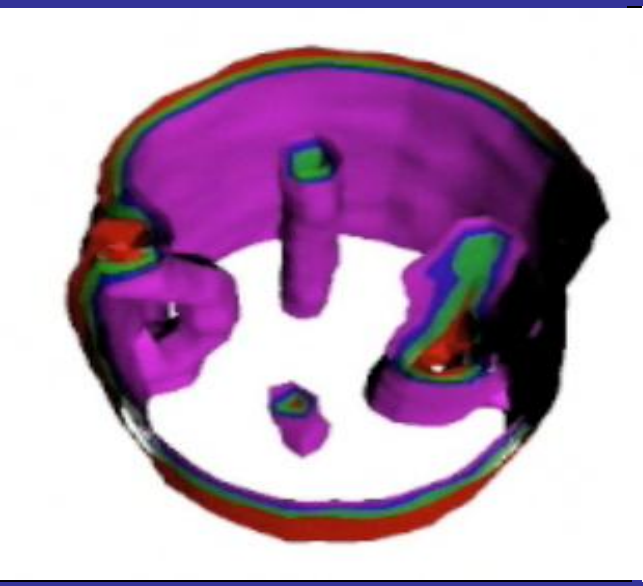
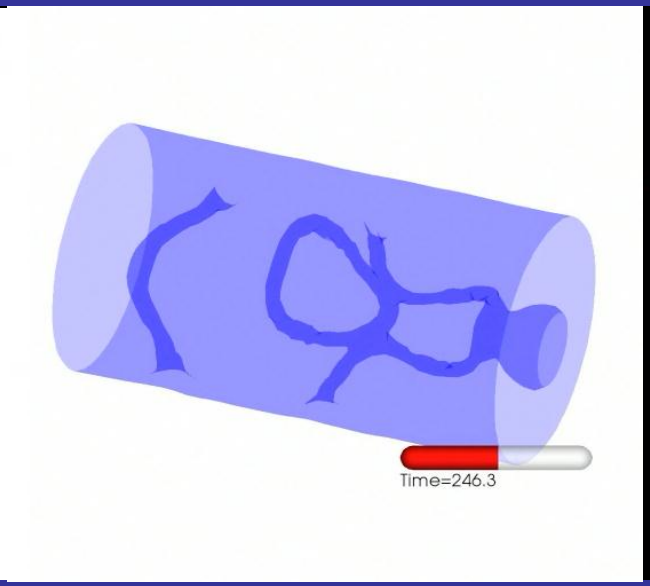
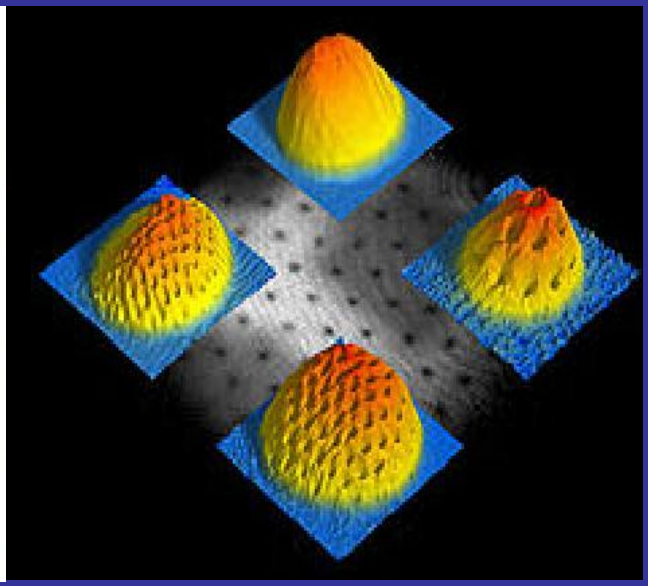
Dynamics of ultracold atomic gases and atomic nuclei within DFT







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GOAL:

Description of fermionic superfluids far from equilibrium.

Theoretical approaches to superfluid dynamics:

- **two-fluid hydrodynamics**
- **Landau-Ginzburg model (or Gross-Pitaevski equations)**
- **Density Functional Theory – extension to superfluid systems and time-dependent phenomena.**

Density Functional Theory (DFT)

Hohenberg-Kohn theorem:

$$E_{gs} = \mathrm{E}[n(\vec{r})]$$

particle density

Local Density Approximation:

$$E_{gs} = \int d^3 r \left\{ \frac{\hbar^2}{2m} \tau(\vec{r}) + \varepsilon[n(\vec{r})] n(\vec{r}) \right\}$$

$$n(\vec{r}) = \sum_{i=1}^{N} |\psi_i(\vec{r})|^2 \qquad \tau(\vec{r}) = \sum_{i=1}^{N} |\vec{\nabla} \psi_i(\vec{r})|^2$$

$$-\frac{\hbar^2 \Delta}{2m} \psi_i(\vec{r}) + U(\vec{r}) \psi_i(\vec{r}) = \varepsilon_i \psi_i(\vec{r})$$

Kohn-Sham equations

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

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

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

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

pairing (anomalous) density

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

Mean-field and pairing field are both local fields!
(for sake of simplicity spin degrees of freedom are not shown)

There is a problem!
The pairing field diverges.

$$\begin{cases} [h(\vec{r}) - \mu]\mathrm{u}_i(\vec{r}) + \Delta(\vec{r})\mathrm{v}_i(\vec{r}) = E_i \mathrm{u}_i(\vec{r}) \\ \Delta^*(\vec{r})\mathrm{u}_i(\vec{r}) - [h(\vec{r}) - \mu]\mathrm{v}_i(\vec{r}) = E_i \mathrm{v}_i(\vec{r}) \end{cases}$$

$$\begin{cases} h(\vec{r}) = -\vec{\nabla}\dfrac{\hbar^2}{2m(\vec{r})}\vec{\nabla} + U(\vec{r}) \\ \Delta(\vec{r}) = -g_{\mathrm{eff}}(\vec{r})\nu_c(\vec{r}) \end{cases}$$

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

$$\rho_c(\vec{r}) = 2\sum_{E_i \le E_c} |\mathrm{v}_i(\vec{r})|^2, \qquad \nu_c(\vec{r}) = \sum_{E_i \le E_c} \mathrm{v}_i^*(\vec{r})\mathrm{u}_i(\vec{r})$$

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

One has to introduce position and momentum dependent running coupling constant.

