Time-Dependent Density Functional Theory and Real-Time Dynamics of Fermi Superfluids

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Athena UW Cluster, Hyak UW cluster,
Franklin and Hopper, NERSC and JaguarPF, NCCS, starting to use Titan, NCCS

Why should one study fermionic superfluidity?

Superconductivity (discovered on April 8th, 1911) and superfluidity in Fermi systems are manifestations of quantum coherence at a macroscopic level

- ✓ **Dilute atomic Fermi gases** $T_c \approx 10^{-9}$ eV
- ✓ **Liquid ^{3}He** $T_c \approx 10^{-7}$ eV
- ✓ **Metals, composite materials** $T_c \approx 10^{-3} – 10^{-2}$ eV
- ✓ **Nuclei, neutron stars** $T_c \approx 10^{5} – 10^{6}$ eV
- **QCD color superconductivity** $T_c \approx 10^{7} – 10^{8}$ eV

units (1 eV ≈ 10^4 K)

Physical systems and processes we are interested in:

- ✓ Collective states in nuclei
- ✓ Nuclear large amplitude collective motion (LACM)
  (Induced) nuclear fission
- ✓ Excitation of nuclei with gamma rays and neutrons
- ✓ Coulomb excitation of nuclei with relativistic heavy-ions
- ✓ Nuclear reactions, fusion between colliding heavy-ions
- ✓ Neutron star crust and dynamics of vortices and their pinning mechanism

- ✓ Dynamics of vortices, Anderson-Higgs Mode
- ✓ Vortex crossing and reconnection and the onset of quantum turbulence
- ✓ Domain wall solitons and shock waves in collision of fermionic superfluid atomic clouds

Near and long term goals:

To describe accurately the time-dependent evolution of externally perturbed Fermi superfluid systems

Tool: a DFT extension to superfluid systems and time-dependent phenomena (and subsequently we have to add quantum fluctuations and extend the theory to a stochastic incarnation)

In order to treat this plethora of phenomena one needs to treat spatially inhomogeneous systems in real time!

Methods?

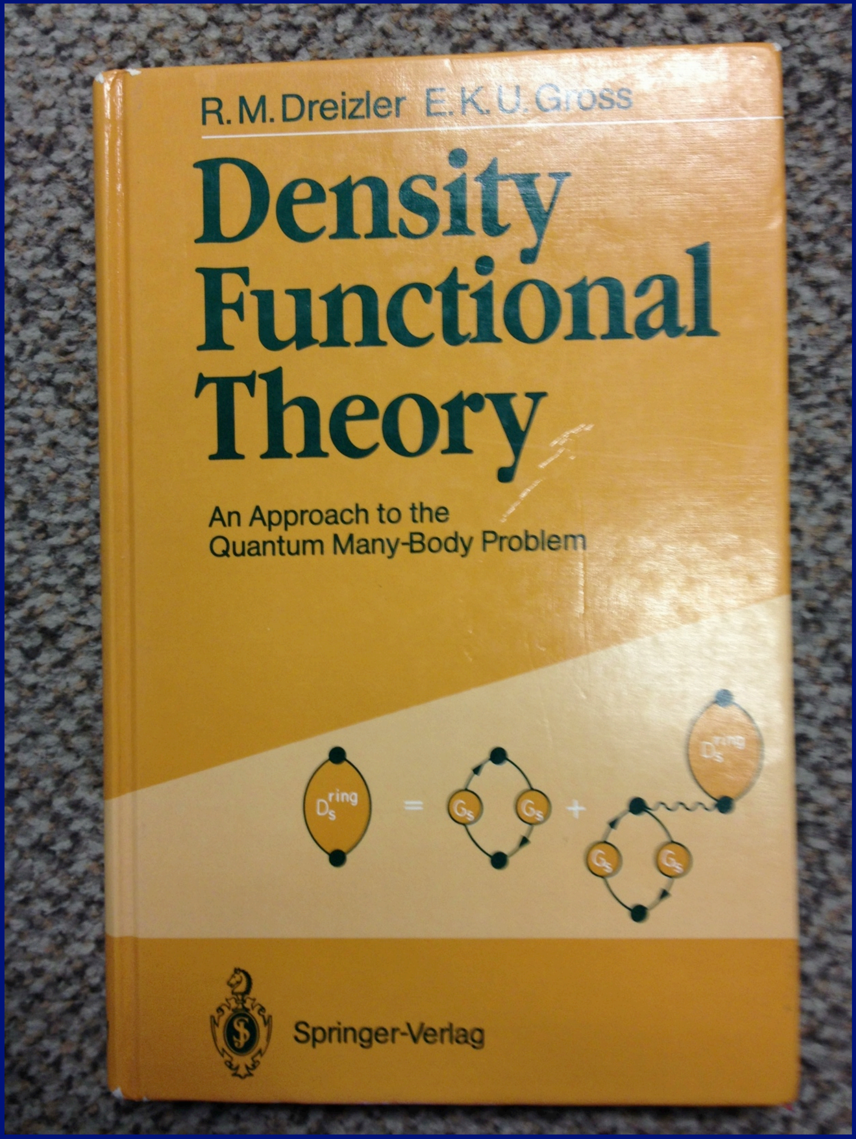
- **Quantum Monte Carlo is feasible for small particle numbers only and has been implemented so far only for static phenomena**

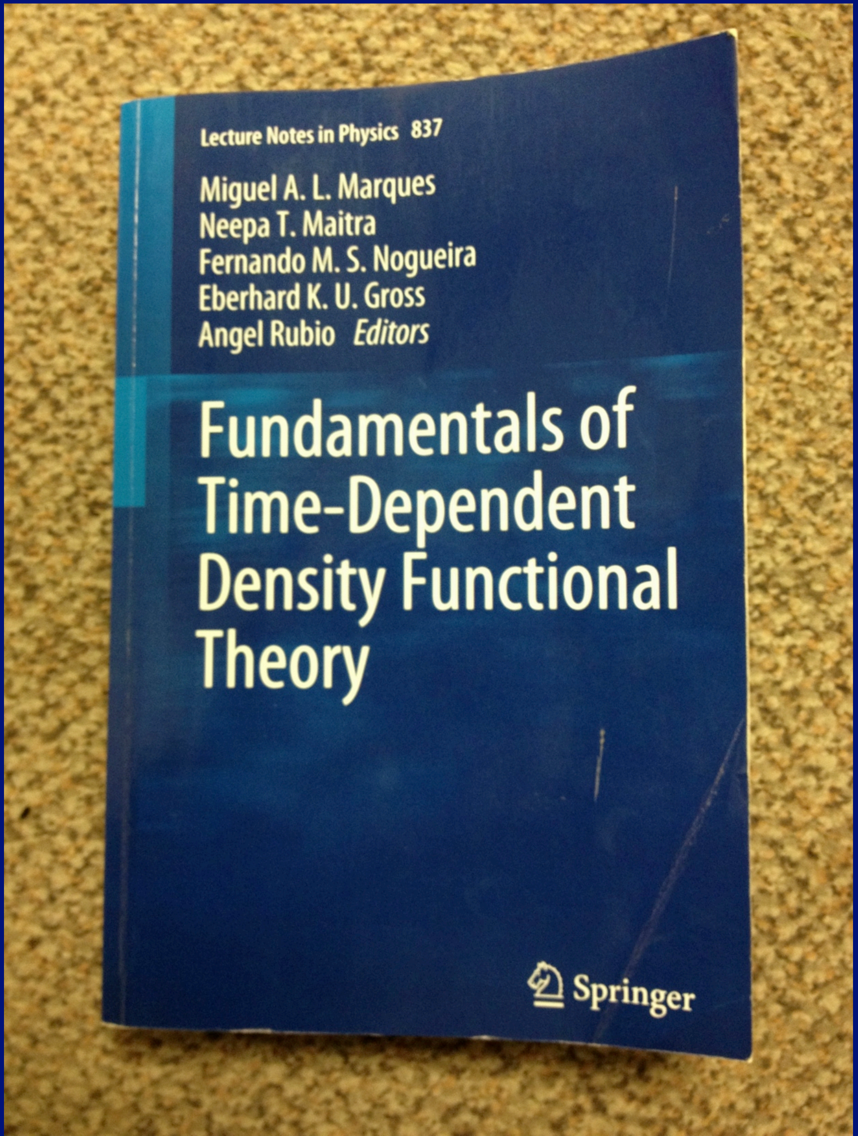
- **<u>Density Functional Theory</u> (large particle numbers)**

  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 (TDSLDA)
  4) to develop a stochastic extension (STDSLDA)

Why Density Functional Theory (DFT)?





One option is the two-fluid hydrodynamics (here at T=0)

N.B. There is no quantum statistics in two-fluid hydrodynamics

$$\frac{\partial n(\vec{r},t)}{\partial t} + \vec{\nabla}\bullet\left[\vec{v}(\vec{r},t)n(\vec{r},t)\right] = 0$$

$$m\frac{\partial \vec{v}(\vec{r},t)}{\partial t} + \vec{\nabla}\left\{\frac{m\vec{v}^2(\vec{r},t)}{2} + \mu\left[n(\vec{r},t)\right] + V_{ext}(\vec{r},t)\right\} = 0$$

Troubles:

- **These are classical equations, <u>no Planck's constant</u>, thus no quantized vortices (unless one imposes by hand quantization)**
- **No physically clear physical mechanism to describe superfluid to normal transition (no role for the critical velocity)**

Two-fluid hydrodynamics + vortex quantization is equivalent to a ``Bohr model" of a superfluid

Another option is the phenomenological Ginzburg-Landau model (or the Gross-Pitaevskii equation, near T=0, only for bosons really):

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2 \Delta \Psi(\vec{r},t)}{2M} + U\left(\left|\Psi(\vec{r},t)\right|^2\right)\Psi(\vec{r},t) + V_{ext}(\vec{r},t)\Psi(\vec{r},t)$$

Troubles:

- Many would rightly claim that such an equation is not valid (as there should be no imaginary unit on the rhs)
- Only for temperatures near and below the critical temperature (or at T=0 for GP equation)
- Even though is a quantum approach, it describes only the superfluid phase. There is no Cooper pair breaking mechanism

Other issues:

There are a number of modes, such as the so called Higgs mode, which cannot be describes in either of these phenomenological approaches.

What is a unitary Fermi gas and why would one want to study it?

One reason:

(for the nerds, I mean the hard-core theorists,
not for the phenomenologists)

Bertsch's Many-Body X challenge, Seattle, 1999

What are the ground state properties of the many-body system composed of spin ½ fermions interacting via a zero-range, infinite scattering-length contact interaction.

What are the scattering length and the effective range?

$$k \text{ cotan } \delta_0 = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + \cdots$$

$$\sigma = \frac{4\pi}{k^2} \sin^2 \delta_0 + \cdots = 4\pi a^2 + \cdots$$

If the energy is small, only the s-wave scattering is relevant.

Let us consider a very old and simple example:

The hydrogen atom.

The ground state energy could only be a function of:

- ✓ Electron charge
- ✓ Electron mass
- ✓ Planck's constant

and then trivial dimensional arguments lead to

$$E_{gs} = \frac{e^4 m}{\hbar^2} \times \frac{1}{2}$$

Only the factor ½ requires some hard work.

Let us turn now to dilute fermion matter

The ground state energy is given by a function:

$$E_{gs} = f(N, V, \hbar, m, a, r_0)$$

Taking the scattering length to infinity and the range of the interaction to zero, we are left with:

$$E_{gs} = F(N, V, \hbar, m) = \frac{3}{5}\varepsilon_F N \times \xi$$

$$\frac{N}{V} = \frac{k_F^3}{3\pi^2}, \qquad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

Pure number (dimensionless)

In 1999 we did not know the sign of ξ!

There were a number of papers making opposite claims around that time.

- **G.A. Baker, Jr (LANL) won the $600 prize**

($300 from George + $300 from V.A. Khodel)

Phys. Rev. C <u>60</u>, 064901 (1999)

The Bertsch, nonparametric model of neutron matter is analyzed and strong indications are found that, in the infinite system limit, the ground state is a Fermi liquid with an effective mass, except for a set of measure zero.

- **H. Heiselberg, second runner-up**

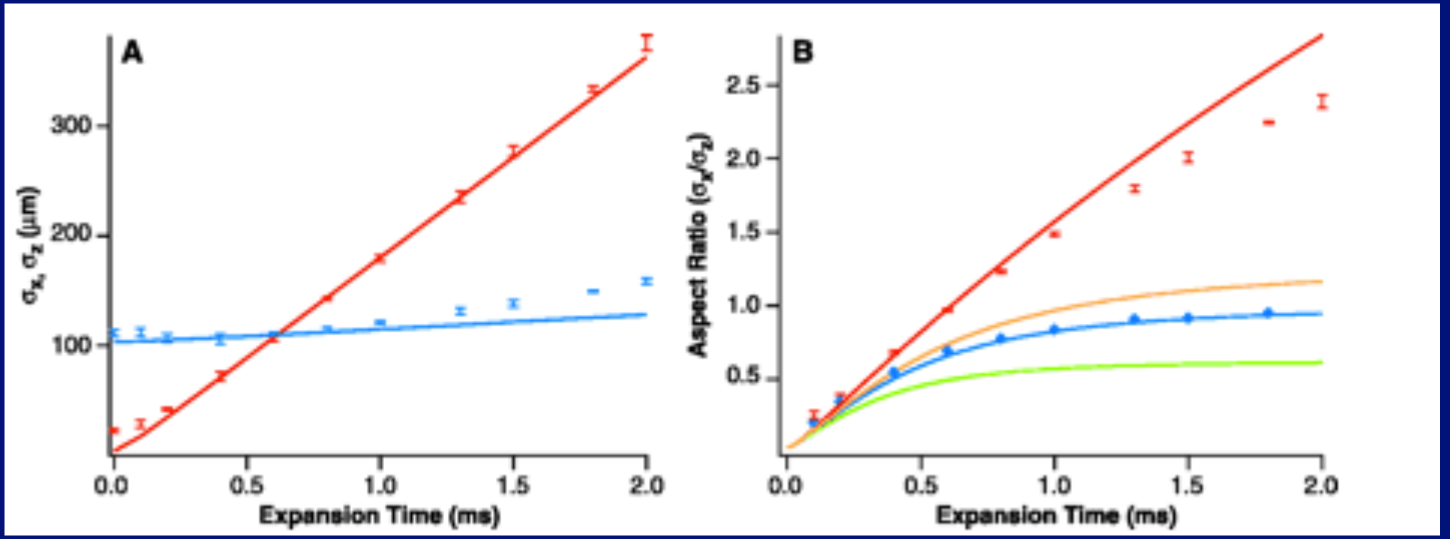
Phys. Rev. A <u>63</u>, 043606 (2001)

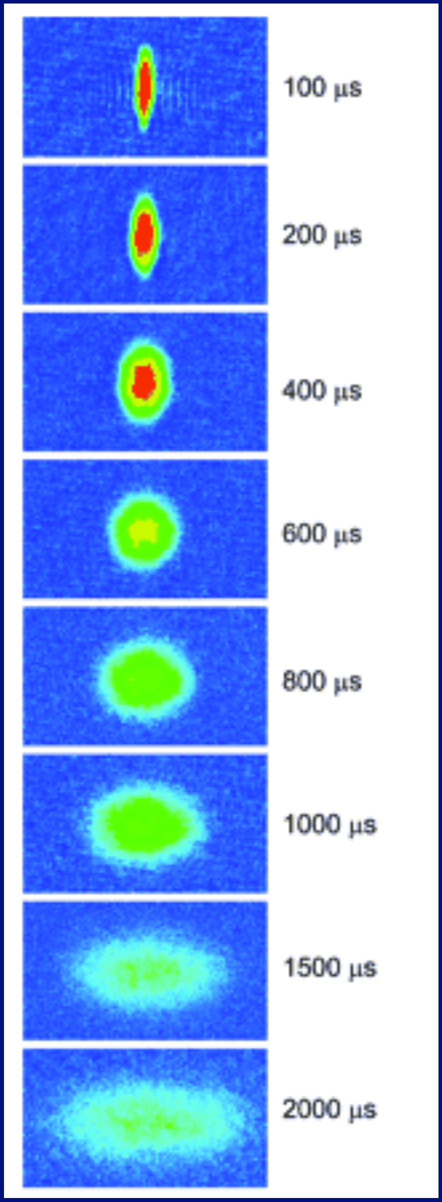
Ground-state energies and superfluid gaps are calculated for degenerate Fermi systems interacting via long attractive scattering lengths such as cold atomic gases, neutron, and nuclear matter. In the Intermediate region of densities, where the interparticle spacing (~$1/k_F$) is longer than the range of the interaction but shorter than the scattering length, the superfluid gaps and the energy per particle are found to be proportional to the Fermi energy and thus differ from the dilute and high-density limits. The attractive potential increase linearly with the spin-isospin or hyperspin statistical factor such that, e.g., symmetric nuclear matter undergoes spinodal decomposition and collapses whereas neutron matter and Fermionic atomic gases with two hyperspin states are mechanically *stable* in the intermediate density region. The regions of spinodal instabilities in the resulting phase diagram are reduced and do not prevent a superfluid transition.

