Real-Time Dynamics of Fermionic Superfluid Systems: from Deterministic Petascale to Stochastic Exascale Simulations

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Near and long term goals:

To describe *accurately* the time-dependent evolution of externally perturbed Fermi superfluid systems (cold atomic clouds, nuclei, neutron star crust, …)

We need 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

Why should one study fermionic superfluidity?

Superconductivity (which turned 100 years old on April 8th, 2011) and superfluidity in Fermi systems are manifestations of quantum coherence at a macroscopic level

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

units (1 eV ~ 10^4 K)

- **What physical problems we are addressing now and in the near future in the petascale regime**
- **What physical problems we plan to attack to solve in the exascale regime**
- **Methods, resources and tools implemented and used so far**
- **New methods which we started implementing with an eye to the exascale regime**
- **What resources we will need in the 3 to 10 year time frame**

Physical systems and processes:

- ✓ Collective states in nuclei
- ✓ Large amplitude collective motion (LACM)
- ✓ Excitation of nuclei with gamma rays and neutrons
- ✓ Coulomb excitation of nuclei with relativistic heavy-ions
- ✓ Nuclear fusion between colliding heavy-ions
- ✓ (Induced) nuclear fission
- ✓ 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
- ✓ Dark solitons and shock waves in collision of fermionic superfluid atomic clouds

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

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

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

- ✓ We developed: the extension of DFT to superfluid systems: (A)SLDA
- ✓ " the extension of SLDA to time-dependent phenomena: TDSLDA
- ✓ " the appropriate accurate numerics for both SLDA and TDSLDA
- ✓ We implemented SLDA/TDSLDA on leadership class supercomputers with massive parallelization, fast I/O, checkpoint/restart, extensive use of the latest advanced visualization techniques for the analysis of results and their presentation

  (the nuclear code is 1,000-2,000 more complex than any existing TDHF code)
- ✓ We have used cca 70M+ CPU hours on Jaguar PF in 2010 and 5M+ CPU hours on Hopper in 2011
- ✓ We established a very accurate relation between *ab initio* QMC results and the energy density functional for the unitary Fermi gas, amply confirmed by experiments
- ✓ We demonstrated the ability to calculate: collective spectra of open shell nuclei, nucleon scattering and capture/knockout, nuclear fission, a limited (so far) number of nuclear reactions
- ✓ We revealed a number of new qualitative physics phenomena

  (superfluid flow at supercritical phenomena, Higgs-Anderson modes, shock waves, dark solitons/domain walls, generation of vortices, vortex rings and their real-time dynamics, the first simulation of the vortex crossing and reconnection and the incipient phases of quantum turbulence in a fermionic superfluid)
- ✓ We have started the study of the feasibility of the stochastic extension of DFT

Capabilities of the SLDA/TDSLDA suite of codes:

(extensively documented in: J. Phys.: Conf. Ser. 125, 012064 (2008), DOE ASCR's GPRA/PMM (Joule) metric for FY 2010, SOM of Science, 332,1288 (2011))

- ✓ full 3D simulations with no symmetry restrictions
- ✓ number of coupled nonlinear time-dependent 3D PDEs for ^{238}U = 546,512
- ✓ high numerical accuracy for spatial derivatives using FFTW
- ✓ for TD high-accuracy and numerically stable 5th order predictor-corrector-modifier algorithm with only 2 evaluations of the rhs per time step and with no matrix operations
- ✓ full diagonalization of Hermitian matrices 409,600x409,600 on JaguarPF (for ^{238}U)
- ✓ Performance:

Static: ins/wall-time = 1.37e19/18,393= 7.46e14, flops/wall-time=9.42e16/18,393= 5.12e13
PEs = 217,800

TD: ins/wall-time = 7.11e17/2,031= 3.50e14, flops/wall-time= 1.89e16/2,031= 0.93e13
PEs = 136,628

- ✓ excellent weak and strong scaling
- ✓ very fast I/O and checkpoint/restart capabilities
- ✓ nuclear volumes (so far) of the order of (L = 40 to 80 fm)^3, larger volumes possible
- ✓ in such volumes one can describe cca 42,000 neutrons at saturation density
- ✓ capable of simulating up to times of the order of 10^{-18} s (a few million time steps)
- ✓ codes written in Fortran90, with many components in C

n := lattice points in one dimension

$$\psi_{\mathbf{i}}(\vec{x}) = \begin{pmatrix} u_{\mathbf{i}}(\vec{x}) \\ v_{\mathbf{i}}(\vec{x}) \end{pmatrix} \rightarrow \begin{pmatrix} u_{\mathbf{i}}(x,y,t)\exp(ik_{\mathbf{i}}z) \\ v_{\mathbf{i}}(x,y,t)\exp(ik_{\mathbf{i}}z) \end{pmatrix}$$

$$m \sim n^3$$

Computation	FP Operations	Data
general solver *	$O(n^9)$	$O(n^6)$
homogeneous solver %	$O(n^6)$	$O(n^6)$
time evolution #	$56mO(mlog_2(m))$	$O(n^6)$

*) per self-consistent iteration; convergence in ~ 10 to 150 iterations
%) solver spatial symmetry to reduce the complexity per iteration; perfect strong scaling
#) per time step ; O(1000) to O(1000000) time steps depending

I/O	Data	Other
Observables	$O(n^3)$	per output event; 10 to 100 ts / output; O(100K) ts ; (4,11) observables for (gases,nuclei); double precision type
Checkpoint / restart	$O(n^6)$	at most 1 cp, 1 rs per execution; scaling constant of (22,44) for (gases,nuclei); double precision complex type

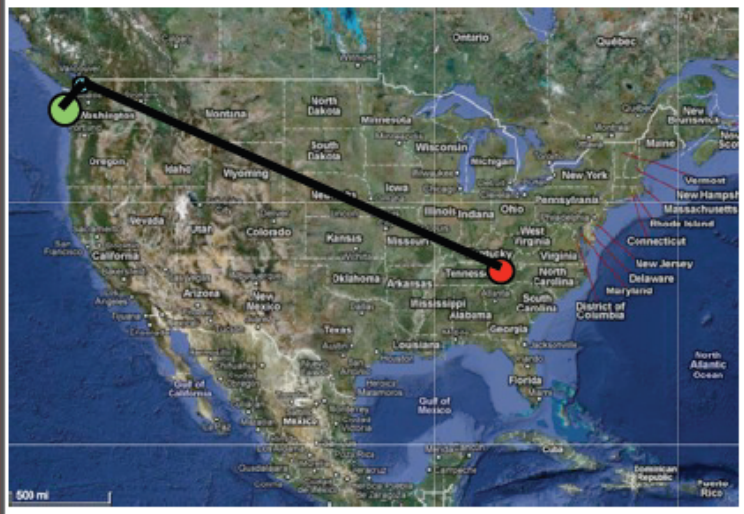
--we accumulate all observables for ~ 10 output events in a single file; number of files and overall amount of stored observable data clearly grows w/ number of time steps

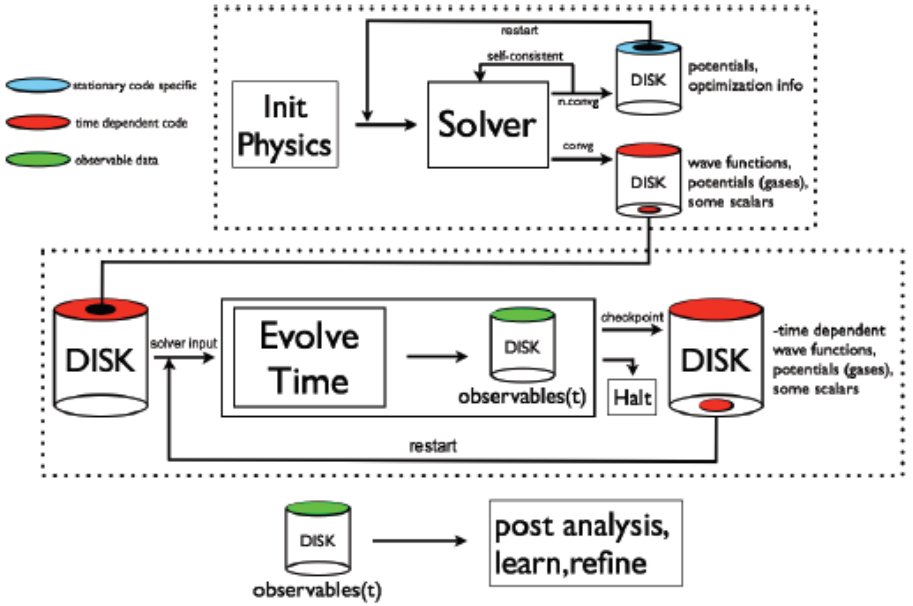
--these are usually O(TB)

Wednesday, June 22, 2011

From a talk given by K.J. Roche on 6/22/2011

O() Data Magnitudes: Supercomputers to Laptops





STAGE	k * O() BYTES	TYPE
problem instantiation	**2^10 (k = 1)**	.txt
program text	**2^40 (k = 100)**	binary
ground state wavefunctions	**2^40 (k = 10)**	.bin (.txt, .dat)
checkpointing / progress	**2^40 (k = 10)**	.bin (.dat)
observables	**2^30 (k = 100)**	.txt, .dat, .bin, .silo
movies , plots, etc	**2^20 (k = 10)**	.jpeg, .eps, .m4v

Wednesday, June 22, 2011

From a talk given by K.J. Roche on 6/22/2011

Application	TD-SLDA	POP	LS3DF	Denovo
Problem	***Q2 : Nuclear 196W study*** • Z=74, N=124 • 40 x 40 x 40 lattice • 7,466 p-quasiparticle • 8,946 n-quasiparticle • 200 time steps • 0.75fm spacing • 100MeV cutoff • n = 256000 ***Q4 : Nuclear 238U study*** • Z=92, N=146 • 40 x 40 x 64 lattice • 67,118 p-quasiparticle • 69,508 n-quasiparticle • 200 time steps • 1.25fm spacing • 100MeV cutoff • n = 409600	***3 simulated days, ocean-only model*** • 0.1-degree tripole global grid (3600×2400) • 42 vertical levels • 10 minute time steps • High-frequency output time slice	***Self-consistent DFT calculation for ZnO nanorod*** • 2776 atoms • 24220 valence electrons, d-electrons in valence band • 720×300×300 numerical grid	***Q2 : Full Core EDF PWR900 benchmark*** • 17x17 fuel assemblies • 17x17 fuel pins per assembly • 2x2 cells per pin cell • 3 fuel enrichments • 45 homogenized pin cell materials per assembly • 135 different pin cell materials • 233,858,800 (578x578x700) cells • 168 angles, 1 moment, 2 energy (fast and thermal) groups • 7.86×10^{10} total unknowns ***Q4 : Full Core EDF PWR900 benchmark*** • 168 angles, 1 moment, 44 energy (fast and thermal) groups • 1.73×10^{12} total unknowns
Hardware (cores)				
Q2	(s)73,728; (td)16,414	4,800	43,200	17,424
Q4	(s)217,800; (td)136,628	9600	86,400	112,200
Time (seconds)				
Q2	(s)6538.5, (td)2084.4	957.8	13,932	11,260.8
Q4	(s)18393.2, (td)2031.5	290.3	5328	1121.6
Metric target	(s)Q2:Q4 efficiency ≥ 1.0 ; (td)Q2:Q4 time ≥ 1.0	Q2:Q4 time ≥ 2.0	Q2:Q4 time ≥ 2.0	Q2:Q4 efficiency ≥ 1.0
Metric result	(s)Q2:Q4 efficiency = 2.11 (td)Q2:Q4 time = 1.026	Q2:Q4 time = 3.2992	Q2:Q4 time = 2.6	Q2:Q4 efficiency = 31

From a talk given by K.J. Roche on 6/22/2011

What is Density Functional Theory (DFT)?

