Quantized superfluid vortices in the unitary Fermi gas within time-dependent Superfluid Local Density Approximation

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Motivation: The Challenge put forward by MIT experiment

Heavy solitons in a fermionic superfluid

Tarik Yefsah[1], Ariel T. Sommer[1], Mark J. H. Ku[1], Lawrence W. Cheuk[1], Wenjie Ji[1], Waseem S. Bakr[1] & Martin W. Zwierlein[1]

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- ^{6}Li atoms near a Feshbach resonance ($N \approx 10^6$) cooled in harmonic trap (axially symmetric)

atoms near a Feshbach resonance
= unitary Fermi gas

$$0 \leftarrow k_F r_0 \ll 1 \ll k_F a \rightarrow \infty$$

System is **dilute** but...

strongly interacting!

- Unitary limit: no interaction length scale...
- Universal physics...
  - Cold atomic gases
  - Neutron matter
  - High-Tc superconductors
- Simple, but hard to calculate!
  (Bertsch Many Body X-challenge)

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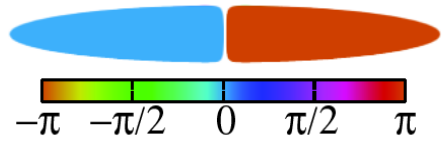
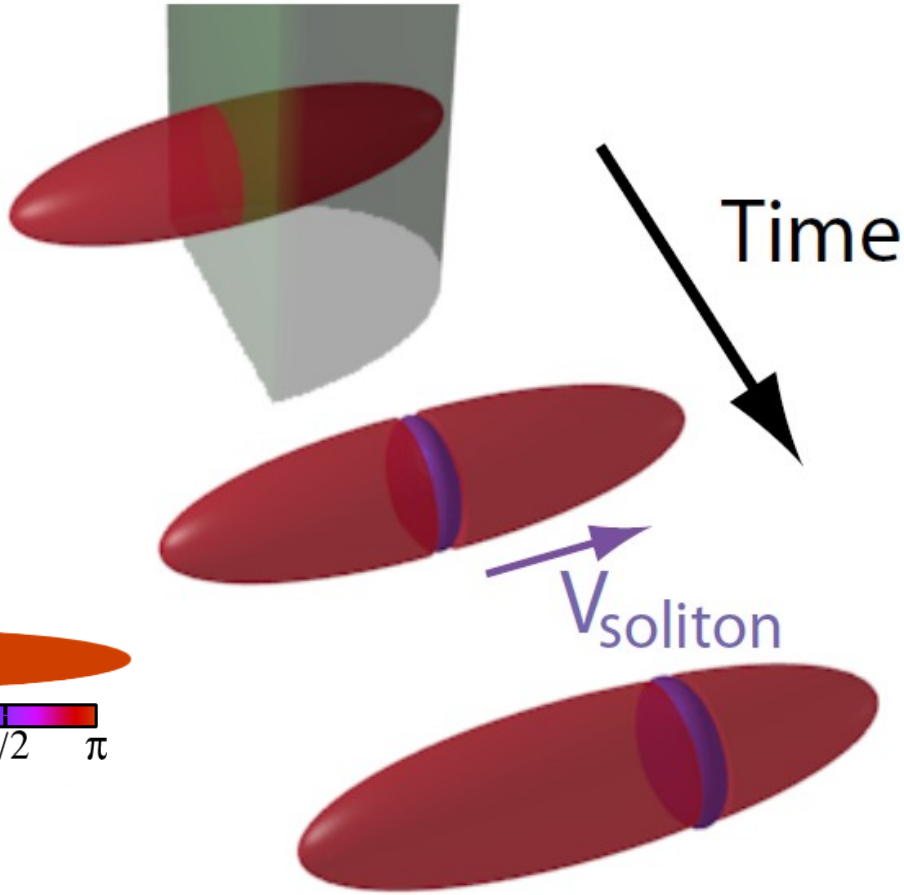
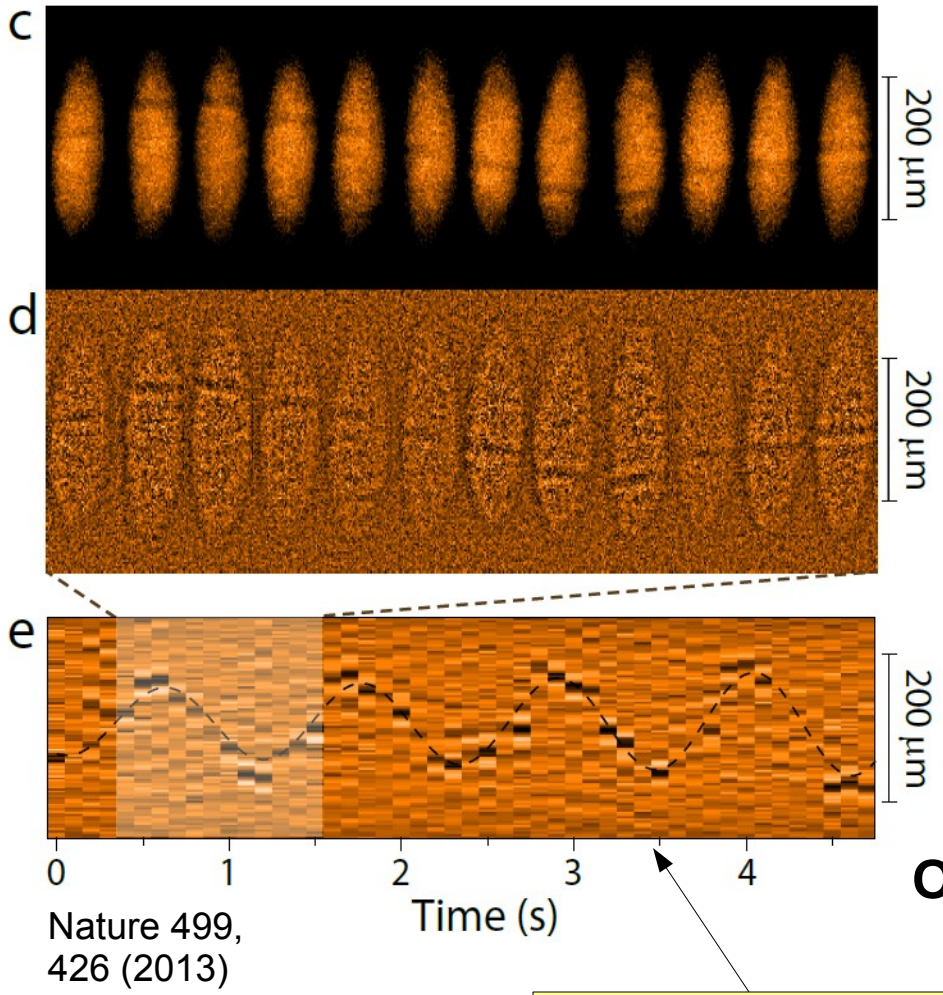
- ^{6}Li atoms near a Feshbach resonance (N≈10^6) cooled in harmonic trap (axially symmetric)
- Step potential used to imprint a soliton (evolve to π phase shift)
- Let system evolve...





Experimental result



Nature 499, 426 (2013)

- Observe an oscillating “soliton” with long period $T \approx 12T_z$
- Inertial mass 200 times larger than the free fermion mass
- Interpreted as “*Heavy Solitons*”

Problem for theory:

- Bosonic solitons (BECs) oscillate with $T \approx 1.4T_z$
- Fermionic solitons (BdG) oscillate with $T \approx 1.7T_z$

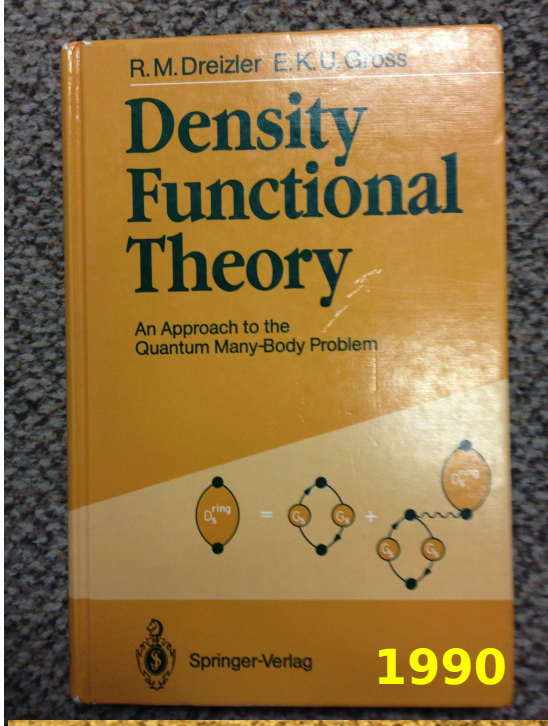
Order of magnitude larger than theory!