Observation of a Strongly Interacting Degenerate Fermi Gas of Atoms

O'Hara, Hemmer, Gehm, Granade, and Thomas

Science, 298, 2179 (2002)





The atomic cloud expansion is similar to that observed in RHIC heavy-ion collisions.

Superfluid Fermi Gases with Large Scattering Length

Carlson, Chang, Pandharipande, and Schmidt

Phys. Rev. Lett. <u>91</u>, 050401 (2003)

*We report quantum Monte Carlo calculations of superfluid Fermi gases with short-range two-body attractive interactions with infinite scattering length. The energy of such gases is estimated to be **0:44 ±0:01** times that of the non-interacting gas, and their pairing gap is approximately twice the energy per particle.*

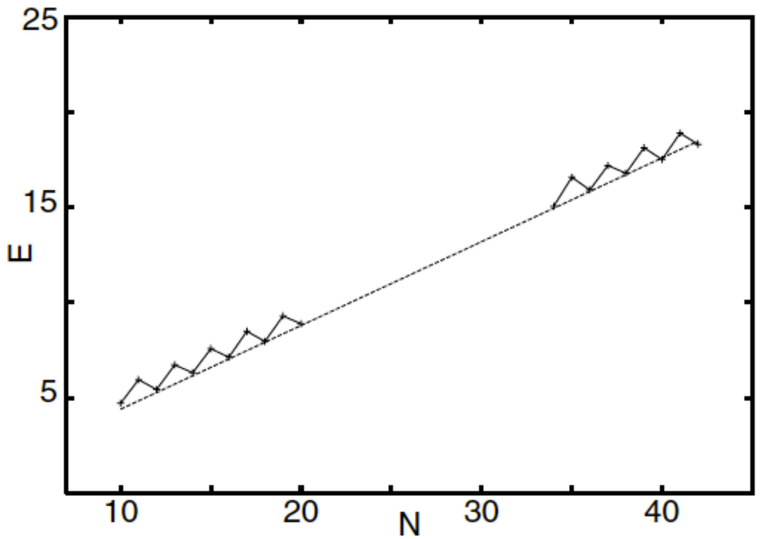


FIG. 3. The $E(N)$ in units of E_{FG}.

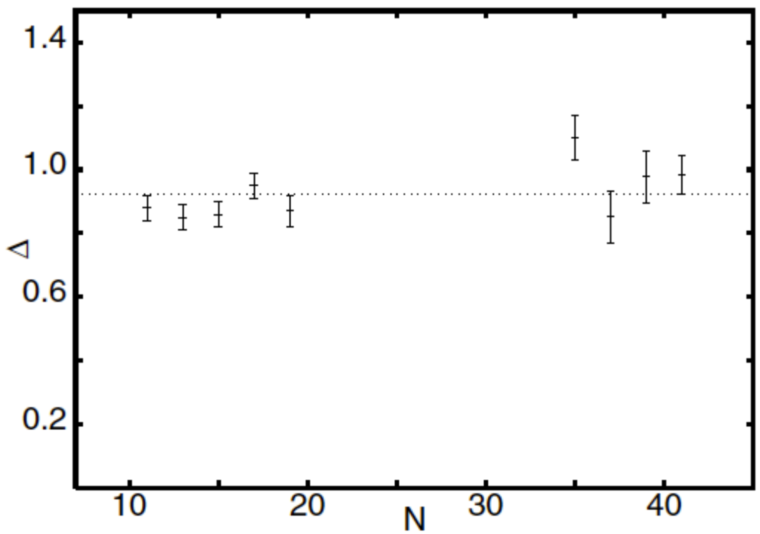
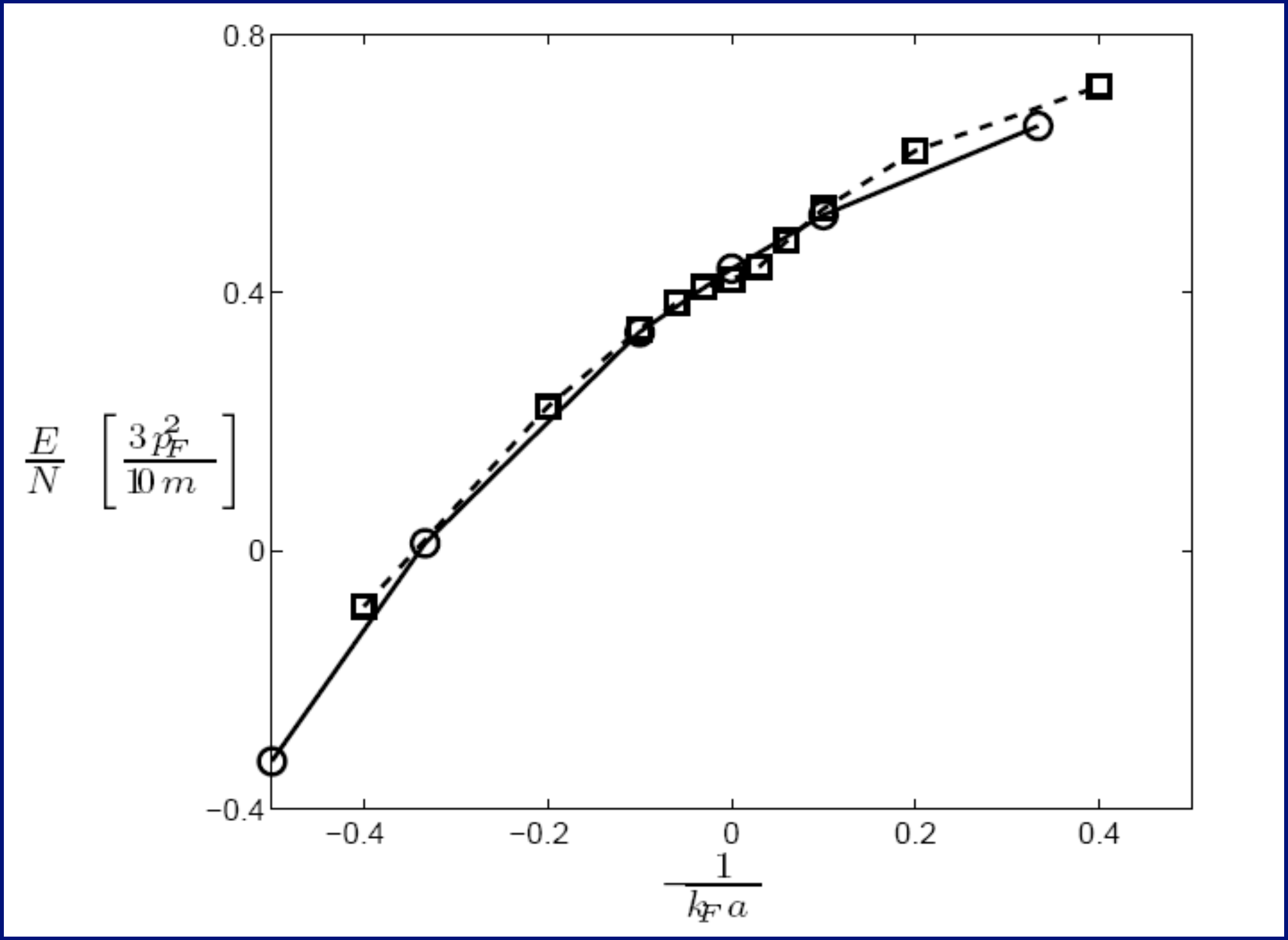


FIG. 4. The gap in units of E_{FG}.

$$E_{FG} = \frac{E}{N} = \frac{3\hbar^2 k_F^2}{10m}, \qquad n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}$$

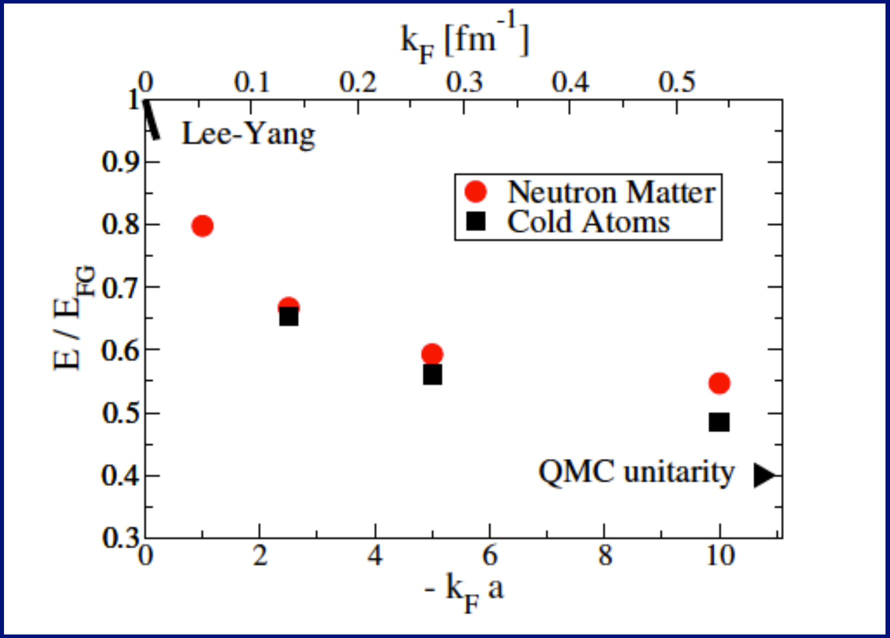
BEC side **BCS side**

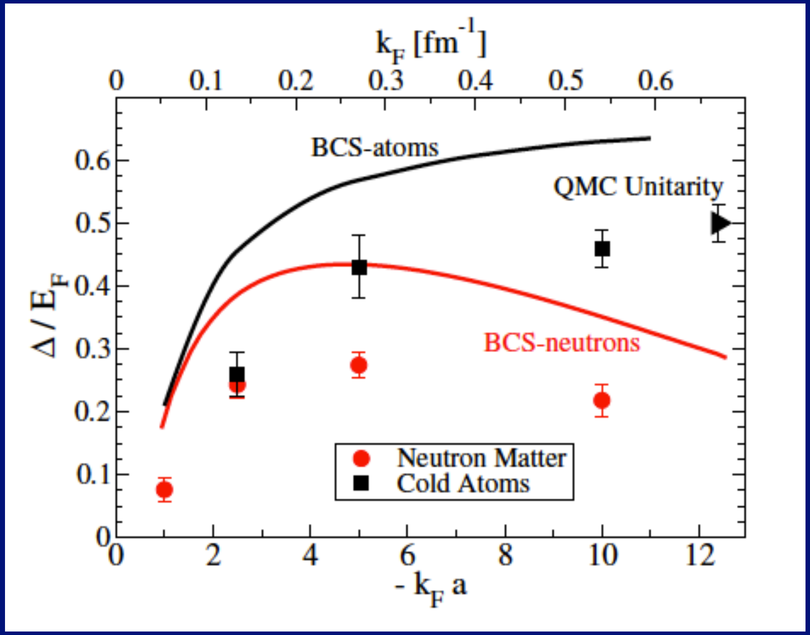


Solid line with open circles – Chang *et al.* PRA, 70, 043602 (2004)
Dashed line with squares - Astrakharchik *et al.* PRL 93, 200404 (2004)

Superfluid pairing in neutrons and cold atoms

Carlson, Gandolfi, and Gezerlis, arXiv:1204.2596





$$E_{FG} = \frac{E}{N} = \frac{3\hbar^2 k_F^2}{10m}, \qquad n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}$$

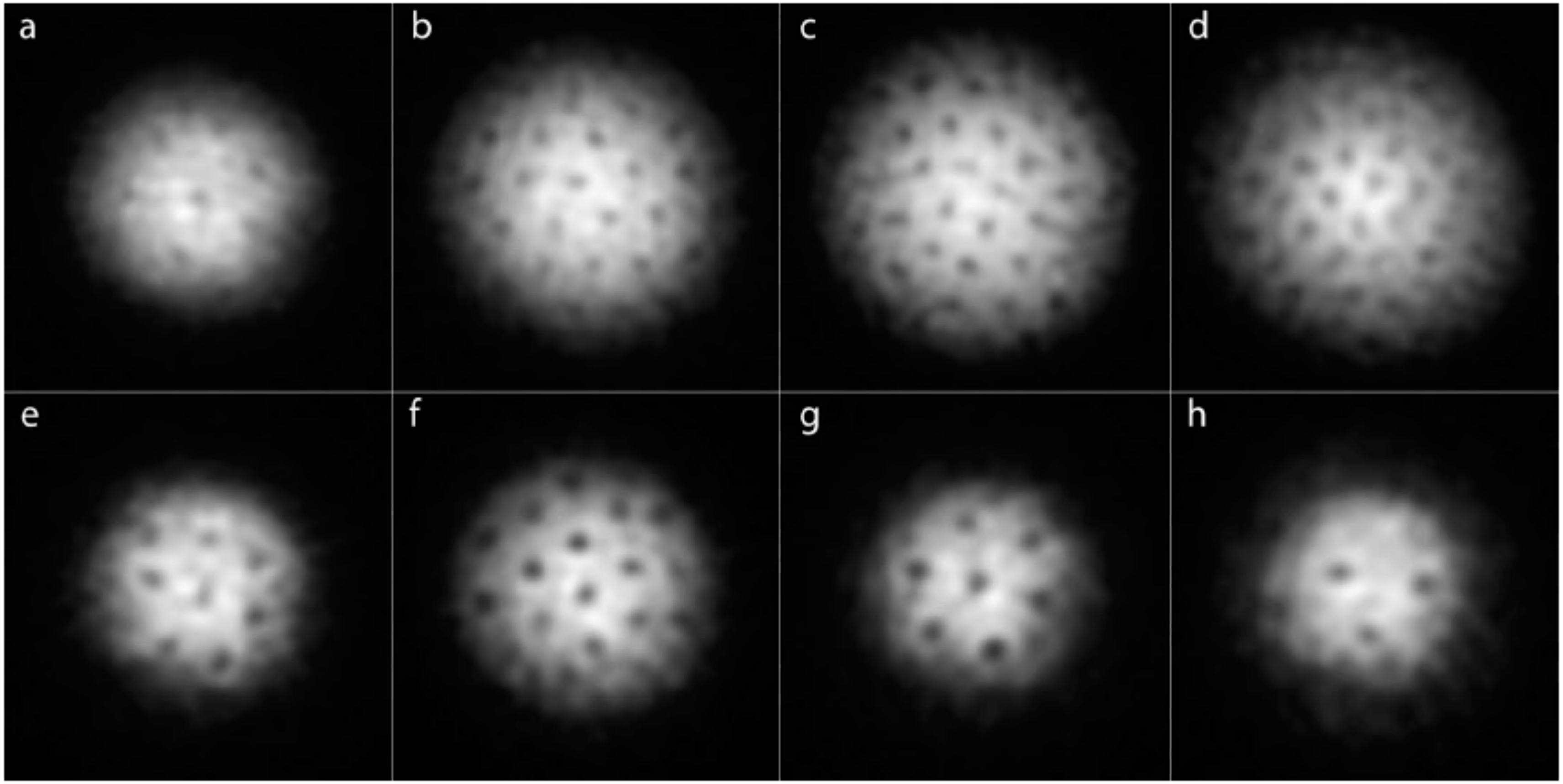


Fig. 2: Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) to 500 ms (b-h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were (a) 740 G, (b) 766 G, (c) 792 G, (d) 812 G, (e) 833 G, (f) 843 G, (g) 853 G and (h) 863 G. The field of view of each image is $880\ \mu m \times 880\ \mu m$.