Kohn-Sham theorem (1965)

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

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

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

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, and Galilean invariance determine the functional

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

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

$$\nu_c(\vec{r}) = \sum_{0<E<E_c} u_k(\vec{r})v_k^*(\vec{r})$$

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

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

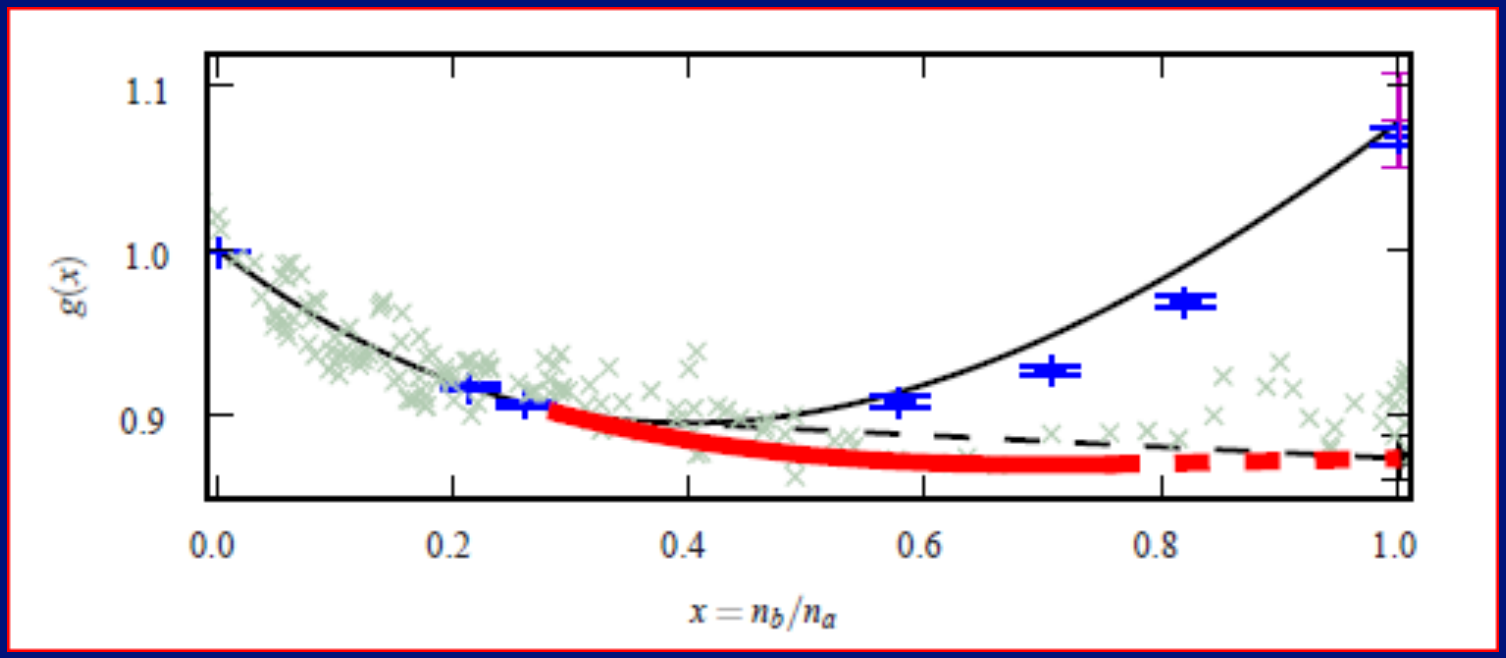
$$\begin{cases} [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu]\mathrm{u}_\mathrm{i}(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)]\mathrm{v}_\mathrm{i}(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{u}_\mathrm{i}(\vec{r},t)}{\partial t} \\ [\Delta^*(\vec{r},t) + \Delta^*_{ext}(\vec{r},t)]\mathrm{u}_\mathrm{i}(\vec{r},t)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

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

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%				

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

EOS for spin polarized systems



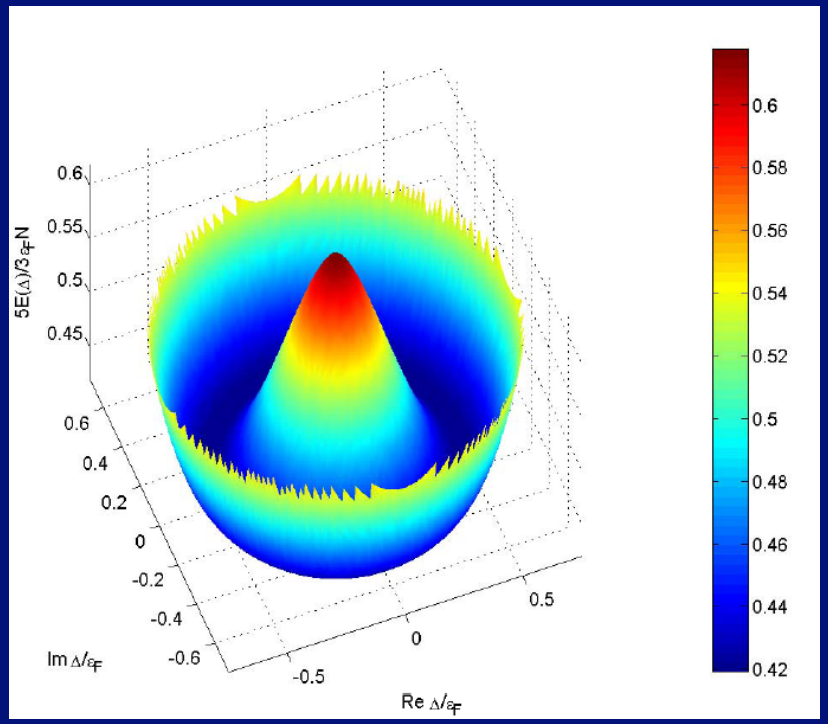
Red line: Larkin-Ovchinnikov phase (unitary Fermi supersolid)

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)

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



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

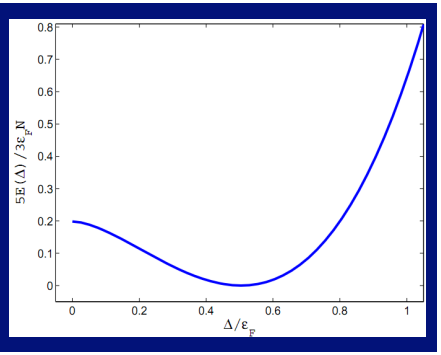
$$m\dot{\vec{\mathrm{v}}} + \vec{\nabla}\left\{\frac{m\vec{\mathrm{v}}^2}{2} + \mu\left[n\right]\right\} = 0$$

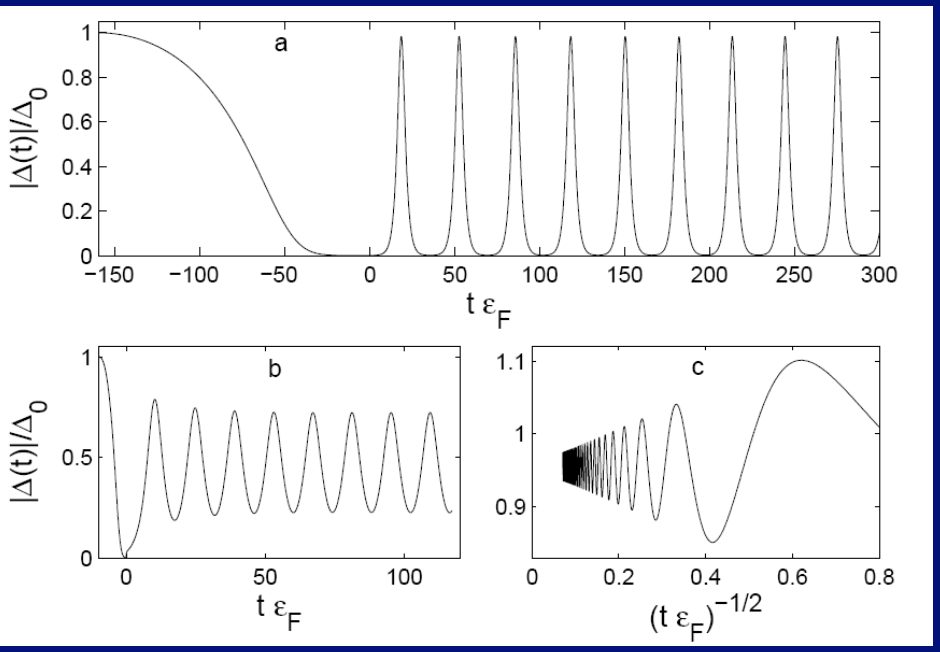
Two-fluid hydrodynamics

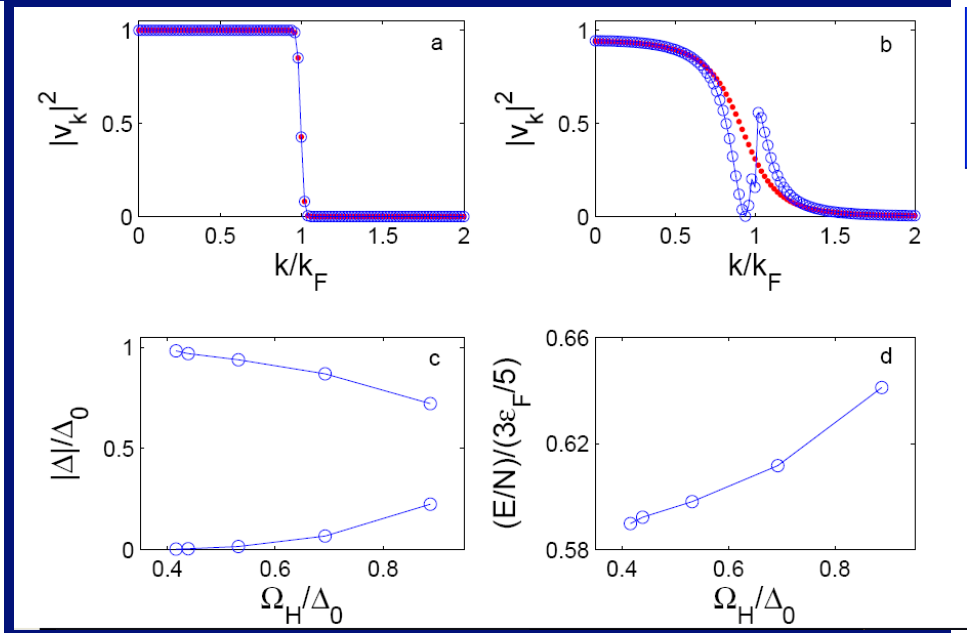
$$i\hbar\dot{\Psi}(\vec{r},t) = -\frac{\hbar^2}{4m}\Delta\Psi(\vec{r},t) + U\left(\left|\Psi(\vec{r},t)\right|^2\right)\Psi(\vec{r},t)$$