Formalism for Time Dependent Phenomena: TDSLDA

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)

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

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

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

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: $O(10^4)$- $O(10^6)$
- ✓ high numerical accuracy for spatial derivatives using FFTW
- ✓ for TD high-accuracy and numerically stable Adams–Bashforth–Milne 5th order predictor-corrector-modifier algorithm with only 2 evaluations of the rhs per time step and with no matrix operations
- ✓ The time step is adjusted so the relative error in ABM method is between 10^{-7} -10^{-15}

  Eg. we evolve 4x136626=546504 coupled eigenvectors for ^{238}U on the lattice: 50x50x80 fm (mesh size: 1.25fm) with energy cutoff 100MeV to an accuracy 10^{-8}
- ✓ very fast I/O capabilities
- ✓ volumes of the order of ($L = 80^3$) capable of simulating time evolution of 42000 neutrons at saturation density (possible application: neutron stars)
- ✓ capable of simulating up to times of the order of 10^{-19} s (a few million time steps)
- ✓ Presented calculations for unitary Fermi gas required over 200,000 cores of JaguarPF

SLDA for unitary Fermi gas

SLDA – Superfluid Local Density Approximation

SLDA energy density functional at unitarity

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

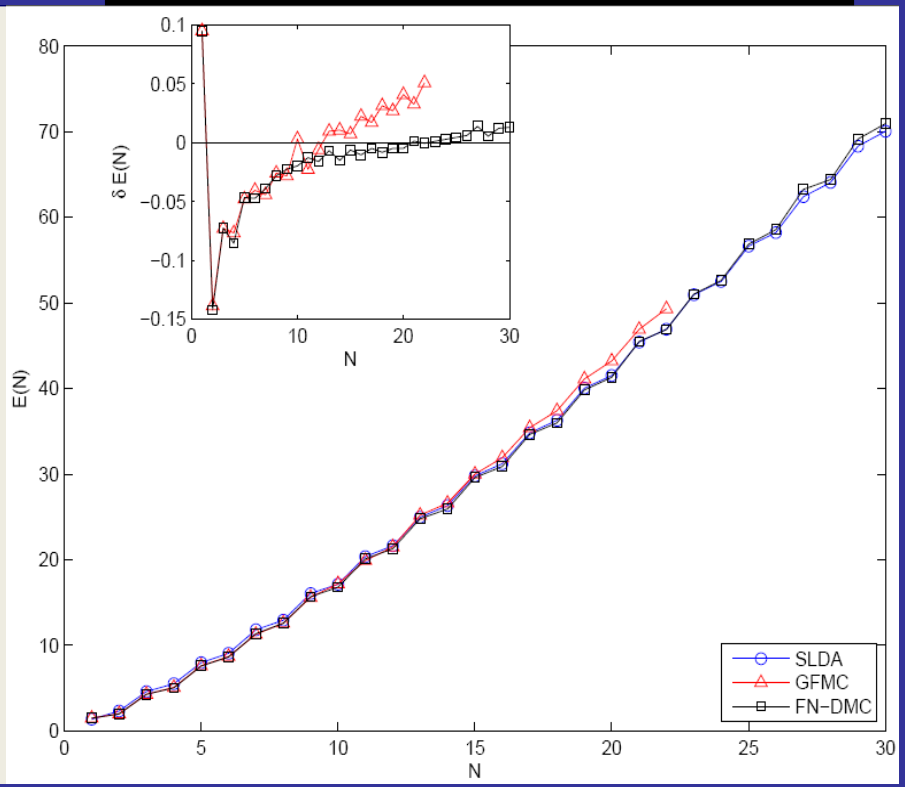
$$n(\vec{r}) = 2\sum_{0<E_k<E_c}\left|\mathrm{v}_k(\vec{r})\right|^2, \quad \tau_c(\vec{r}) = 2\sum_{0<E_k<E_c}\left|\vec{\nabla}\mathrm{v}_k(\vec{r})\right|^2,$$

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

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

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

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)

Normal State				Superfluid State			
(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)	(N_a, N_b)	E_{FNDMC}	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%				

A. Bulgac, M.M. Forbes, P. Magierski, *in* BCS-BEC crossover and the Unitary Fermi gas „Lecture Notes in Physics" v.836, p. 305, ed. W. Zwerger (2012)