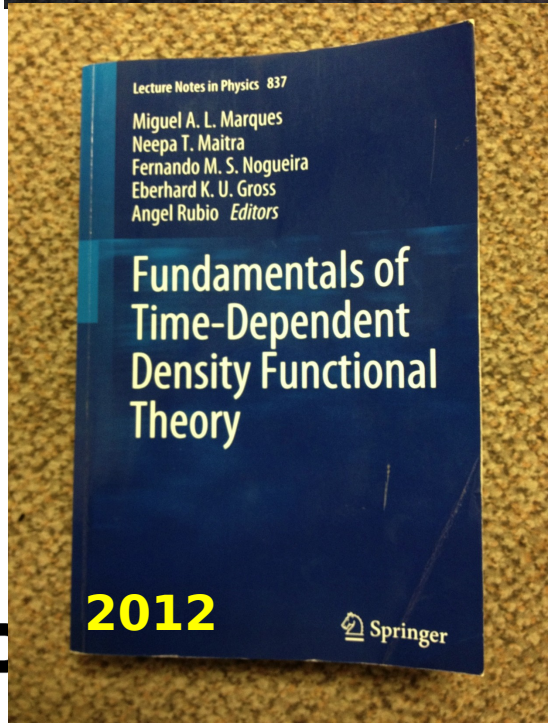
Subtle imaging needed:
- needed expansion
- must ramp to specific value of magnetic field

DFT: workhorse for electronic structure simulations

- The Hohenberga-Kohn theorem assures that the theory can reproduce exactly the ground state energy if the “exact” Energy Density Functional (EDF) is provided
- Often called as *ab initio* method
- Extension to Time-Dependent DFT is straightforward
- Very successful – DFT industry (commercial codes for quantum chemistry and solid-state physics)
- Can be extended to superfluid systems...

  (numerical cost increases dramatically)





EDF for UFG: Superfluid Local Density Approximation (SLDA)

Dimensional arguments, renormalizability, Galilean invariance, and symmetries (translational, rotational, gauge, parity) determine the functional (energy density)

Only local densities

unique combination of the kinetic and anomalous densities required by the renormalizability of the theory

$$\mathcal{E}\left[n(\vec{r},t),\tau(\vec{r},t),\vec{j}(\vec{r},t),\nu(\vec{r},t)\right]=\alpha\left[\frac{\hbar^2}{2m}\tau(\vec{r},t)-\Delta(\vec{r},t)\nu^*(\vec{r},t)\right]+$$

$$\beta\frac{3(3\pi^2)^{2/3}\hbar^2}{10m}n^{5/3}(\vec{r},t)+\lambda\frac{\hbar^2|\vec{\nabla}n(\vec{r},t)|^2}{m\,n(\vec{r},t)}+(1-\alpha)\frac{|\vec{j}(\vec{r},t)|^2}{m\,n(\vec{r},t)}.$$

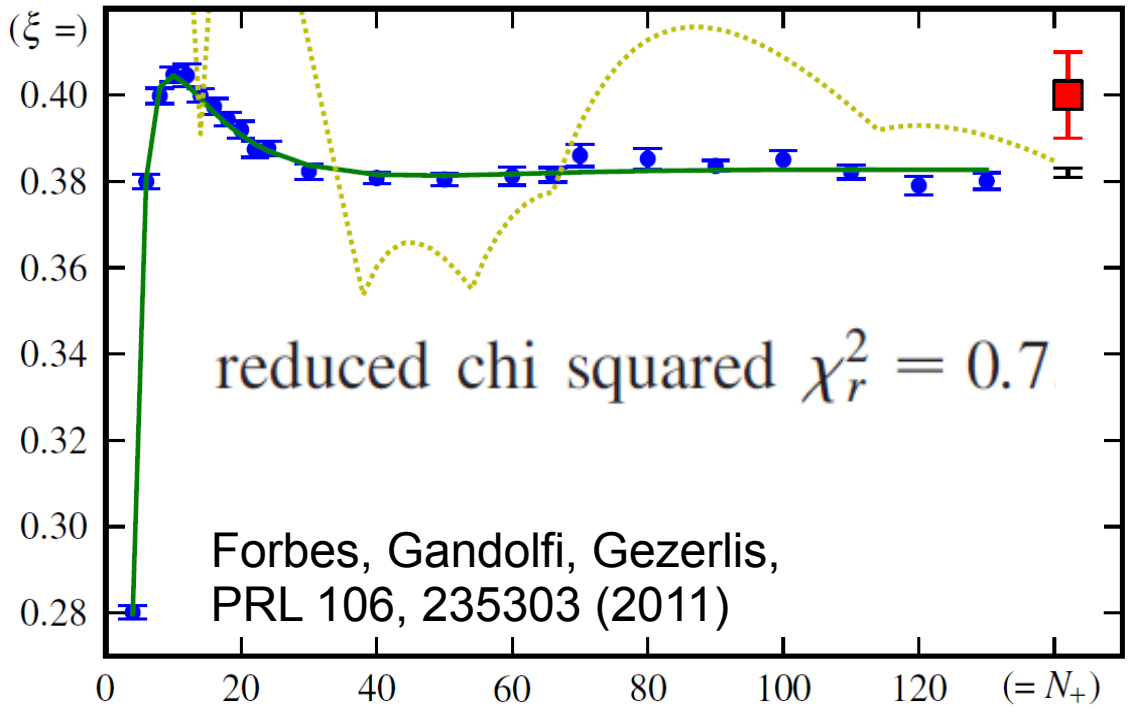
Self-energy term - the only function of the density alone allowed by dimensional arguments

lowest gradient correction- negligible

required by Galilean invariance

$$\mathcal{E}(\mathbf{r}) = \alpha \frac{\tau(\mathbf{r})}{2} + \beta \frac{3(3\pi^2)^{2/3} n^{5/3}(\mathbf{r})}{10} + \gamma \frac{|\nu(\mathbf{r})|^2}{n^{1/3}(\mathbf{r})} + \cdots,$$

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.
NOTE: there is no fit to experimental results

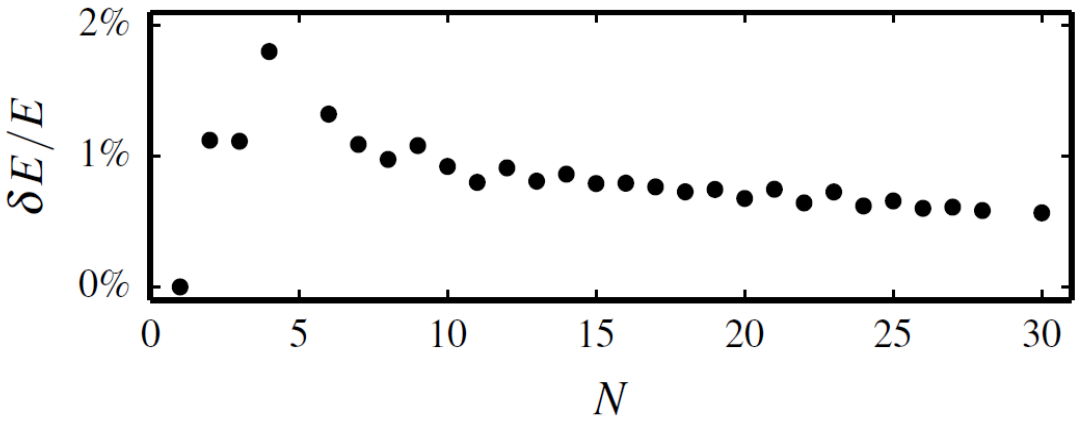


SLDA has been verified and validated against a large number of quantum Monte Carlo results for inhomogeneous systems and experimental data as well

$$\mathcal{E}(\mathbf{r}) = \alpha\frac{\tau(\mathbf{r})}{2} + \beta\frac{3(3\pi^2)^{2/3}n^{5/3}(\mathbf{r})}{10} + \gamma\frac{|\nu(\mathbf{r})|^2}{n^{1/3}(\mathbf{r})} + \cdots,$$

Set to α=1

$$+ (1-\alpha)\frac{|\vec{j}(\vec{r},t)|^2}{m\,n(\vec{r},t)}$$



So simple ...
... so accurate!

Figure 5. (color online) Relative energy change (in %) between simulations with $\alpha = 1$ and $\alpha = 1.14$ that compute the energy of N fermions (both even and odd particle numbers) in the unitary Fermi gas trapped in an isotropic harmonic oscillator.

Time-dependent extension

The real-time dynamics is given by equations, which are formally equivalent to the Time-Dependent HFB (TDHFB) or Time-Dependent Bogolubov-de Gennes (TDBdG) equations:

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) & 0 & 0 & \Delta(\boldsymbol{r},t) \\ 0 & h_b(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h_a^*(\boldsymbol{r},t) & 0 \\ \Delta^*(\boldsymbol{r},t) & 0 & 0 & -h_b^*(\boldsymbol{r},t) \end{pmatrix} \begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix}$$

The mean field potentials $h_i(\boldsymbol{r},t)$ are derived from the EDF as functional derivative $h_i = \frac{\delta E}{\delta n_i}$ and they explicitly depends on local densities $n(\boldsymbol{r})$, $\tau(\boldsymbol{r})$, etc. The set of 4-component "wave functions" is in turn related to the densities and the pairing field $\Delta(r)$

$$\begin{aligned} n_i(\boldsymbol{r}) &= \sum_{E_n<E_c} |v_{n,i}(\boldsymbol{r})|^2, \\ \tau_i(\boldsymbol{r}) &= \sum_{E_n<E_c} |\nabla v_{n,i}(\boldsymbol{r})|^2, \\ \nu(\boldsymbol{r}) &= \sum_{E_n<E_c} u_{n,a}(\boldsymbol{r}) v^*_{n,b}(\boldsymbol{r}), \\ \Delta(\mathbf{r}) &= -g_{\rm eff}(\mathbf{r})\nu(\mathbf{r}). \end{aligned}$$

nonlinear coupled 3D Partial Differential Equations

Supercomputing

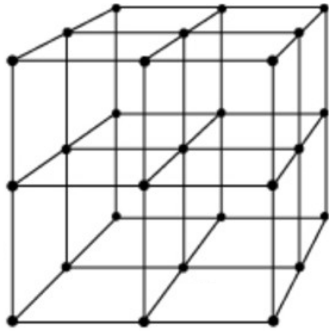
"The time-dependent density functional theory is viewed in general as a reformulation of the exact quantum mechanical time evolution of a many-body system when only one-body properties are considered."

http://www.tddft.org

Solving...