Landau-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

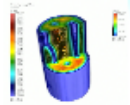
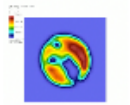
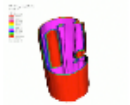
- None of these modes can be described either within two-fluid hydrodynamics or Landau-Ginzburg like approaches

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

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

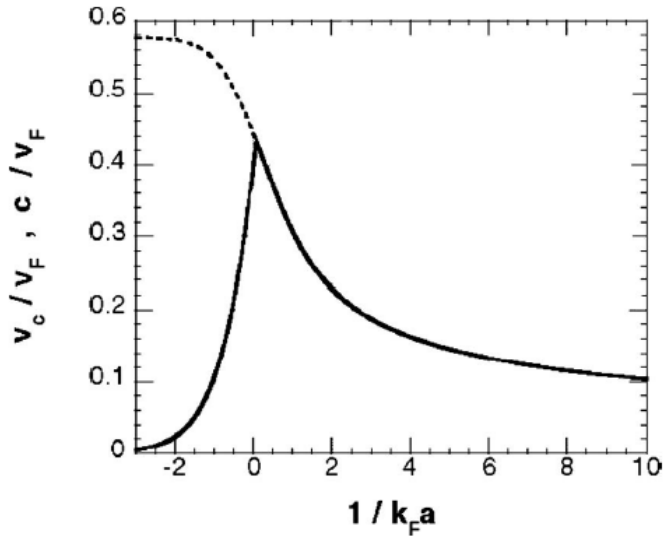


FIG. 20. Landau's critical velocity (in units of the Fermi velocity) calculated along the crossover using BCS mean-field theory. The critical velocity is largest near unitarity. The dashed line is the sound velocity. From Combescot, Kagan, and Stringari, 2006.

$$c_s = 0.370(5)\mathrm{v}_\mathrm{F}$$

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

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

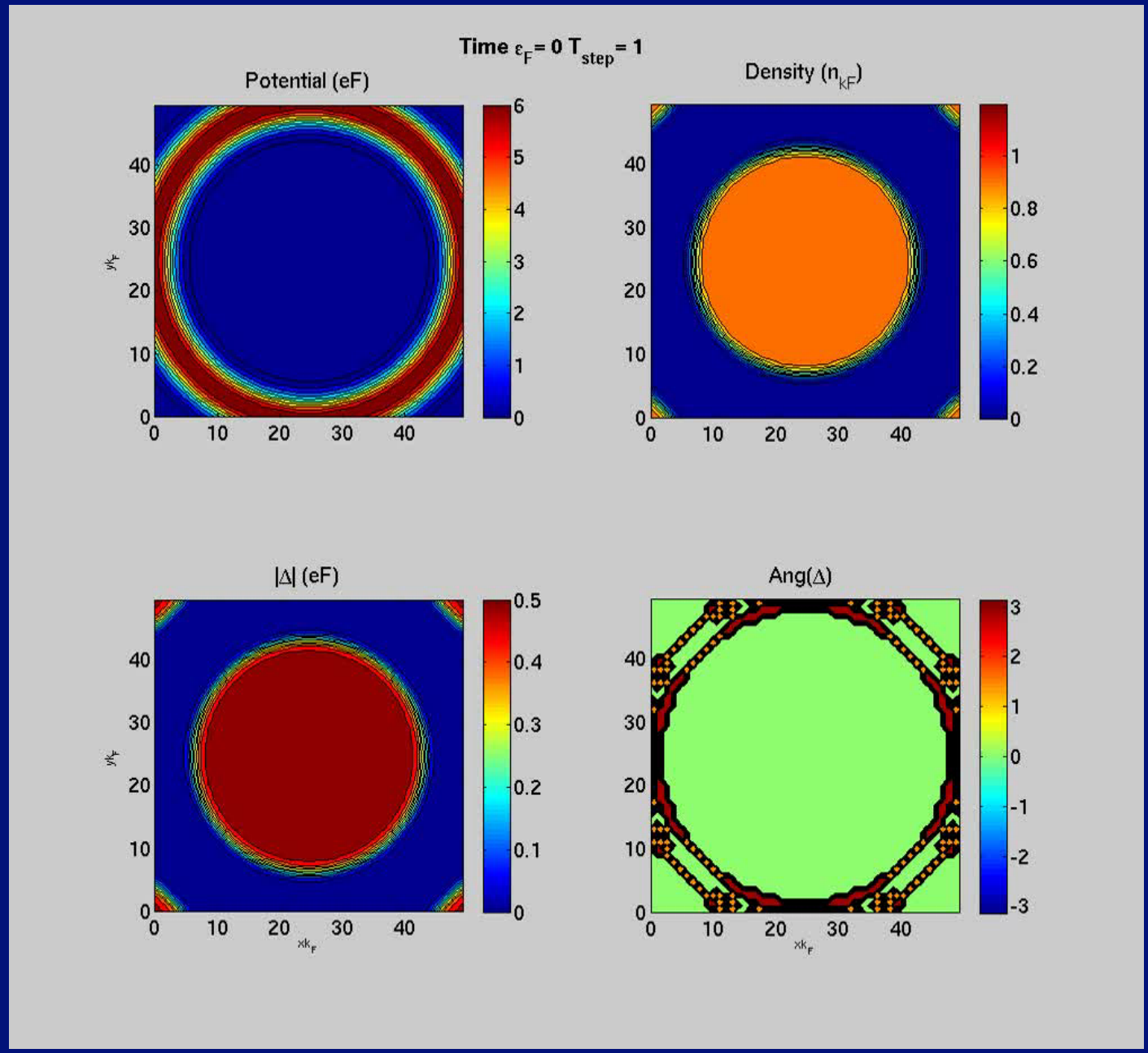
Values obtained using QMC data

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

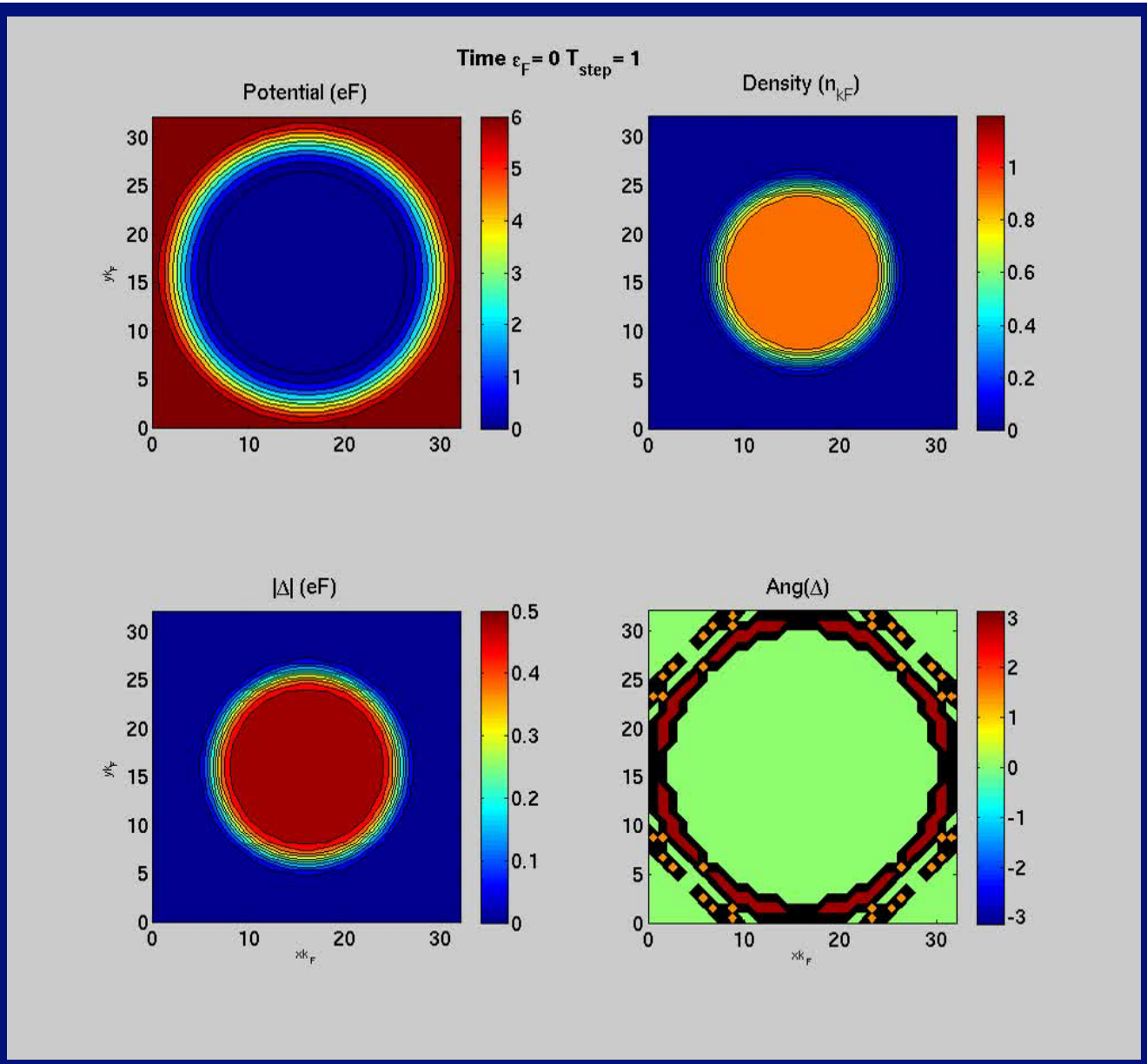
$$\mathrm{v}_c \approx 0.25(3)\mathrm{v}_F$$

Miller et al. (MIT, 2007)