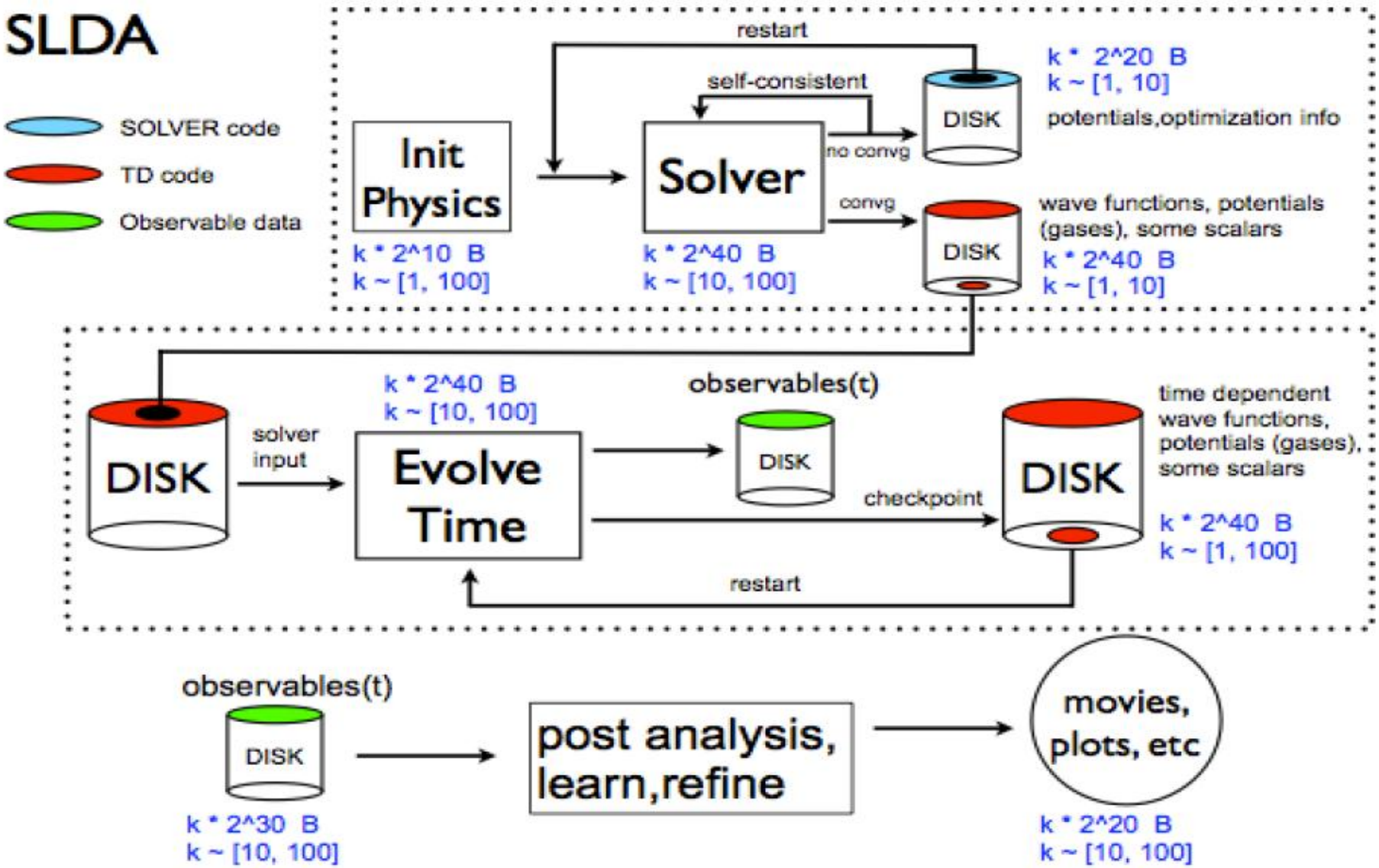
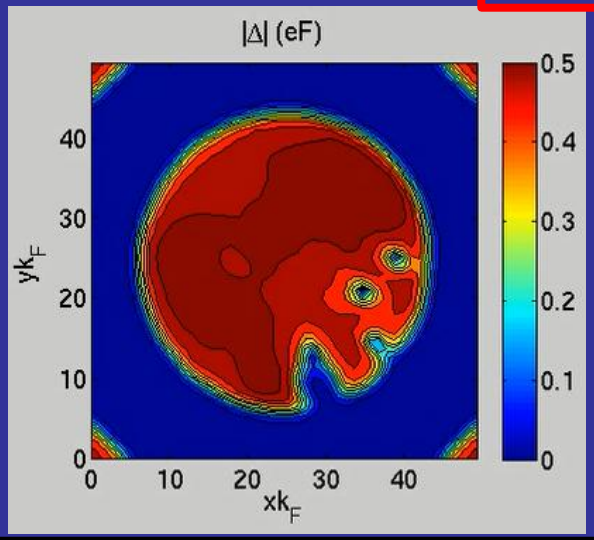
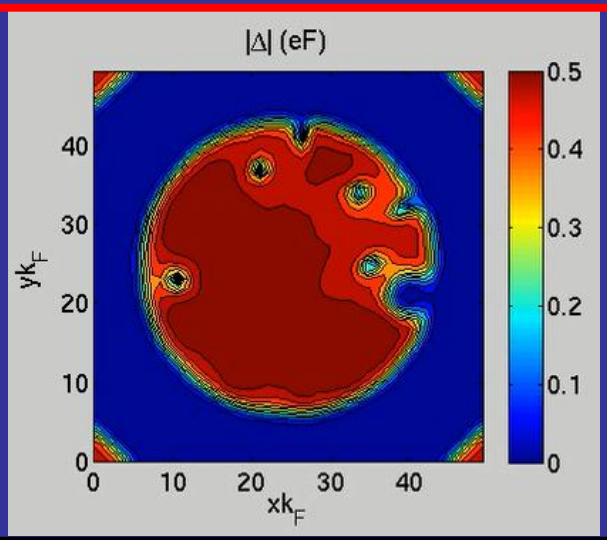
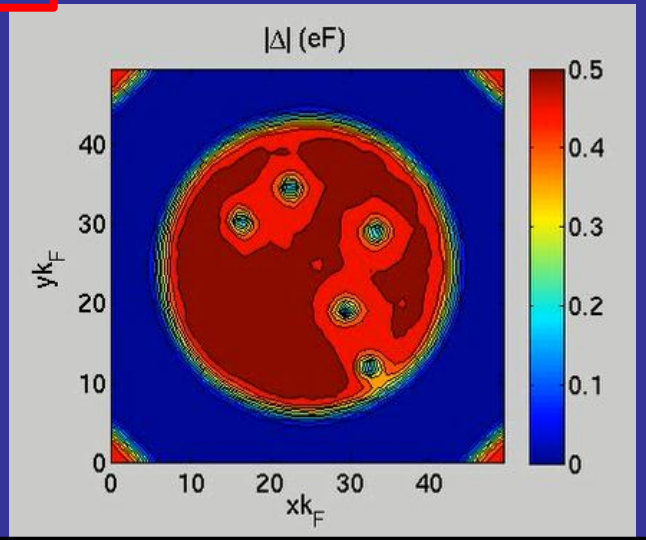


Figure 4: Structure of the (TD)SLDA production software and workflow. Data data magnitudes per analysis stage are printed blue and range from kilobytes to describe a problem, to hundreds of terabytes in memory, to tens of terabytes for checkpoint / restart, to up to nearly a hundred gigabytes data for post analysis.