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) & 0 & 0 & \Delta(\boldsymbol{r},t) \\ 0 & h_b(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h_a^*(\boldsymbol{r},t) & 0 \\ \Delta^*(\boldsymbol{r},t) & 0 & 0 & -h_b^*(\boldsymbol{r},t) \end{pmatrix} \begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix}$$

- The system is placed on a large 3D spatial lattice of size $N_x \times N_y \times N_z$
  - Discrete Variable Representation (DVR) - solid framework (see for example: Bulgac, Forbes, Phys. Rev. C 87, 051301(R) (2013))
  - Errors are well controlled – exponential convergence
  - No symmetry restrictions



- Number of PDEs is of the order of the number of spatial lattice points
  - Typically (for cold atoms problems): 10^5 - 10^6

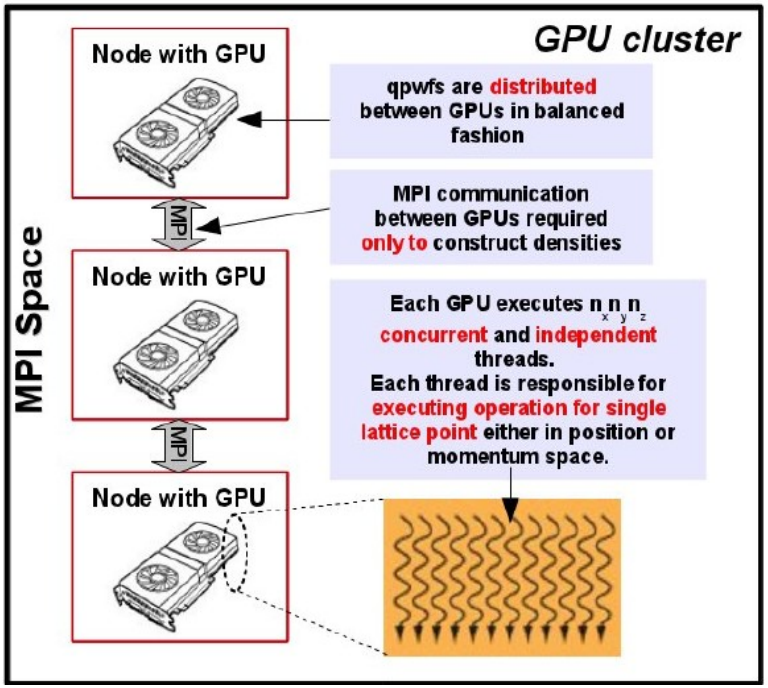
Solving...

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) & 0 & 0 & \Delta(\boldsymbol{r},t) \\ 0 & h_b(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h_a^*(\boldsymbol{r},t) & 0 \\ \Delta^*(\boldsymbol{r},t) & 0 & 0 & -h_b^*(\boldsymbol{r},t) \end{pmatrix} \begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix}$$

- Derivatives are computed with FFT
  - insures machine accuracy
  - very fast
- Integration methods:
  - Adams-Bashforth-Milne fifth order predictor-corrector-modifier integrator – very accurate but memory intensive
  - Split-operator method that respects time-reversal invariance (third order) – very fast, but can work with simple EDF

The spirit of SLDA is to exploit only local densities...

- Suitable for efficient parallelization (MPI)
- Excellent candidate for utilization multithreading computing units like GPUs