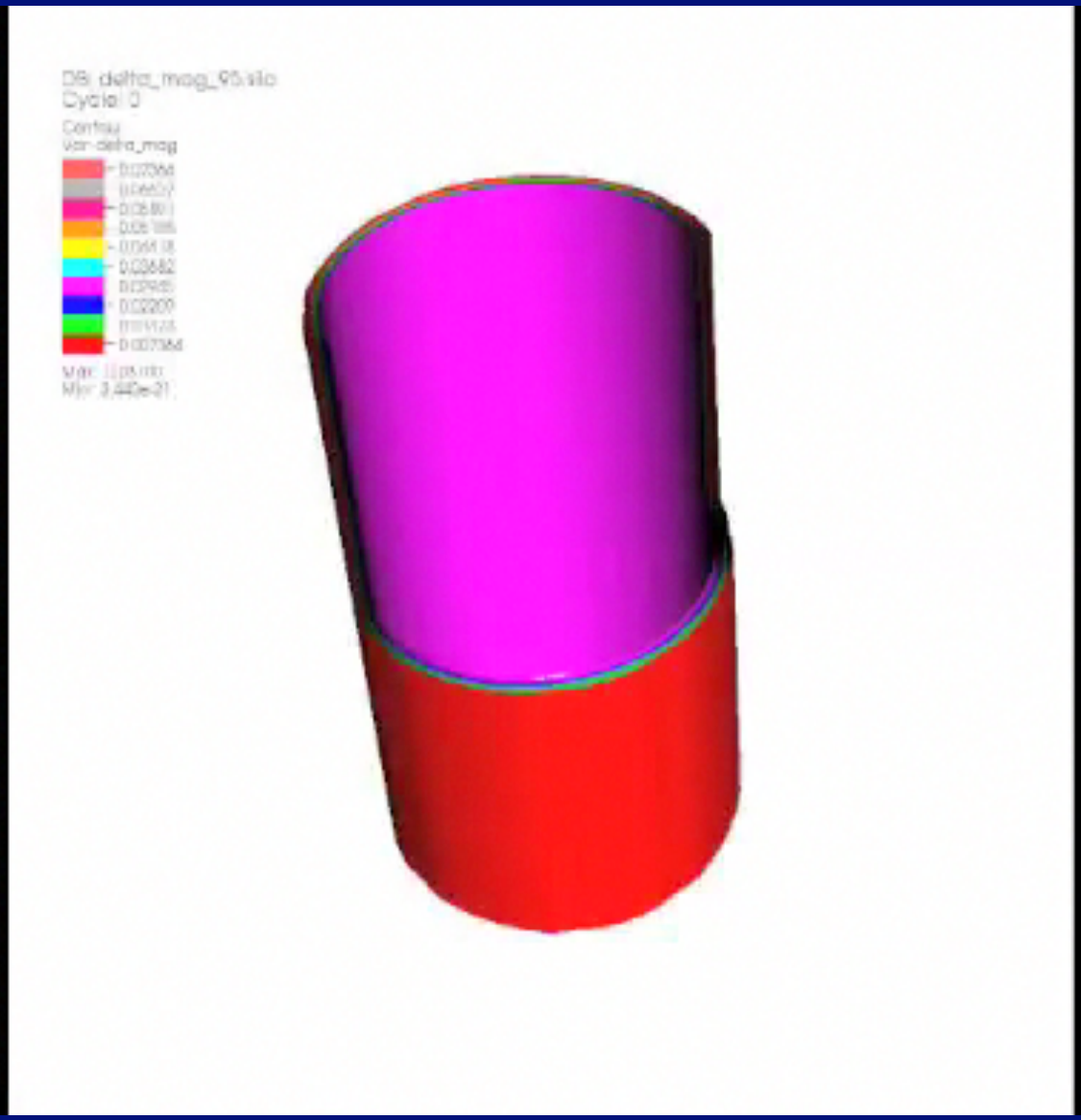
Study based on BCS/Leggett approximation


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

Movie


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

Movie



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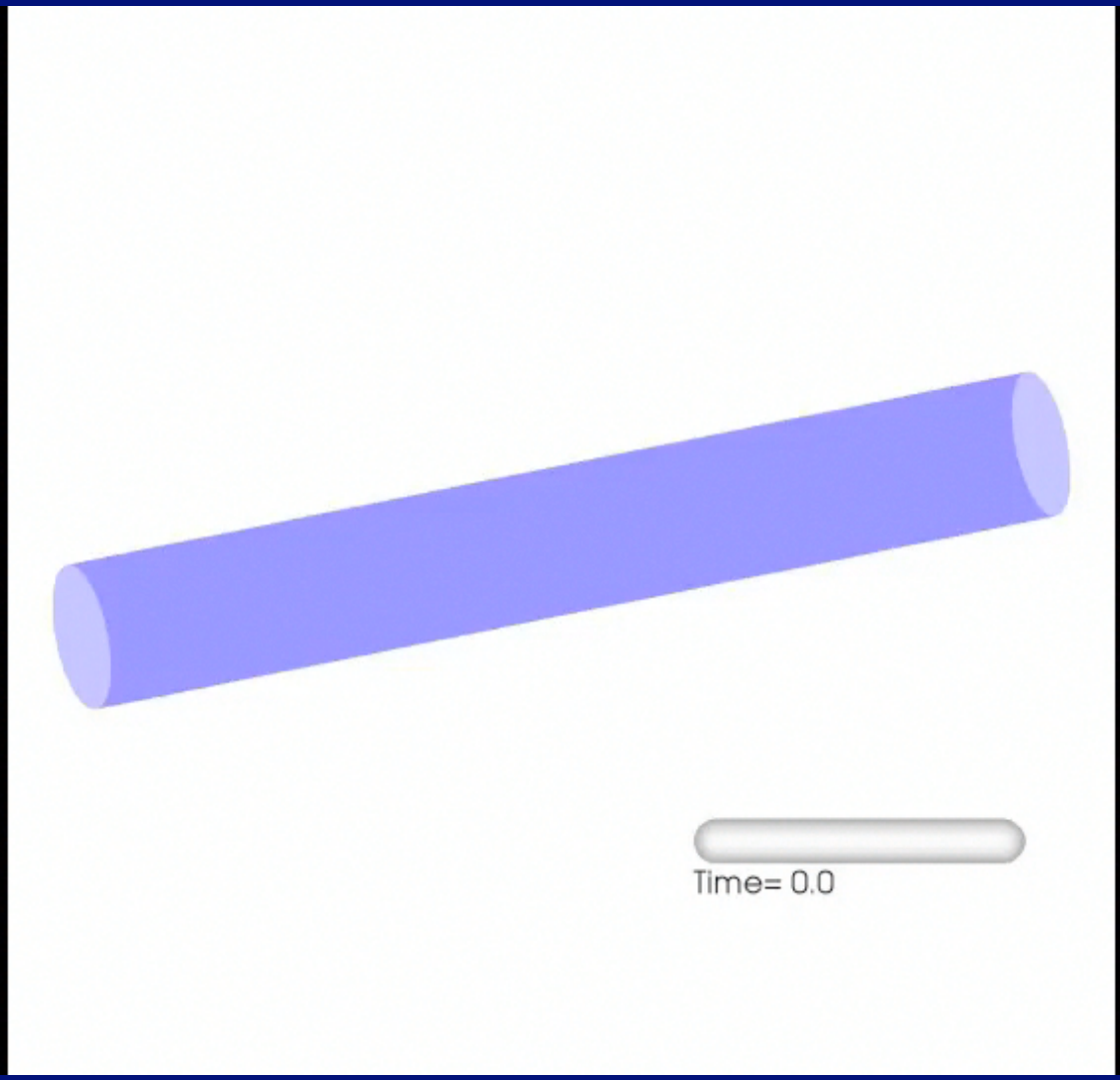

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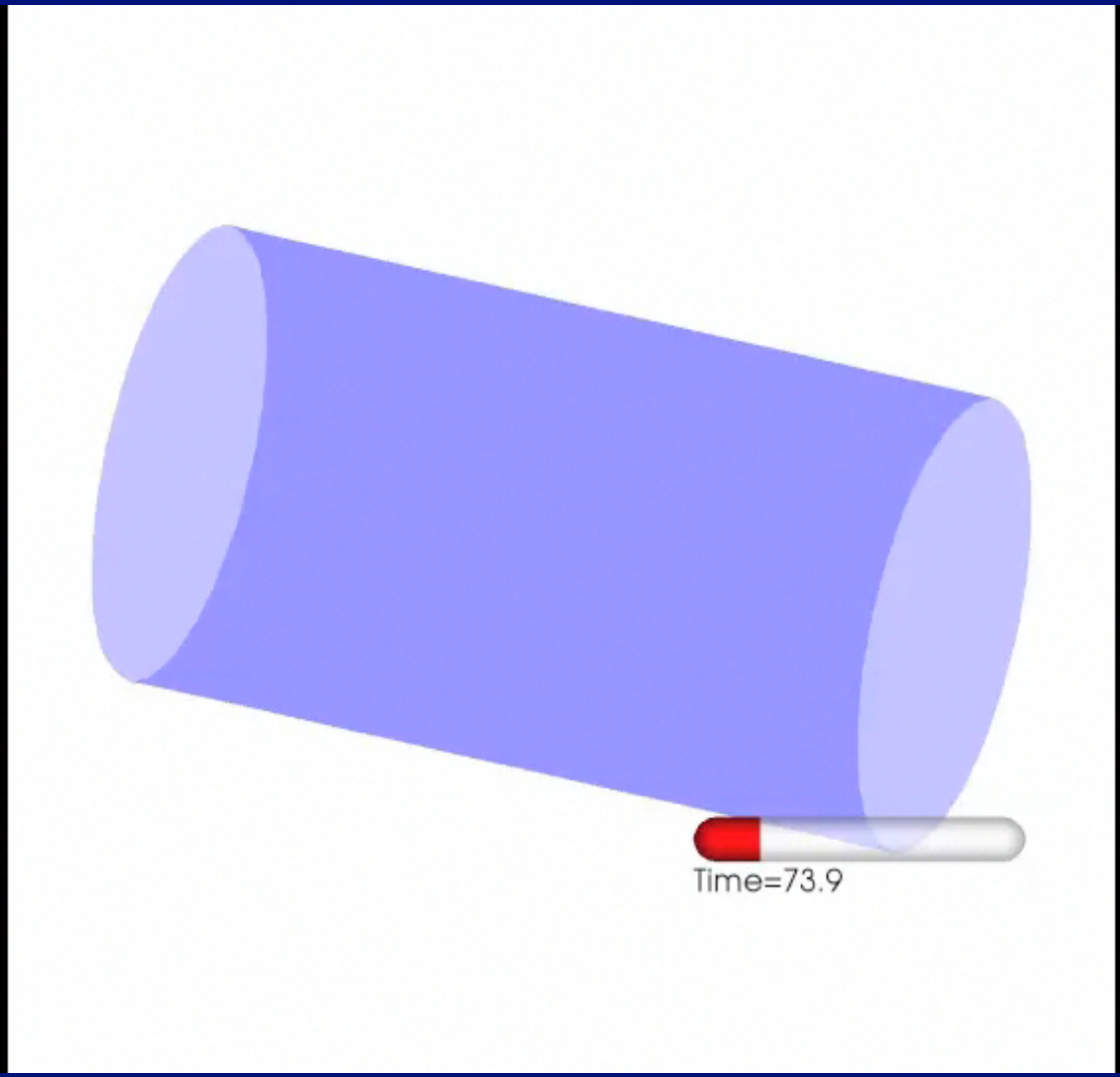

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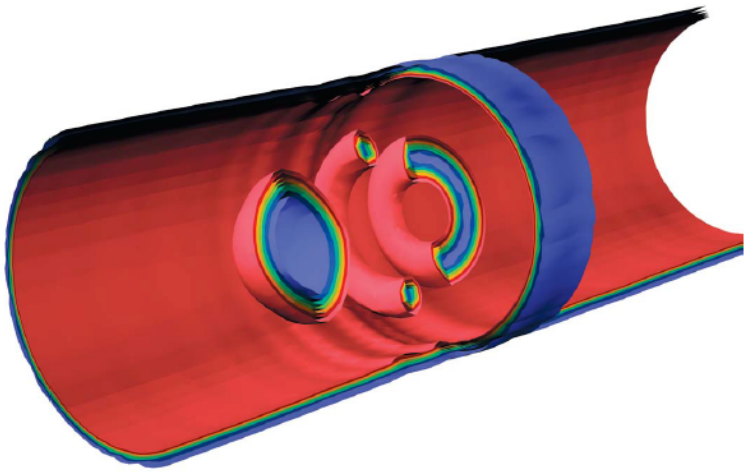


Fig. 2. A spherical projectile flying along the symmetry axis leaves in its wake two vortex rings.

