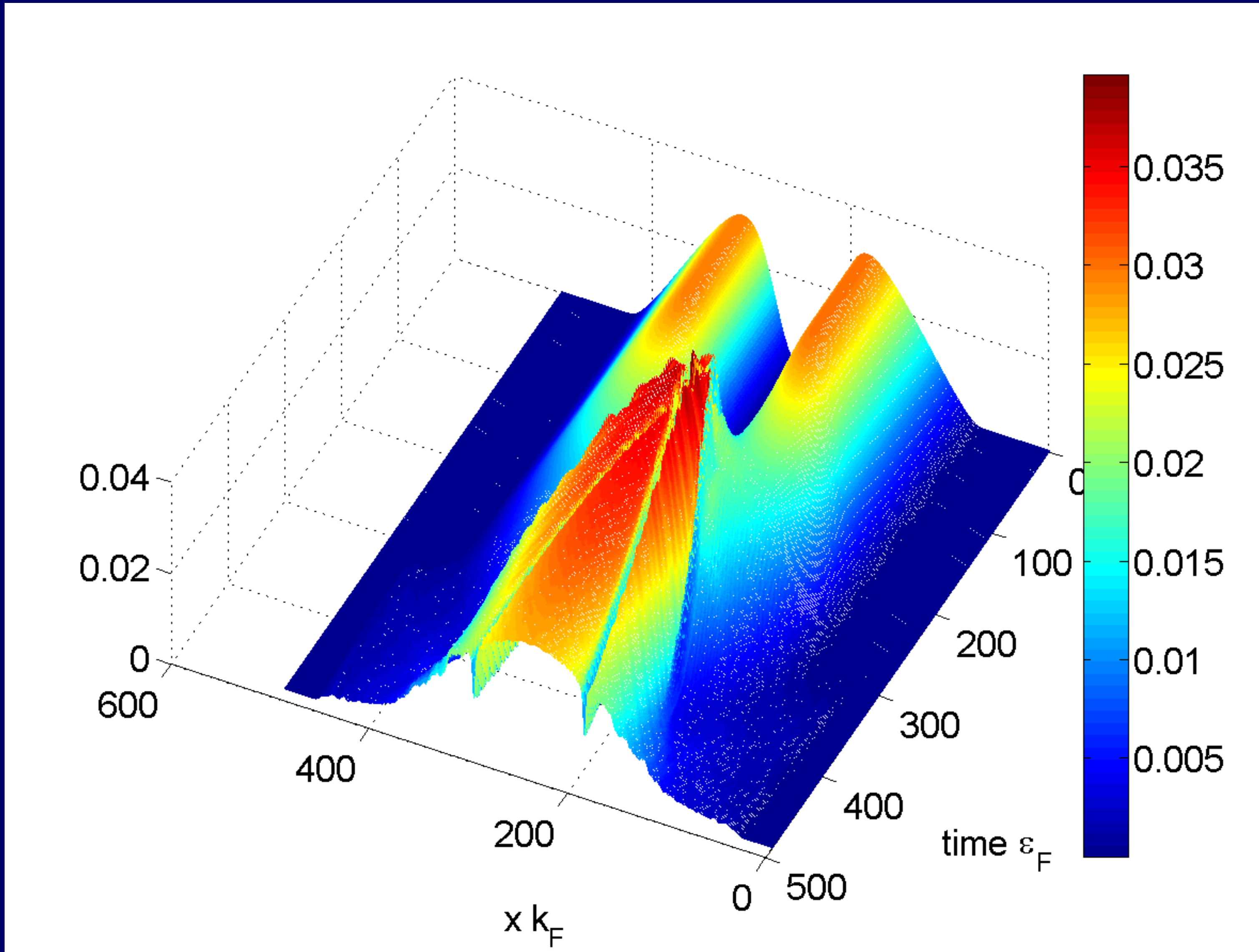
$$\partial_t v = -\partial_z \left(\frac{v^2}{2} + C n^{\frac{2}{5}} + \frac{1}{2} \omega_z^2 z^2 \right) + \nu \frac{\partial_z (n \partial_z v)}{n},$$

NB! There is no $\hbar$ in these equations.