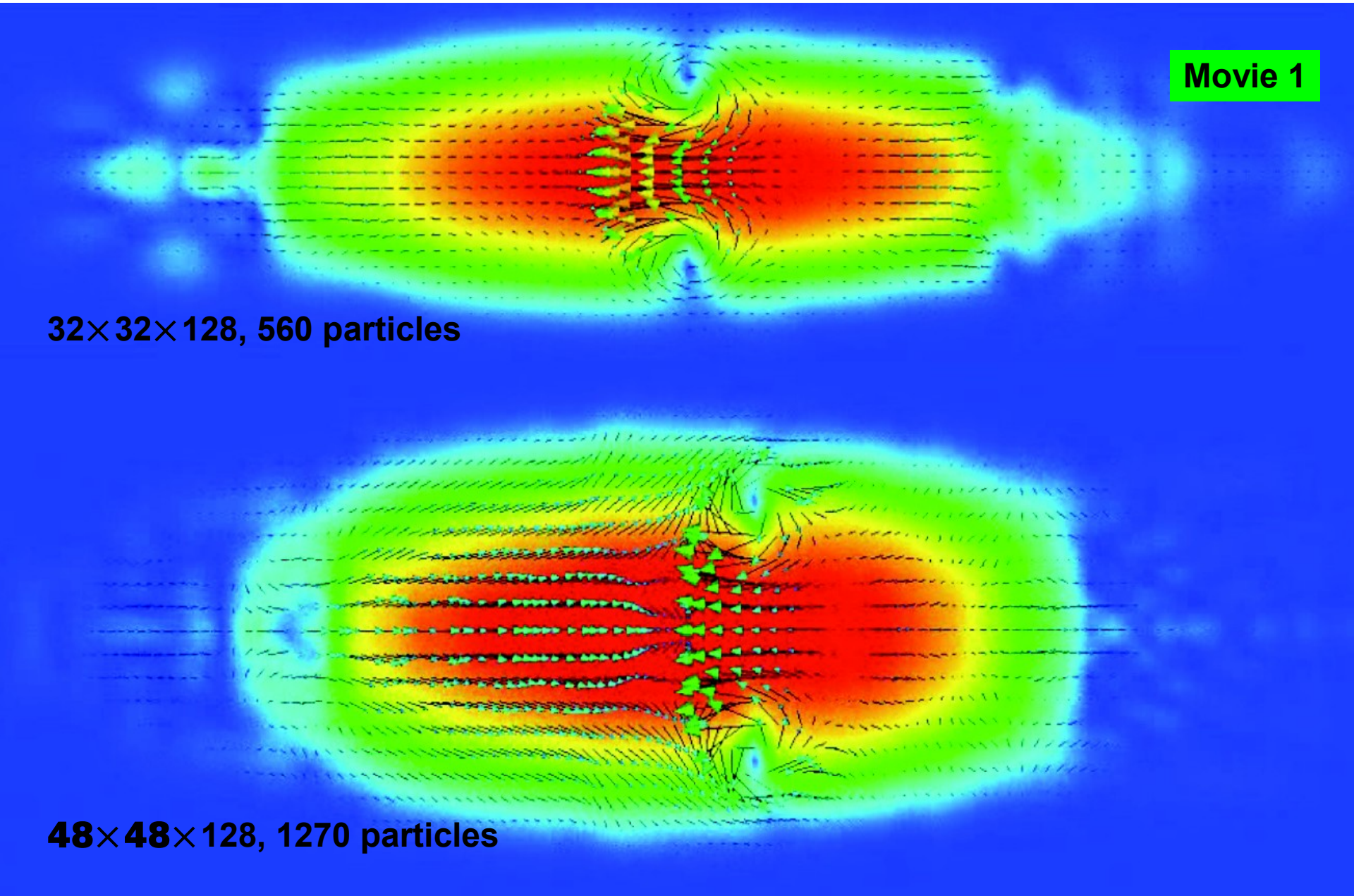


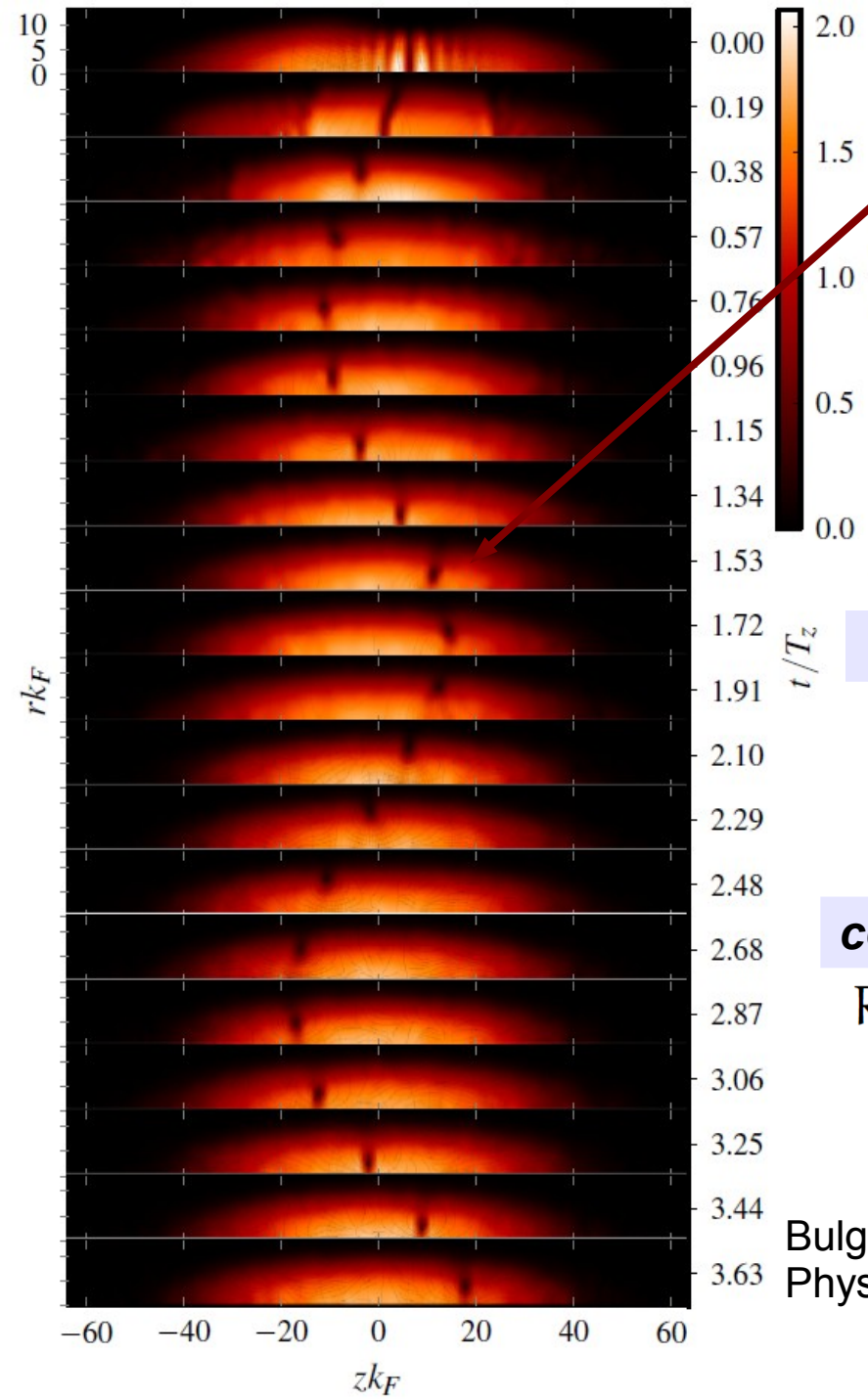
Lattice	# of GPUs	# of qpwfs	time per step [s]
24x24x96	64	24425	0.33
24x24x96	128	24425	0.17
24x24x96	256	24425	0.09
24x24x96	512	24425	0.06
32x32x128	256	57849	0.32
32x32x128	313	57849	0.25
48x48x128	512	129881	0.95
48x48x128	1024	129881	0.50
48x48x128	2048	129881	0.27
48x48x128	4096	129881	0.16
48x48x128	8192	129881	0.10

Lattice 64^3, 137,062 (2-component) wave functions, ABM
CPU version running on 16x4096=65,536 cores
GPU version running on 4096 GPUs

15 times Speed-up!!!

What do fully 3D simulations see?





Vortex Ring Oscillation!
(near-harmonic motion)

Can vortex ring explain
long periods?

Thin vortex approximation in infinite matter

dispersion $\varepsilon(p)$, and speed $v = d\varepsilon(p)/dp$

Vortex radius ***circulation***

$$\varepsilon \sim \frac{mn\kappa^2 R}{2} \ln \frac{R}{l_{coh}}, \qquad v \sim \frac{\kappa}{4\pi R} \ln \frac{R}{l_{coh}}$$

coherence length

$$R \gg l_{coh} \sim k_F^{-1}$$

Speed decreases as radius increases!
(sets correct orders)

Bulgac, Forbes, Kelley, Roche,Wlazłowski,
Phys. Rev. Lett. 112, 025301 (2014)

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Simulate larger systems – Extended Thomas-Fermi model

Fermionic simulations – numerically expensive, cannot reach 10^6 particles...

Our solution: match ETF model (essentially a bosonic theory for the dimer/Cooper-pair wavefunction) with DFT...

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{4m}\vec{\nabla}^2\Psi + 2\frac{\partial\mathcal{E}_h(n,a)}{\partial n}\Psi + 2V_{ext}\Psi$$

$$\mathcal{E}_h(n,a) = \frac{3}{5}\varepsilon_F n\xi\frac{\xi+x}{\xi+x(1+\zeta)+3.0\pi\xi x^2} - \frac{\hbar^2}{2ma^2}n$$

$$x = 1/k_F a$$
$$\xi = 0.370$$
$$\zeta = 0.901 \text{ (the contact)}$$

- Accurate Equation of State state for a>0, speed of sound, phonon dispersion, static response, respects Galilean invariance
- Ambiguous role played by the ‘’wave function,” as it describes at the same time both the number density and the order parameter.
- Density depletion at vortex/soliton core exaggerated! Systematically underestimates time scales by a factor of close to 2

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PROBLEMS:

- lacks a mechanisms for the superfluid to relax
- **not suitable for the period shortly after the imprint** where the system exhibits significant relaxation