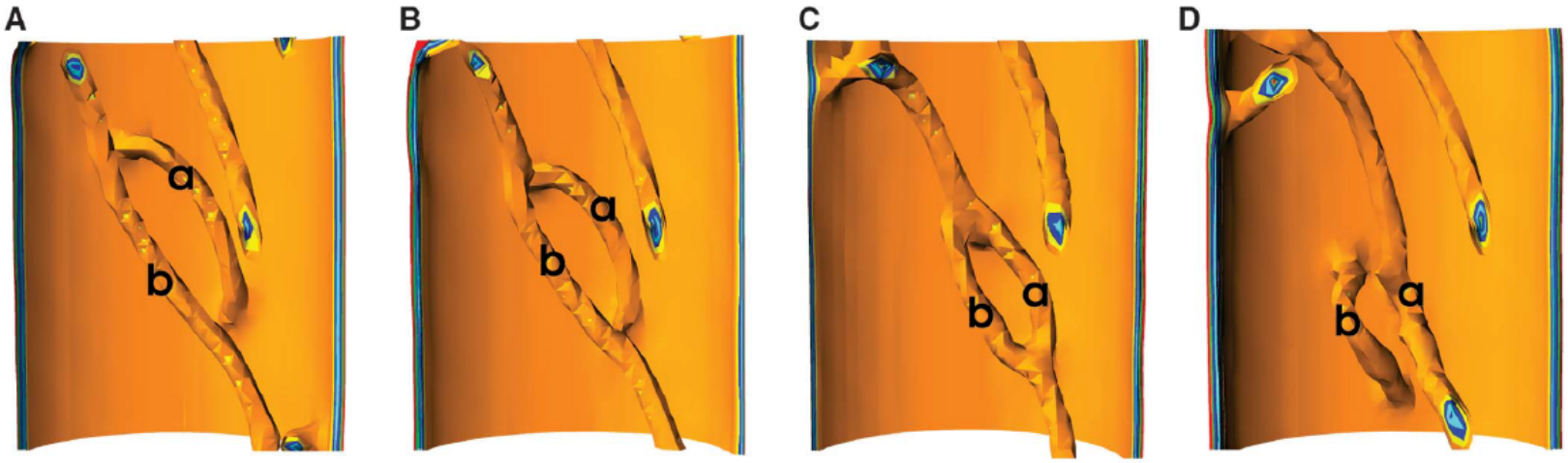
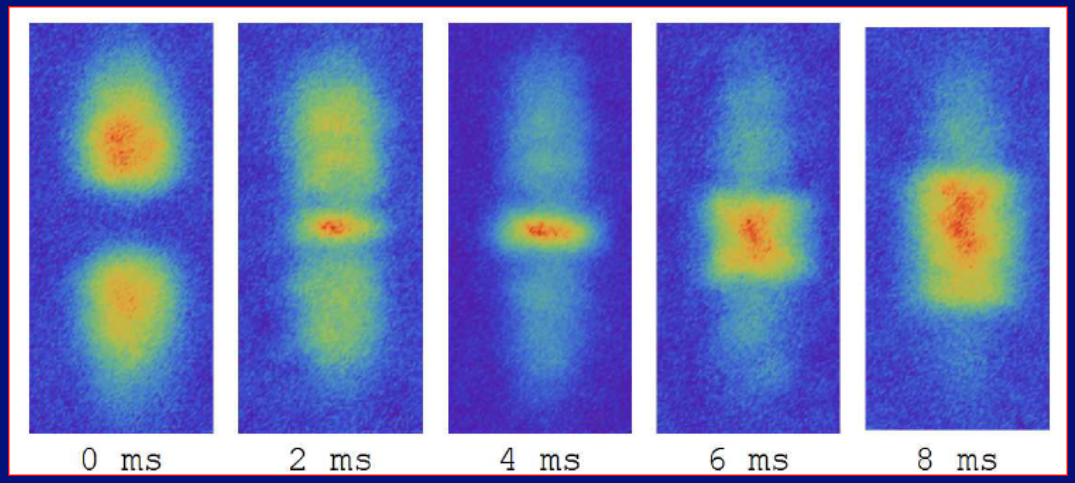
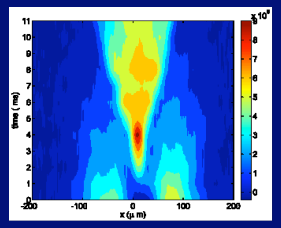


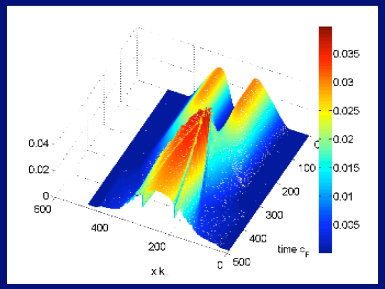
Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b)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





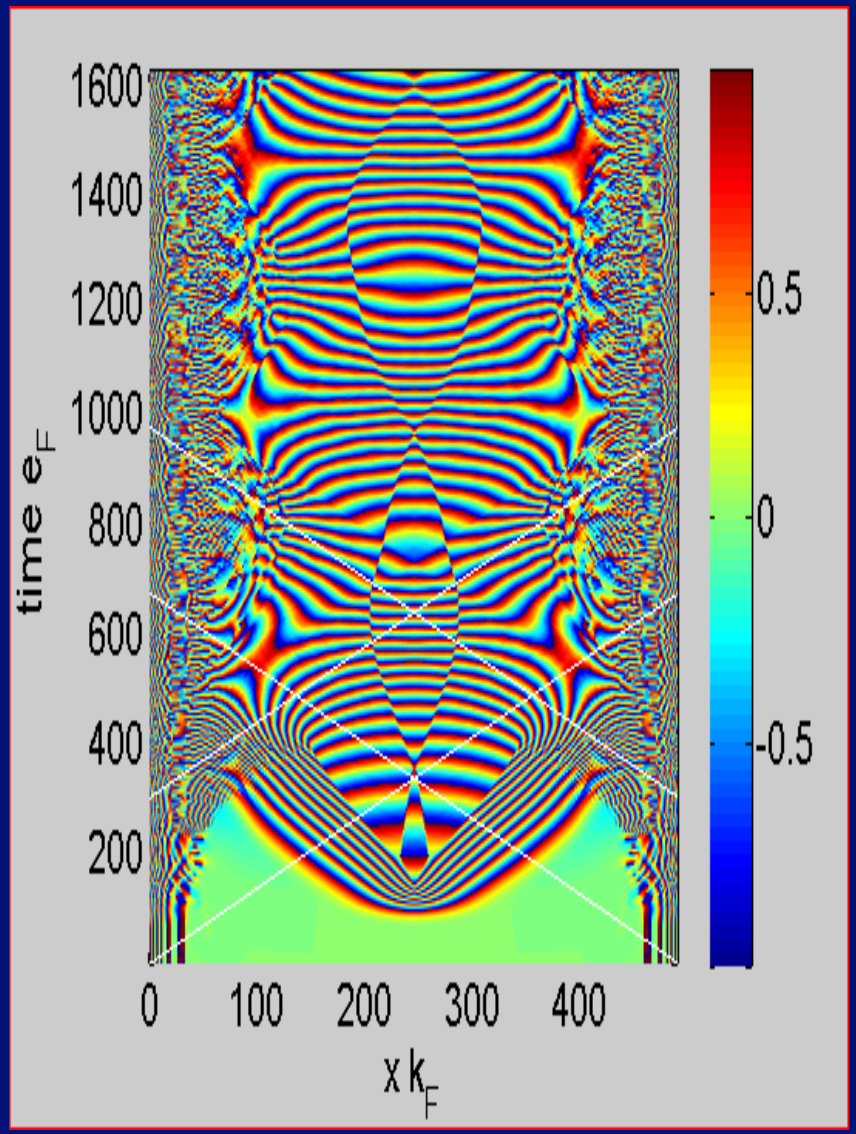
Observation of shock waves in a strongly interacting Fermi gas

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

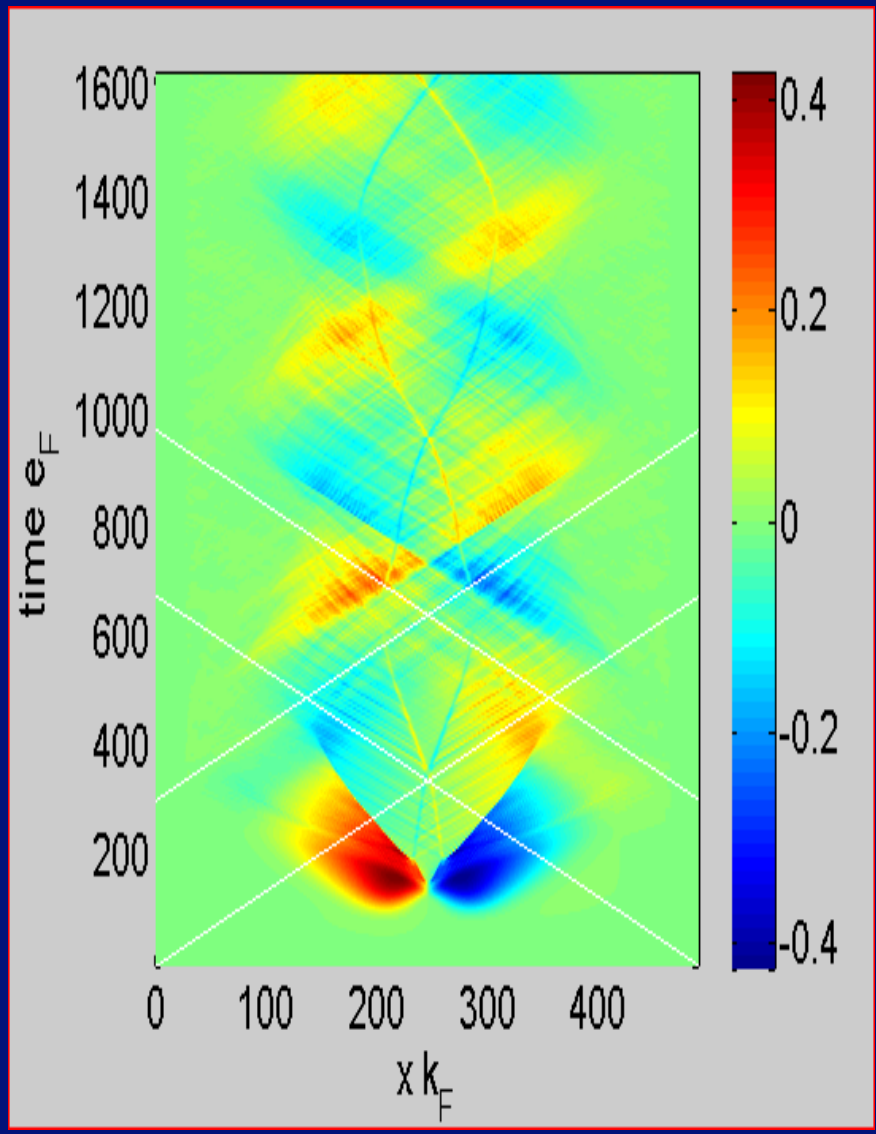


Number density of two colliding cold Fermi gases in TDSLDA

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



Phase of the pairing gap normalized to



Local velocity normalized to Fermi velocity

The main 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.)