Let us find out what TDSLDA tell us about this collision.

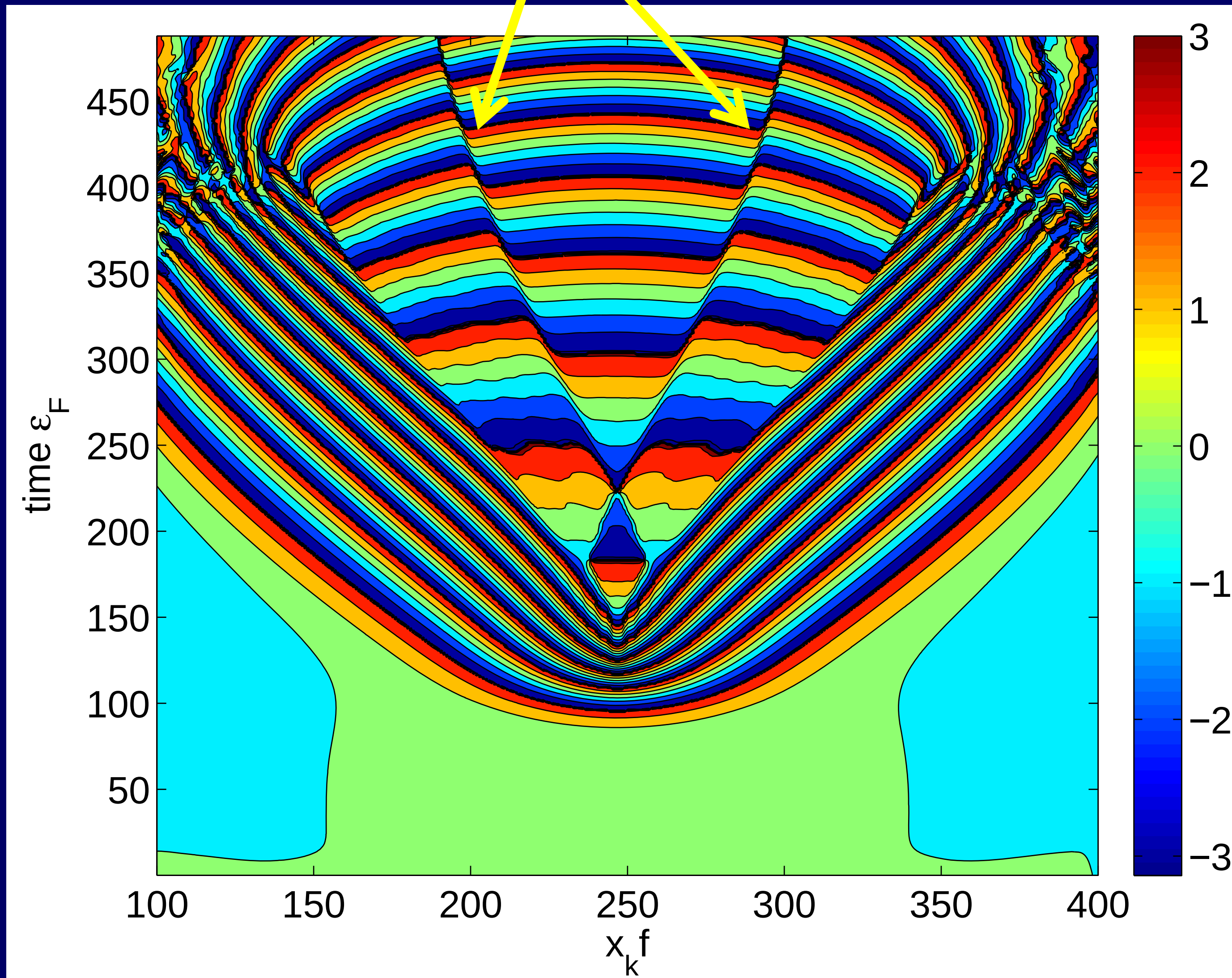


