

The Unitary Fermi Gas: From Quantum Monte Carlo to Density Functional Theory, to Real Time Dynamics

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Goal:

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

What options exist out there?

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

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

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

Troubles:

- **These are classical equations, no Planck's constant, 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 + quantization
is the 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):

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

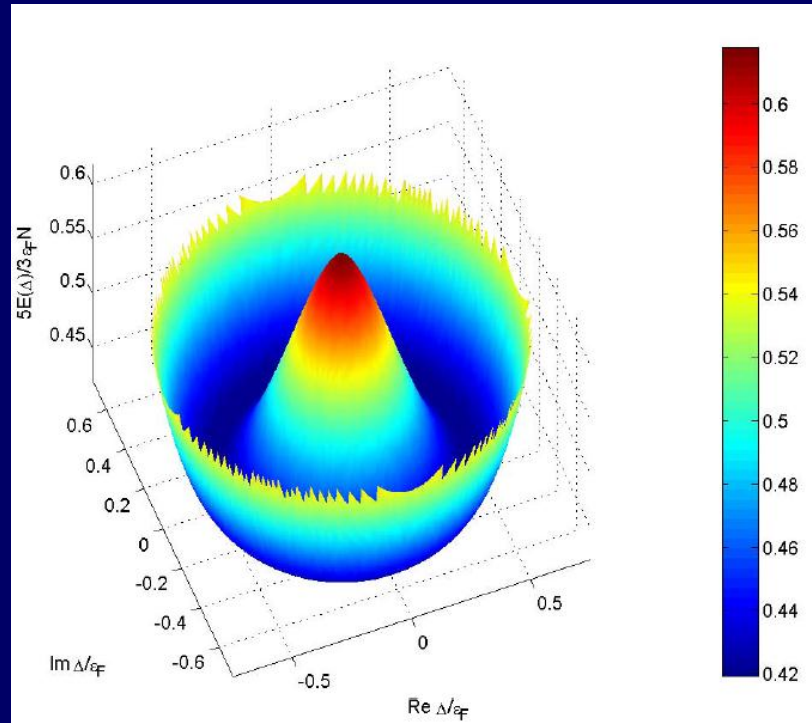
Troubles:

- **Even though is a quantum approach, it describes only the superfluid phase**
- **Only for temperatures near and below the critical temperature (or at T=0 for GP equation)**
- **There is 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.

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



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

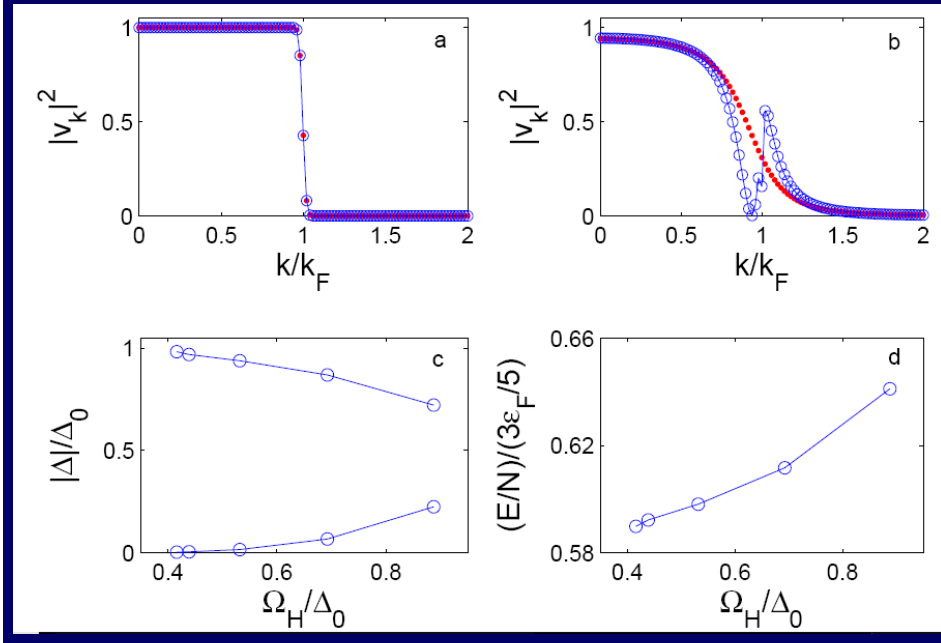
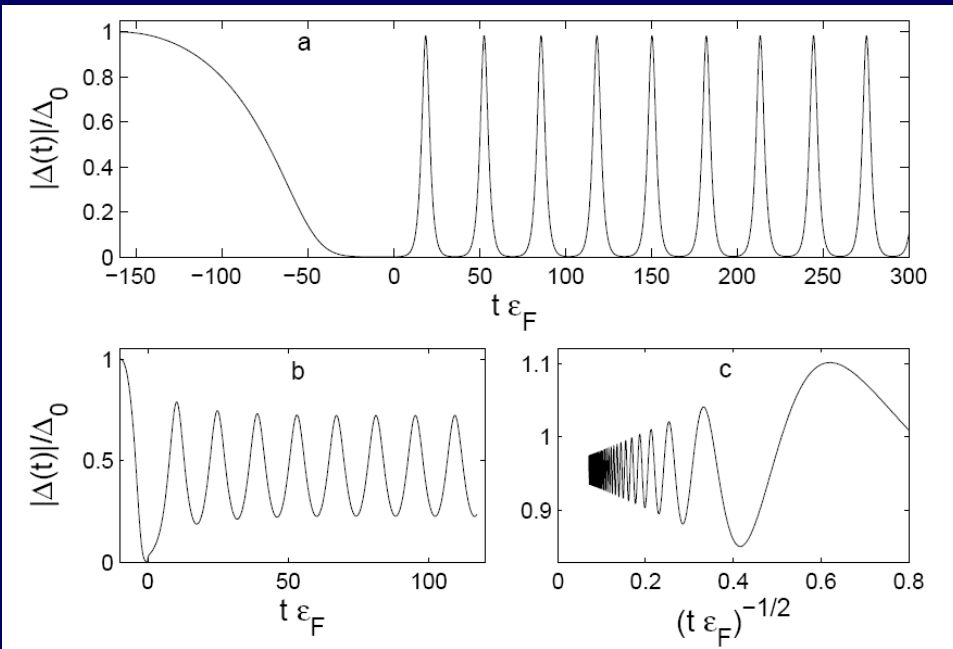
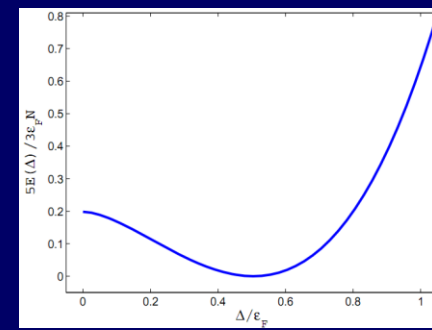
$$m\dot{\vec{v}} + \vec{\nabla} \cdot \left\{ \frac{m\vec{v}^2}{2} + \mu[n] \right\} = 0$$