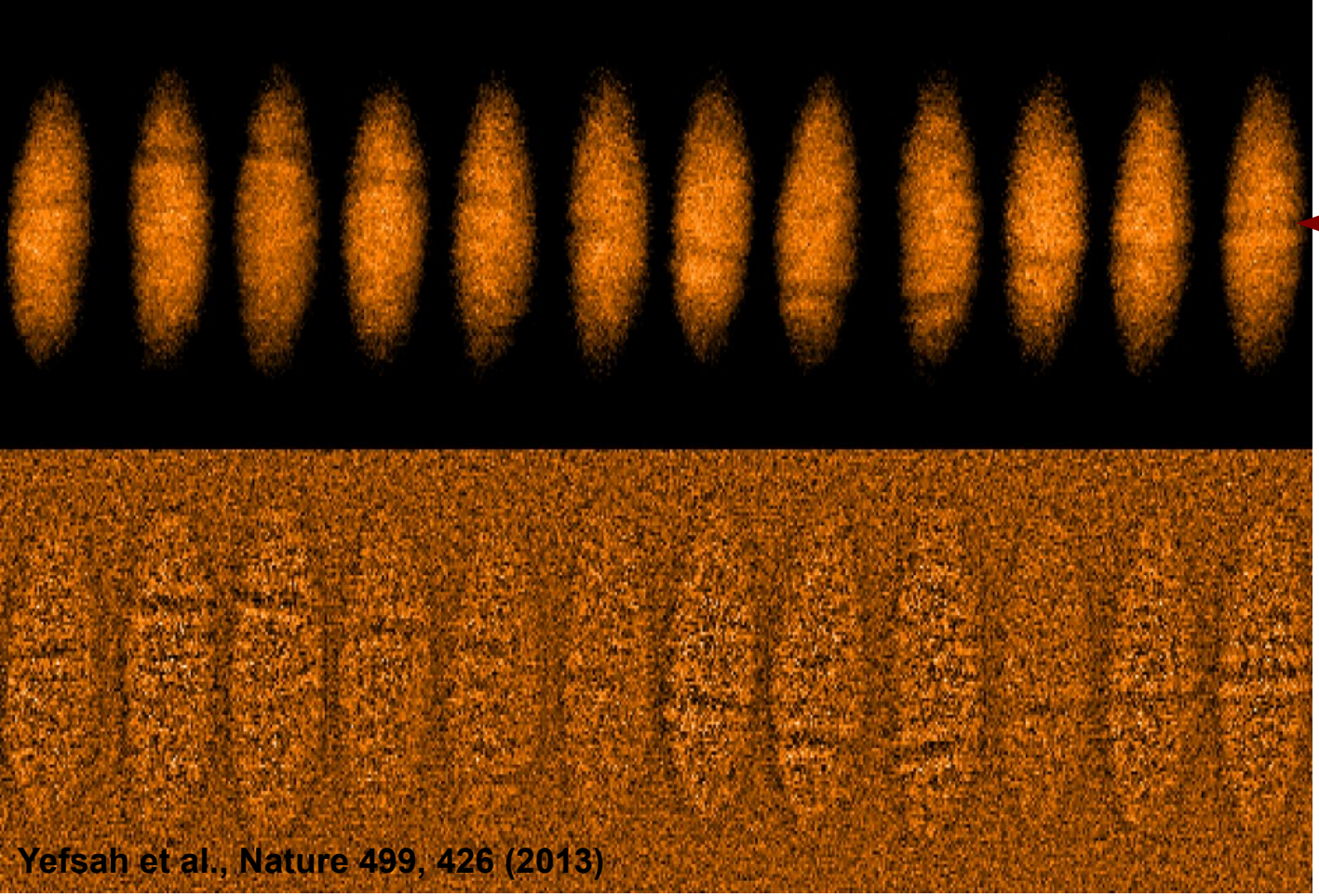
Movie 2

- suitable for studying the qualitative dynamics of vortex motion in large traps

Note: factor 2 for

$$\frac{\text{(EFT Period)}}{\text{(Exp. Period)}}$$

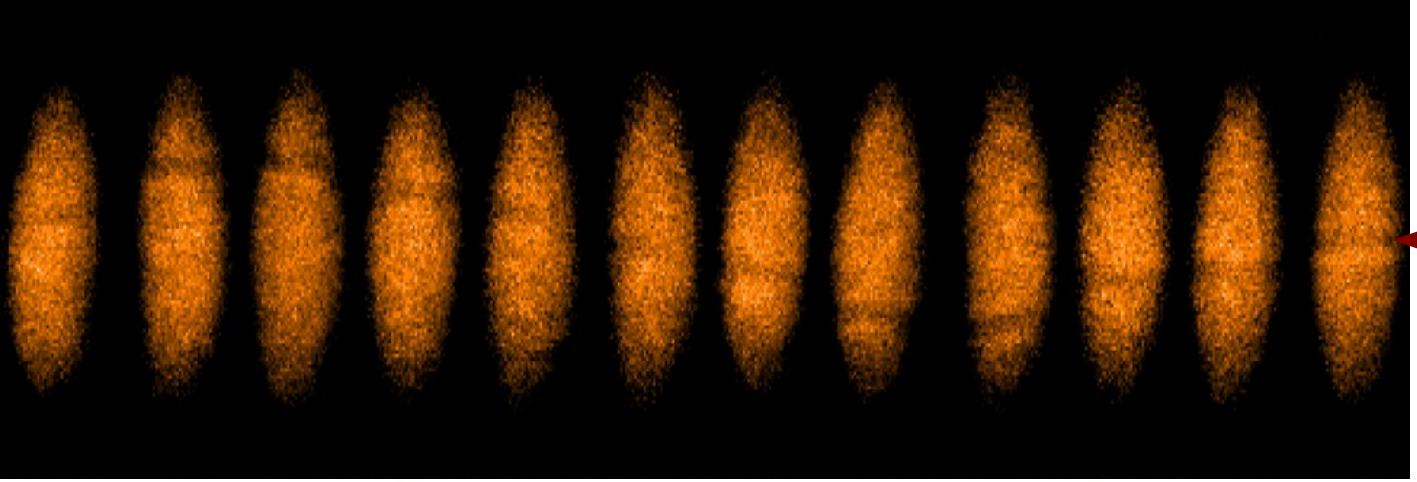
Aspect Ratio	ETF Period	Observed Period [1]
$\lambda = 3.3$	$T = 9.9\ T_z$	$T = 18(2)T_z$
$\lambda = 6.2$	$T = 8.4\ T_z$	$T = 14(2)T_z$
$\lambda = 15$	$T = 6.7\ T_z$	$T = 12(2)T_z$



Yefsah et al., Nature 499, 426 (2013)

Is it a vortex ring? (looks like a domain wall)

Subtle imaging:
- needed expansion
- must ramp to specific value of magnetic field



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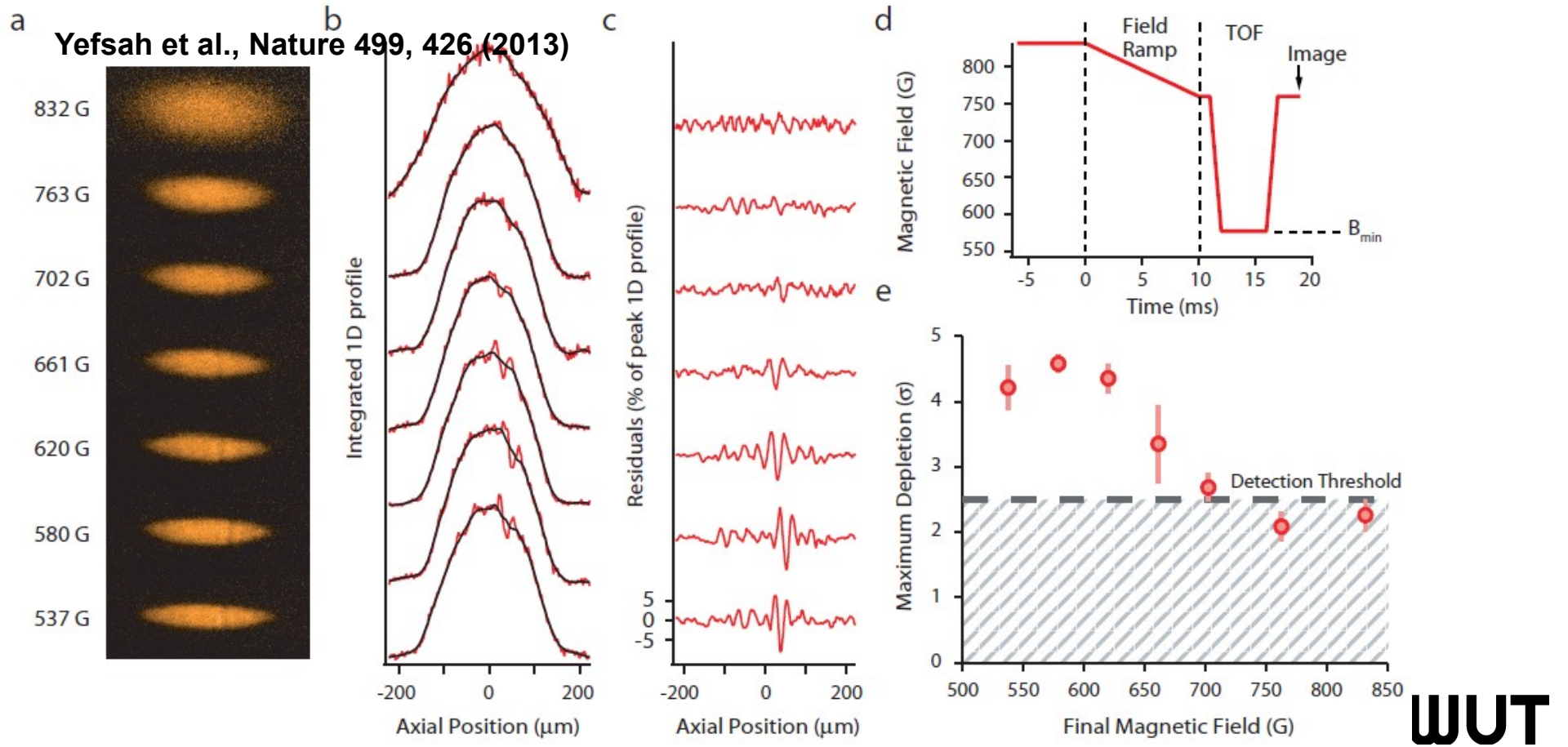

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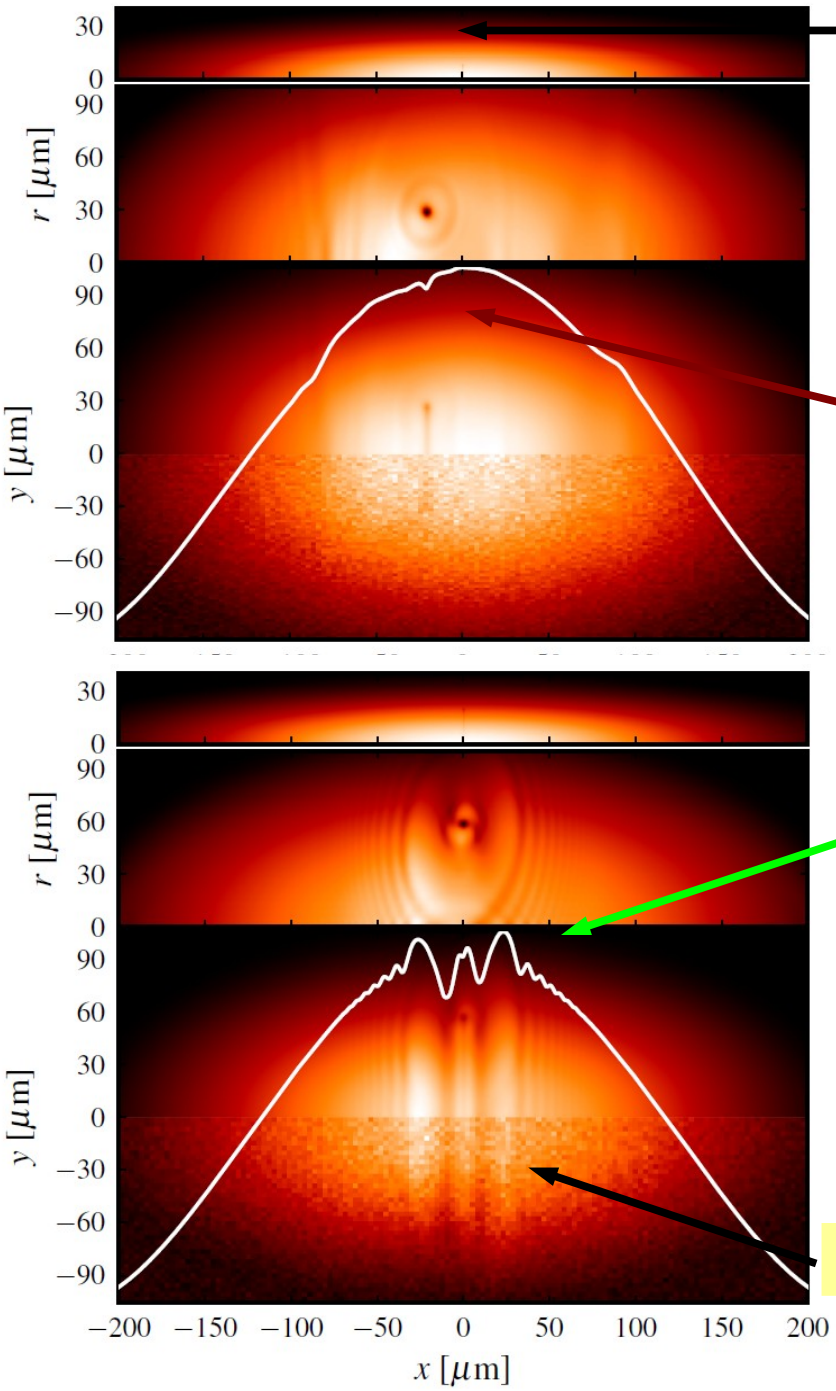
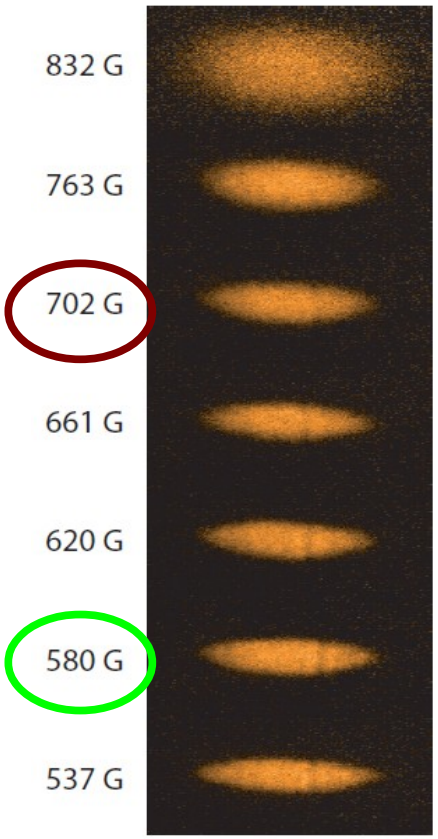
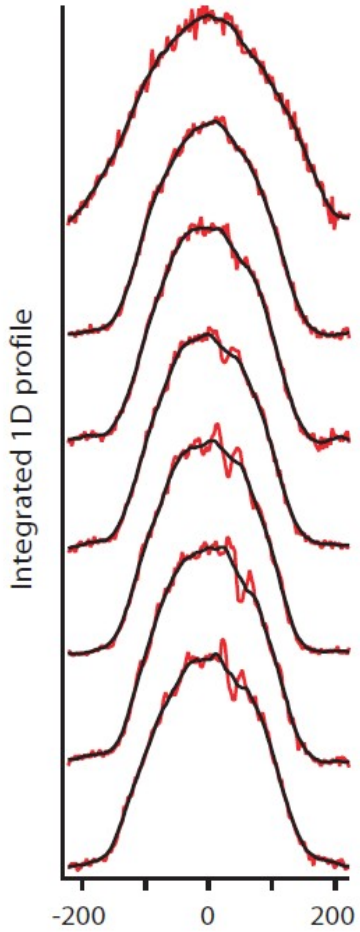