Zwierlein *et al.* Nature 435, 1047 (2005)

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)

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

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

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

Universal functional of particle density alone

Independent of external potential

Normal Fermi systems only!

However, not everyone is normal!

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

***Dimensional arguments, renormalizability, Galilean invariance, and symmetries** determine the functional (energy density)*

$$\varepsilon(\vec{r}) = \frac{\hbar^2}{m}\left\{\left[\alpha\frac{\tau_c(\vec{r})}{2} - \tilde{\Delta}(\vec{r})\nu_c(\vec{r})\right] + \beta\frac{3(3\pi^2)^{2/3}n^{5/3}(\vec{r})}{5}\right\} - \frac{\hbar^2}{m}(\alpha-1)\frac{\vec{j}^2(\vec{r})}{2n(\vec{r})}$$

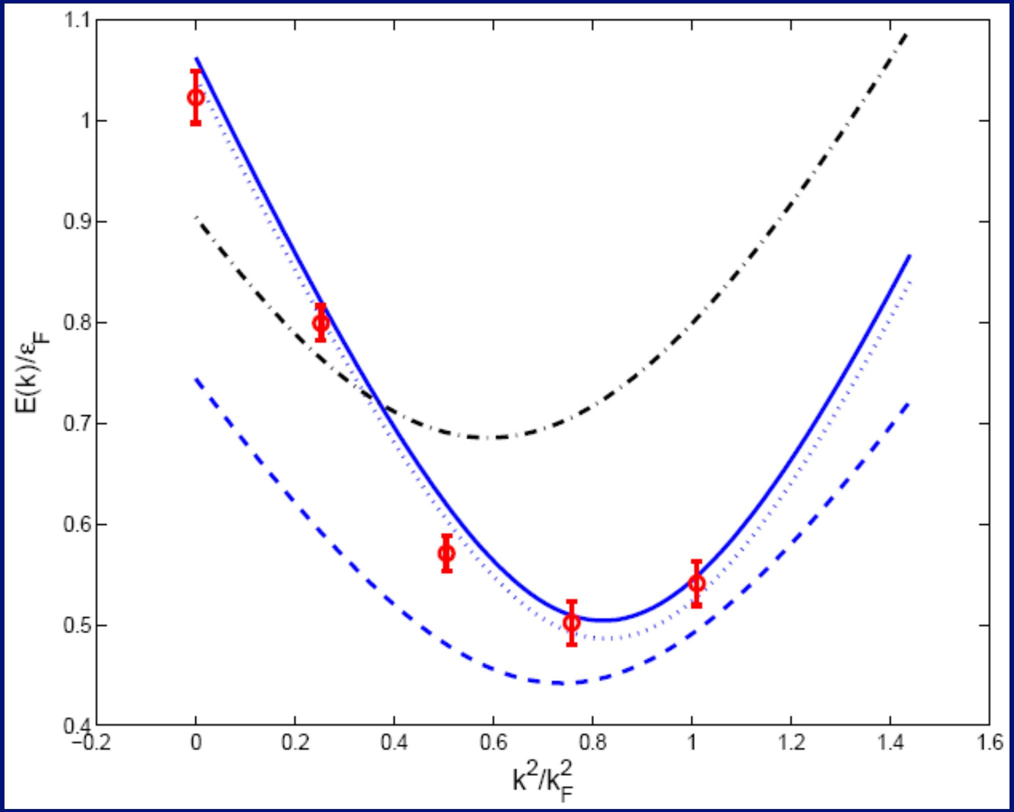
$$\Delta(\vec{r}) = \frac{\hbar^2}{m}\tilde{\Delta}(\vec{r})$$

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

$$\nu_c(\vec{r}) = \sum_{0<E<E_c}\mathrm{u}_\mathrm{k}(\vec{r})\mathrm{v}^*_\mathrm{k}(\vec{r}) \quad \Leftarrow \text{ divergent without a cutoff, need RG}$$

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

Quasiparticle spectrum in homogeneous matter



solid/dotted blue line - SLDA based on homogeneous GFMC due to Carlson *et al*
red circles - GFMC due to Carlson and Reddy
dashed blue line - SLDA, homogeneous MC due to Juillet
black dashed-dotted line – meanfield at unitarity

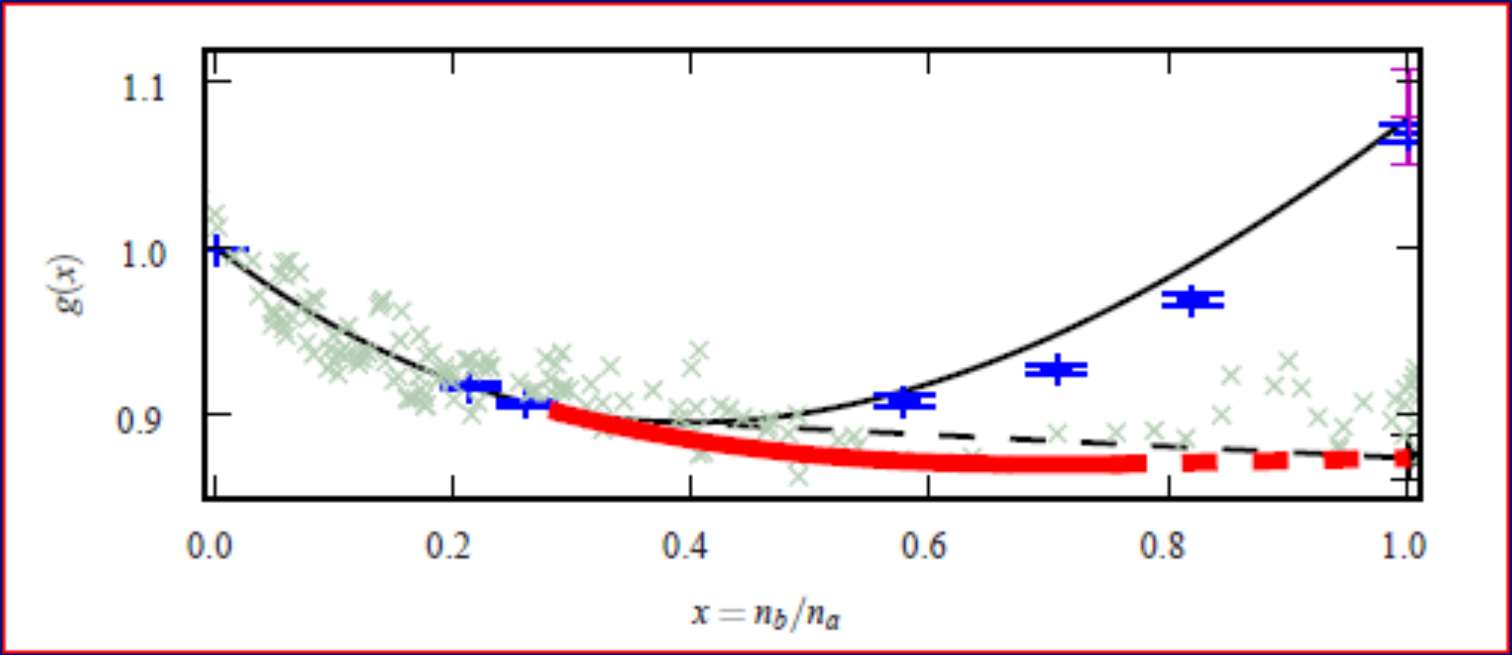
Bulgac, PRA 76, 040502(R) (2007)

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, Lecture Notes in Physics (2012)

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)

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)

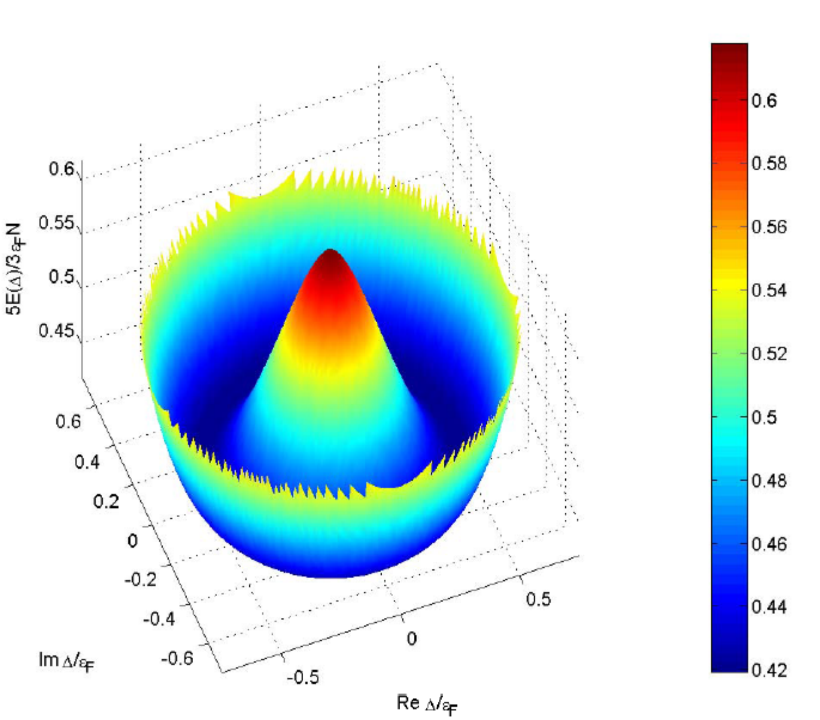
http://www.tddft.org

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

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

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

Energy of a Fermi system as a function of the pairing gap



$$\dot{n} + \vec{\nabla} \cdot \left[\vec{\mathrm{v}} n \right] = 0$$

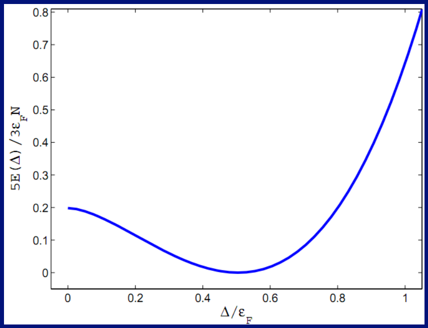
$$m\dot{\vec{\mathrm{v}}} + \vec{\nabla} \left\{ \frac{m\vec{\mathrm{v}}^2}{2} + \mu\left[n \right] \right\} = 0$$

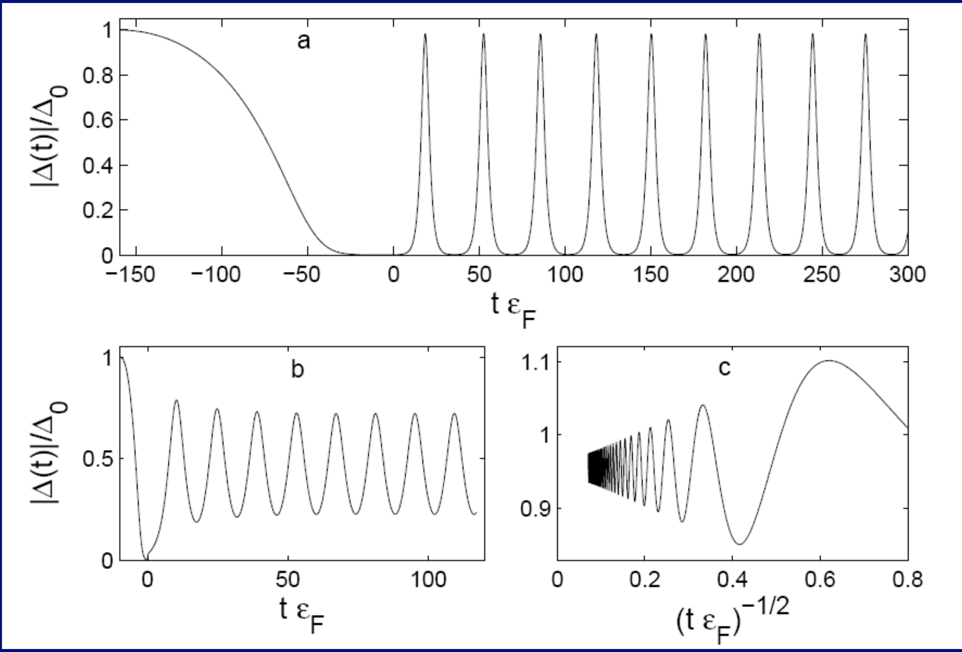
$$i\hbar\dot{\Psi}(\vec{r},t) = -\frac{\hbar^2}{4m}\Delta\Psi(\vec{r},t) + U\left(\left| \Psi(\vec{r},t) \right|^2 \right)\Psi(\vec{r},t)$$

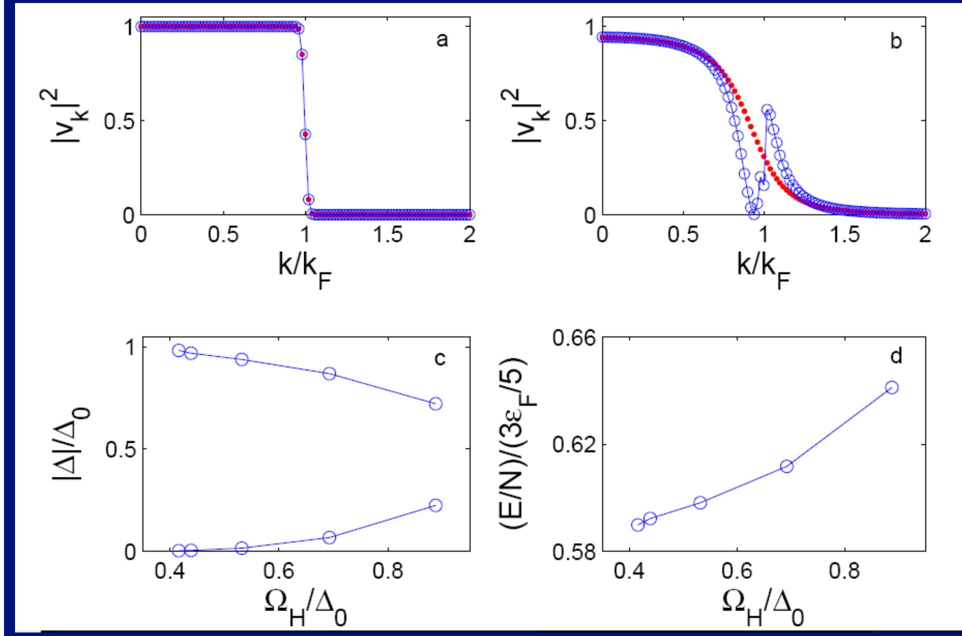
Landau's two-fluid hydrodynamics

Landau-Ginzburg-like equation

Response of a unitary Fermi system to changing the scattering length with time







- All these modes have a very low frequency below the pairing gap, a very large amplitude and very large excitation energy