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

Two-fluid hydrodynamics

“Landau-Ginzburg” 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

Outline:

- **What is a unitary gas?**
- **DFT extension to superfluid systems and its further extension to time-dependent phenomena**
- **The birth and life of vortices in a unitary Fermi gas in real time, superfluid to normal transformation, vortex reconnection and onset of quantum turbulence**

Why would one want to study a unitary gas?

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 $1/2$ fermions interacting via a zero-range, infinite scattering-length contact interaction.

What are the scattering length and the effective range?

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

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

If the energy is small only the s-wave 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 1/2 requires some hard work.

Let us turn now to dilute fermion matter

The ground state energy is given by a function:

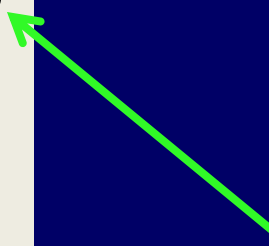
$$E_{gs} = f(N, V, \hbar, m, a, r_0)$$

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

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

$$\frac{N}{V} = \frac{k_F^3}{3\pi^2},$$

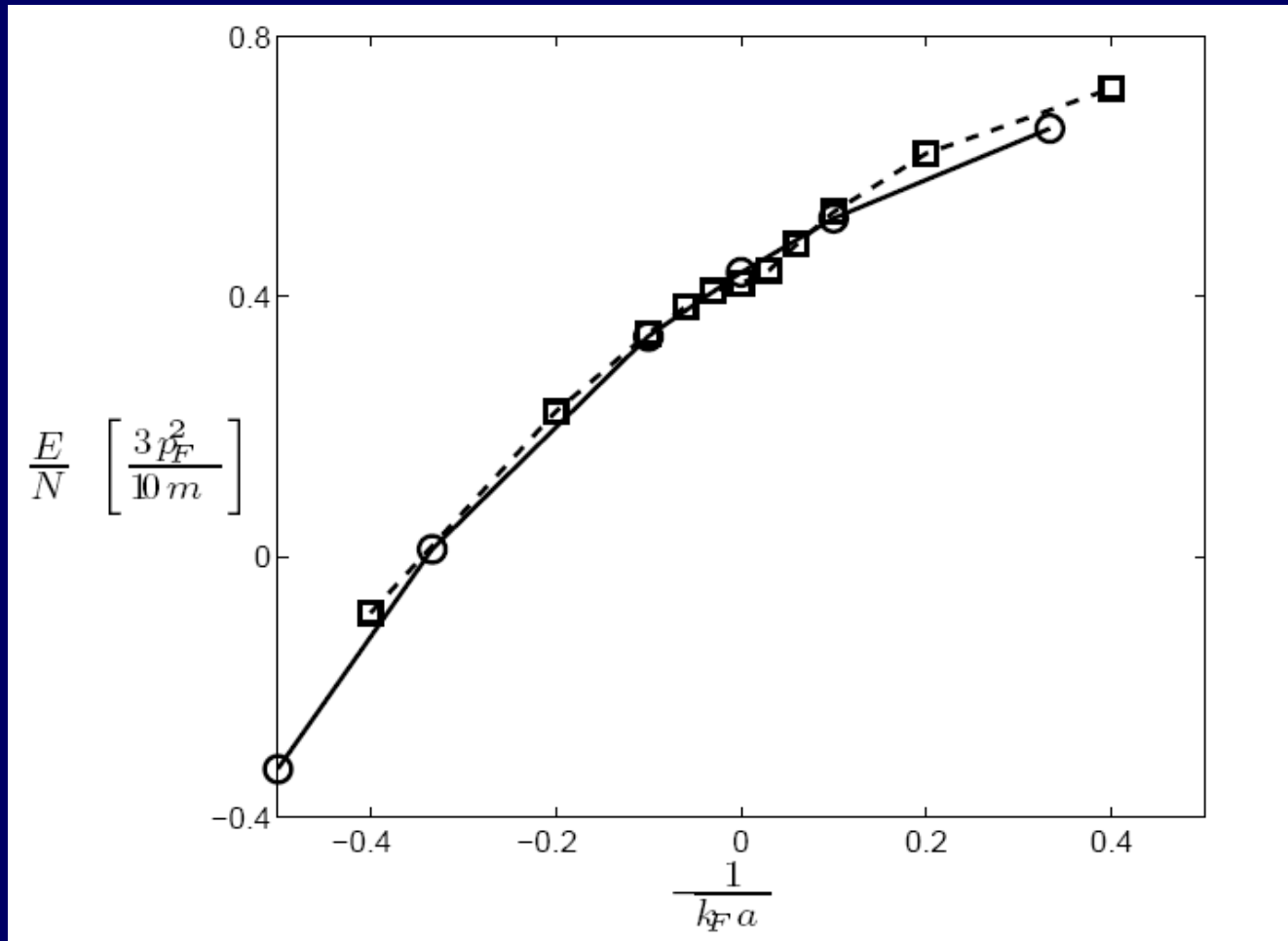
$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$



Pure number
(dimensionless)