Number density contour plot

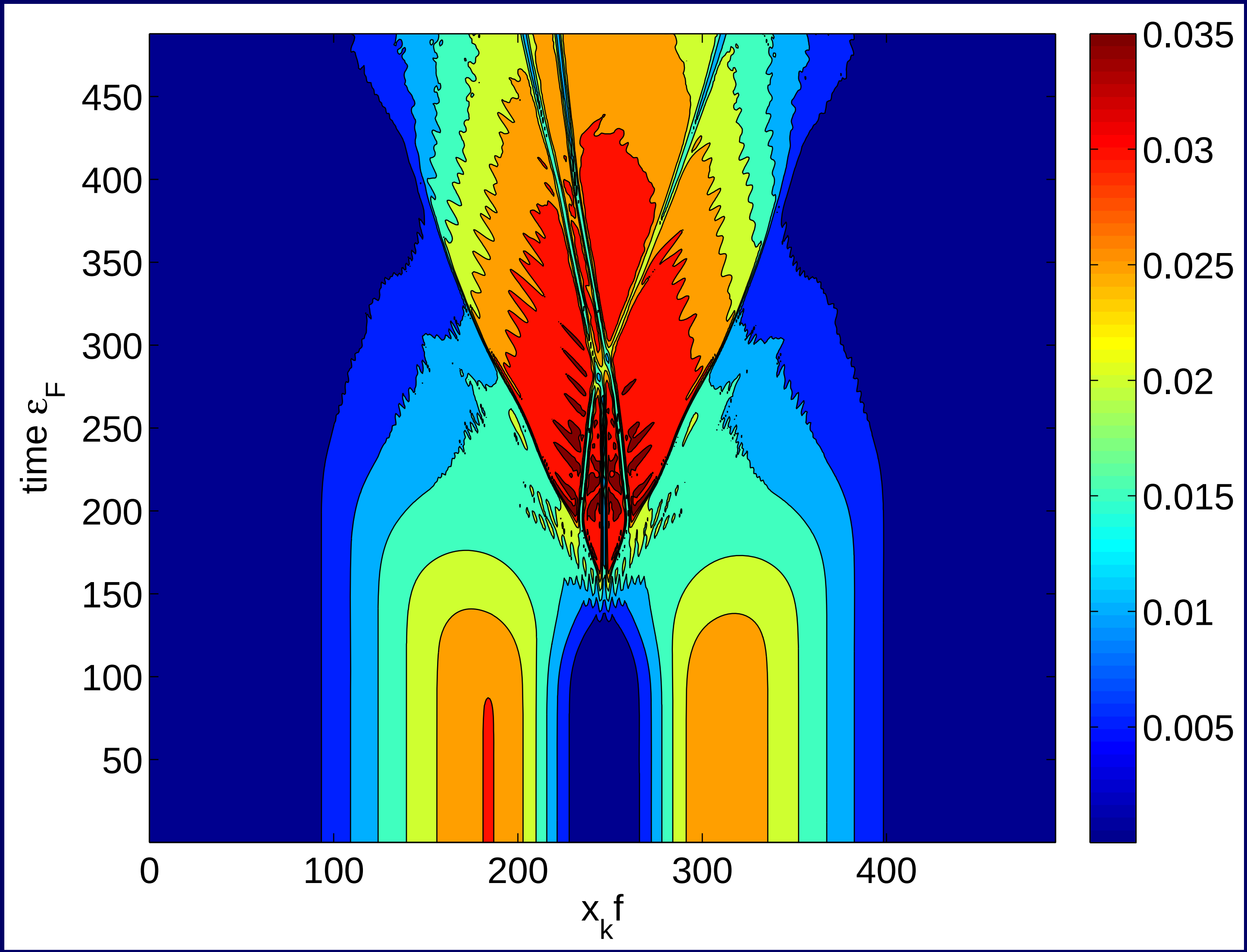


Number density
(Pairing gap has a very similar behavior)