Excitation of vortices through stirring

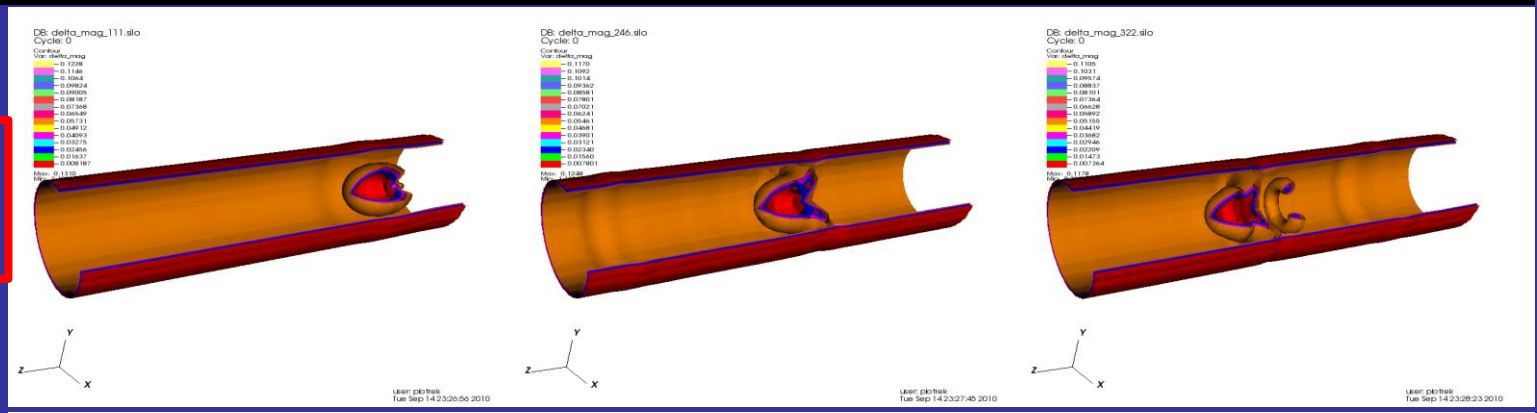


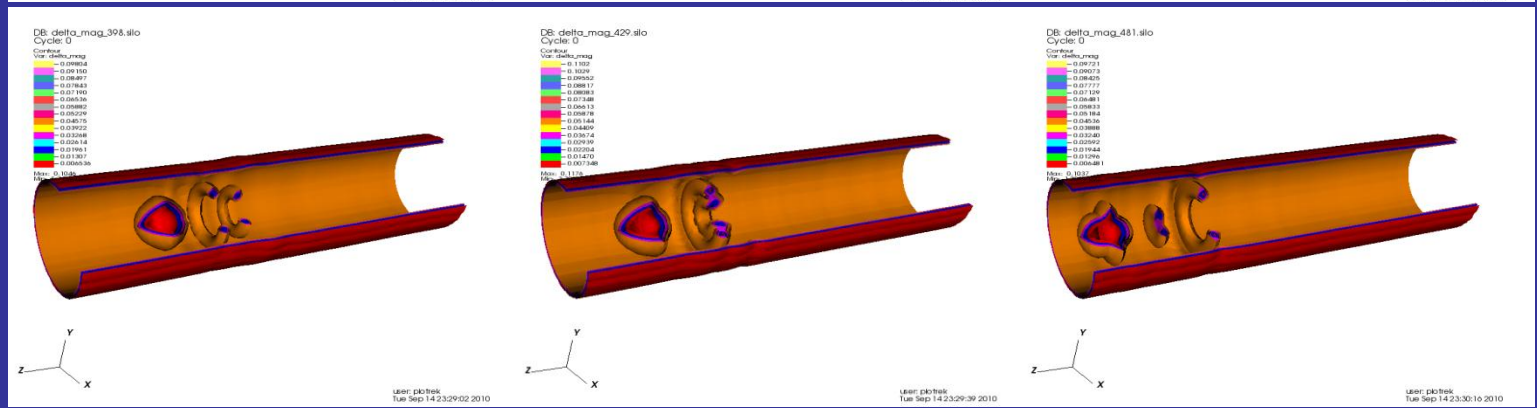




dynamics of vortex rings

Heavy spherical object moving through the superfluid unitary Fermi gas





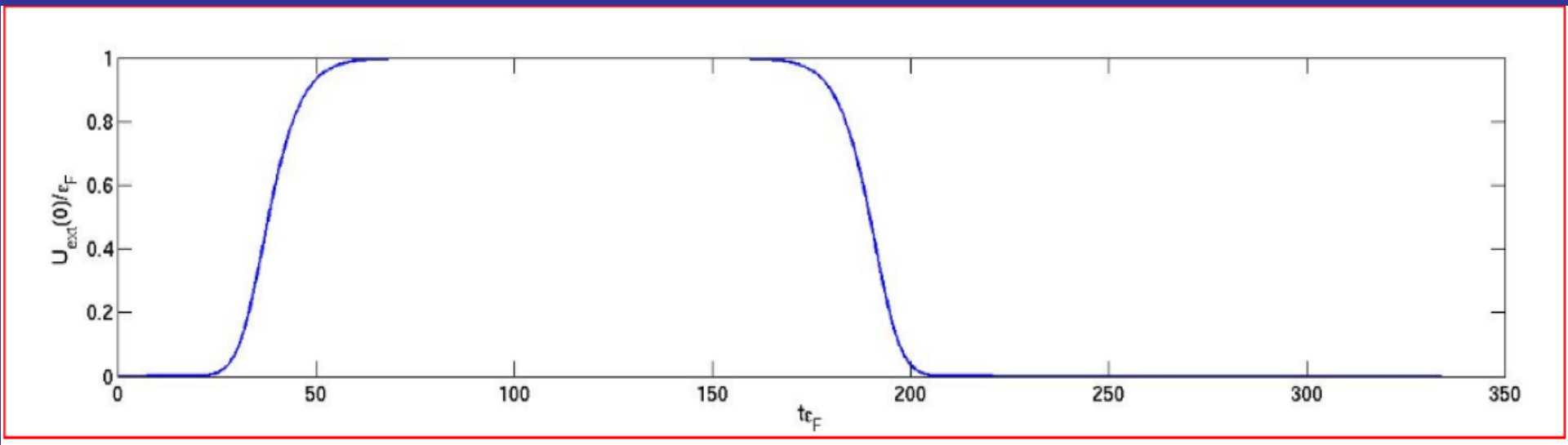


Figure 4. The strength of the external stirrer as a function of time in a typical simulation.