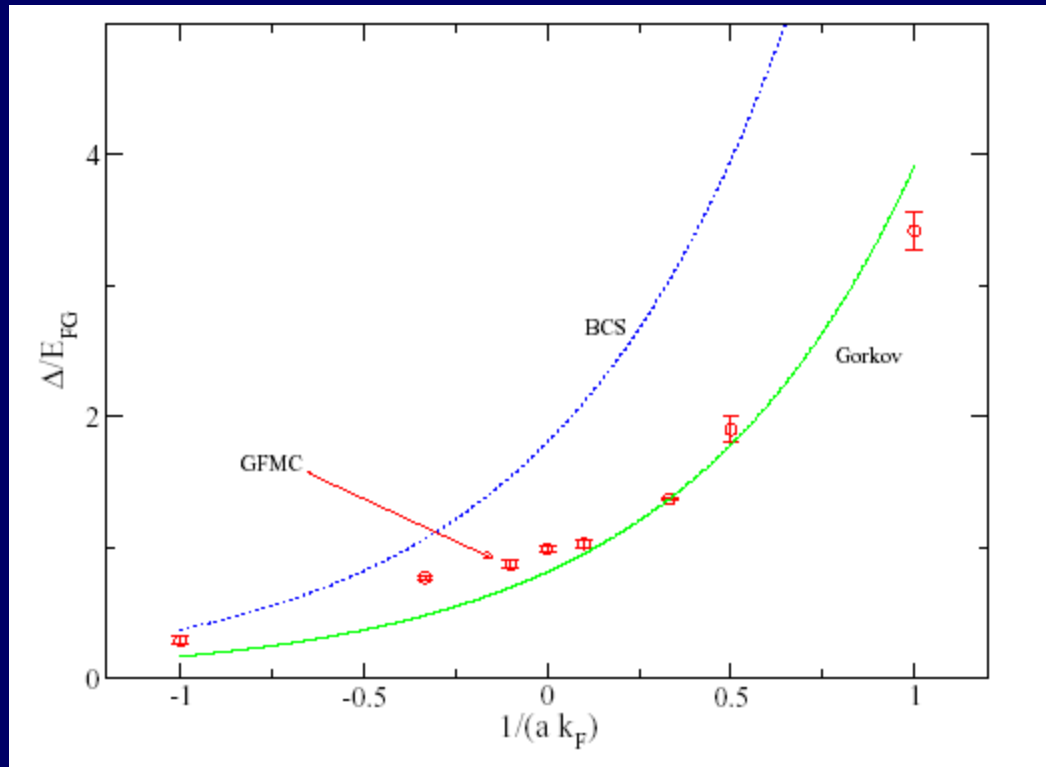
BEC side

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)



$$\Delta_{Gorkov} = \left(\frac{2}{e}\right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp\left(\frac{\pi}{2k_F a}\right)$$

$$\Delta_{BCS} = \frac{8}{e^2} \frac{\hbar^2 k_F^2}{2m} \exp\left(\frac{\pi}{2k_F a}\right)$$

Fixed node GFMC results: S.-Y. Chang *et al.* PRA 70, 043602 (2004)

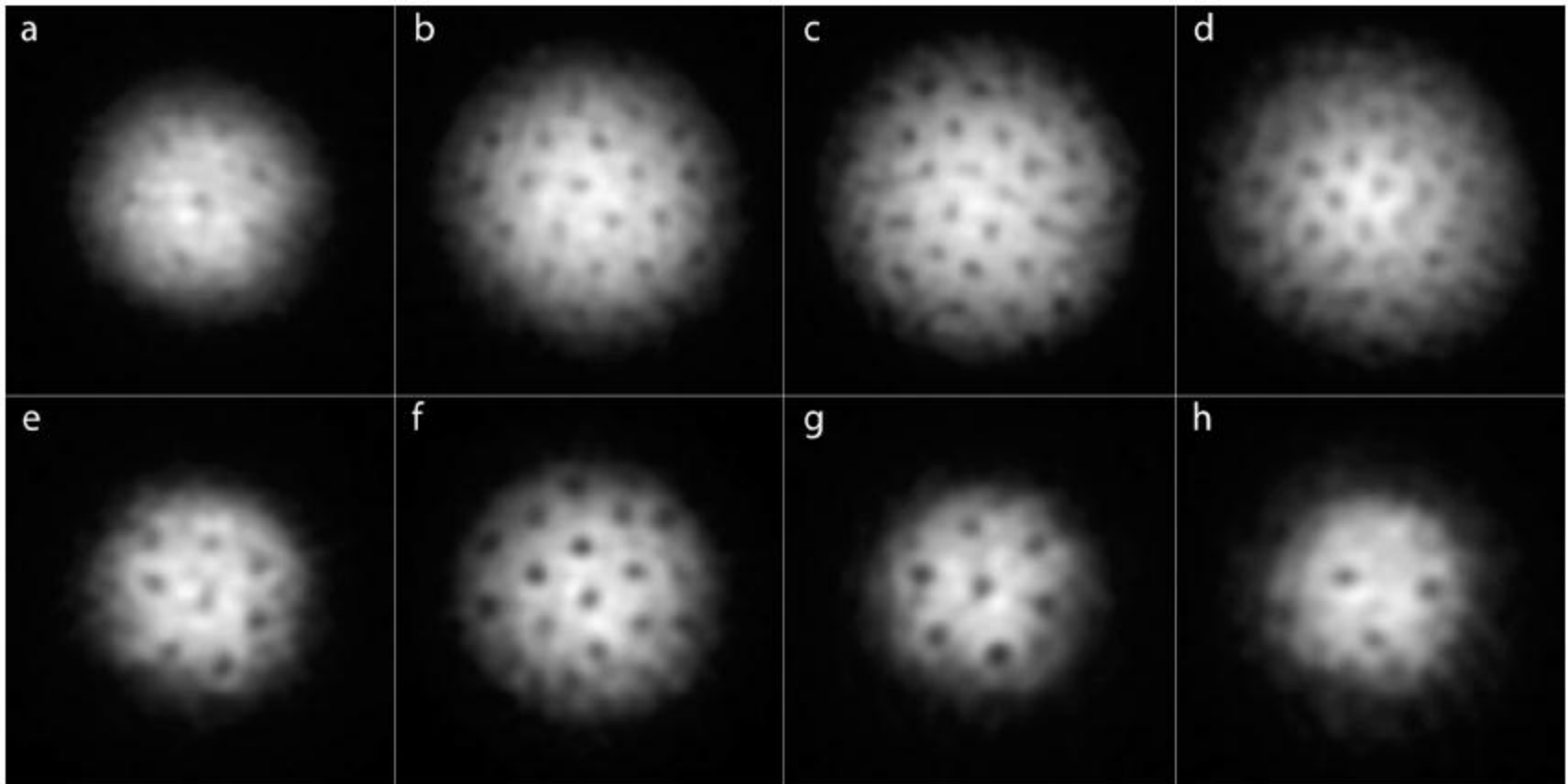


Fig. 2: Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) to 500 ms (b-h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic 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 $880 \mu\text{m} \times 880 \mu\text{m}$.