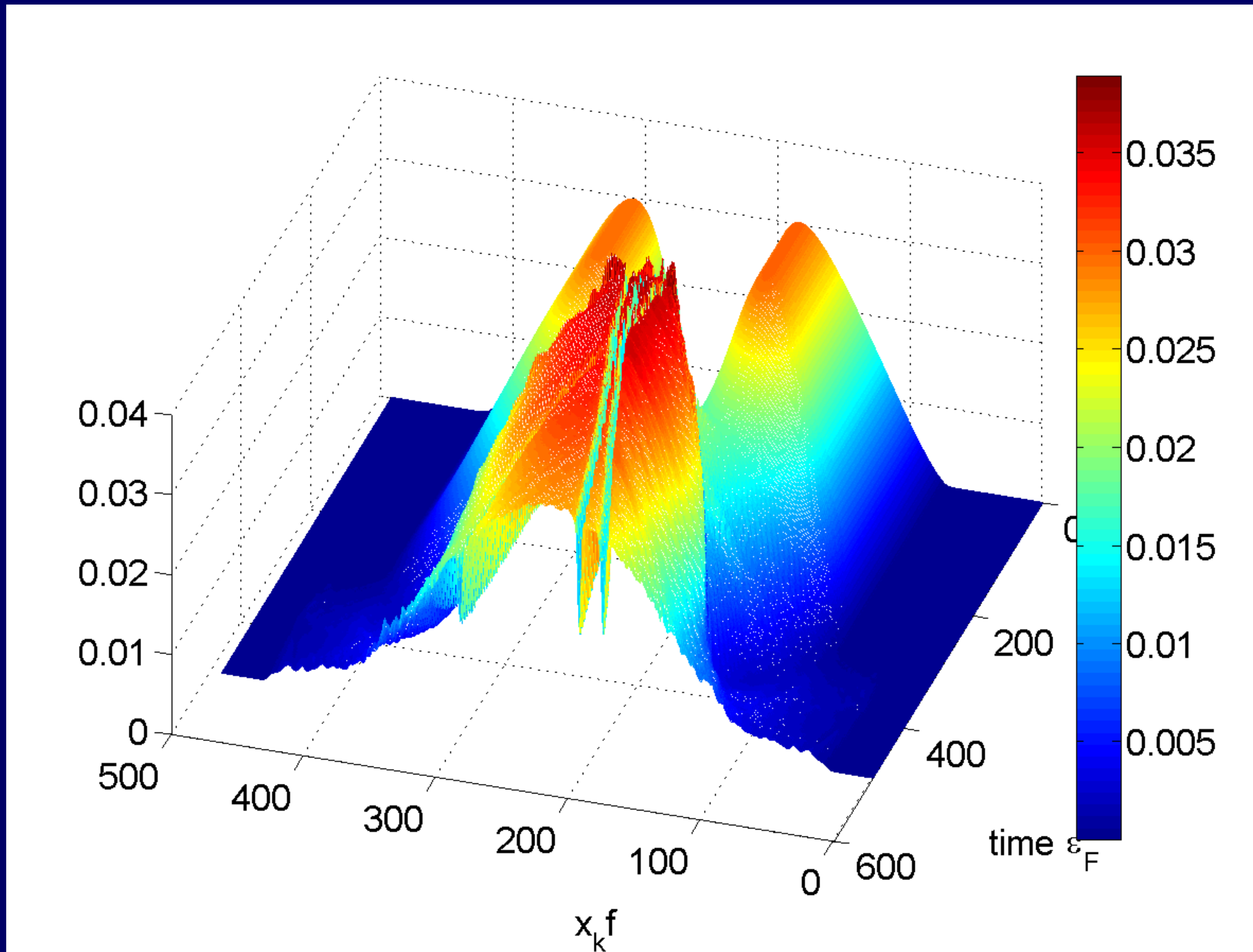
These are dark solitons!