- None of these modes can be described either within two-fluid hydrodynamics or Landau-Ginzburg like approaches

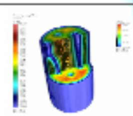
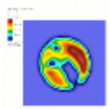
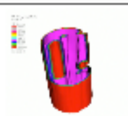
Bulgac and Yoon, Phys. Rev. Lett. 102, 085302 (2009)

About 4 hours of videos

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

A. Bulgac, Y.-L. Luo, P. Magierski, K.J. Roche, Y. Yu
Science, 332, 1288 (2011)

Critical velocity in a unitary gas

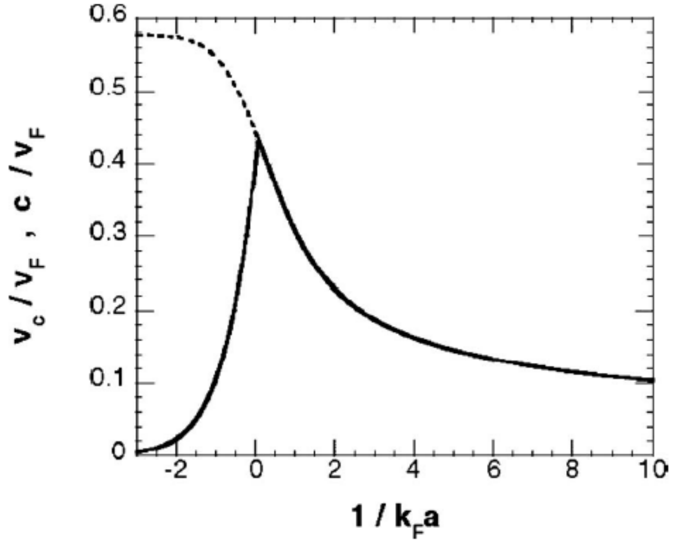


FIG. 20. Landau's critical velocity (in units of the Fermi velocity) calculated along the crossover using BCS mean-field theory. The critical velocity is largest near unitarity. The dashed line is the sound velocity. From Combescot, Kagan, and Stringari, 2006.

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

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

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

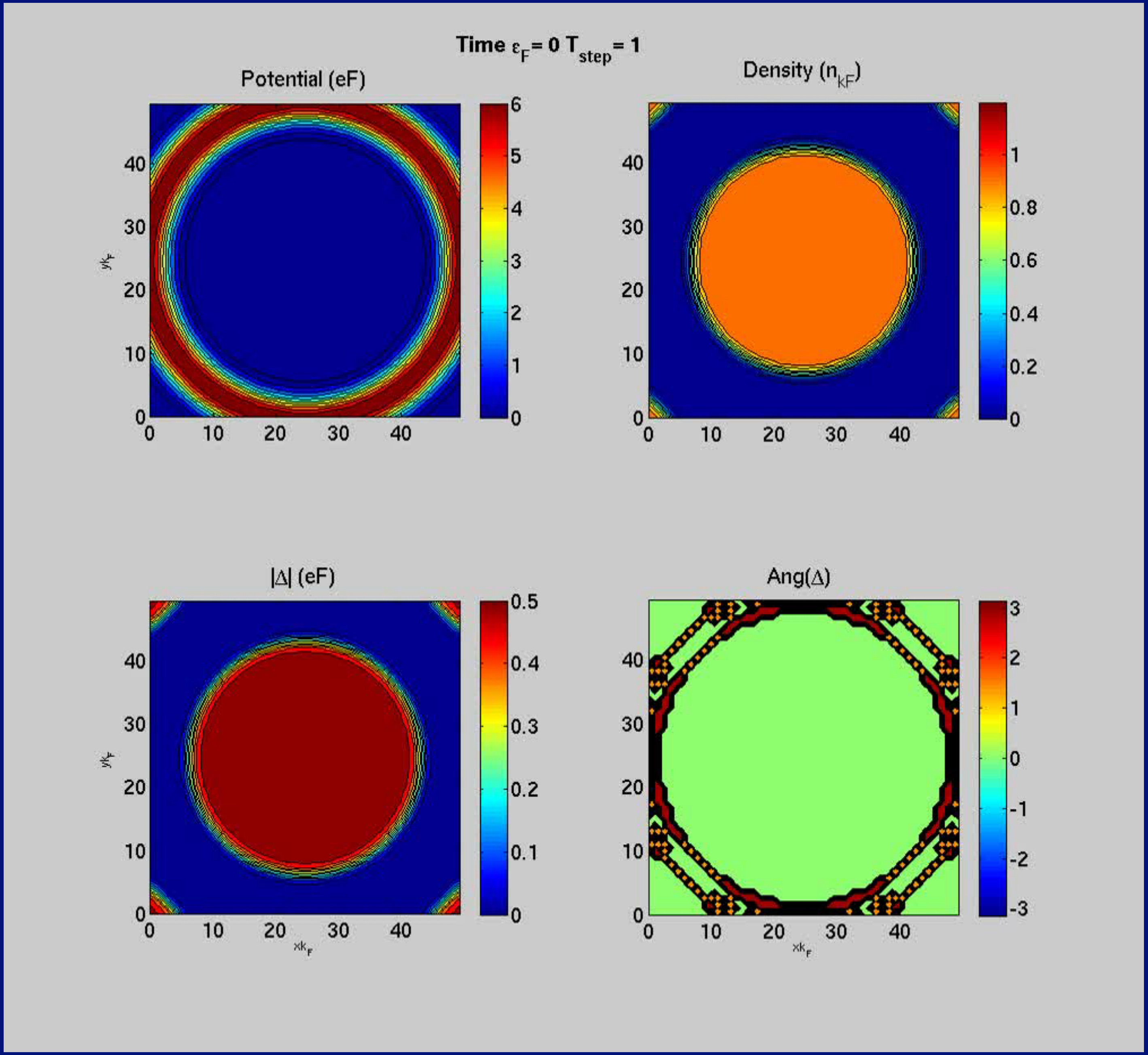
Values obtained using QMC data

Figure from Giorgini, Pitaevskii and Stringari, Rev. Mod. Phys., 80, 1215 (2008)
See also, Sensarma, Randeria, Ho Phys. Rev. Lett. 96, 090403 (2006)

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

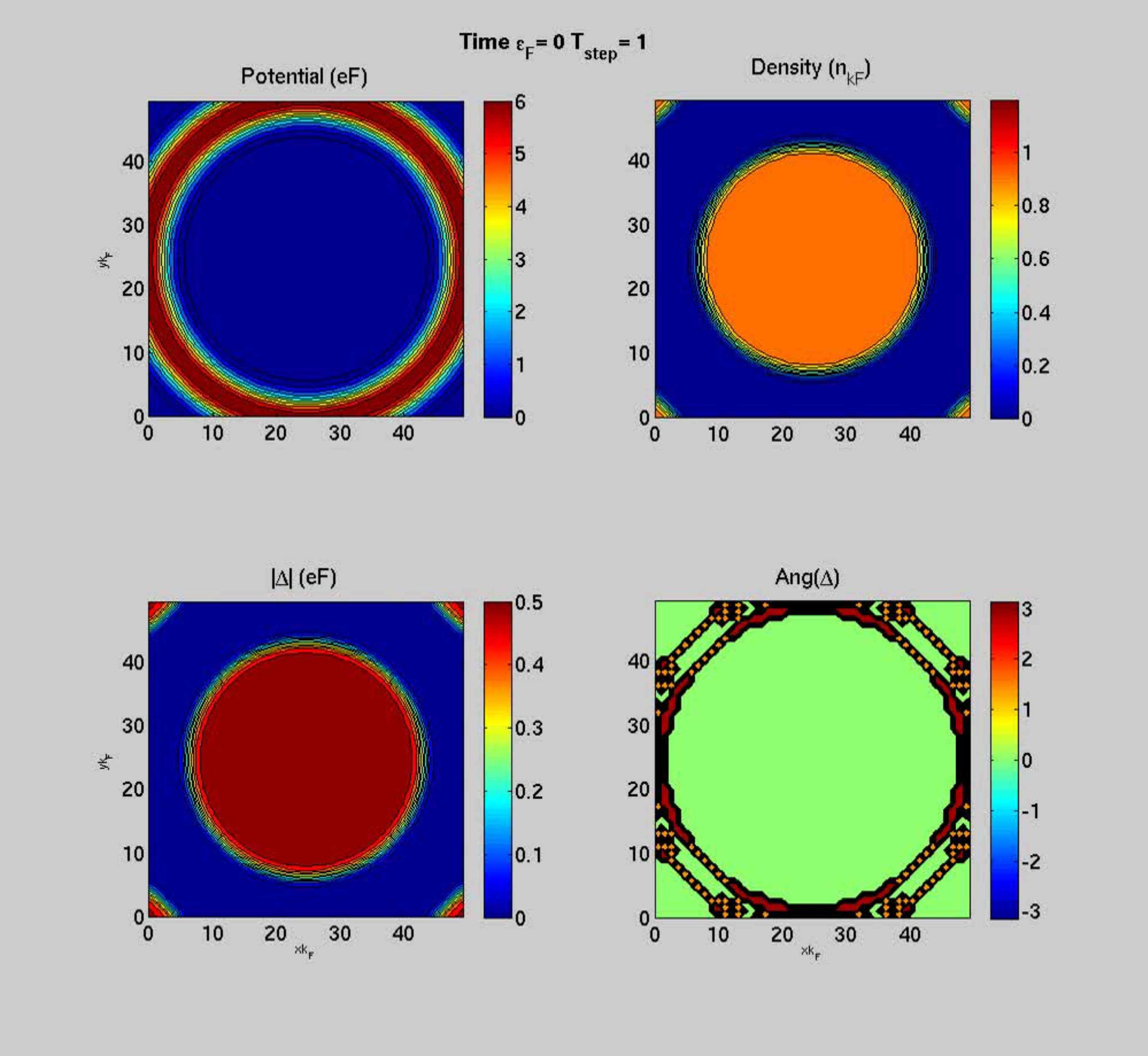
Miller et al. (MIT, 2007)

Study based on BCS/Leggett approximation



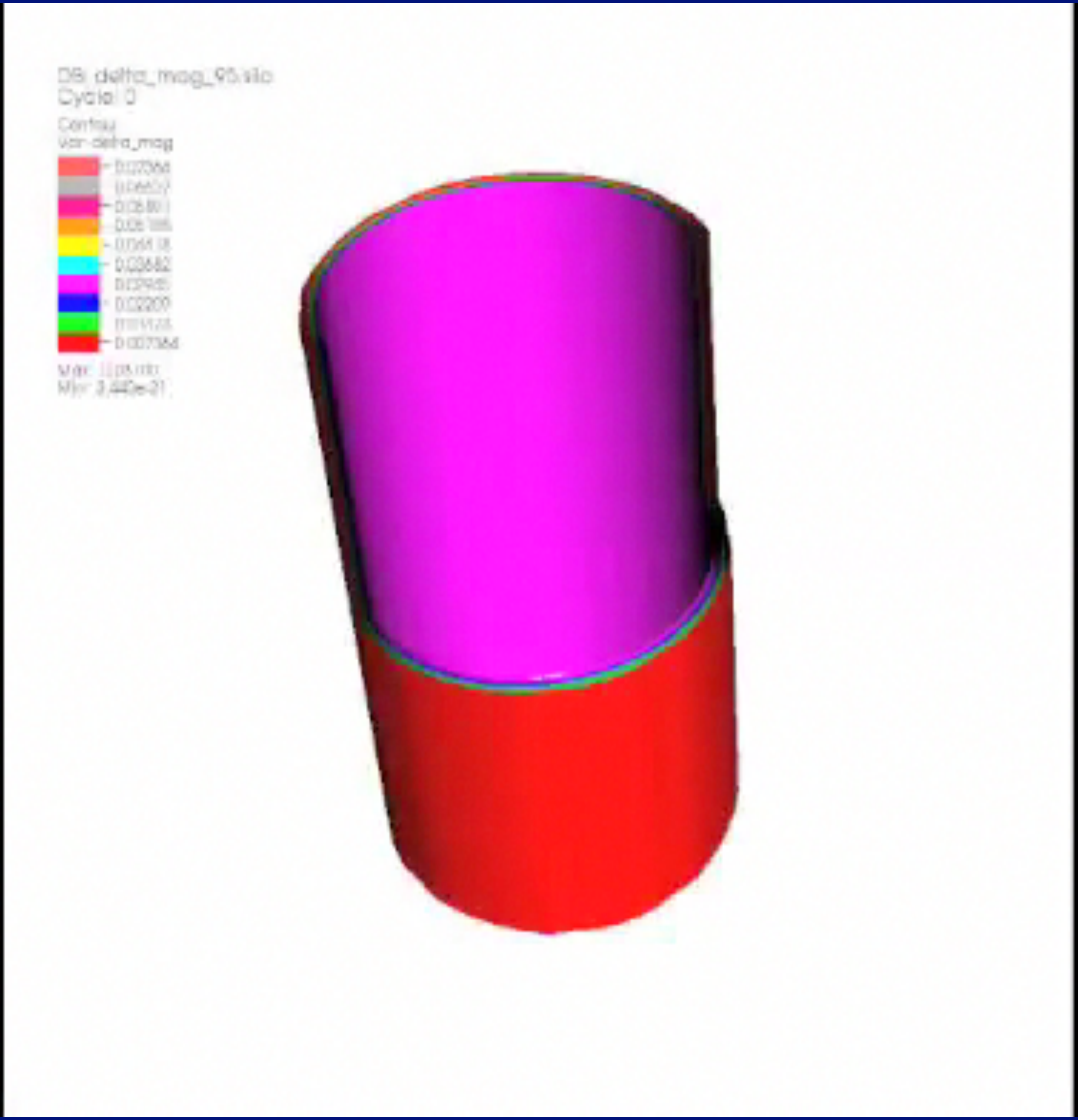
Time ε_F= 0 T_{step}= 1
Potential (eF)
Density (n_{kF})
|Δ| (eF)
Ang(Δ)
yk_F
xk_F