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

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

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

$$n(\vec{r}) = \langle \Psi_0 | \sum_i^N \delta(\vec{r} - \vec{r}_i) | \Psi_0 \rangle$$

**Injective map
(one-to-one)**

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

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

$$n(\vec{r}) = \sum_i^N |\varphi_i(\vec{r})|^2, \quad \tau(\vec{r}) = \sum_i^N |\vec{\nabla} \varphi_i(\vec{r})|^2$$

Universal functional of particle density alone
Independent of external potential

Normal Fermi systems only!

However, not everyone is normal!

Superconductivity and superfluidity in Fermi systems

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

units (1 eV \approx 10⁴ K)

Superfluid LDA (SLDA)

Extension of Kohn-Sham approach (LDA) to superfluid Fermi systems

$$E_{gs} = \int d^3r \varepsilon[n(\vec{r}), \tau(\vec{r}), \nu(\vec{r})]$$

$$n(\vec{r}) = 2 \sum_k |\mathbf{v}_k(\vec{r})|^2, \quad \tau(\vec{r}) = 2 \sum_k |\vec{\nabla} \mathbf{v}_k(\vec{r})|^2$$

$$\nu(\vec{r}) = \sum_k \mathbf{u}_k(\vec{r}) \mathbf{v}_k^*(\vec{r})$$

$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} \mathbf{u}_k(\vec{r}) \\ \mathbf{v}_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} \mathbf{u}_k(\vec{r}) \\ \mathbf{v}_k(\vec{r}) \end{pmatrix}$$

Mean-field and pairing field are both local fields!

(for the sake of simplicity spin degrees of freedom are not shown)

There is a little problem! The pairing field Δ diverges.

The SLDA (renormalized) equations

$$E_{gs} = \int d^3r \left\{ \underline{\varepsilon_N [n(\vec{r}), \tau(\vec{r})]} + \underline{\varepsilon_S [n(\vec{r}), \nu(\vec{r})]} \right\}$$

$$\varepsilon_S [n(\vec{r}), \nu(\vec{r})] \stackrel{\text{def}}{=} -\Delta(\vec{r})\nu_c(\vec{r}) = g_{\text{eff}}(\vec{r})|\nu_c(\vec{r})|^2$$

$$\begin{cases} [h(\vec{r}) - \mu]u_i(\vec{r}) + \Delta(\vec{r})v_i(\vec{r}) = E_i u_i(\vec{r}) \\ \Delta^*(\vec{r})u_i(\vec{r}) - [h(\vec{r}) - \mu]v_i(\vec{r}) = E_i v_i(\vec{r}) \end{cases} \quad \begin{cases} h(\vec{r}) = -\vec{\nabla} \frac{\hbar^2}{2m(\vec{r})} \vec{\nabla} + U(\vec{r}) \\ \Delta(\vec{r}) = -g_{\text{eff}}(\vec{r})\nu_c(\vec{r}) \end{cases}$$

$$\frac{1}{g_{\text{eff}}(\vec{r})} = \frac{1}{g[n(\vec{r})]} - \frac{m(\vec{r})k_c(\vec{r})}{2\pi^2\hbar^2} \left\{ 1 - \frac{k_F(\vec{r})}{2k_c(\vec{r})} \ln \frac{k_c(\vec{r}) + k_F(\vec{r})}{k_c(\vec{r}) - k_F(\vec{r})} \right\}$$

$$\rho_c(\vec{r}) = 2 \sum_{E_i \geq 0} |v_i(\vec{r})|^2, \quad \nu_c(\vec{r}) = \sum_{E_i \geq 0} v_i^*(\vec{r})u_i(\vec{r})$$

$$E_c + \mu = \frac{\hbar^2 k_c^2(\vec{r})}{2m(\vec{r})} + U(\vec{r}), \quad \mu = \frac{\hbar^2 k_F^2(\vec{r})}{2m(\vec{r})} + U(\vec{r})$$

Position and momentum dependent running coupling constant
Observables are (obviously) independent of cut-off energy (when chosen properly).

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

Only this combination is cutoff independent

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

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

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

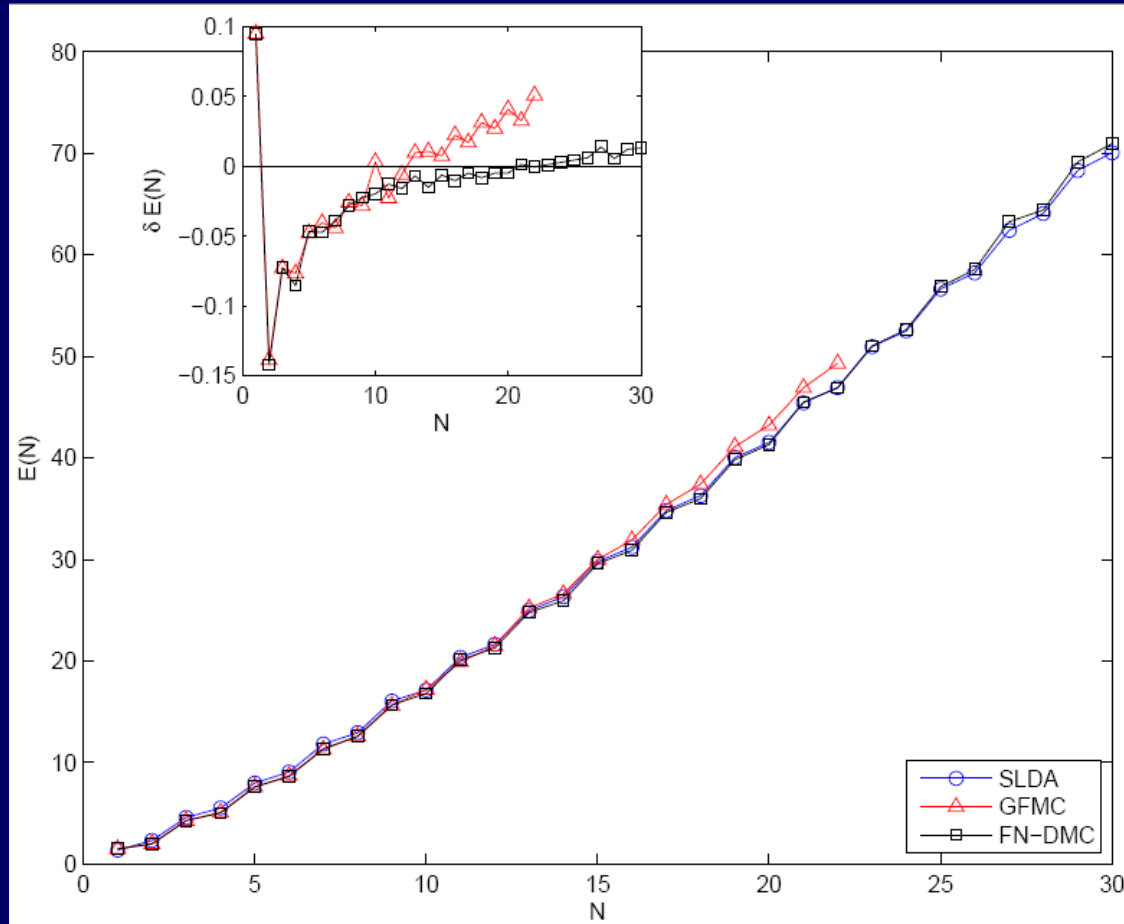
$$U(\vec{r}) = \beta \frac{(3\pi^2)^{2/3} n^{2/3}(\vec{r})}{2} - \frac{|\Delta(\vec{r})|^2}{3\gamma n^{2/3}(\vec{r})} + V_{ext}(\vec{r})$$