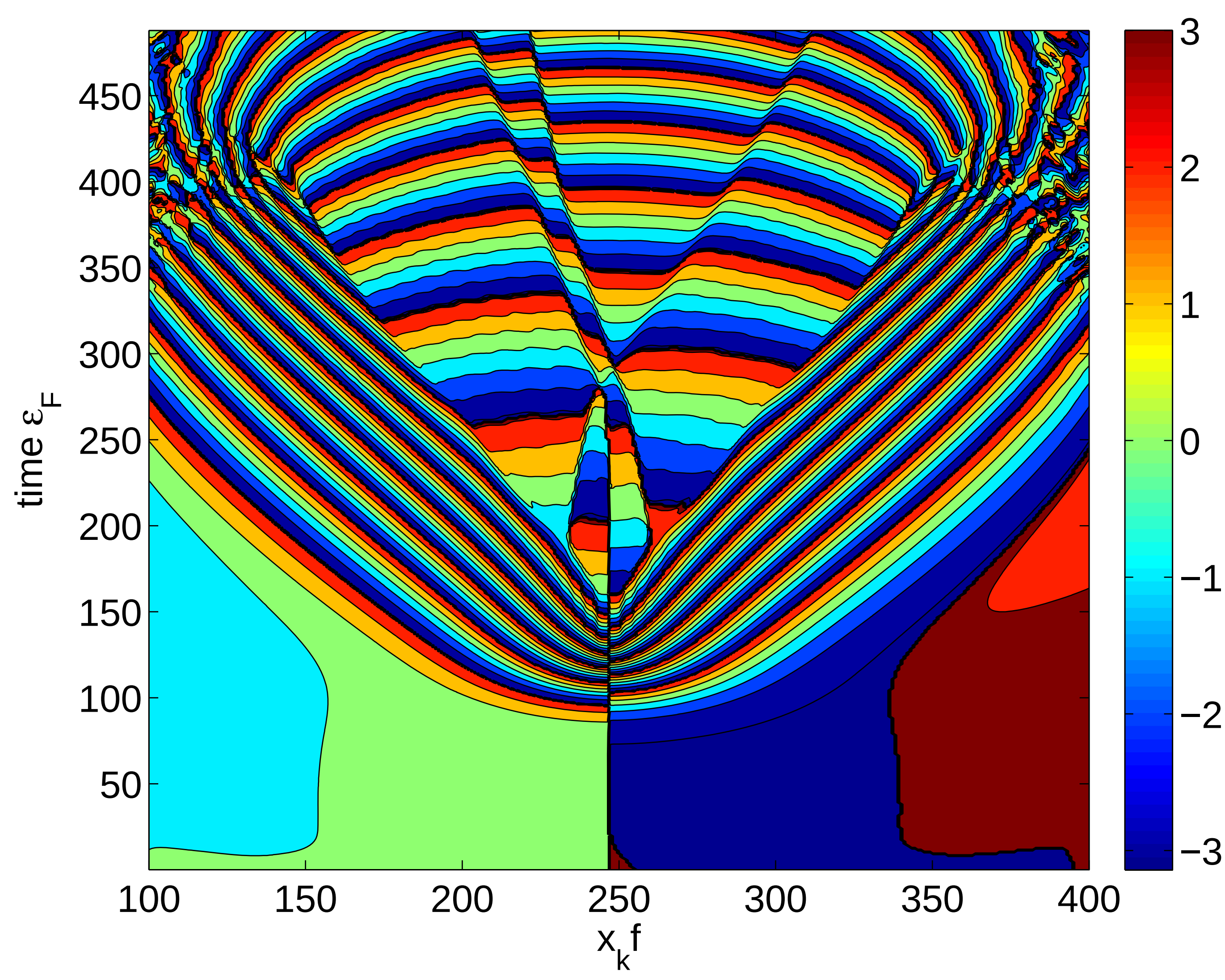
Phase of the pairing gap contour plot



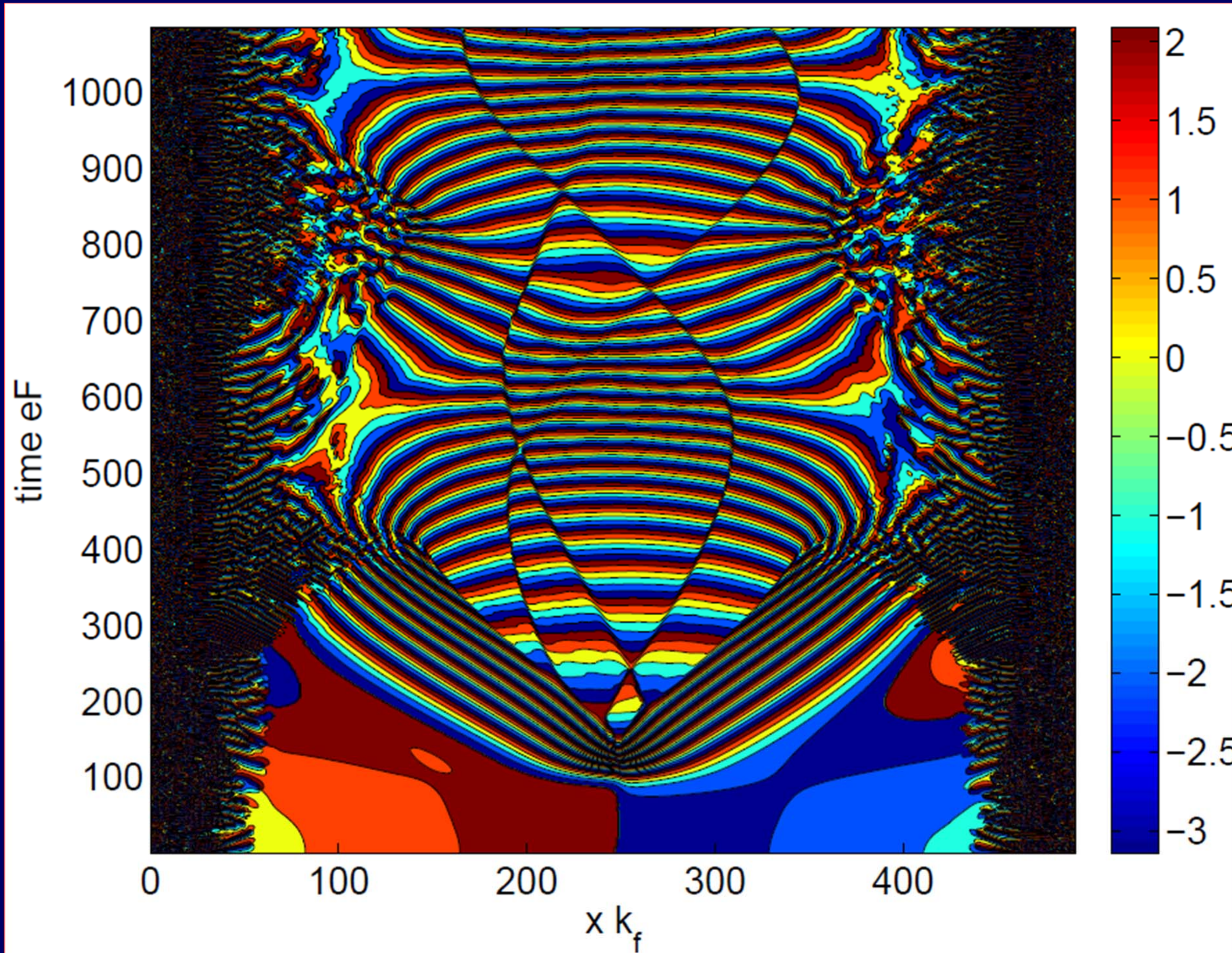
Number density contour plot



Number density



Phase of the pairing gap contour plot



Phase of the pairing gap contour plot

Summary

- ✓ Full 3D real-time simulations of the dynamics of a superfluid Fermi gas are now feasible
- ✓ A number of new phenomena were observed:
Higgs modes, superfluid to normal transition under the action of external quantum stirrers, generation of quantized vortices, supercritical superfluid flow, crossing and reconnection of vortex lines (quantum turbulence), excitation of vortex rings, …
- ✓ Excitation of dark solitons in the collision of unitary Fermi gas clouds are predicted
- ✓ One can study a large variety of time-dependent phenomena when basically any