Movie

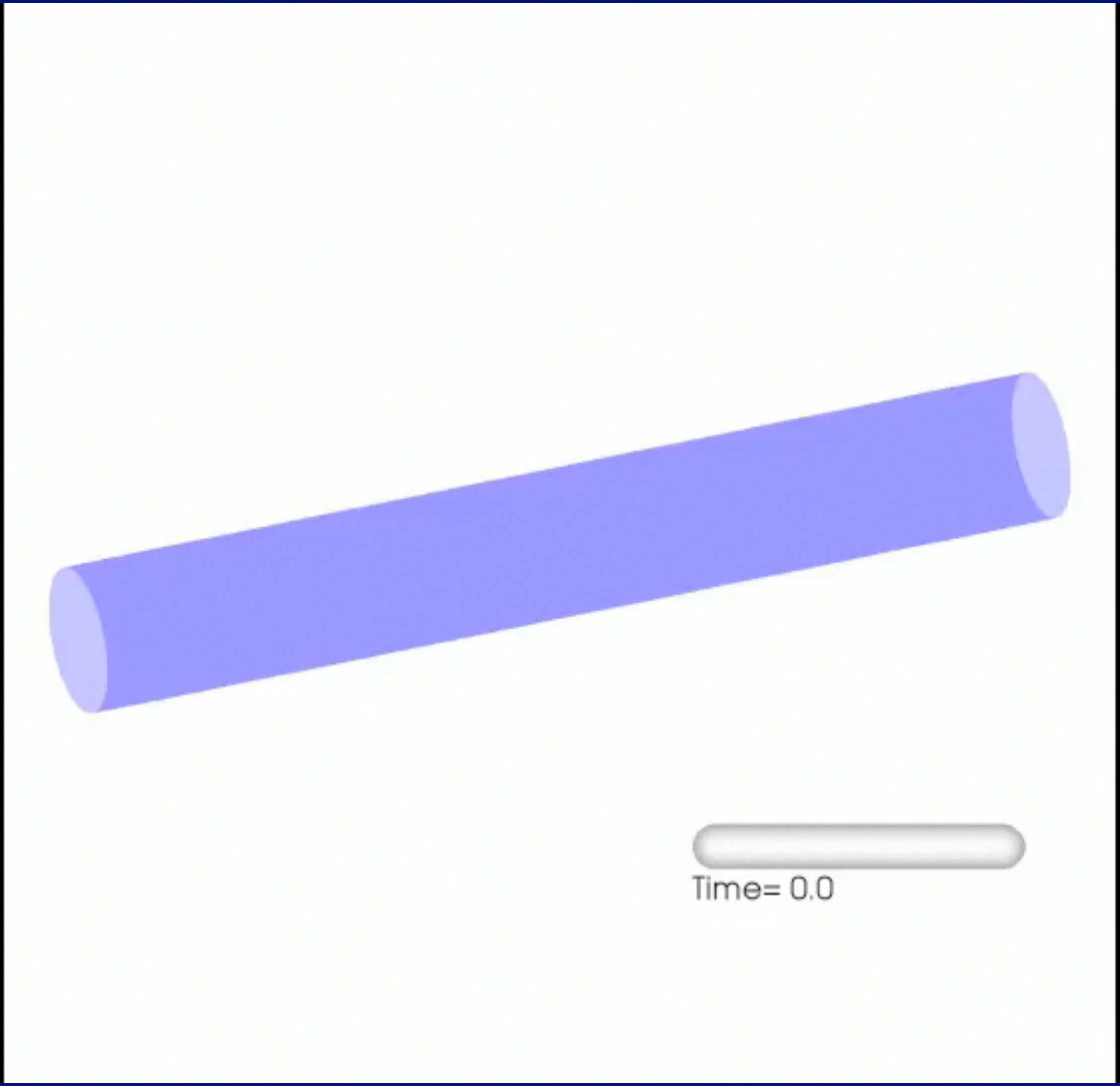


Time ε_F = 0 T_{step} = 1
Potential (eF)
Density (n_{kF})
|Δ| (eF)
Ang(Δ)
yk_F
xk_F

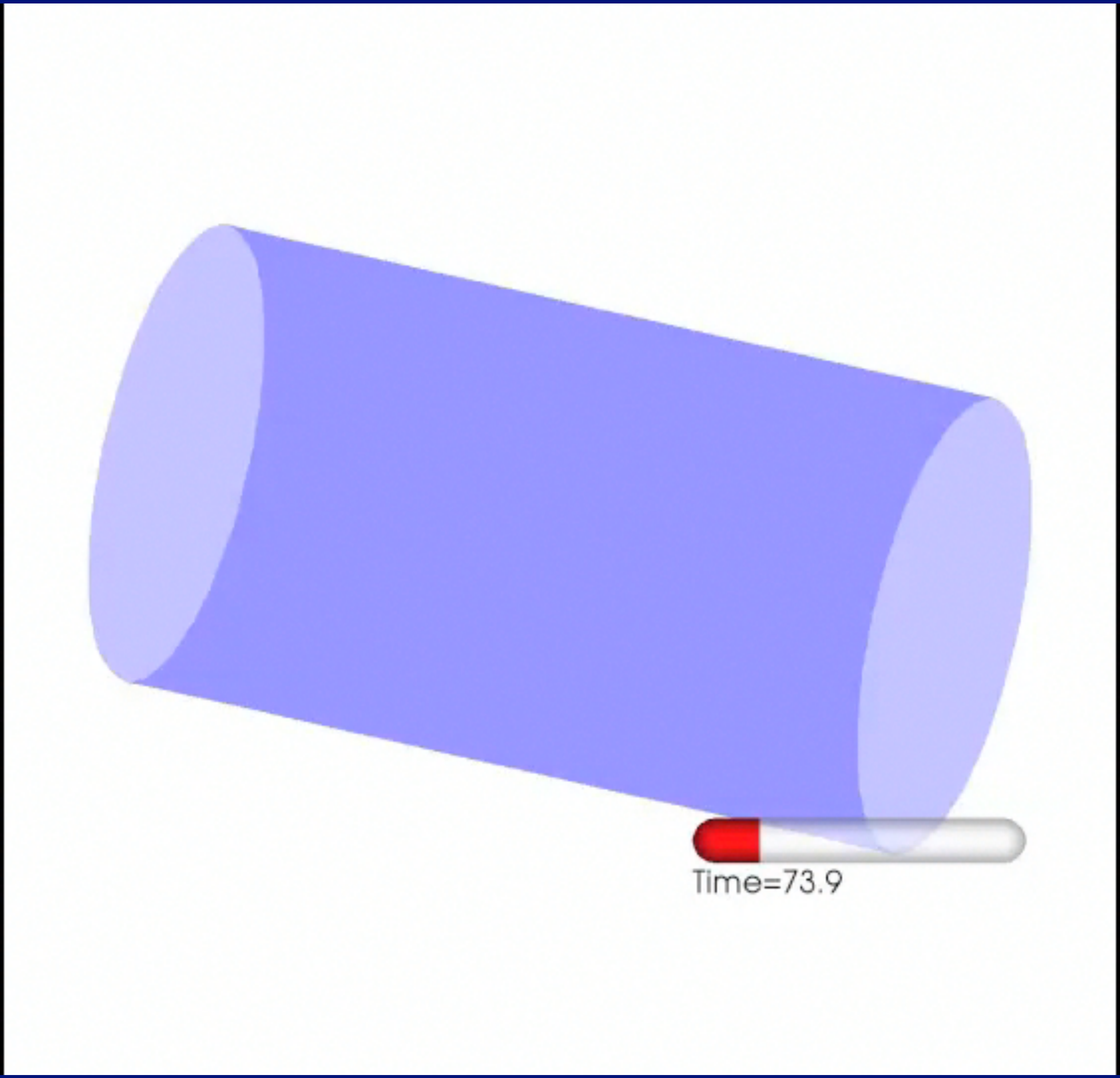
Movie



Movie



Movie



Movie

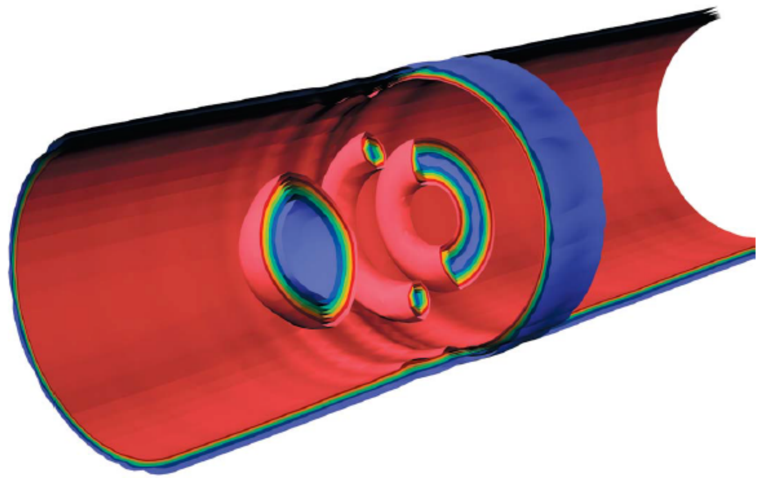


Fig. 2. A spherical projectile flying along the symmetry axis leaves in its wake two vortex rings.

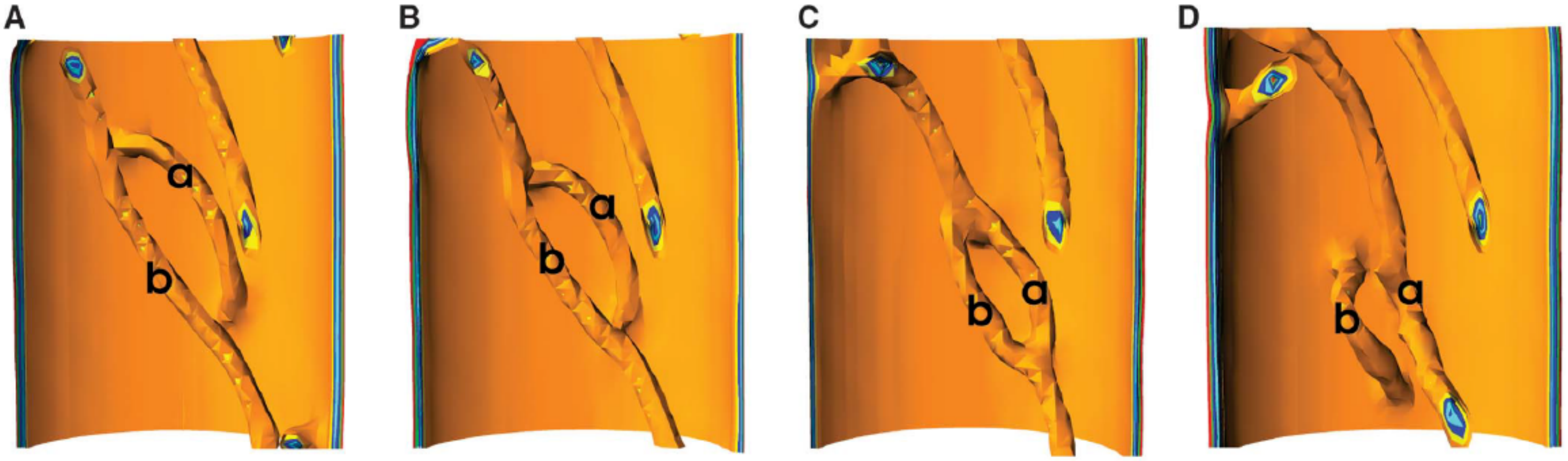
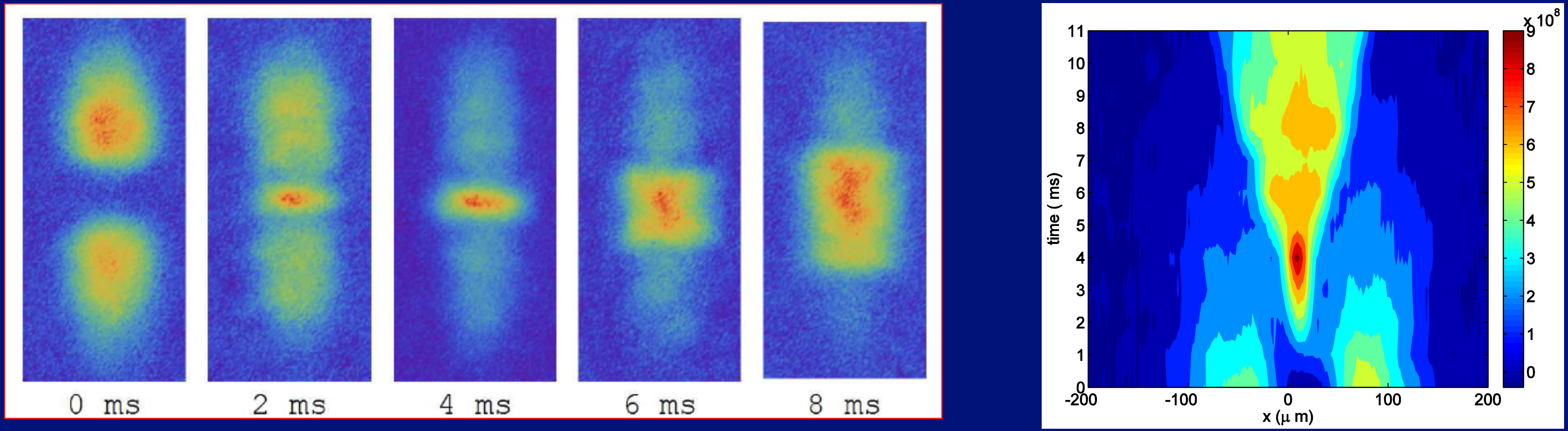
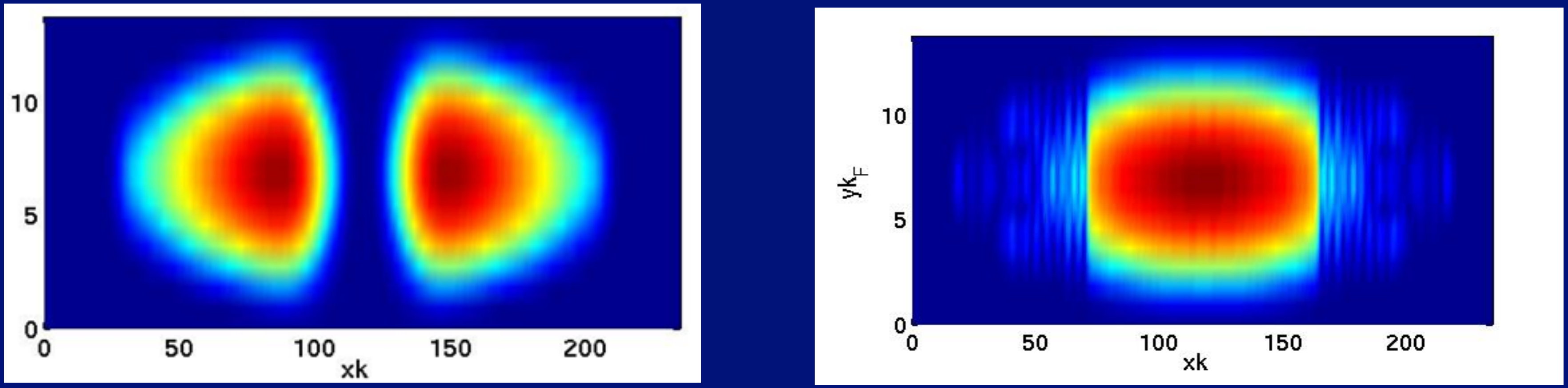


Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b) after reconnection and vice versa.