$$\Delta(\vec{r}) = -g_{eff}(\vec{r})\nu_c(\vec{r})$$

α can take any positive value,
but the best results are obtained when α is fixed by the qp-spectrum

Fermions at unitarity in a harmonic trap

Total energies $E(N)$



GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)

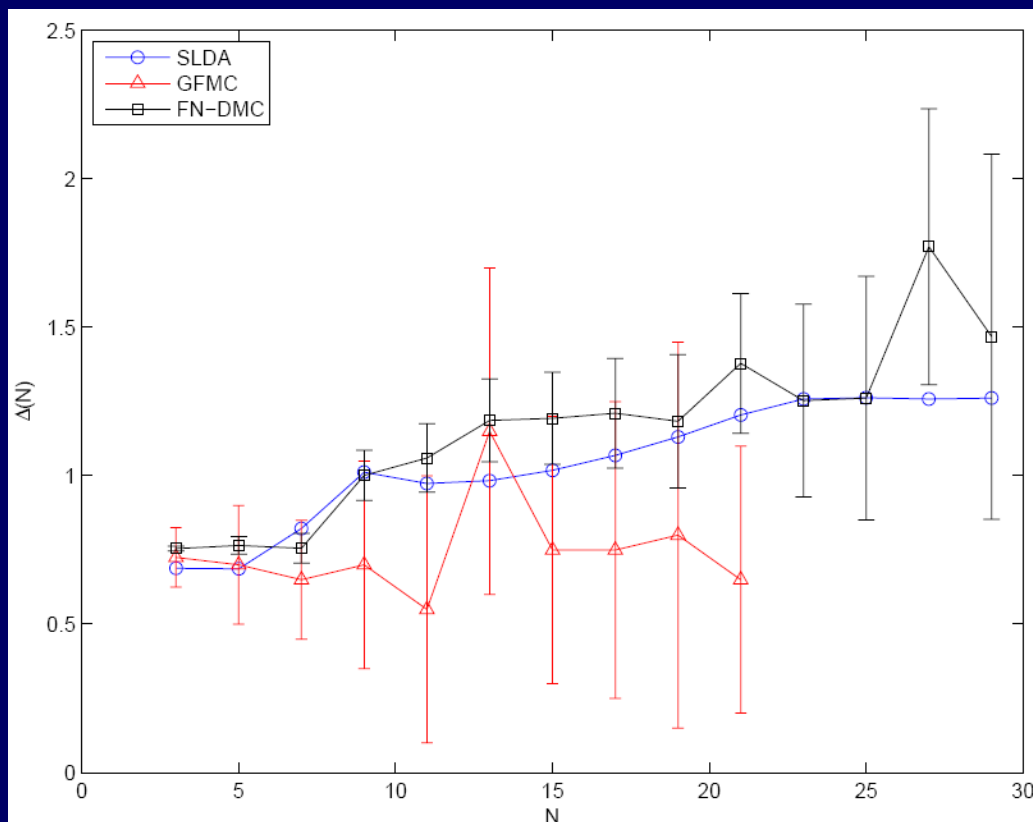
FN-DMC - von Stecher, Greene and Blume, PRL 99, 233201 (2007)

PRA 76, 053613 (2007)