the vortex ring is barely visible





Imaging limitations -
Better imaging procedure needed
to solve the "puzzle"

vortex rings appear as "solitons"

Movie 3

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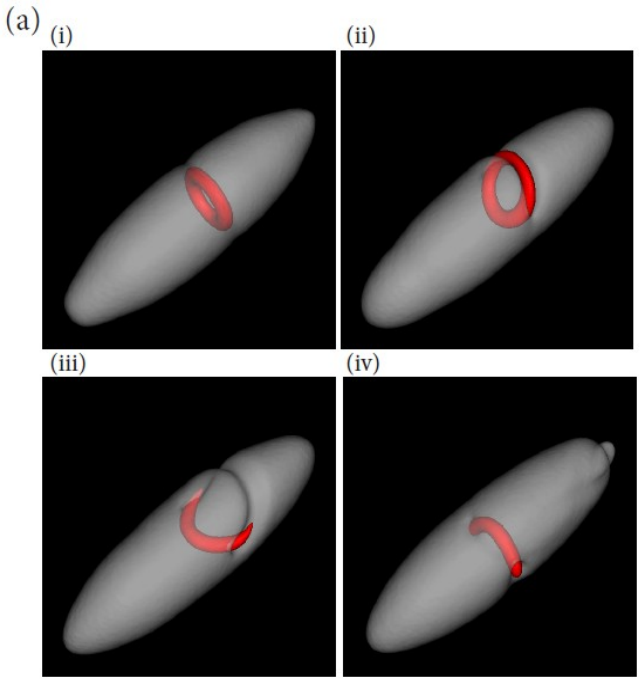
“Heavy Solition” = Superfluid Vortex

SIMILAR CONCLUSIONS:

- Matthew D. Reichl and Erich J. Mueller , Phys. Rev. A 88, 053626 (2013)
- Wen Wen, Changqing Zhao, and Xiaodong Ma, Phys. Rev. A 88, 063621 (2013)
- Lev P. Pitaevskii, arXiv:1311.4693
- Peter Scherpelz et al., arXiv:1401.8267
  (vortex ring is unstable
  and converts into vortex line)



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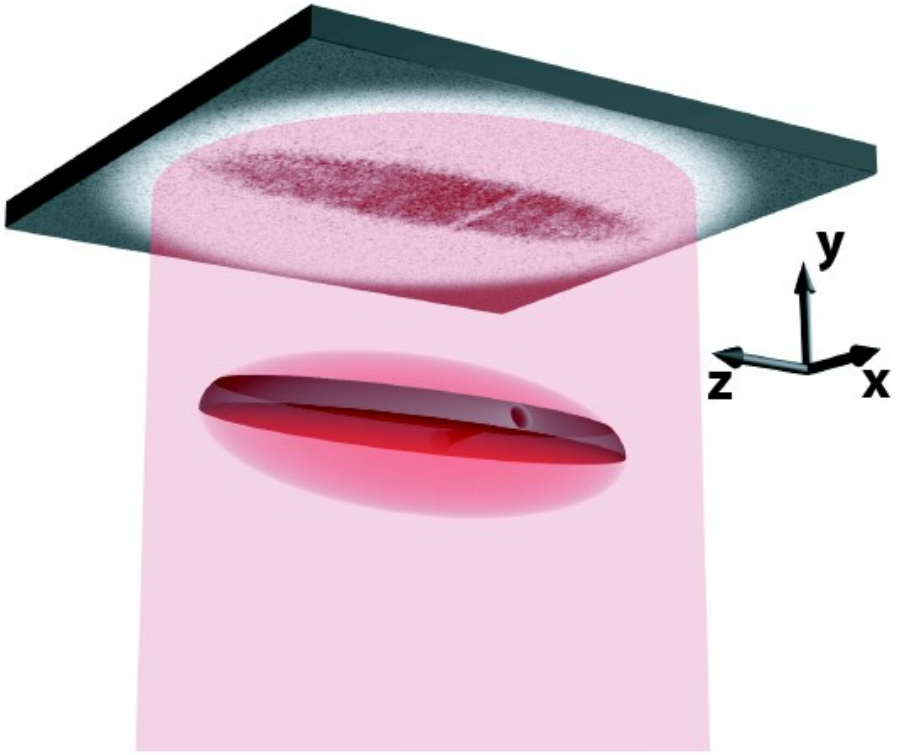
Mark J.H. Ku et. al., arXiv:1402.7052



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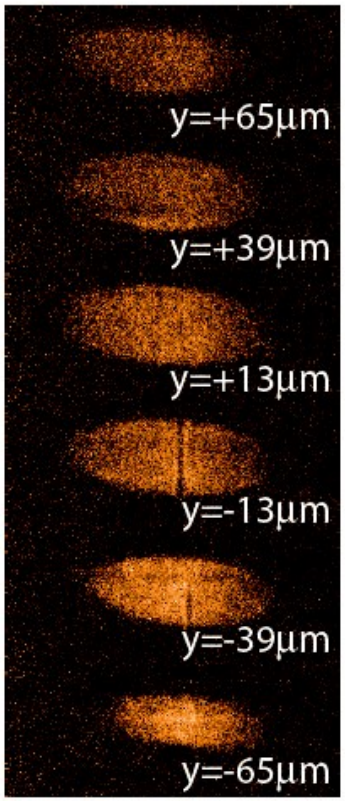


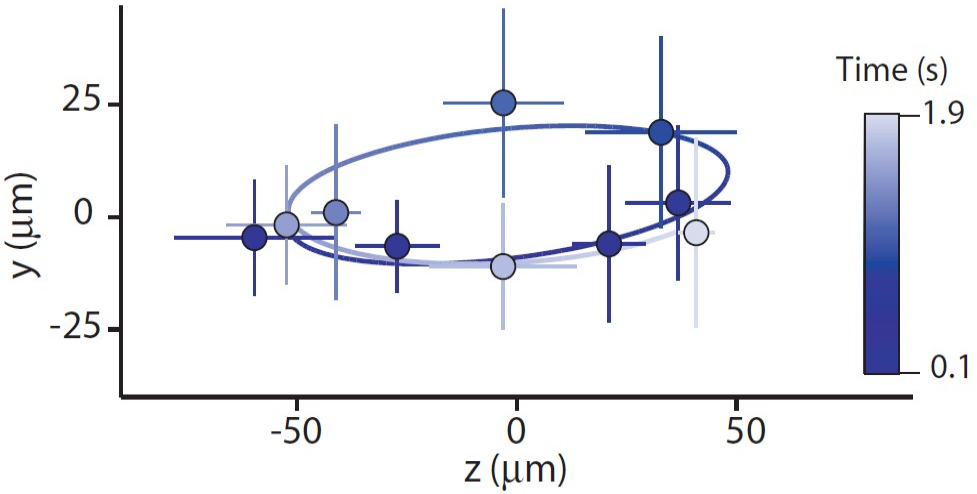
Update of the experiment

$$\omega_y/\omega_x - 1 \approx 5\%$$

Anisotropy:
Due to gravity

RESULTS:

- Observe an oscillating **vortex line** with long period
- Always aligned along the short axis
- Precessional motion



anisotropy and anharmonicity

Trapping potential:

$$V(x,y,z) = \frac{m\omega_z^2 z^2}{2} + \mathcal{O}(z^4) + \\ + V_0\left[1 - \exp\left(-\frac{m\omega_x^2(x^2+y^2)}{2V_0}\right)\right] + mgy. \quad (1)$$

Shifting $y \to y + y_0$ where y_0 is the new minimum gives the following effective trapping potential

$$V(x,y+y_0,z) \approx \frac{m\omega_z^2 z^2}{2} + \mathcal{O}(z^4) + \\ \frac{m\omega_x^2 x^2}{2} + \frac{m\omega_y^2 y^2}{2} + Cy^3 + \mathcal{O}(\delta^2) + \text{const} \quad (2)$$

Needed to generate single vortex line!
(breaking of mirror symmetry)

where $\delta = 3mg^2/4\omega_x^2 V_0$ is treated perturbatively, and

$$\omega_y \approx \omega_x(1-\delta), \quad C \approx \frac{2m\omega_x^4}{3g}\delta. \quad (3)$$

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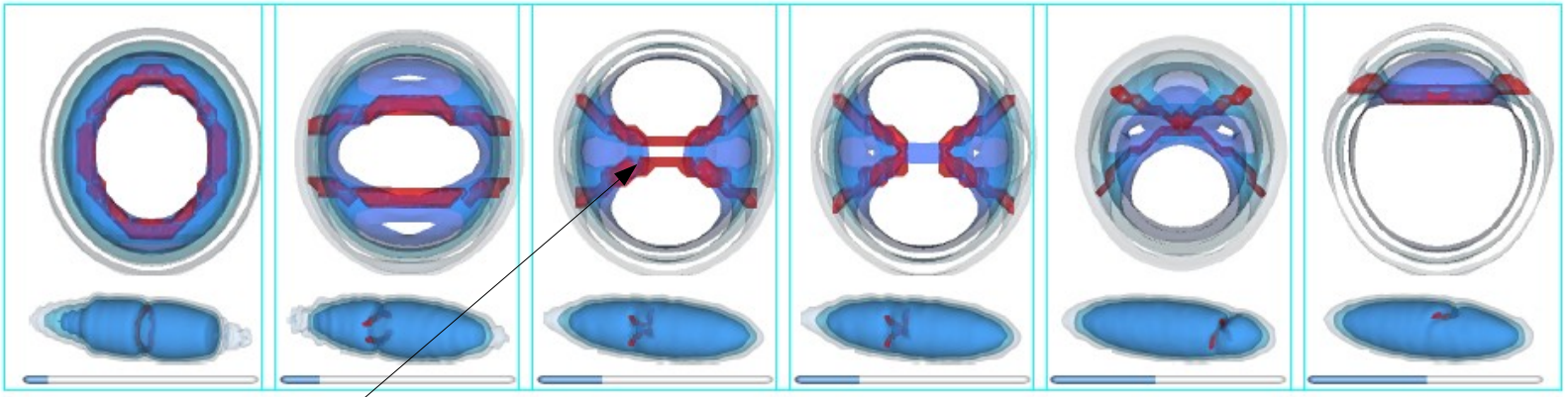
What do fully 3D simulations see?

Wlazłowski,Bulgac, Forbes, Roche, arXiv:1404.1038

Movie 4

$\delta \approx 10\%$

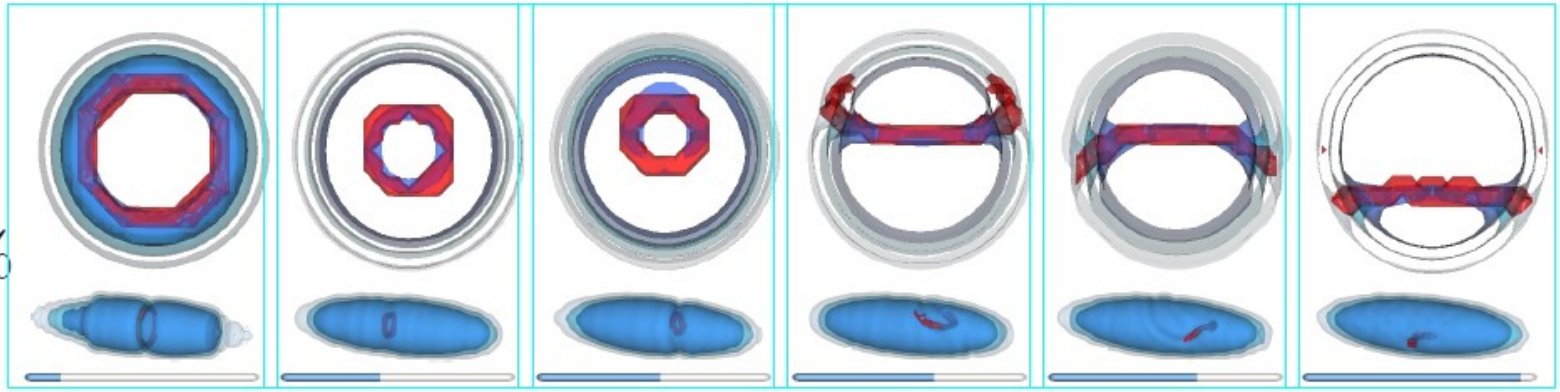
$\frac{C}{C_0} \approx 3\%$



Crossing and reconnection!

$\delta \approx 0.5\%$

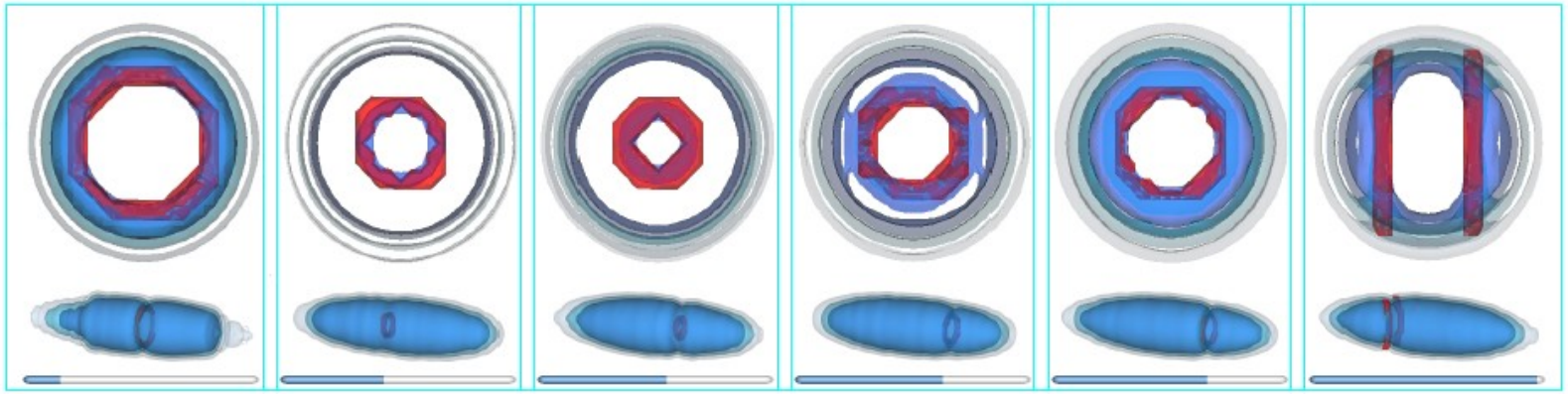
$\frac{C}{C_0} \approx 0.15\%$



Movie 5

$\delta \approx 0.5\%$

$\frac{C}{C_0} \approx 0$



Needed to get single vortex line, as seen in experiment.

CONCLUSIONS:

- DFT capable to explain all aspects of the experiment
  - Long periods of oscillation...
  - Vortex alignment...
- Correctly describes generation, dynamics, evolution, and eventual decay - large number of degrees of freedom in the SLDA permit many mechanisms for superfluid relaxation: *various phonon processes, Cooper pair breaking,* and *Landau damping*
- Validates (TD)DFT...
- Can be used to engineer interesting scenarios: colliding of vortices, QT, vortex interactions... **Movie 6**

Computational challenge: Finding initial (ground) state?