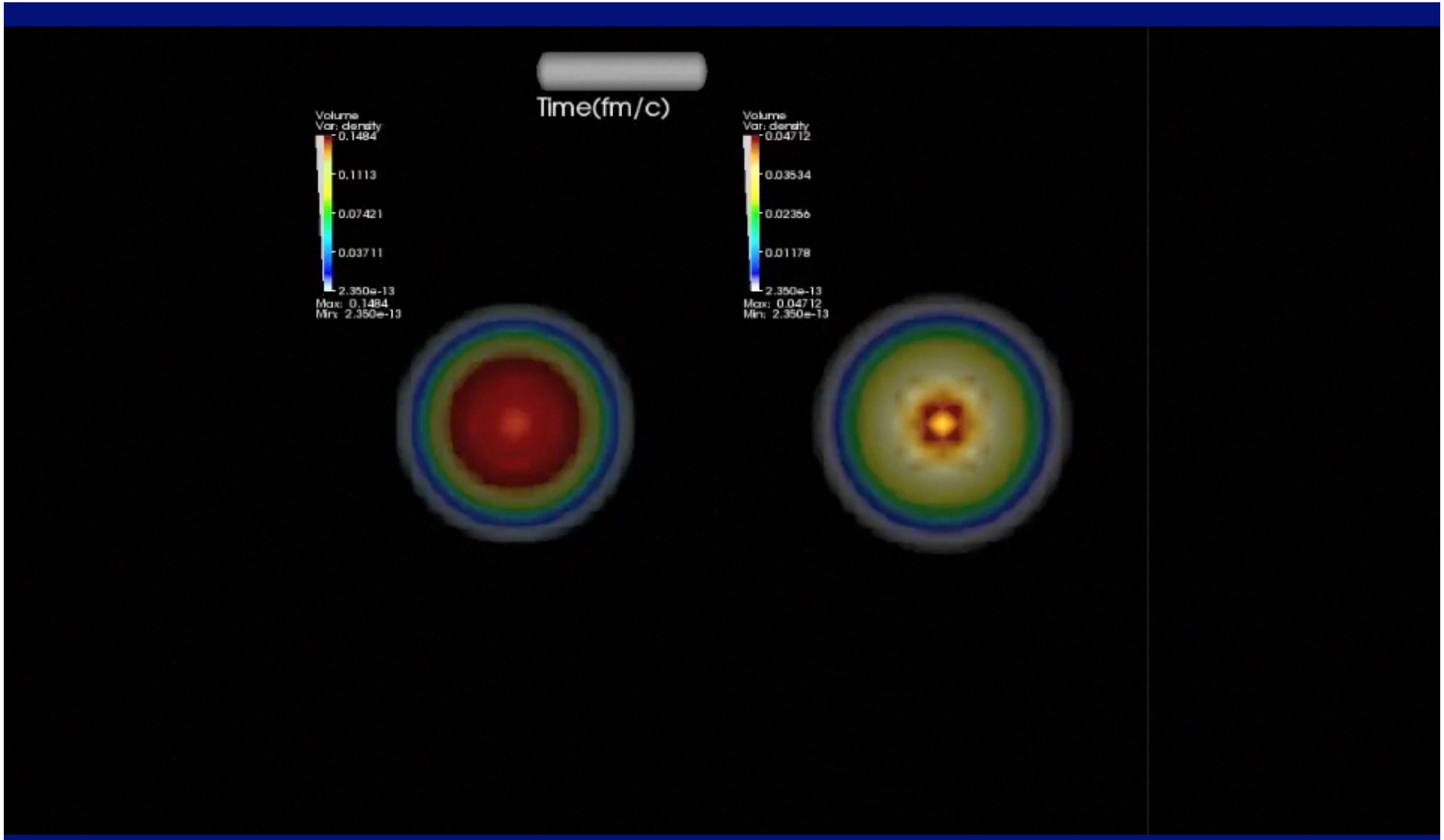
$$\varepsilon_S\left[\rho_n, \rho_p, \nu_p, \nu_n\right] = g(\rho_p, \rho_n)[|\nu_p|^2 + |\nu_n|^2] + f(\rho_p, \rho_n)[|\nu_p|^2 - |\nu_n|^2] \quad \frac{\rho_p - \rho_n}{\rho_p + \rho_n}$$

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

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

Nuclear TDSLDA equations

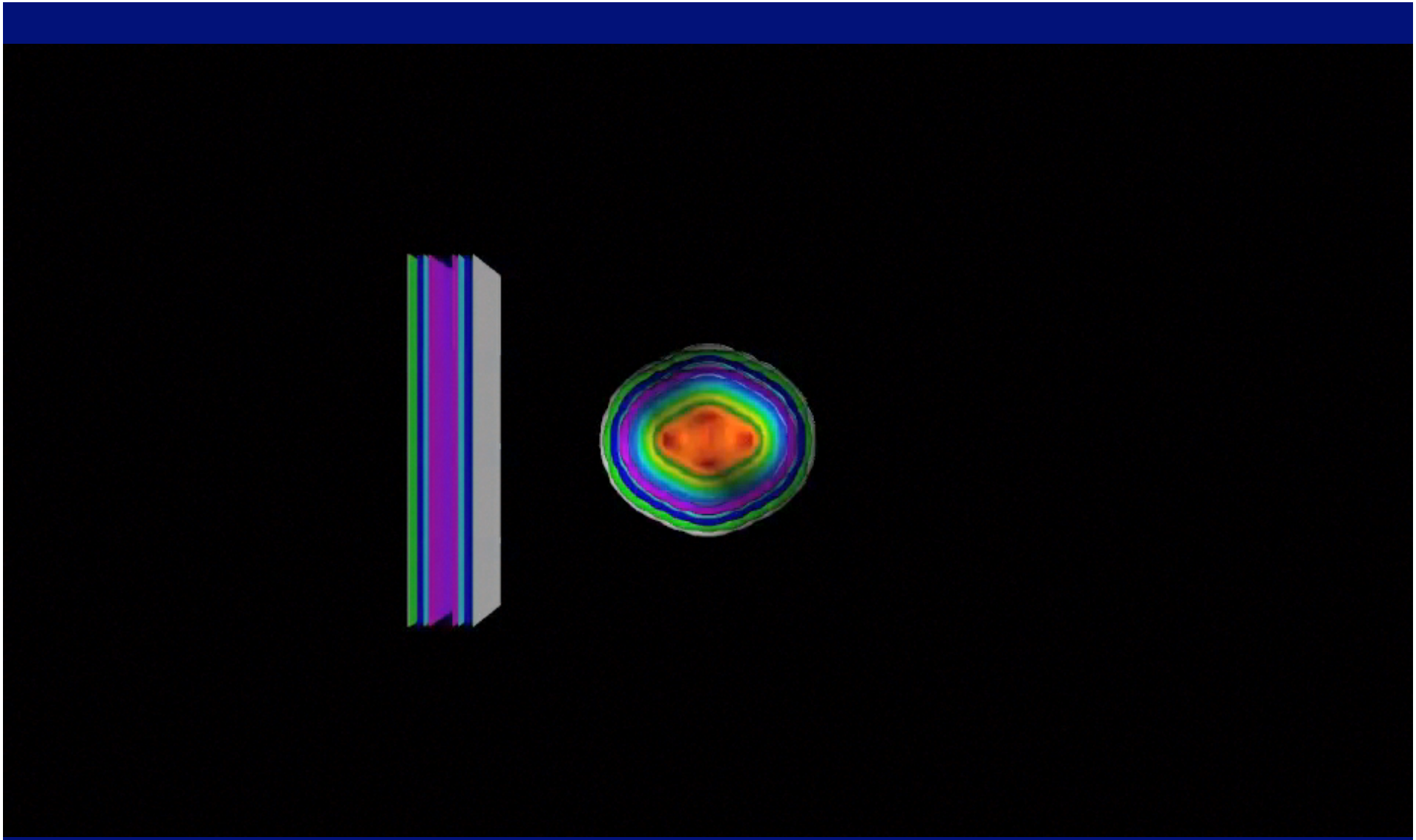
$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{h}_{\uparrow\uparrow}(\vec{r},t)-\mu & \hat{h}_{\uparrow\downarrow}(\vec{r},t) & 0 & \Delta(\vec{r},t)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



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

Movie

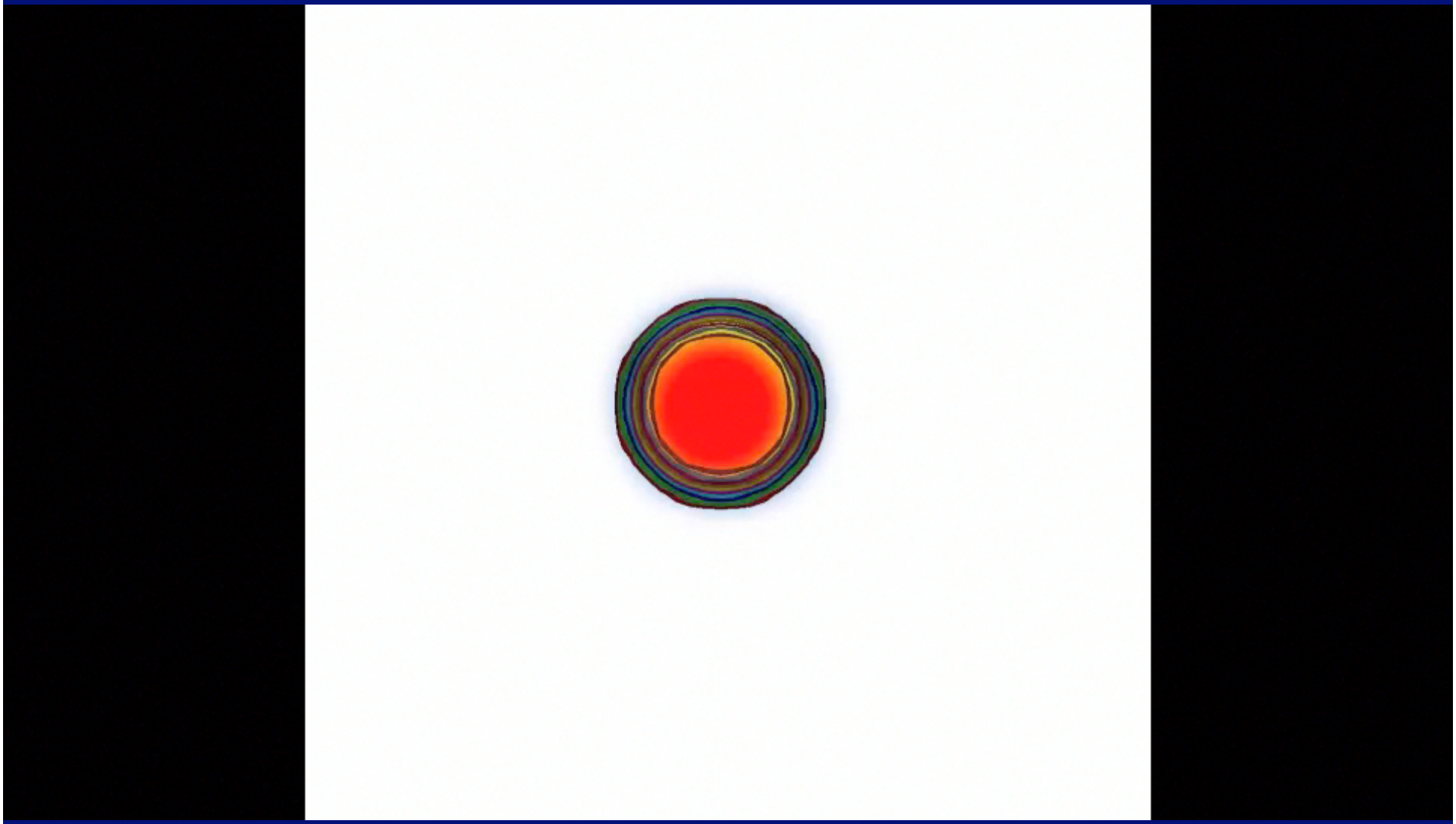
I. Stetcu, A. Bulgac, P. Magierski, K.J. Roche