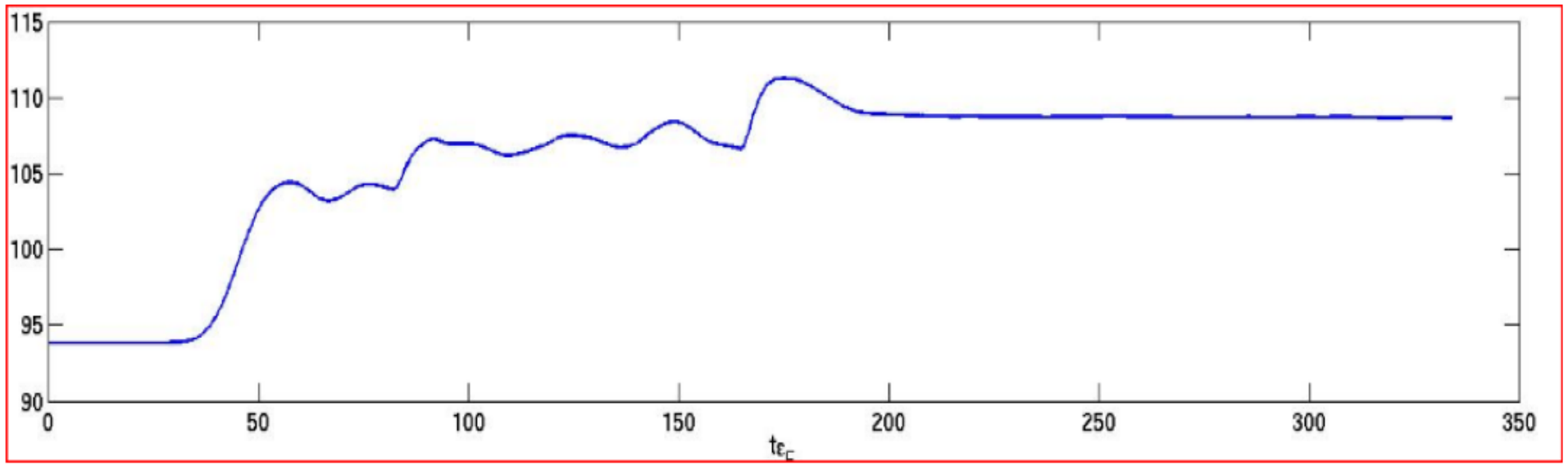


Figure 5. The total energy of 300 particles as a function of time in a typical stirring simulation.

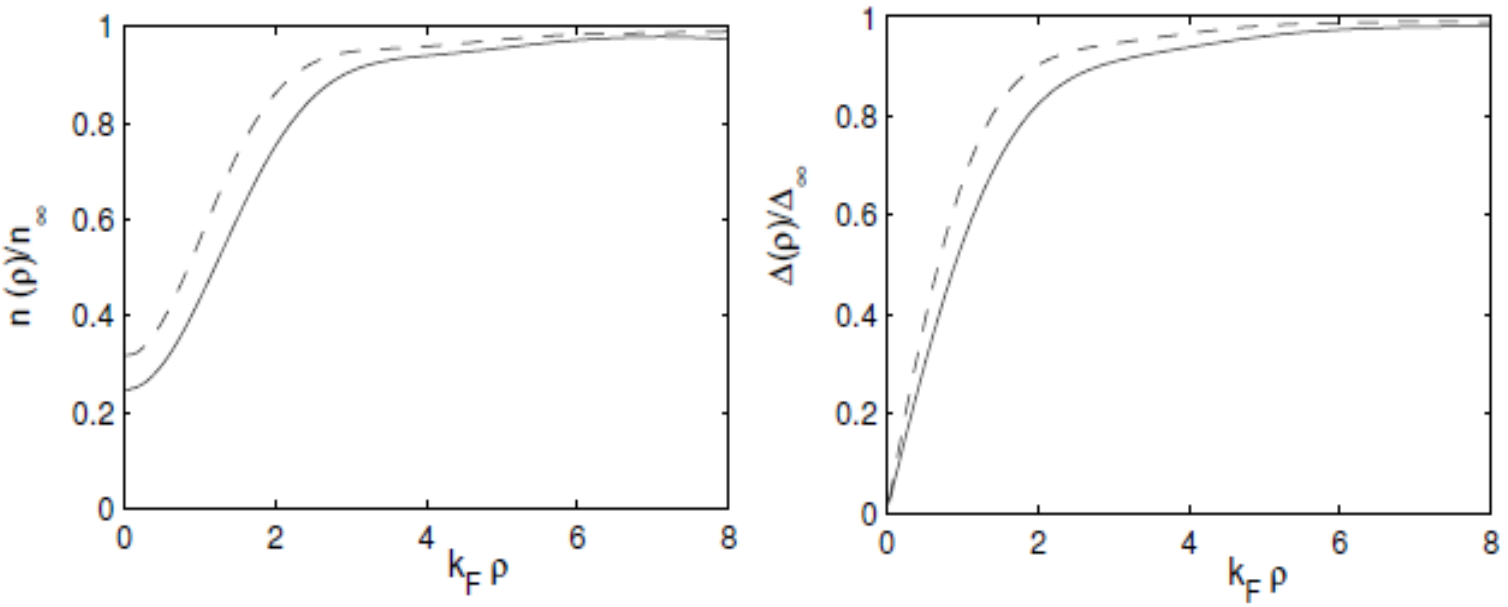


Fig. 9.13 Density profile (left) and gap parameter (right) from [60] for a superfluid vortex in the symmetric $n_a = n_b$ unitary Fermi gas with unit circulation. The solid curve corresponds to a parametrization of the SLDA with no self-energy $\beta = 0$ but including an effective mass correction. The dotted curve corresponds to a version with unit effective mass $\alpha = 1$. The other two parameters were fixed to reproduce the best approximation to energies of the normal and superfluid states known at the time: $\xi_N = 0.54$ and $\xi_{SF} = 0.44$. The current parameter set (9.95) should be preferred, but gives similar results. Note: The solid curve does not have the required currents to restore Galilean invariance (see Sec. 9.4.2), but the effect should be small here. Since the dotted curve has no effective mass correction, Galilean corrections are not required.