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) & 0 & 0 & \Delta(\boldsymbol{r},t) \\ 0 & h_b(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h_a^*(\boldsymbol{r},t) & 0 \\ \Delta^*(\boldsymbol{r},t) & 0 & 0 & -h_b^*(\boldsymbol{r},t) \end{pmatrix} \begin{pmatrix} u_{n,a}(\boldsymbol{r},t) \\ u_{n,b}(\boldsymbol{r},t) \\ v_{n,a}(\boldsymbol{r},t) \\ v_{n,b}(\boldsymbol{r},t) \end{pmatrix}$$

E_n

Real time evolution scaling: $O(N^2 \ln N)$
$N = N_x N_y N_z$

- Diagonalization:
  - requires repeatedly diagonalizing the NxN single-particle Hamiltonian (an **O(N^3)** operation) for the **hundreds of iterations** required to converge to the self-consistent ground state
  - only suitable for small problems or if symmetries can be used
- Imaginary time evolution:
  - Non-unitary: spoils orthogonality of wavefunctions
  - Re-orthogonalization unfeasible (communication)

Quantum friction

Single particle Hamiltonian

Energy density functional

$$\mathcal{H} = \frac{\delta \mathcal{E}}{\delta \mathcal{R}^T}$$

Generalized density matrix

Equation of motion

$$i\dot{\mathcal{R}} = [\mathcal{H}, \mathcal{R}]$$

$$E = \int d^3\boldsymbol{r}\, \mathcal{E}(\boldsymbol{r})$$

Energy of the system

$$\frac{dE}{dt} = \mathrm{Tr}\left\{\mathcal{H}\dot{\mathcal{R}}\right\} = -i\mathrm{Tr}\left\{\mathcal{H}[\mathcal{H}, \mathcal{R}]\right\} = 0$$

Consider evolution with “external” potential: $\mathcal{H} \to \mathcal{H} + \mathcal{V}_t$

$$i\dot{\mathcal{R}} = [\mathcal{H} + \mathcal{V}_t, \mathcal{R}]$$

$$\frac{dE}{dt} = \mathrm{Tr}\left\{\mathcal{H}\dot{\mathcal{R}}\right\} = -i\mathrm{Tr}\left\{\mathcal{H}[\mathcal{H} + \mathcal{V}_t, \mathcal{R}]\right\} = i\mathrm{Tr}\left\{[\mathcal{H}, \mathcal{R}]\mathcal{V}_t\right\}$$

Quantum friction

$$\frac{dE}{dt} = \mathrm{Tr}\left\{\mathcal{H}\dot{\mathcal{R}}\right\} = -i\mathrm{Tr}\left\{\mathcal{H}[\mathcal{H}+\mathcal{V}_t,\mathcal{R}]\right\} = i\mathrm{Tr}\left\{[\mathcal{H},\mathcal{R}]\mathcal{V}_t\right\}$$

Note: $\mathrm{Tr}\left\{AA^\dagger\right\} = \sum |A_{kl}|^2 \geqslant 0$

$$\mathcal{V}_t \propto i[\mathcal{H},\mathcal{R}]^\dagger \Rightarrow \frac{dE}{dt} \leqslant 0$$

Non-local potential equivalent to “complex time” evolution

Not suitable for fermionic problem

“Local” option: $\mathrm{Tr}\left\{A\,\mathrm{diag}[A^\dagger]\right\} = \sum |A_{kk}|^2 \geqslant 0$

$$\mathcal{V}_t \propto i\mathrm{diag}\left[[\mathcal{H},\mathcal{R}]^\dagger\right] = -\hbar\boldsymbol{\nabla}\cdot\boldsymbol{j}_t(\boldsymbol{r})$$

current

$$\mathcal{V}_t = -\beta\frac{\hbar\boldsymbol{\nabla}\cdot\boldsymbol{j}_t(\boldsymbol{r})}{n_t(\boldsymbol{r})}$$

dimensionless constant of order unity

removes any irrotational currents in the system, damping currents by being repulsive where they are converging

Quantum friction

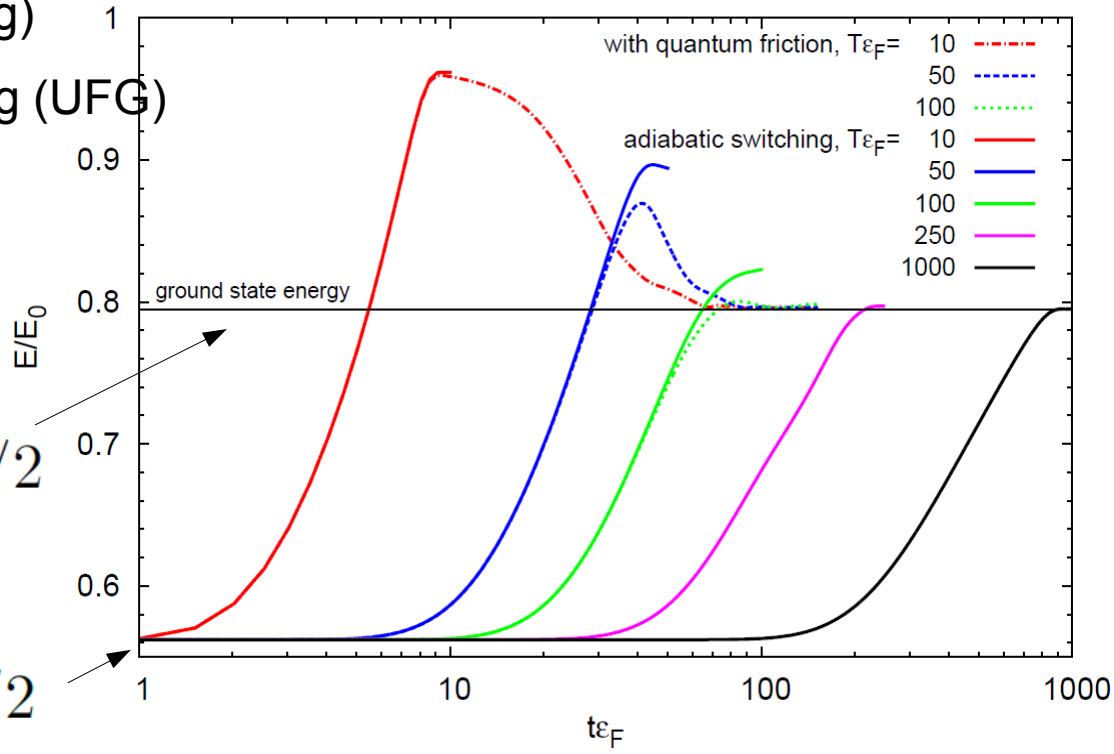
$$\mathcal{V}_t = -\beta \frac{\hbar \nabla \cdot \boldsymbol{j}_t(\boldsymbol{r})}{n_t(\boldsymbol{r})}$$

- Does not guarantee convergence to ground state
  - proceed with adiabatic state preparation $H_t = s_t H_1 + (1 - s_t) H_0$
  - generally much faster than pure adiabatic state preparation
- Gain: computational scaling: $O(N^2 \ln N)$
- Works well for: **Movie 7**
  - Normal systems (no pairing)
  - Systems with strong pairing (UFG)
- Additional "cooling" potential can be added in pairing channel (ongoing work)

$$V_1(x,y,z) = m\omega_\perp^2 (x^2+y^2)/2 + m\omega_\parallel^2 z^2/2$$

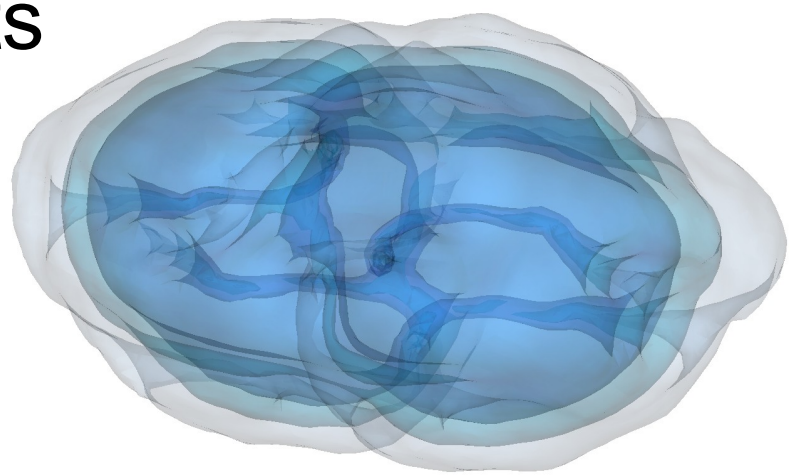
$$V_0(x,y) = m\omega_\perp^2 (x^2+y^2)/2$$

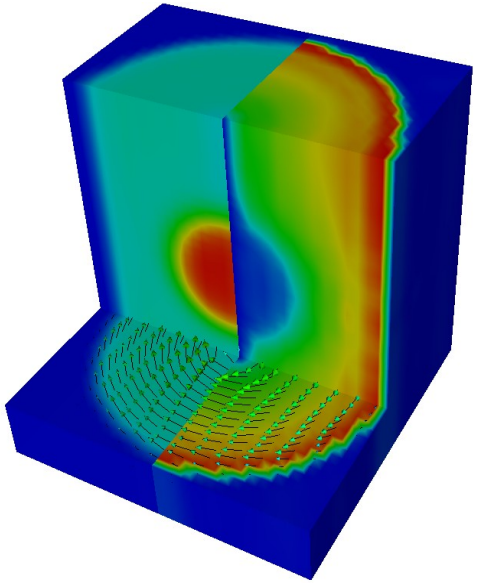
Bulgac, Forbes,Roche, and Wlazłowski, arXiv:1305.6891



Related ongoing projects

- Quantum turbulence in UFG
- Pinning of vortices
  in neutron matter to nuclei
- Fission of a heavy nucleus





Collaboration

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Thank you

physics wut