Neutron scattering of ^{238}U computed in TDSLDA

I. Stetcu, A. Bulgac, P. Magierski, K.J. Roche

Movie



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

I. Stetcu, A. Bulgac, P. Magierski, K.J. Roche

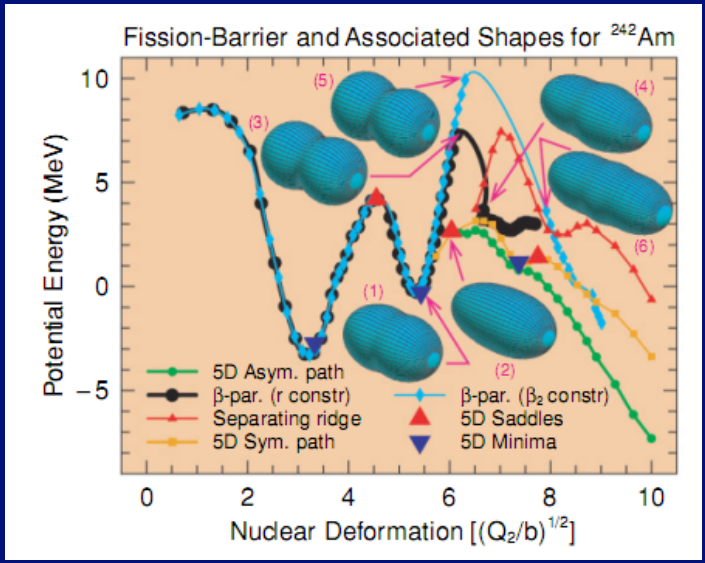
Movie

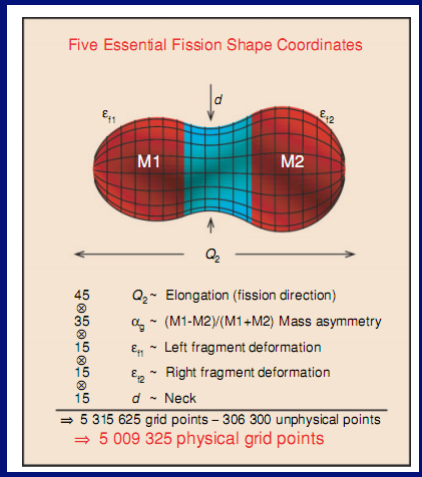
Why we need exascale and the extension of the TDSLDA to the Stochastic TDSLDA?

Nuclear LACM and fission studies using a GCM type of many-body wave function:

$$\int \prod_{i=1}^{n} dq_i \Phi_{\text{Coll.}}(q_1,\ldots,q_n)\Psi_{\text{Slater det.}}(x_1,\ldots,x_A,\{q_1,\ldots,q_n\})$$

P. Moller and collaborators need more than 5,000,000 shapes in a five dimensional space.



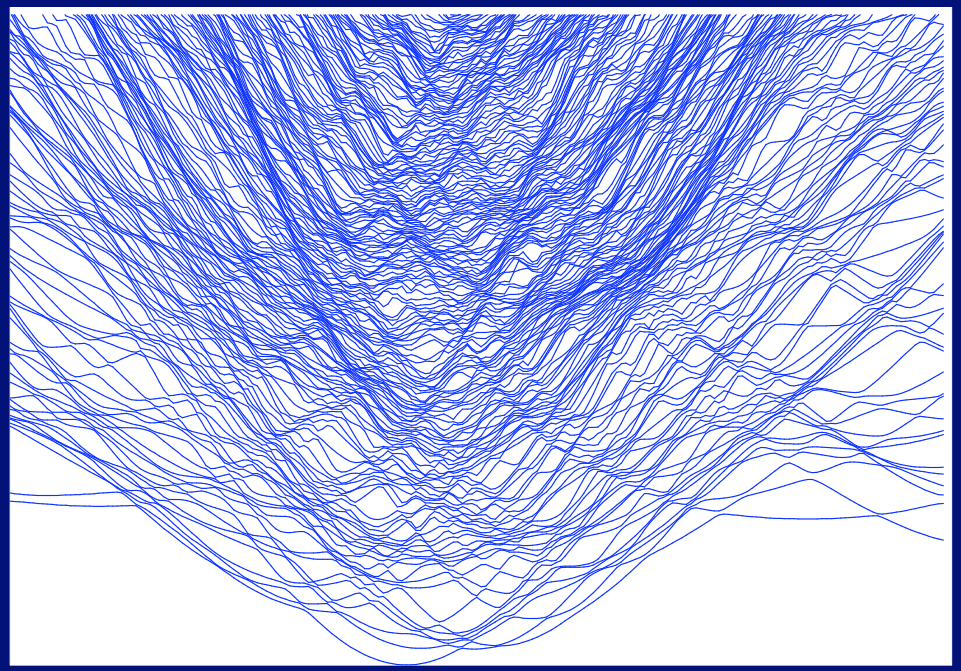


P.Moller *et al.* Phys. Rev. C 79, 064304 (2009)

Why this is inadequate? (just a few reasons)

- **Many more collective degrees of freedom needed, theoretical accuracy hard to quantify**
- **Only one potential energy surface, while many are needed**
- **Inertia tensor difficult to calculate, ambiguous prescriptions**
- **Adiabaticity is definitely violated, unclear how to describe dissipation within LACM**
- **Theory becomes impractical (even at exascale) for many collective degrees of freedom**

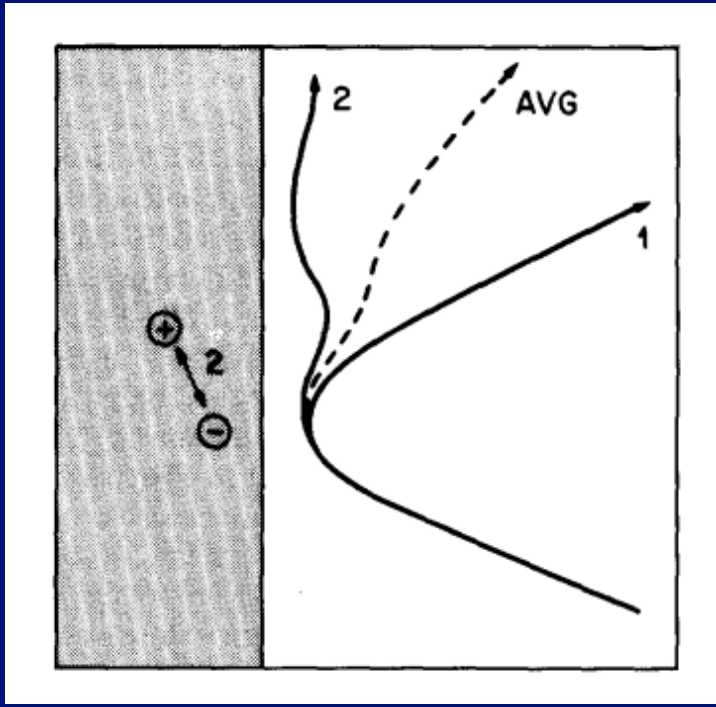
We need to consider the generic situation with multiple potential energy surfaces.



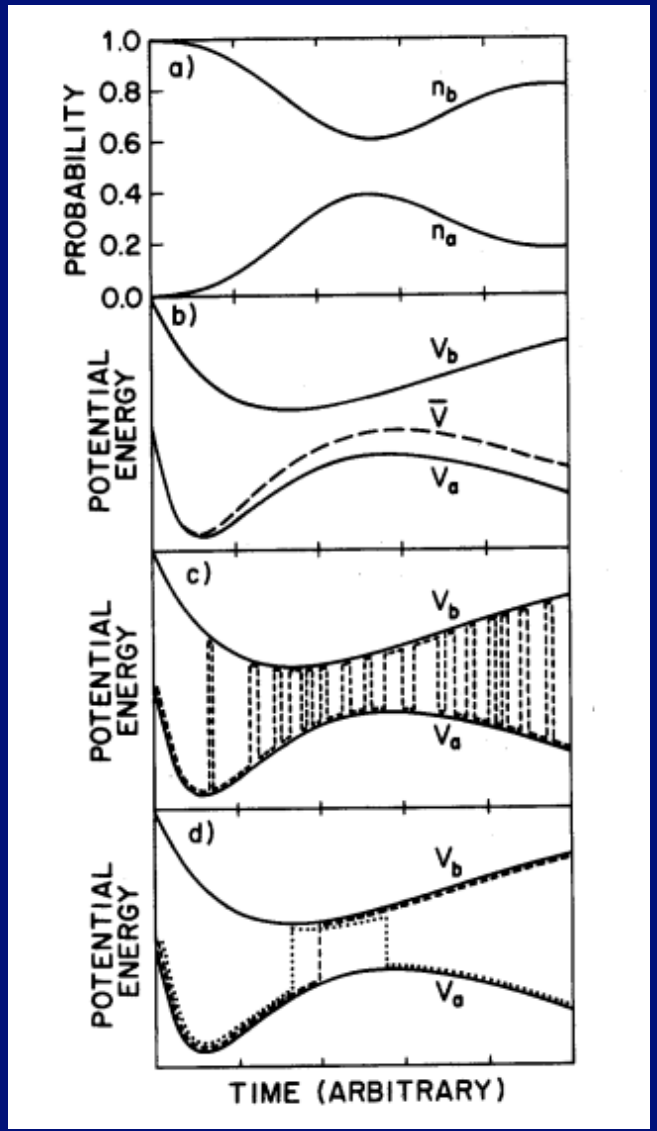
Energy

Deformation

John C. Tully suggested the following recipe for condensed matter and chemistry applications
J. Chem. Phys. 93, 1061 (1990)



$$\psi(\vec{r},\vec{R},t) = \sum_i c_i(\vec{R},t)\varphi_i\left(\vec{r}\,\middle|\,\vec{R}\right)$$



Evolution operator of an interacting many-body system

(after a Trotter expansion and a Hubbard-Stratonovich transformation, from Negele and Orland, *Quantum Many-Particle Systems*, 1988)