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

Fermions at unitarity in a harmonic trap

Pairing gaps



$$\Delta(N) = \frac{E(N+1) - 2E(N) + E(N-1)}{2}, \quad \text{for odd } N$$

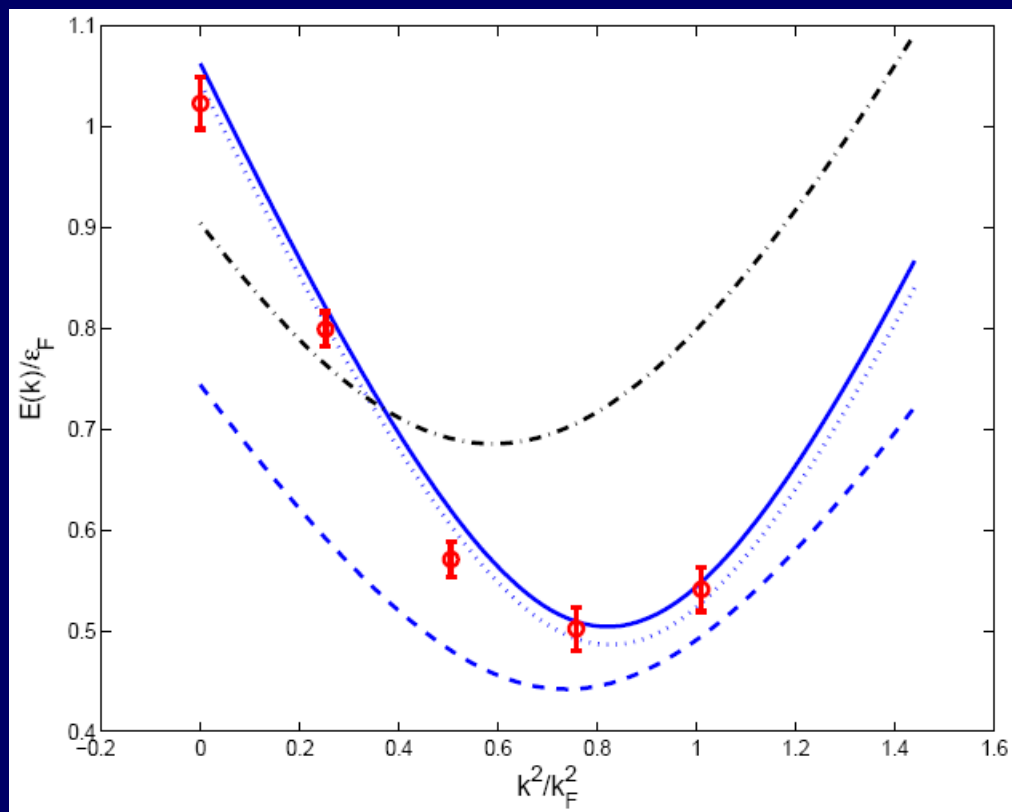
GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)

FN-DMC - von Stecher, Greene and Blume, PRL 99, 233201 (2007)

PRA 76, 053613 (2007)

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

Quasiparticle spectrum in homogeneous matter

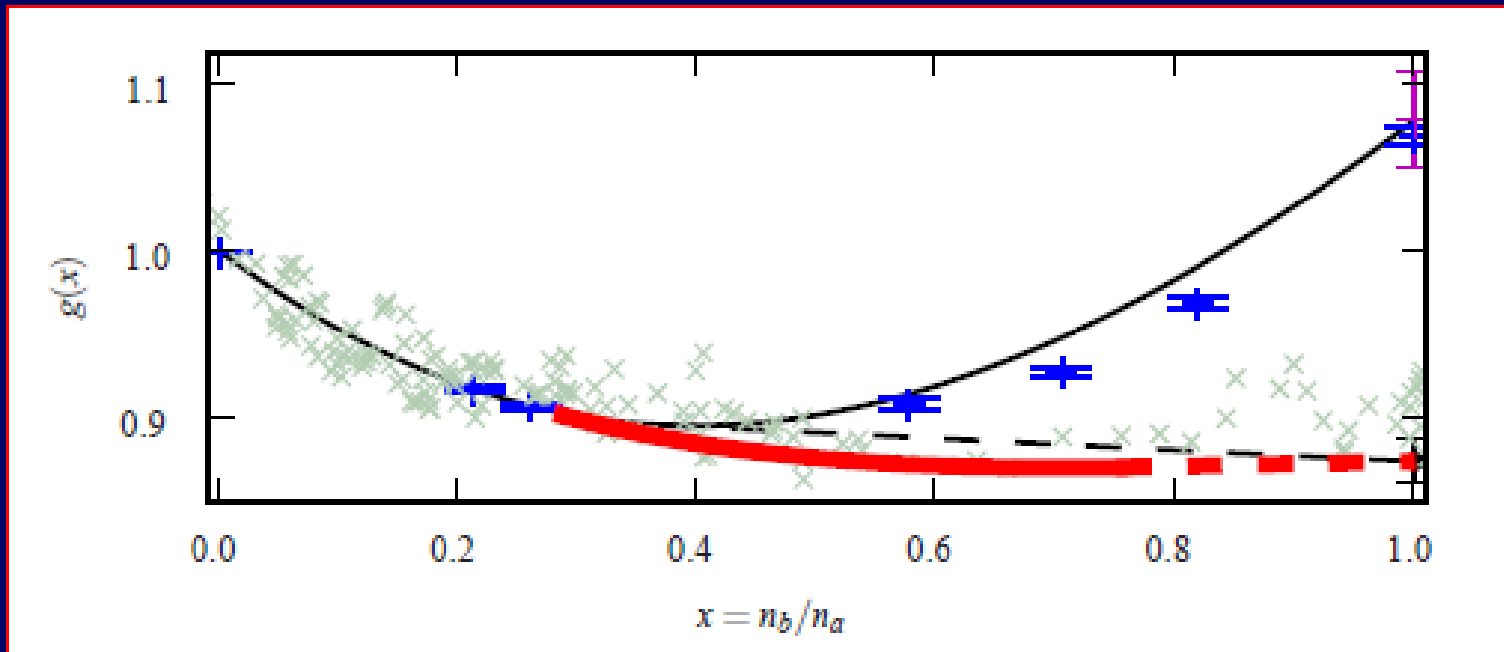


NB! In DFT one does not try to reproduce the single-particle spectrum (only the Fermi level)

- solid/dotted blue line** - SLDA, 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

Normal State				Superfluid State			
(N_a, N_b)	E_{FNDCMC}	E_{ASLDA}	(error)	(N_a, N_b)	E_{FNDCMC}	E_{ASLDA}	(error)
(3, 1)	6.6 ± 0.01	6.687	1.3%	(1, 1)	2.002 ± 0	2.302	15%
(4, 1)	8.93 ± 0.01	8.962	0.36%	(2, 2)	5.051 ± 0.009	5.405	7%
(5, 1)	12.1 ± 0.1	12.22	0.97%	(3, 3)	8.639 ± 0.03	8.939	3.5%
(5, 2)	13.3 ± 0.1	13.54	1.8%	(4, 4)	12.573 ± 0.03	12.63	0.48%
(6, 1)	15.8 ± 0.1	15.65	0.93%	(5, 5)	16.806 ± 0.04	16.19	3.7%
(7, 2)	19.9 ± 0.1	20.11	1.1%	(6, 6)	21.278 ± 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 ± 0.1	22.42	2.4%	(8, 8)	30.876 ± 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 ± 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 ± 0.1	29.41	0.034%	(14, 14)	64.388 ± 0.31	62.52	2.9%
(10, 2)	29.9 ± 0.1	30.05	0.52%	(15, 15)	70.927 ± 0.3	68.72	3.1%
(10, 6)	35 ± 0.1	35.93	2.7%	(1, 0)	1.5 ± 0.0	1.5	0%
(20, 1)	73.78 ± 0.01	73.83	0.061%	(2, 1)	4.281 ± 0.004	4.417	3.2%
(20, 4)	73.79 ± 0.01	74.01	0.3%	(3, 2)	7.61 ± 0.01	7.602	0.1%
(20, 10)	81.7 ± 0.1	82.57	1.1%	(4, 3)	11.362 ± 0.02	11.31	0.49%
(20, 20)	109.7 ± 0.1	113.8	3.7%	(7, 6)	24.787 ± 0.09	24.04	3%
(35, 4)	154 ± 0.1	154.1	0.078%	(11, 10)	45.474 ± 0.15	43.98	3.3%
(35, 10)	158.2 ± 0.1	158.6	0.27%	(15, 14)	69.126 ± 0.31	62.55	9.5%
(35, 20)	178.6 ± 0.1	180.4	1%				