Observation of shock waves in a strongly interacting Fermi gas

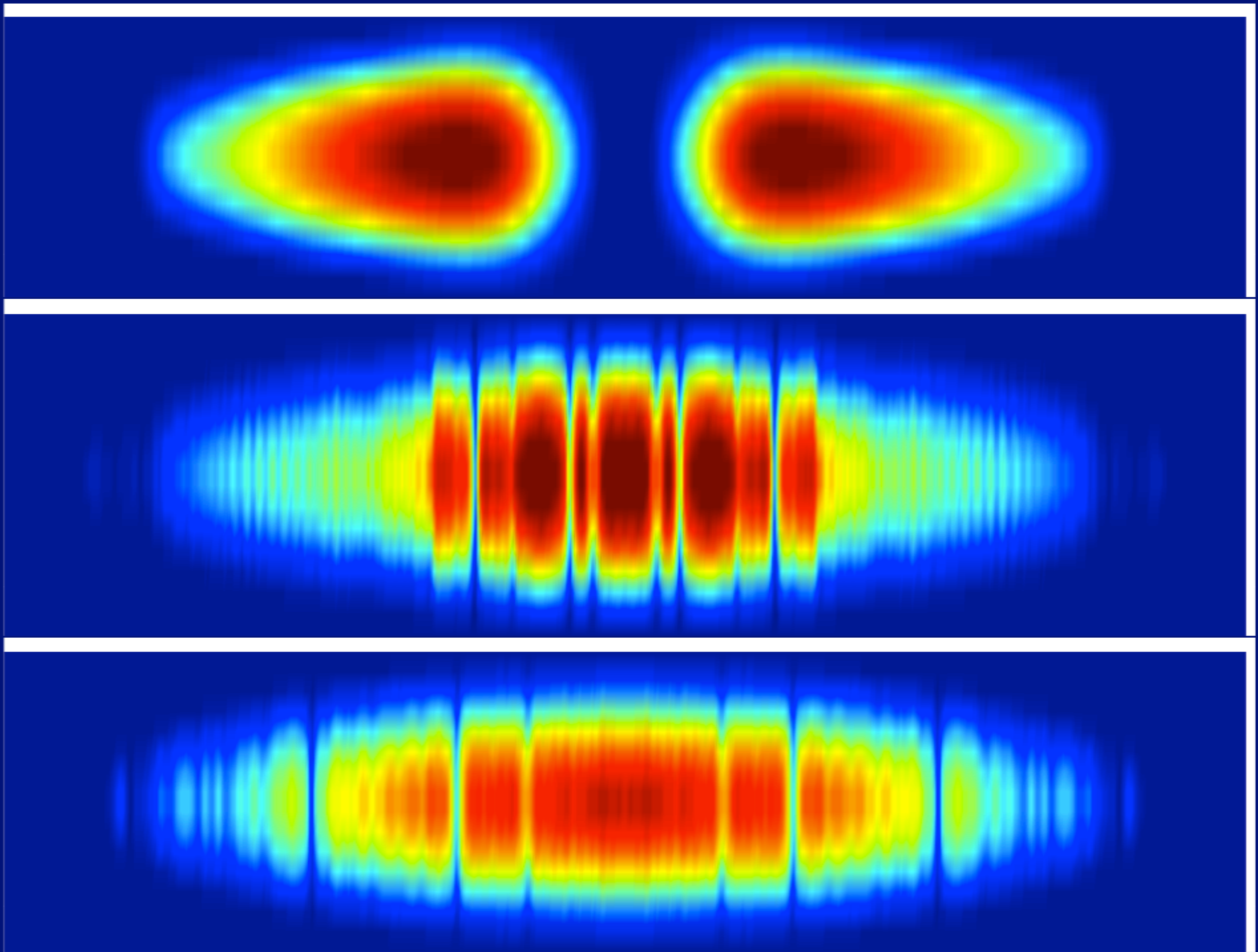
J. Joseph, J.E. Thomas, M. Kulkarni, and A.G. Abanov PRL 106, 150401 (2011)



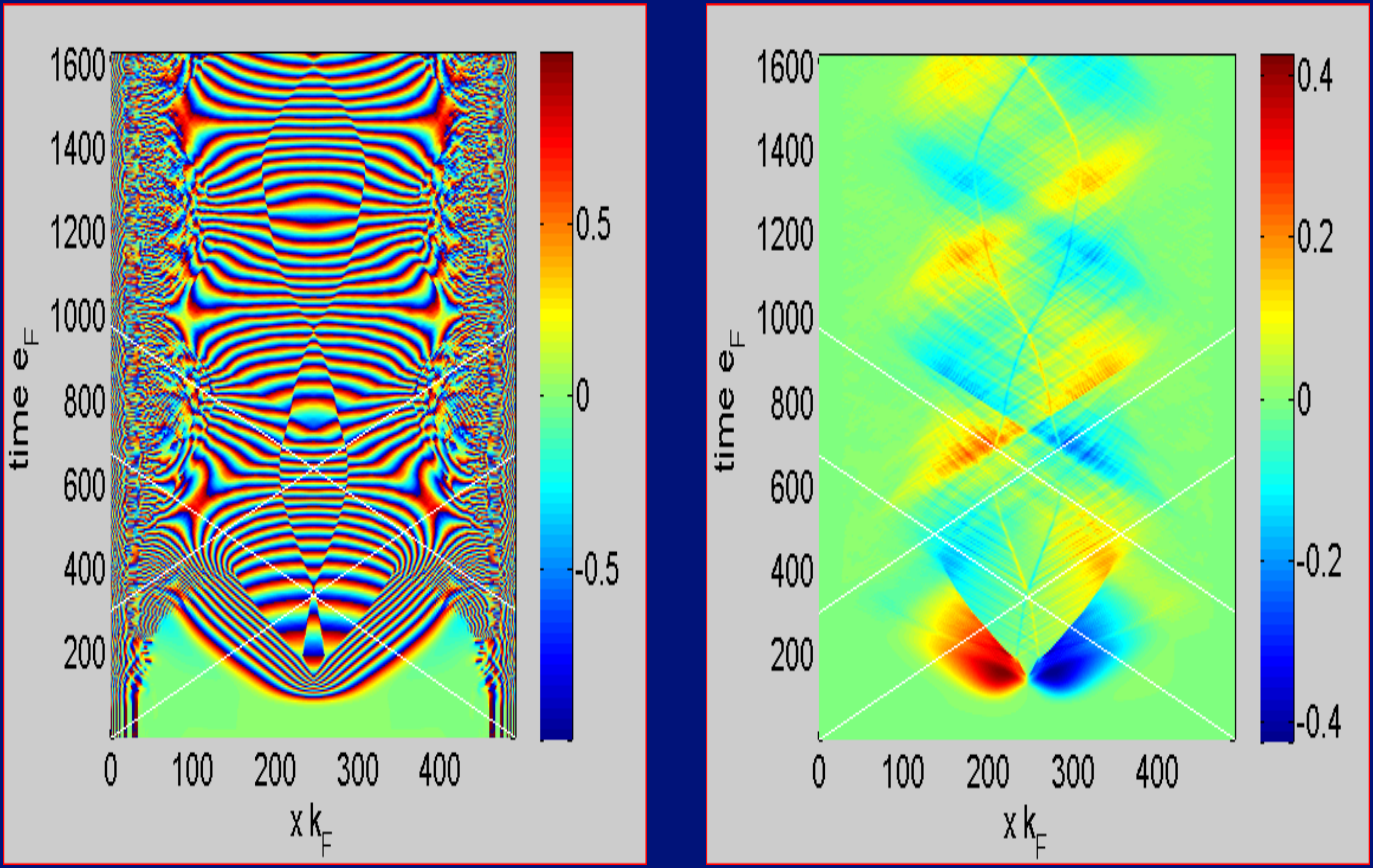
Number density of two colliding cold Fermi gases in TDSLDA

Bulgac, Luo, and Roche, Phys. Rev. Lett. 108, 150401 (2012)

Collision of clouds with larger aspect ratio



Dark solitons/domain walls and shock waves in the collision of two UFG clouds



Phase of the pairing gap normalized to ε_F

Local velocity normalized to Fermi velocity

JETP LETTERS VOLUME 68, NUMBER 3 10 AUGUST 1998

Towards a universal nuclear density functional

S. A. Fayans
Kurchatov Institute Russian Science Center, 123182 Moscow, Russia

The total energy density of a nuclear system is represented as

$$\varepsilon = \varepsilon_{\mathrm{kin}} + \varepsilon_v + \varepsilon_s + \varepsilon_{\mathrm{Coul}} + \varepsilon_{sl} + \varepsilon_{\mathrm{anom}}, \qquad (1)$$

where $\varepsilon_{\mathrm{kin}}$ is the kinetic energy term which, since we are constructing a Kohn–Sham type functional, is taken with the free operator $t = p^2/2m$, i.e., with the effective mass $m^* = m$; all the other terms are discussed below.

The volume term in (1) is chosen to be in the form

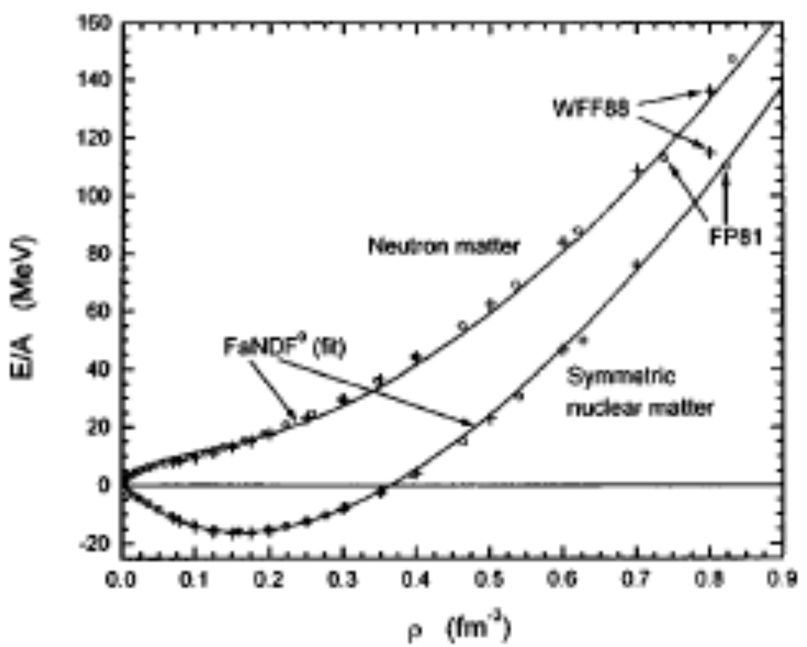
$$\varepsilon_v = \frac{2}{3}\epsilon_F^0 \rho_0 \left[a_+^v \frac{1 - h_{1+}^v x_+^\sigma}{1 + h_{2+}^v x_+^\sigma} x_+^2 + a_-^v \frac{1 - h_{1-}^v x_+}{1 + h_{2-}^v x_+} x_-^2 \right].$$

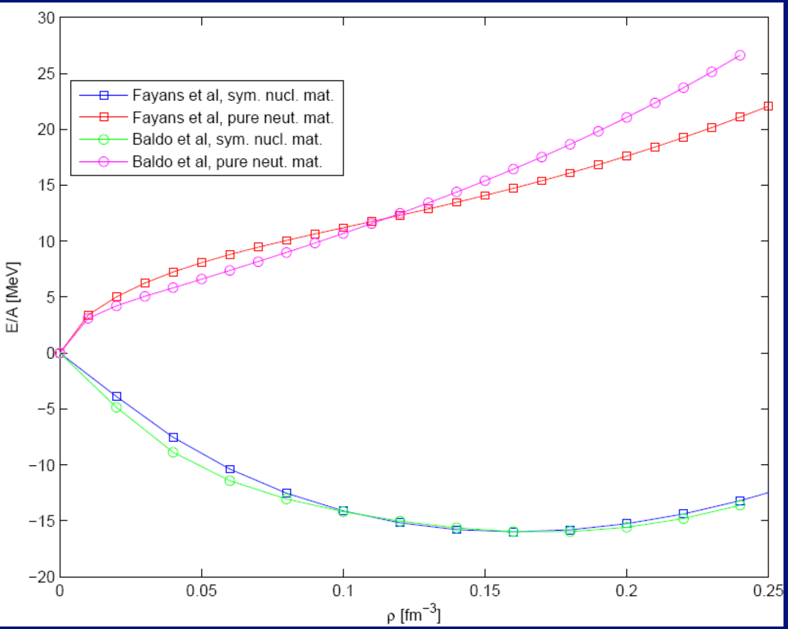
Here and in the following $x_\pm = (\rho_n \pm \rho_p)/2\rho_0$, $\rho_{n(p)}$ is the neutron (
$2\rho_0$ is the equilibrium density of symmetric nuclear matter wit

The surface part in Eq. (1) is meant to describe the finite-range and nonlocal in-medium effects which may presumably be incorporated phenomenologically within the EDF framework in a localized form by introducing a dependence on density gradients. It is taken as follows:

$$\varepsilon_s = \frac{2}{3}\epsilon_F^0 \rho_0 \frac{a_+^s r_0^2 (\nabla x_+)^2}{1 + h_+^s x_+^\sigma + h_\nabla^s r_0^2 (\nabla x_+)^2}, \qquad (3)$$

with $h_+^s = h_{2+}^v$, a_+^s, and h_∇^s the two free parameters. Such a form is obtained by adding





Baldo, Schuck, and Vinas, arXiv:0706.0658

Let us summarize some of the ingredients of the SLDA in nuclei

Energy Density (ED) describing the normal system

ED contribution due to superfluid correlations

$$E_{gs} = \int d^3r \left\{ \varepsilon_N[\rho_n(\vec{r}),\rho_p(\vec{r})] + \varepsilon_S[\rho_n(\vec{r}),\rho_p(\vec{r}),\nu_n(\vec{r}),\nu_p(\vec{r})] \right\}$$

$$\begin{cases} \varepsilon_N[\rho_n(\vec{r}),\rho_p(\vec{r})] = \varepsilon_N[\rho_p(\vec{r}),\rho_n(\vec{r})] \\ \varepsilon_S[\rho_n(\vec{r}),\rho_p(\vec{r}),\nu_n(\vec{r}),\nu_p(\vec{r})] = \varepsilon_S[\rho_p(\vec{r}),\rho_n(\vec{r}),\nu_p(\vec{r}),\nu_n(\vec{r})] \end{cases}$$

Isospin symmetry constraints
(Coulomb energy and other relatively small terms not shown here.)