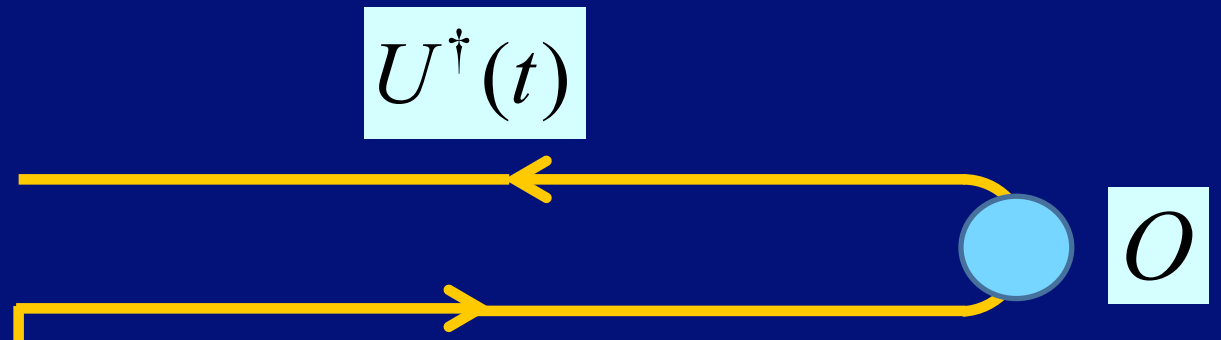
$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i\frac{\Delta t}{2} \sum_{abcd} \sigma_{ab}(n) V_{abcd} \sigma_{cd}(n) \right] \times$$

$$\exp\left[i\Delta t \sum_{ab} \left(T_{ab} + \sum_{cd} V_{abcd} \sigma_{cd}(n) \right) \alpha_a^\dagger \alpha_b \right]$$

This representation is not unique, the one-body evolution operator is arbitrary!!!
Kerman, Levit, and Troudet, Ann. Phys. 148, 443 (1983)

This looks much worse that the infamous fermion sign problem!!!

What we need is a bit more complicated, to simulate dynamics along the Keldysh-Schwinger complex time-ordered contour



$$\rho_0 = \frac{\exp(-\beta H_0)}{Z}$$

Initial state preparation (equilibrium at finite T)

$$U(t) = T_t \exp\left[-i\int_0^t dt H(t)\right]$$

$$H(t) = H_0 + V_{ext}(t), \qquad t>0$$

$$i\hbar\frac{\partial\rho(t)}{\partial t} = \left[H(t),\rho(t)\right], \qquad \rho(0)=\rho_0$$

$$O(t) = \mathrm{Tr}\left[O\rho(t)\right] = \mathrm{Tr}\left[\rho_0 U^{\dagger}(t) O U(t)\right]$$

Here is how this can be done and has already been implemented numerically on Hyak-UW (MRI-NSF funded cluster, Intel chips, 1120 cores, 3Gb RAM/core)

We place several fermions on a square lattice

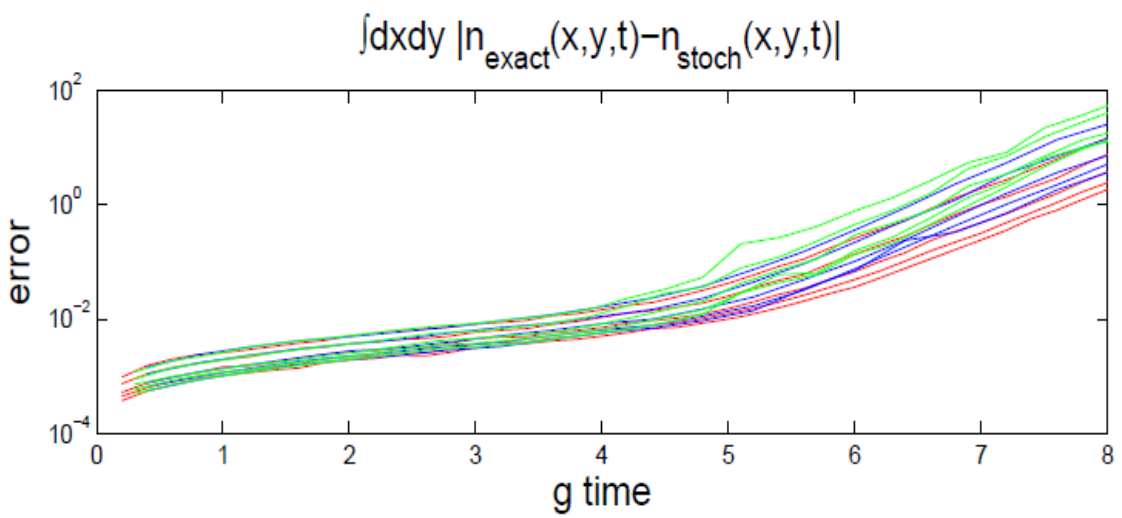
$$H = \sum_{k,\sigma} \frac{\vec{k}^2}{2} \alpha^{\dagger}_{\vec{k},\sigma} \alpha_{\vec{k},\sigma} + g \sum_{\vec{r}} \alpha^{\dagger}_{\vec{r},\uparrow} \alpha^{\dagger}_{\vec{r},\downarrow} \alpha_{\vec{r},\downarrow} \alpha_{\vec{r},\uparrow}$$

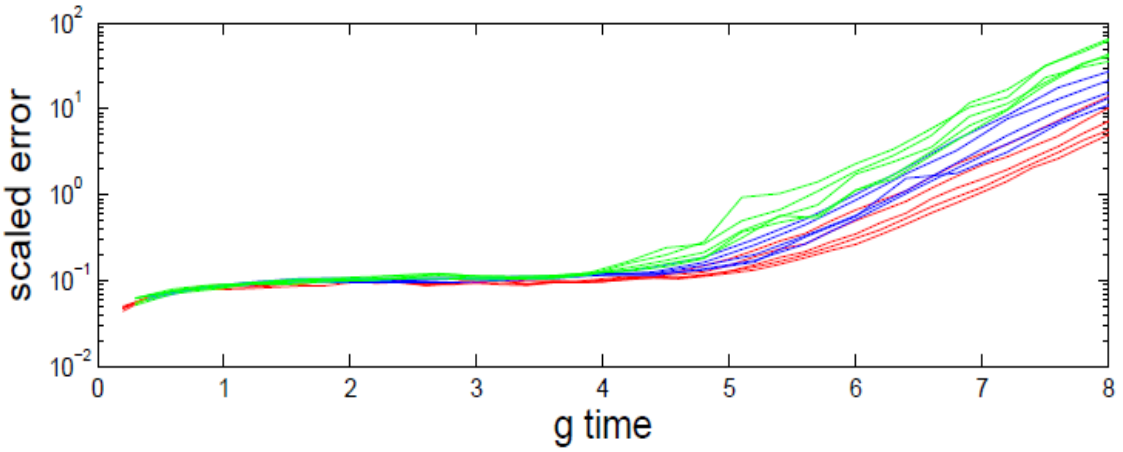
NB The coordinate and momentum creation/anihilation operators are linked by the usual unitary transformations.

We evolve an initial many-fermion wave function using independent real-time path integral representations of the propagators for the bra (backward in time) and ket (forward in time) many-body wave functions:

$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i \frac{\Delta t}{2} \sum_{abcd} \sigma_{ab}(n) V_{abcd} \sigma_{cd}(n) \right] \times \exp\left[i\Delta t \sum_{ab} \left(T_{ab} + \sum_{cd} V_{abcd} \sigma_{cd}(n) \right) \alpha^{\dagger}_a \alpha_b \right]$$

We used both discrete and continuous HS transformations, and simulated up to 6 fermions.





Results for two fermions, for g=1 (red), 2 (blue), and 3 (green), and a 16x16 lattice
Sample sizes for the propagator M= 2,500, 5,000, 10,000 and 20,000.
Lower plot shows that error scales as theoretically expected

$$\propto \exp(gt/2)/\sqrt{M}.$$

Theoretical analysis and further numerical simulations show that for N interacting fermions the simulation error behaves as

$$\propto \exp(Ngt/2)/\sqrt{M}.$$

NB The error is independent of:

- the dimensionality of the space
- the spatial volume/size of lattice
- a relatively small number of samples is needed for a decent accuracy

What we could in principle be able to calculate?

- **We do not need to determine any collective coordinates, potential energy surfaces, inertia tensor, non-abelian gauge fields, etc. as the system will find naturally the right collective manifold**
- **We will not need to assume either isentropic, isothermal, … meanfield solutions. Instead the temperature and entropy of the collective subsystem will evolve according to the rules of QM. This will be the most natural framework to describe dissipation in large amplitude collective nuclear motion.**
- **We should be able to compute directly the mass, charge distributions and the excitation energy, and maybe even quantum number distributions of each fragment**
- **We should be able to follow in real time a real experimental situation, such as induced fission or fusion**
- **This kind of simulations will answer in particular real needs of national security (nuclear forensics)**
- **New theoretical techniques however would allow us to address new types of theoretical questions, in particular we would be able to study, with quantifiable theoretical errors, very fast non-equilibrium processes in strongly interacting many-fermion systems**

All this is naturally not limited to nuclear physics alone, this is a general approach to solve a large class of many-body problems numerically exactly, with quantifying errors, within the next decade … or sooner.

Plans for the next few years:

- Improve performance and numerical accuracy of the codes, study alternative numerical methods, improve the treatment of the absorbing boundary conditions, extend calculations to larger nuclear simulation volumes and longer times)
- Systematic calculations of collective states in nuclei across the periodic table (likely new collaboration with K. Nakatsukasa and his colleagues)
- Perform real-time calculations of excitation of nuclear reaction with neutrons and excitation of nuclei with gamma rays
- Simulate the excitation of single, double and triple GDR with relativistic heavy ions (new collaboration with C. Bertulani, GSI experiment)
- Simulate the induced nuclear fission with relativistic heavy ions (new collaboration with C. Bertulani, GSI experiment)
- Simulate the dynamics of vortices in neutron star crust and attempt to finally elucidate the pinning mechanism of vortices and their role in starquakes (new collaboration with S. Reddy)
- Study the dissipation in spontaneous fission by simulating the real-time dynamics of a fissioning nucleus from the scission point onward
- Extend/apply TDSLDA approach to nuclear reactions
- Further studies of the unitary Fermi gas
- Vigorously pursue the Stochastic extension of TDSLDA and prepare the grounds for doing nuclear physics in the exascale regime (new collaborations envisioned with G.F. Bertsch, M.M. Forbes, S. Moroz, …)

Computational and Computer Science needs:

- Next three years between 100-200 M CPU hours/year
- 3-5 years 1-20 billion CPU hours/year (assuming the 10-100 petascale regime)
- 5-7 and after 20-200 billion CPU hours/year (assuming the exascale regime)
- Likely we will need to perform a large number of calculations in extended/mixed precision
- We will vigorously examine the use of GPUs (K.J. Roche + S. Cohen (postdoc))

Summary

- ✓ Full 3D real-time simulations of the dynamics of a range of superfluid Fermi systems 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 (incipient phase of quantum turbulence), excitation of vortex rings, …
- ✓ Excitation of dark solitons and shock waves in the collision of unitary Fermi gas clouds are predicted
- ✓ One can study a large variety of time-dependent phenomena in nuclear systems (nuclei, reactions, neutron star crust)
- ✓ The stochastic extension of TDSLDA appears feasible, thus the solution of the time-dependent Schrödinger equation for interacting fermions is possible in the exascale regime