A. Bulgac, M.M. Forbes, P. Magierski, *in* BCS-BEC crossover and the Unitary Fermi gas „Lecture Notes in Physics" v.836, p. 305, ed. W. Zwerger (2012)

Details of simulations of unitary Fermi gas:

Lattice sizes: 48x48x48, 32x32x(96-196)
Number of particles: 300-1800
Number of evolved q.p. wave functions: 9500 - 41000

Road to quantum turbulence

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

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

E – kinetic energy per unit mass associated with the scale 1/k
ε - energy rate (per unit mass) transfered 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 → Kelvin waves → phonon radiation

Vortex reconnections

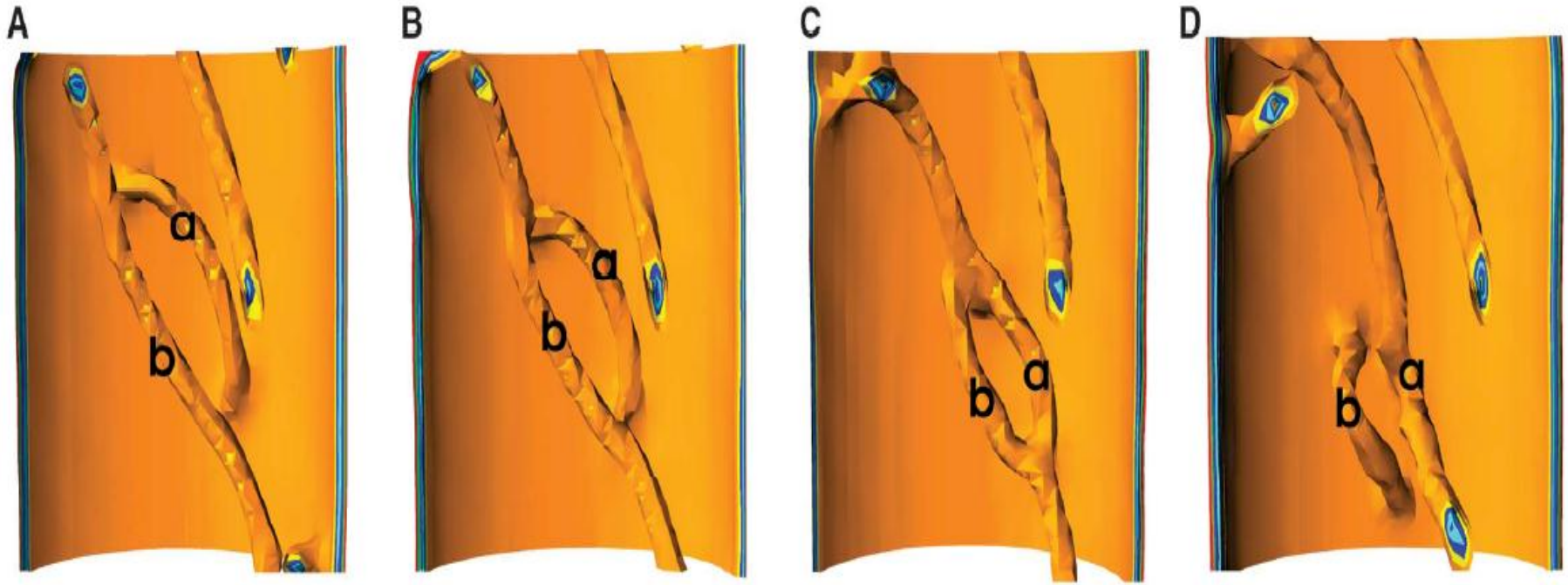


Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b)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

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

More movies here: www.phys.washington.edu/groups/qmbnt/UFG/

Nuclear DFT

$$E = \int d^3r \mathcal{H}(\mathbf{r})$$

where

$$\begin{aligned}\mathcal{H}(\mathbf{r}) &= C^{\rho}\rho^2 + C^{s}\vec{s}\cdot\vec{s} + C^{\Delta\rho}\rho\nabla^2\rho + C^{\Delta s}\vec{s}\cdot\nabla^2\vec{s} + C^{\tau}(\rho\tau - \vec{j}\cdot\vec{j}) + \\ &+ C^{sT}(\vec{s}\cdot\vec{T} - \mathbf{J}^2) + C^{\nabla J}(\rho\vec{\nabla}\cdot\vec{J} + \vec{s}\cdot(\vec{\nabla}\times\vec{j})) + C^{\nabla s}(\vec{\nabla}\cdot\vec{s})^2 + C^{\gamma}\rho^{\gamma} - \Delta\chi^*\end{aligned}$$

where

$$\begin{aligned}J_i &= \sum_{k,l}\epsilon_{ikl}\mathbf{J}_{kl} \\ \mathbf{J}^2 &= \sum_{k,l}\mathbf{J}_{kl}^2\end{aligned}$$

- density: $\rho(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin density: $\vec{s}(\mathbf{r}) = \vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- current: $\vec{j}(\mathbf{r}) = \frac{1}{2i}(\vec{\nabla} - \vec{\nabla}')\rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin current (2nd rank tensor): $\mathbf{J}(\mathbf{r}) = \frac{1}{2i}(\vec{\nabla} - \vec{\nabla}')\otimes\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- kinetic energy density: $\tau(\mathbf{r}) = \vec{\nabla}\cdot\vec{\nabla}'\rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
- spin kinetic energy density: $\vec{T}(\mathbf{r}) = \vec{\nabla}\cdot\vec{\nabla}'\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
- anomalous (pairing) density: $\chi(\mathbf{r}) = \chi(\mathbf{r},\mathbf{r}')|_{r=r'}$

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow,\uparrow}(\mathbf{r},t) & h_{\uparrow,\downarrow}(\mathbf{r},t) & 0 & \Delta(\mathbf{r},t) \\ h_{\downarrow,\uparrow}(\mathbf{r},t) & h_{\downarrow,\downarrow}(\mathbf{r},t) & -\Delta(\mathbf{r},t) & 0 \\ 0 & -\Delta^*(\mathbf{r},t) & -h^*_{\uparrow,\uparrow}(\mathbf{r},t) & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & 0 & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) & -h^*_{\downarrow,\downarrow}(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix}, \qquad (12)$$

where $h_i(\mathbf{r},t)$ (i stands for neutron or protons) is given by (5) and depends on both neutron and proton densities. The 4-component "wave function" is in turn related to the densities and the pairing field $\Delta_i(\mathbf{r})$ (we omit the time variable):