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>

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

$$\begin{cases} [h(\vec{r}, t) + V_{ext}(\vec{r}, t) - \mu]u_i(\vec{r}, t) + [\Delta(\vec{r}, t) + \Delta_{ext}(\vec{r}, t)]v_i(\vec{r}, t) = i\hbar \frac{\partial u_i(\vec{r}, t)}{\partial t} \\ [\Delta^*(\vec{r}, t) + \Delta_{ext}^*(\vec{r}, t)]u_i(\vec{r}, t) - [h(\vec{r}, t) + V_{ext}(\vec{r}, t) - \mu]v_i(\vec{r}, t) = i\hbar \frac{\partial v_i(\vec{r}, t)}{\partial t} \end{cases}$$

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

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

TDSLDA

(equations look like TDHFB/TDBdG)

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

- The system is placed on a 3D spatial lattice
- Derivatives are computed with FFTW
- Fully self-consistent treatment with Galilean invariance
- No symmetry restrictions
- Number of quasiparticle wave functions is of the order of the number of spatial lattice points
- Initial state is the ground state of the SLDA (formally like HFB/BdG)
- The code was implemented on JaguarPf (NCCS), Franklin (NERSC), Athena (UW), and Hyak (UW)

Critical velocity in a unitary gas

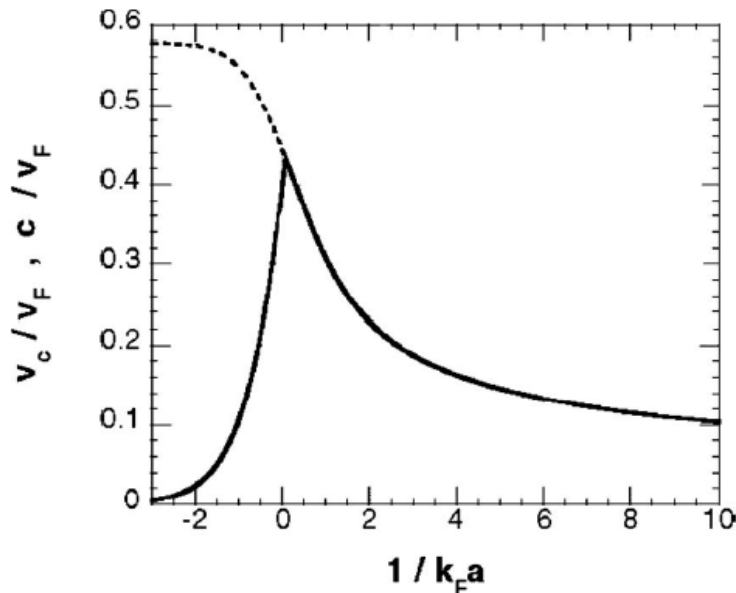


FIG. 20. Landau's critical velocity (in units of the Fermi velocity) calculated along the crossover using BCS mean-field theory. The critical velocity is largest near unitarity. The dashed line is the sound velocity. From [Combescot, Kagan, and Stringari, 2006](#).

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

Study based on BCS/Leggett approximation

$$c_s = 0.370(5)v_F$$

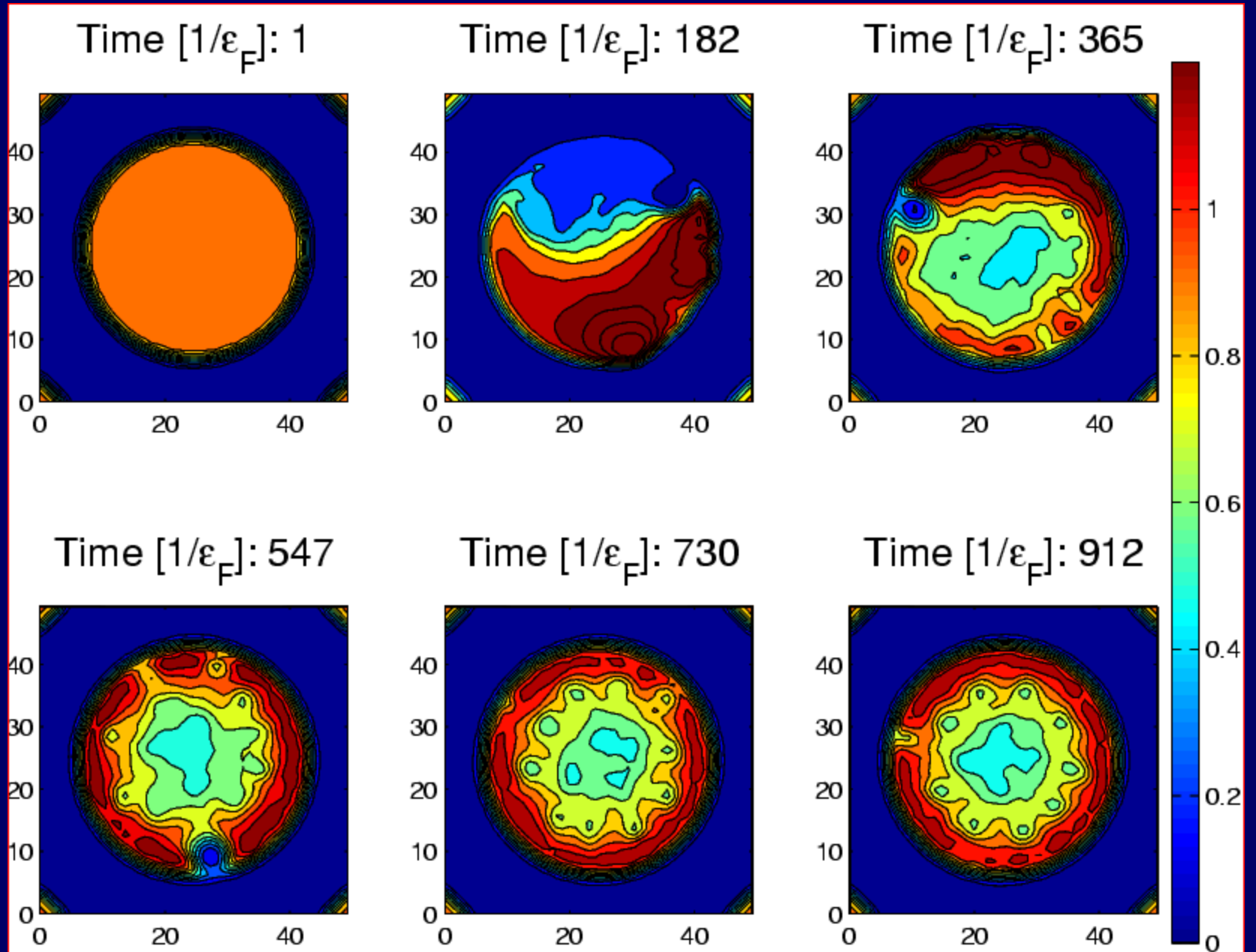
$$\min\left(\frac{\varepsilon_{qp}}{k}\right) = 0.385(3)$$