$$\varepsilon_S\left[\rho_n,\rho_p,\nu_p,\nu_n\right] = g(\rho_p,\rho_n)[|\nu_p|^2 + |\nu_n|^2] + f(\rho_p,\rho_n)[|\nu_p|^2 - |\nu_n|^2]\ \frac{\rho_p-\rho_n}{\rho_p+\rho_n}$$

where $g(\rho_p,\rho_n) = g(\rho_n,\rho_p)$

and $f(\rho_p,\rho_n) = f(\rho_n,\rho_p)$

Nuclear energy functionals

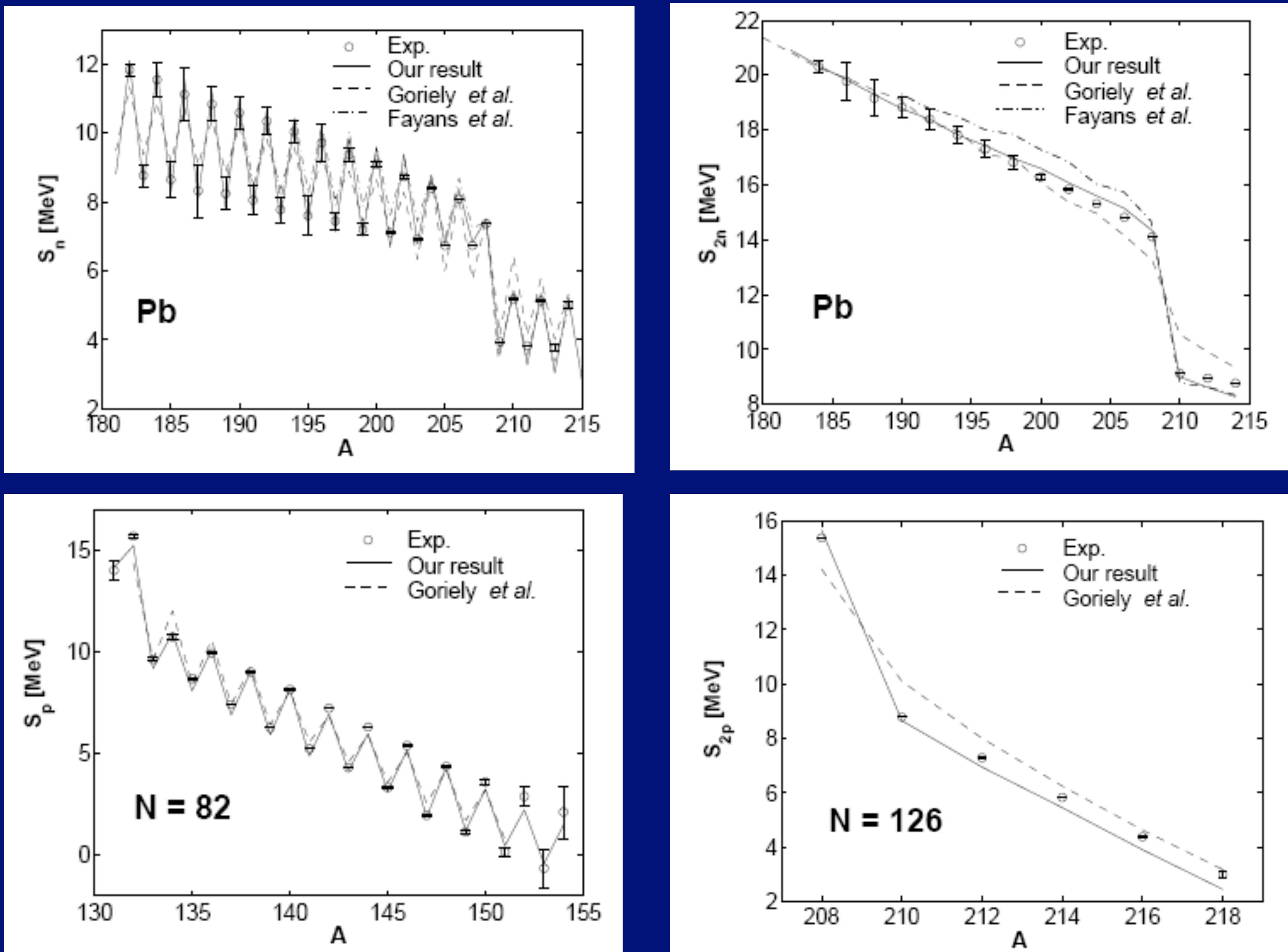
- Ab initio: DME (Negele, Vautherin, Furnstahl , Bogner, …)
- Phenomenological functionals:

$$\mathcal{E}(\vec{r}) = \frac{1}{2M_n}\tau_n(\vec{r}) + \frac{1}{2M_p}\tau_p(\vec{r}) - \Delta(\vec{r})\nu_c(\vec{r})$$
$$+ \sum_{T=0,1} \Big(C_T^{\rho}\rho_T^2 + C_T^{\Delta}\rho_T\nabla^2\rho_T + C_\gamma\rho_0^\gamma\rho_T^2$$
$$+ C_T^{\tau}(\rho_T\tau_T - \vec{j}_T^2) + C_T^{\nabla J}(\rho_T\vec{\nabla}\cdot\vec{J} + \vec{s}_T \times \vec{j}_T)\Big)$$

Galilean invariance

$$h(\vec{r}) = -\nabla\frac{\hbar^2}{2m(\vec{r})}\nabla + U(\vec{r}) + i\vec{\sigma}\cdot\vec{V}(\vec{r}) + i\vec{V}_1(\vec{r})\cdot\nabla + i\vec{W}(\vec{r})\cdot(\vec{\sigma}\times\nabla)$$

From a talk given by Ionel Stetcu recently at LANL



A single universal parameter for pairing!

TDSLDA equations

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{h}_{\uparrow\uparrow}(\vec{r},t)-\mu & \hat{h}_{\uparrow\downarrow}(\vec{r},t) & 0 & \Delta(\vec{r},t) \\ \hat{h}_{\downarrow\uparrow}(\vec{r},t) & \hat{h}_{\downarrow\downarrow}(\vec{r},t)-\mu & -\Delta(\vec{r},t) & 0 \\ 0 & -\Delta^*(\vec{r},t) & -\hat{h}^*_{\uparrow\uparrow}(\vec{r},t)+\mu & -\hat{h}^*_{\uparrow\downarrow}(\vec{r},t) \\ \Delta^*(\vec{r},t) & 0 & -\hat{h}^*_{\downarrow\uparrow}(\vec{r},t) & -\hat{h}^*_{\downarrow\downarrow}(\vec{r},t)+\mu \end{pmatrix}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix}$$

- **The system is placed on a 3D spatial lattice**
- **Derivatives are computed with FFTW**
- **Fully self-consistent treatment with Galilean invariance**
- **Adams-Bashforth-Milne fifth order preditor-corrector-modifier integrator**
- **No symmetry restrictions**
- **Number of PDEs is of the order of the number of spatial lattice points**
  - **from $O(10^4)$ to $O(10^6)$**
- **Initial state is the ground state of the SLDA (formally like HFB/BdG)**
- **The code was implementated on JaguarPF, Franklin, Hopper, Hyak, Athena**
- **TDSLDA is about <u>1,000 times more complex</u> than existing TDHF codes**
- **We used in 2010 and early 2011 about <u>75 million CPU hours</u> on JaguarPF and Hopper alone, and over 217,000 cores on JaguarPF. Starting to use Titan, NCCS.**

TD formalism applications

- Nuclear physics:
  - induced fission
  - heavy-ion collisions
  - neutron scattering/capture
  - pairing vibrations
  - electromagnetic response
- Neutron star crust: dynamics of vortices, vortex pinning mechanism
- Cold atoms physics, optical lattices

Limitations:

- only one-body observables can be described accurately
- the results depend on how good the functional is
- large computational resources necessary

Several slides from a talk given by Ionel Stetcu recently at LANL

RPA and linear response

RPA: small correlations on top of mean-field + excited states 1p-1h

$$|\psi_0\rangle = |HF\rangle + |2p-2h\rangle$$

$$|\nu\rangle \approx |1p-1h\rangle$$

$$\langle\nu|F|\psi_0\rangle = \sum_{ph}(F_{hp}X^{\nu}_{ph} + F_{ph}X^{\nu}_{ph})$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix} = E_\nu \begin{pmatrix} X_\nu \\ -Y_\nu \end{pmatrix}$$

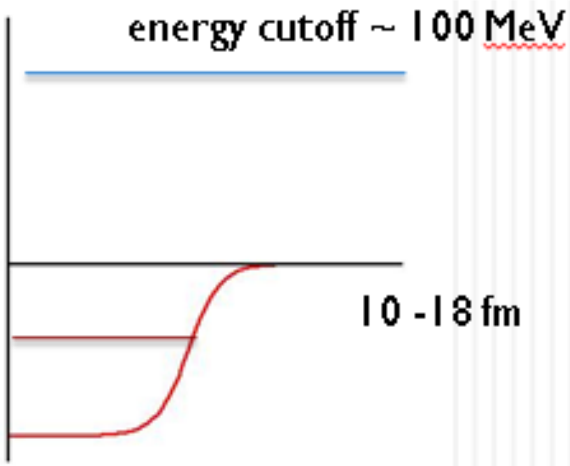
- violates the Pauli principle mainly for non-collective states
- separates the spurious states associated w/ broken symmetry in mean field

Linear response from TD-DFT: exclusively a model for excited states

$$i\hbar\dot{\rho} = [h[\rho] + f(t), \rho] \longrightarrow \left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - E\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} \delta\rho^{ph} \\ \delta\rho^{hp} \end{pmatrix} = -\begin{pmatrix} f^{ph} \\ f^{hp} \end{pmatrix}$$

- Pauli principle preserved
- separates the spurious states associated w/ broken symmetries in mean field

Challenges for QRPA



Terasaki and Engel, PRC **82** (2010) 034326
QRPA w/ axial symmetry for ^{172}Yb
dimension ~ 160,000 (j-dependent)

HF: #s.p. states = # particles

HFB: #q.p. >> # particles
~ 2,500

QRPA: dimension ~ (# q.p.)^2 ~ 10^7

very difficult for today's computers:
- non-Hermitian matrix
- middle of the spectrum

in TDHFB:

$$\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} \approx \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \exp(-iEt) + \begin{pmatrix} \delta u(t) \\ \delta v(t) \end{pmatrix}$$

# of evolved wfs. = # of q.p.
numerical advantage: can be easily parallelized

need latest generation computers to run

QRPA and TD

	QRPA	TD-SLDA
Dimensions	# qp. squared	# qp
Truncation	identification of spurious states difficult	N/A
Galilean invariance	(usually) not implemented	trivial (in functional)

Terasaki and Engel, PRC **82** (2010) 034326
QRPA w/ axial symmetry for ^{172}Yb
Energies of spurious states: 0.3 – 1.5 MeV

Terasaki, Engel, Bertsch, PRC **78** (2008) 044311

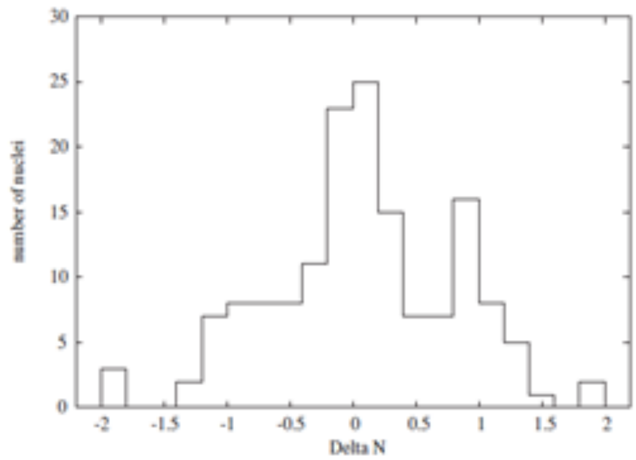


FIG. 1. Particle-hole character of the lowest 2^+ solutions. The histogram displays the quantity ΔN defined in Eq. (1) for 155 nuclei in the SLy4 data set (one of which we drop—see text). The values $-2, 0, +2$ correspond to excitations of hole-hole, particle-hole, and particle-particle character, respectively.

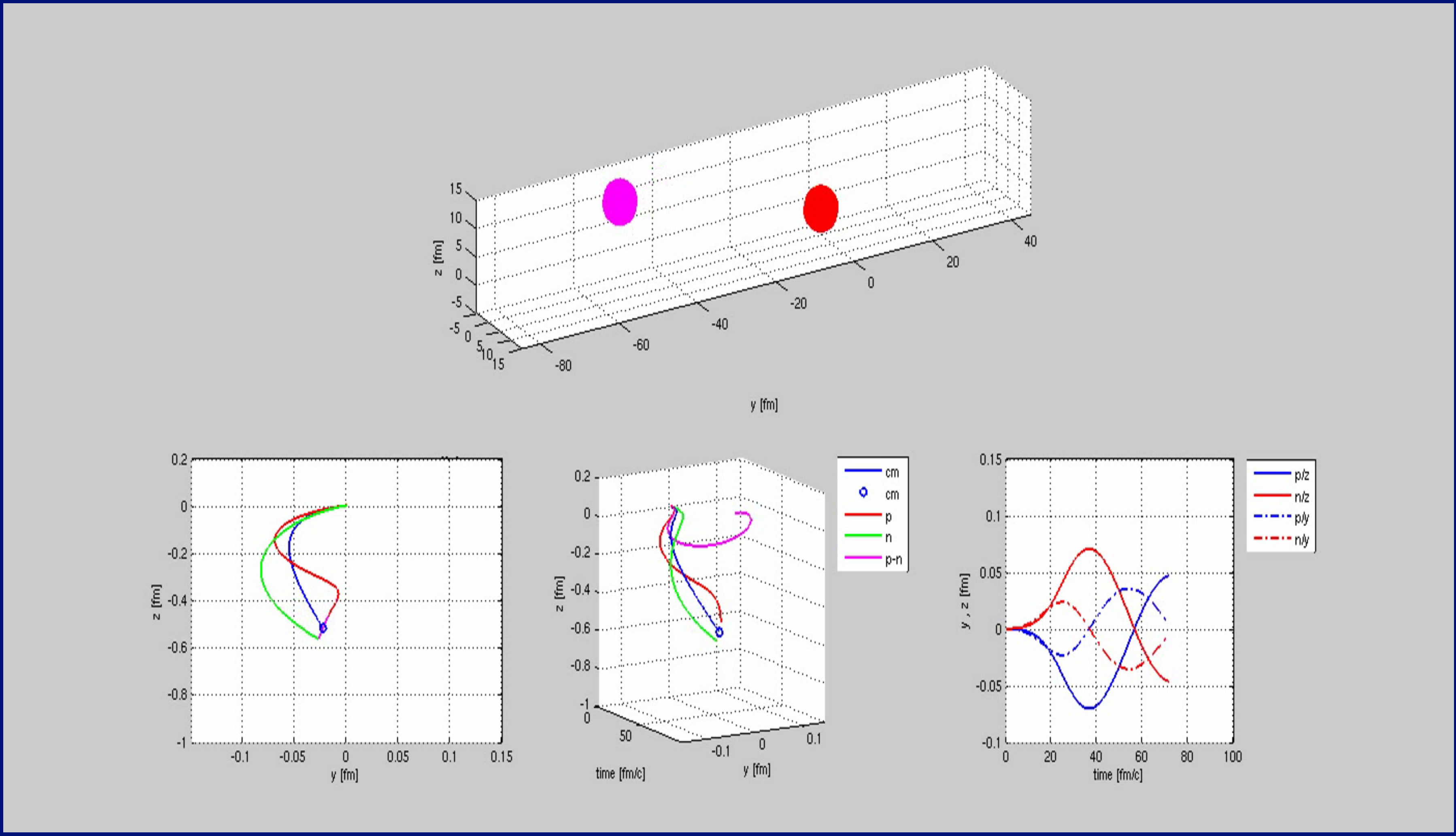
Formalism

$$H_0\Psi(\vec{r}_1,\cdots,\vec{r}_A)=E_0\Psi(\vec{r}_1,\cdots,\vec{r}_A)$$

$$V_{ext}(\vec{r},t)=O(\vec{r})f(t)$$

$$\tilde{O}(\omega)=\int d^3r\,O^*(\vec{r})\,\delta\rho(\vec{r},\omega)$$

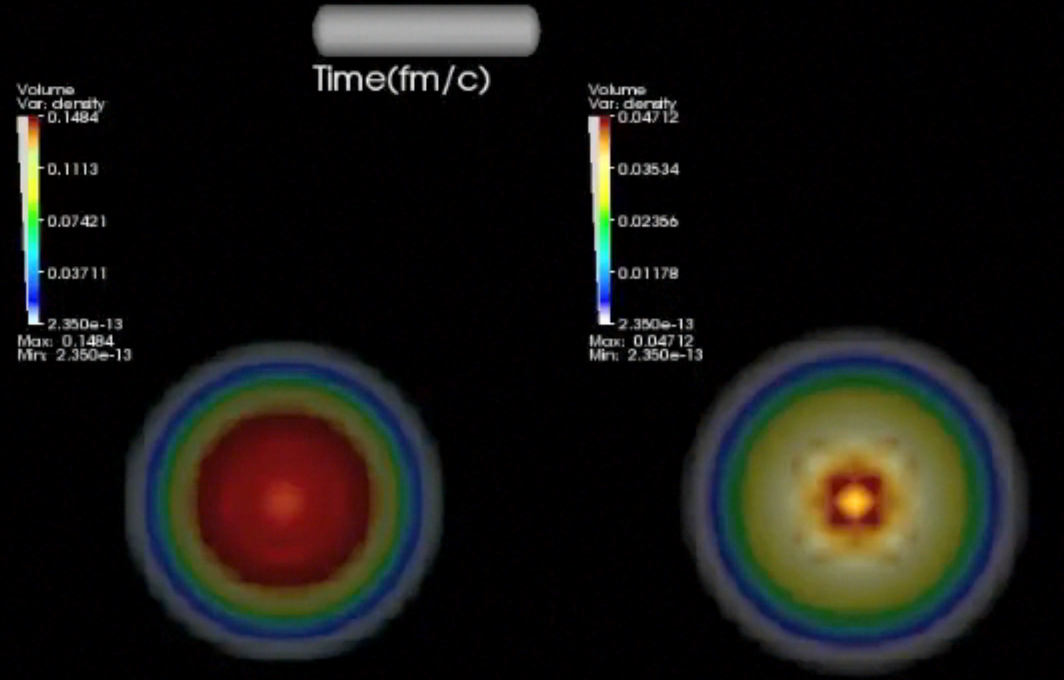
$$S(\omega)=\sum_n\langle\Psi_0|O|\Psi_n\rangle|^2\delta(\omega-\omega_n)=-\frac{1}{\pi}\Im\left(\frac{\tilde{O}(\omega)}{\tilde{f}(\omega)}\right)$$