$$\begin{aligned}
\rho(\mathbf{r},\mathbf{r}') &= \sum_k \left(v^*_{k\uparrow}(\mathbf{r})v_{k\uparrow}(\mathbf{r}') + v^*_{k\downarrow}(\mathbf{r})v_{k\downarrow}(\mathbf{r}')\right) \\
s_x(\mathbf{r},\mathbf{r}') &= \sum_k \left(v^*_{k\uparrow}(\mathbf{r})v_{k\downarrow}(\mathbf{r}') + v^*_{k\downarrow}(\mathbf{r})v_{k\uparrow}(\mathbf{r}')\right) \\
s_y(\mathbf{r},\mathbf{r}') &= i\sum_k \left(v^*_{k\uparrow}(\mathbf{r})v_{k\downarrow}(\mathbf{r}') - v^*_{k\downarrow}(\mathbf{r})v_{k\uparrow}(\mathbf{r}')\right) \\
s_z(\mathbf{r},\mathbf{r}') &= \sum_k \left(v^*_{k\uparrow}(\mathbf{r})v_{k\uparrow}(\mathbf{r}') - v^*_{k\downarrow}(\mathbf{r})v_{k\downarrow}(\mathbf{r}')\right) \\
\chi(\mathbf{r}) &= \sum_{k<k_c} v^*_{k\uparrow}(\mathbf{r})u_{k\downarrow}(\mathbf{r}) \\
\Delta(\mathbf{r}) &= -g_{eff}(\mathbf{r})\chi(\mathbf{r})
\end{aligned}$$

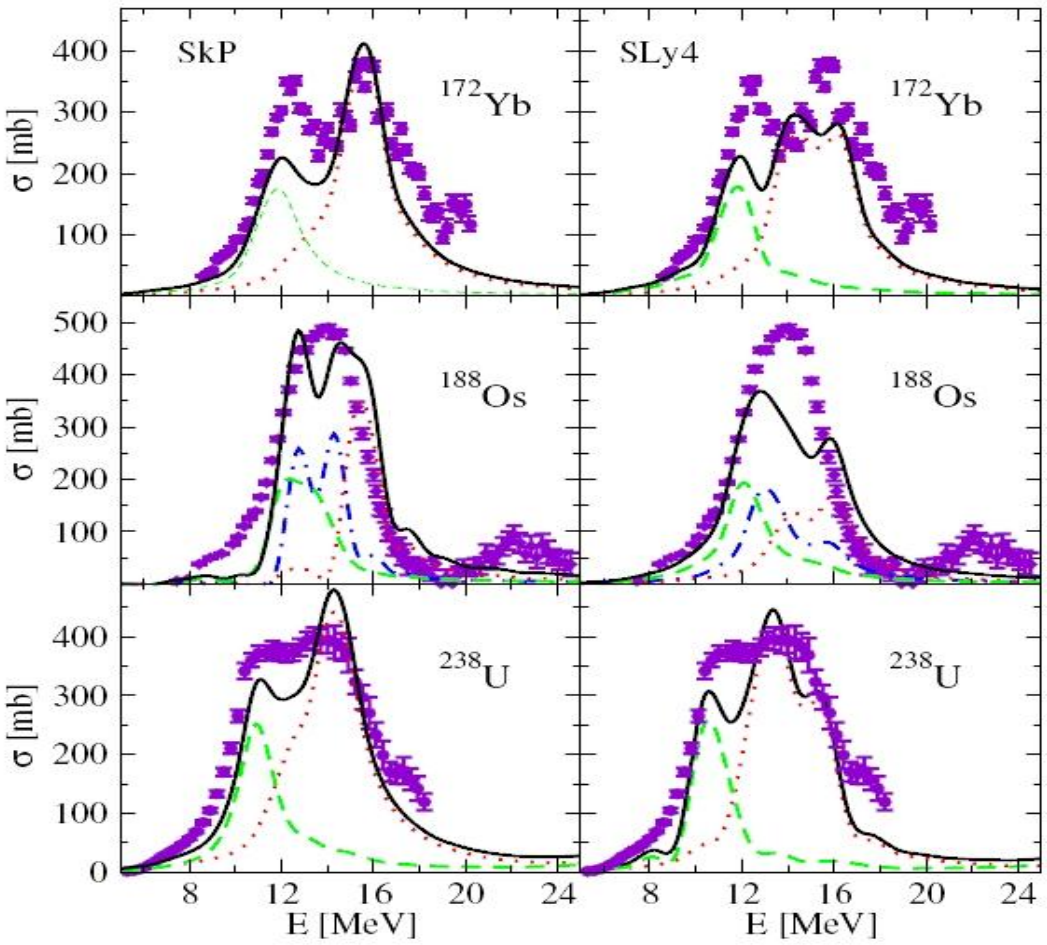
Nuclear dynamics from time dependent density functional theory