$$\Rightarrow v_c = 0.370(5)v_F$$

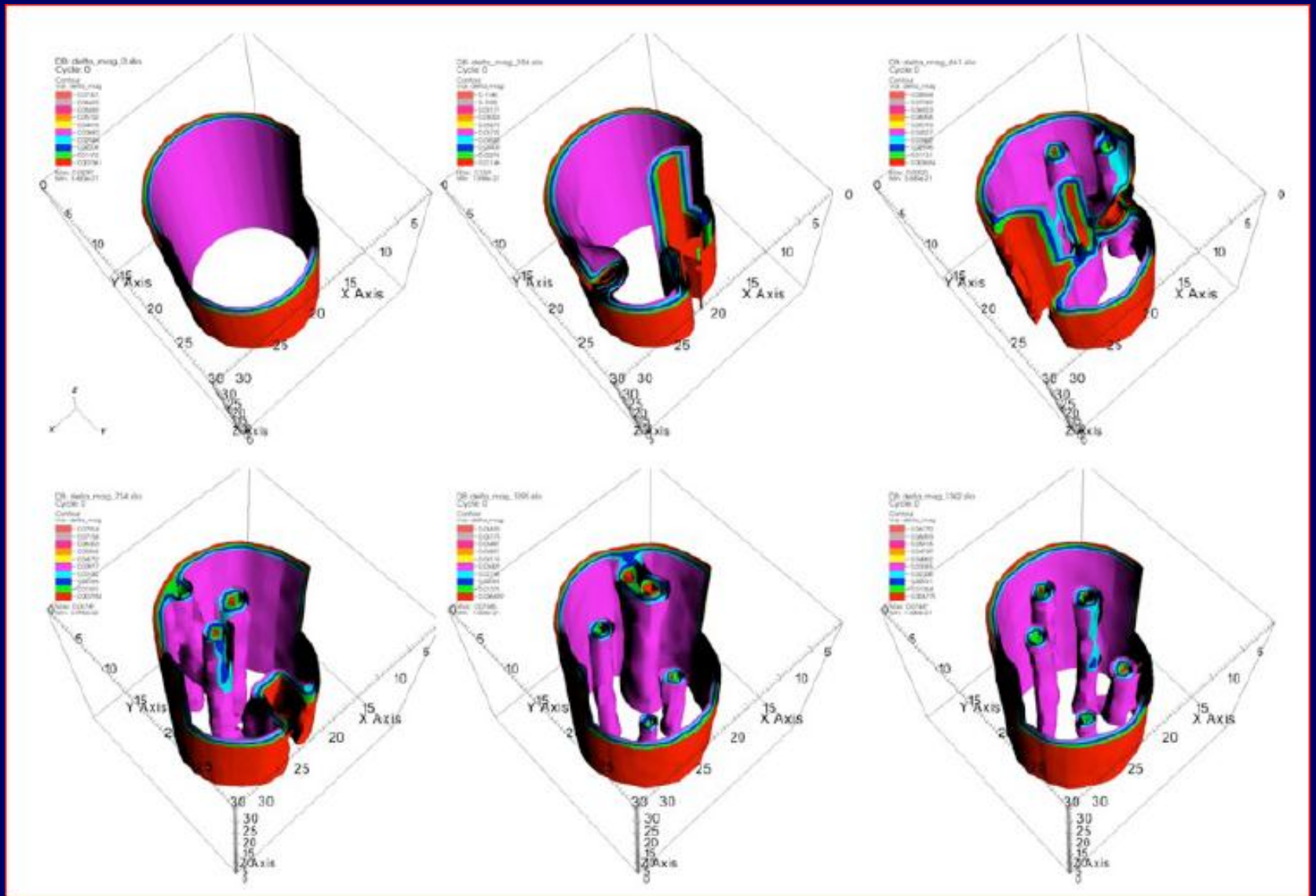
Values obtained using QMC data

$$v_c \approx 0.25(3)v_F$$

Miller et al. (MIT, 2007)



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



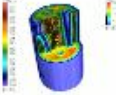
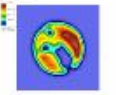
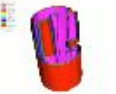
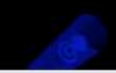
Profile of the pairing gap of a stirred unitary Fermi gas at various times.



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
<i>Ball and Rod</i>		
	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)
<i>Centered Ball</i>		
	nt-ball-c.m4v	density contour plot of magnitude of pairing field focused on vortices; full geometry ; 3m29s