Geometry of the collision of a relativistic heavy-ion with a nucleus

I. Stetcu *et al.*

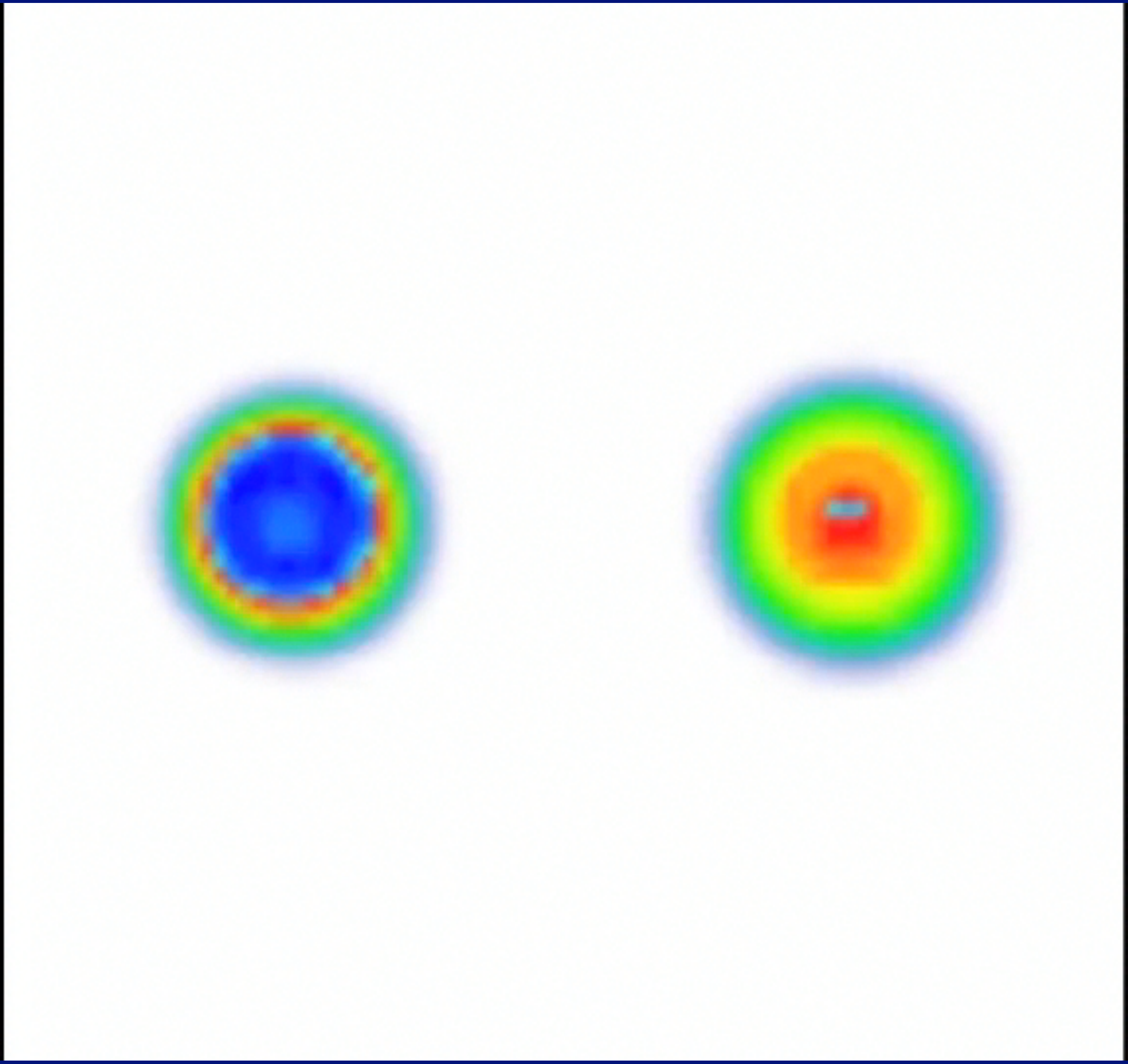
Movie



Coulomb excitation of GDR with a relativistic heavy-ion computed in TDSLDA

I. Stetcu *et al.*

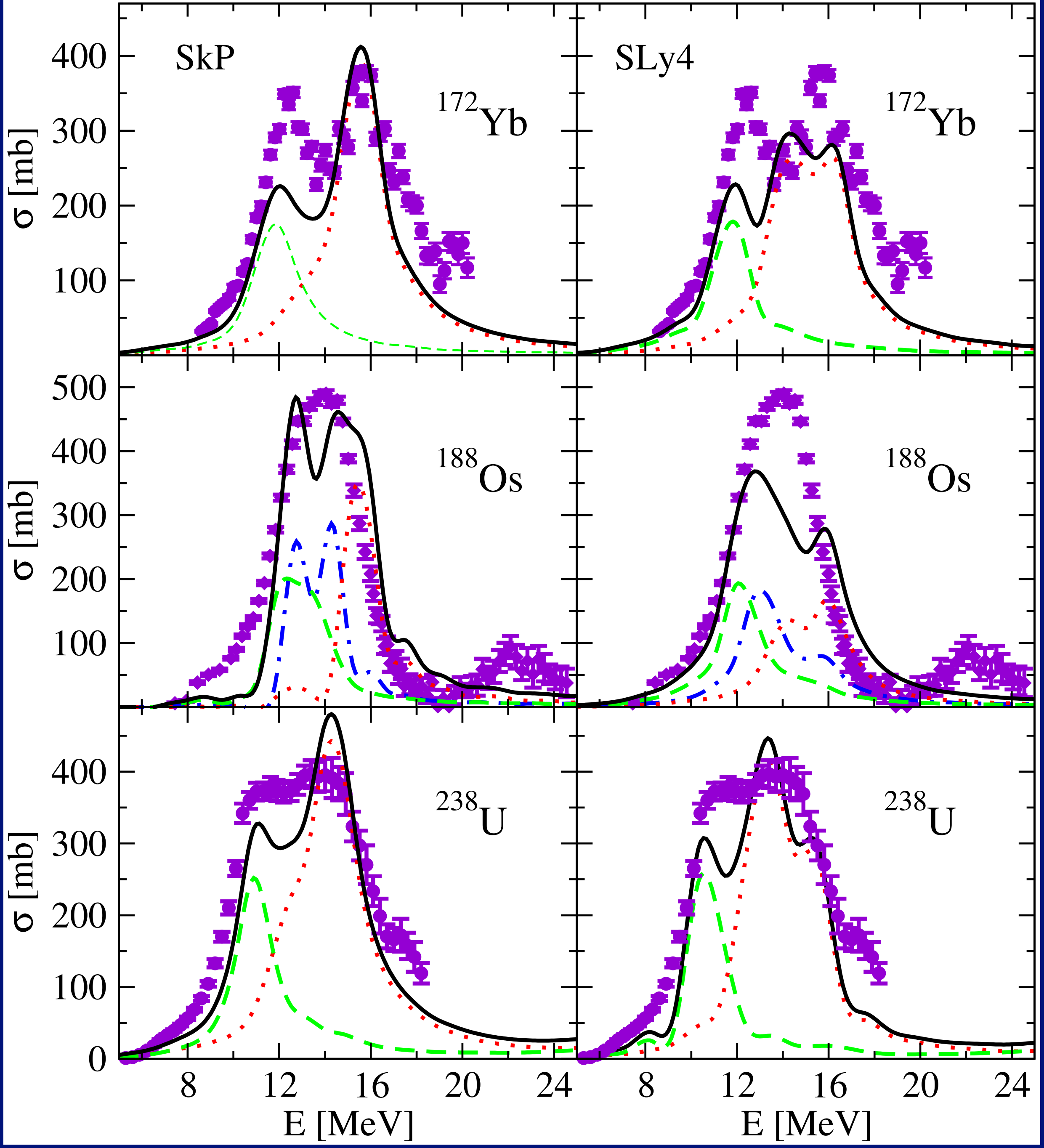
Movie



Coulomb excitation of GDR with relativistic heavy-ions computed in TDSLDA

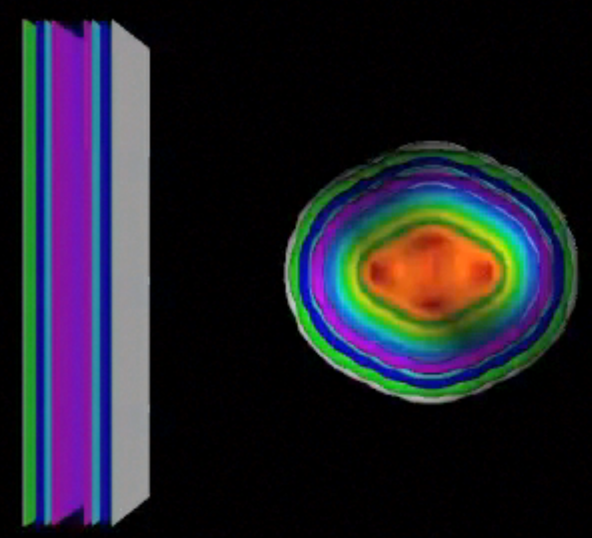
Movie

I. Stetcu *et al.*



Osmium is triaxial, and both protons and neutrons are superfluid.

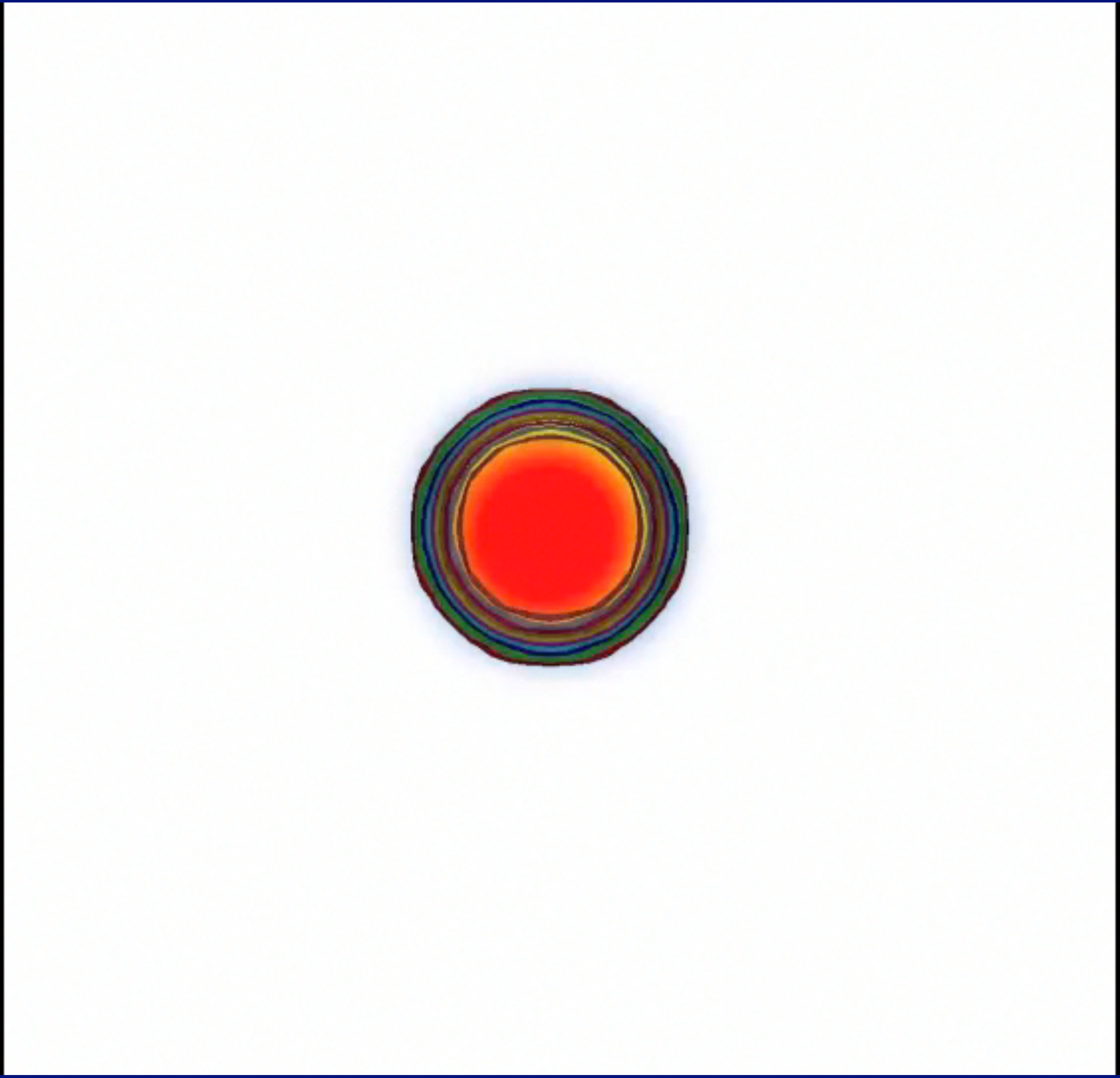
Stetcu, Bulgac, Magierski, and Roche, Phys. Rev. C 84, 051309(R) (2011)



Neutron scattering of ^{238}U computed in TDSLDA

I. Stetcu *et al.*

Movie



Real-time induced fission of ^{280}Cf computed in TDSLDA

I. Stetcu *et al.*

Movie