$$S(E) = \sum_\nu |\langle \nu | \hat{F} | 0 \rangle|^2 \delta(E - E_\nu)$$

$$S(\omega) = \mathrm{Im}\{\delta F(\omega)/[\pi f(\omega)]\}$$

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

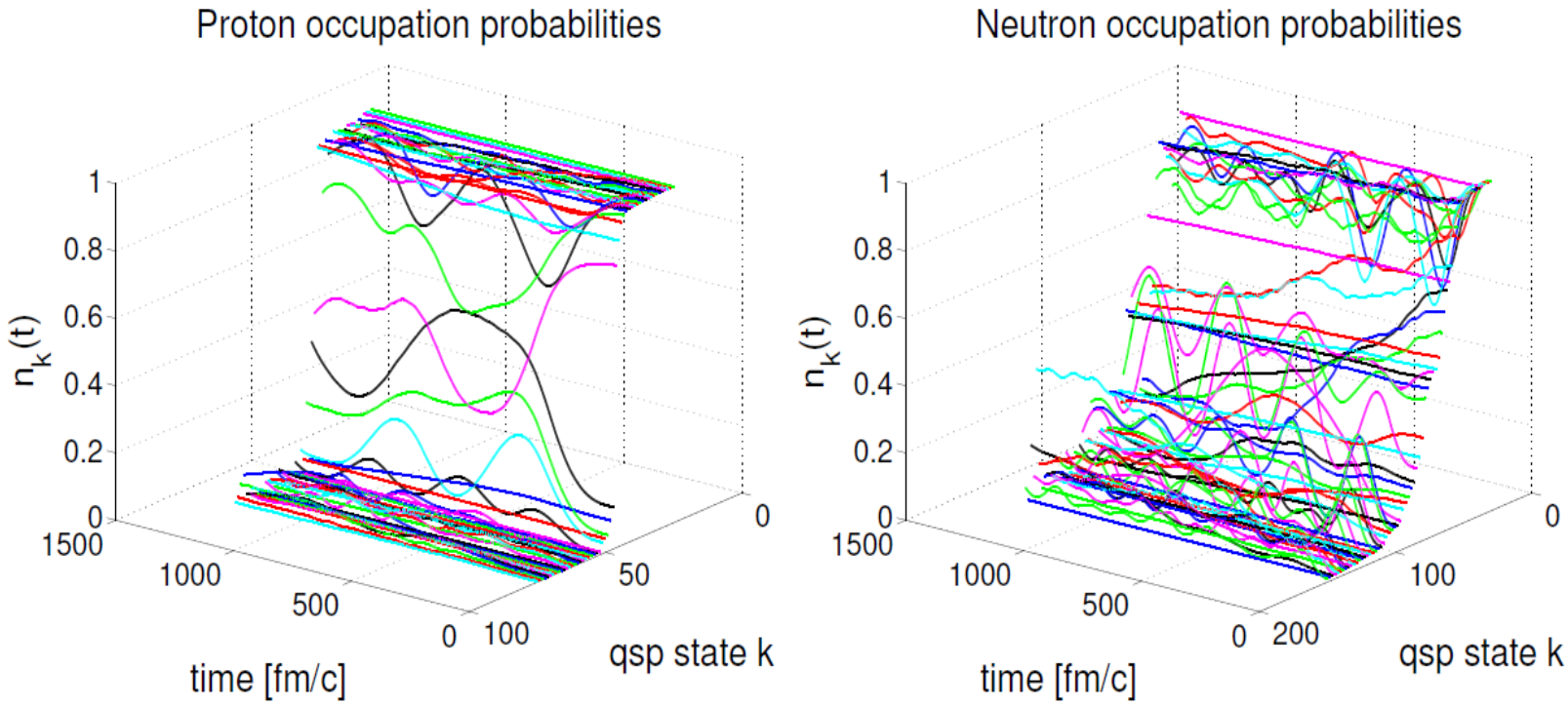


FIG. 1. (Color online) The time-dependent proton and neutron occupation probabilities of a a number of quasiparticle states around the Fermi level for ^{238}U calculated as described in the main text with SLy4.

Box size: 32.5fm (mesh size: 1.25fm)
Energy deposited into a nucleus: 45-50MeV
Adiabatic switching of external perturbation: C*exp[-(t-10)^2/2]
Time window for Fourier transform: 1600 fm/c
Time step: 0.12fm/c -> relative accuracy: 10^(-7)

Coupling to e.m. field:

$$\vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$
$$\vec{B} = \vec{\nabla} \times \vec{A}$$

$$\vec{\nabla}\psi \to \vec{\nabla}_A\psi = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right)\psi$$
$$\vec{\nabla}\psi^* \to \vec{\nabla}_{-A}\psi^* = \left(\vec{\nabla} + i\frac{e}{\hbar c}\vec{A}\right)\psi^*$$
$$i\hbar\frac{\partial}{\partial t}\psi \to \left(i\hbar\frac{\partial}{\partial t} - e\phi\right)\psi$$

which implies that $\vec{\nabla}\psi\psi^* \to \vec{\nabla}\psi\psi^*$.

Consequently the densities change according to:

- density: $\rho_A(\mathbf{r}) = \rho_A(\mathbf{r})$
- spin density: $\vec{s}_A(\mathbf{r}) = \vec{s}(\mathbf{r})$
- current: $\vec{j}_A(\mathbf{r}) = \vec{j}(\mathbf{r}) - \frac{e}{\hbar c}\vec{A}\rho(\mathbf{r})$
- spin current (2nd rank tensor): $\mathbf{J}_A(\mathbf{r}) = \mathbf{J}(\mathbf{r}) - \frac{e}{\hbar c}\vec{A} \otimes \vec{s}(\mathbf{r})$
- spin current (vector): $\vec{J}_A(\mathbf{r}) = \vec{J}(\mathbf{r}) - \frac{e}{\hbar c}\vec{A} \times \vec{s}(\mathbf{r})$
- kinetic energy density: $\tau_A(\mathbf{r}) = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right) \cdot \left(\vec{\nabla}' + i\frac{e}{\hbar c}\vec{A}\right)\rho(\mathbf{r},\mathbf{r}')|_{r=r'}$
  $= \tau(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}\cdot\vec{j}(\mathbf{r}) + \frac{e^2}{\hbar^2c^2}|\vec{A}|^2\rho(\mathbf{r}) = \tau(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}\cdot\vec{j}_A(\mathbf{r}) - \frac{e^2}{\hbar^2c^2}|\vec{A}|^2\rho(\mathbf{r})$
- spin kinetic energy density: $\vec{T}_A(\mathbf{r}) = \left(\vec{\nabla} - i\frac{e}{\hbar c}\vec{A}\right) \cdot \left(\vec{\nabla}' + i\frac{e}{\hbar c}\vec{A}\right)\vec{s}(\mathbf{r},\mathbf{r}')|_{r=r'}$
  $= \vec{T}(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}^T\cdot\mathbf{J}(\mathbf{r}) + \frac{e^2}{\hbar^2c^2}|\vec{A}|^2\vec{s}(\mathbf{r}) = \vec{T}(\mathbf{r}) - 2\frac{e}{\hbar c}\vec{A}^T\cdot\mathbf{J}_A(\mathbf{r}) - \frac{e^2}{\hbar^2c^2}|\vec{A}|^2\vec{s}(\mathbf{r})$

- 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 implementation on JaguarPf (NCCS) and Franklin (NERSC)

Future plans:

- Ultrarelativistic Coulomb excitation (nuclear code)
- Investigation of quantum turbulence (unitary gas code)
- Dynamics of vortices in the inner crust of neutron star (nuclear code)
- Induced fission process (nuclear code)
- Extension to stochastic TDSLDA to include the effects of energy dissipation

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