Quantum turbulence, superfluidity, non-Markovian dynamics and wave function thermalization

The Unitary Fermi gas and a bit about nuclear systems

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- Quantum turbulence occurs in the presence of quantized vortices, which cross and reconnect almost in a random manner.
- Quantum gases are compressible.
- In an isolated system the volume occupied by the gas in the presence of vortices is smaller than the volume of the volume of a quasi-homogeneous gas (due to the presence of vortex cores).
- After a crossing and reconnection of two vortices phonons are emitted and the separating vortices are receding faster from each other than when they were approaching each other.
- If the system is isolated and no energy is pumped into the system, the energy “stored” in the quantized vortices and their lengths are expected to decrease and therefore the average temperature of the system increases.
- The non-equilibrium time evolution is related with question raised in literature for a very long time by

  v. Neuman (1929), M. Berry (1977), Scrednicki (1994) ...

An isolated system thermalizes. → **Eigenstate Thermalization Hypothesis (ETH).**

I will illustrate several new aspects of non-equilibrium real-time dynamics in the case of two superfluid systems: Unitary Fermi Gas (UFG) and two nuclear phenomena.

UFG exhibits several universal properties:

- UFG properties depend on only one scale, the average interparticle separation, and UFG is a strongly interacting system.

- The single particle momentum distribution has power law behavior at large momenta at all energies, a clear non-Maxwellian behavior at any energy or temperature!

- UFG is a superfluid at low temperatures with the largest pairing gaps of any known systems (in appropriate units).

- UFG experiences quantum turbulence conjectured by Feynman in 1955.

- UFG has no classical nor semiclassical limits and an unexpected thermalization dynamics of the many-body wave functions and thus the range of validity of the ETH is questionable.

  v. Neuman (1929), M. Berry (1977), Scrednicki (1994), …

Chapter I: Unitary Fermi gas

Unitary Fermi Gas (UFG),
introduced by G.F. Bertsch (1999)

Pure numbers (dimensionless) determined/known from QMC (DMC) calculations of infinite systems

$$k \cot an\, \delta_0 = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + \cdots$$

$$E_{gs} = \frac{\hbar^2}{m} \int \mathcal{E}(\mathbf{r}) d^3 r$$

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

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

In the UFG limit (zero range and infinite scattering length)

number density
anomalous density

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

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

Dimensional arguments imply that this is
the only form allowed for the UFG energy density functional.

QMC - homogeneous

All these are simulations of finite systems.
SLDA and ASLDA are predictions.

QMC - in trap

Dates of submission on arXiv

QMC/DMC
Bertsch & Chang, 3/19/2007
Blume et al, 5/4/2007

SLDA
Bulgac, SLDA, 3/20/2007

Bulgac, Forbes, Magierski chapter 9, pages 305-373 in
BCS-BEC Crossover and the Unitary Fermi Gas (Lecture Notes in Physics, Vol. 836),
edited by W. Zwerger (Springer Heidelberg Dordrecht London New York, 2012)

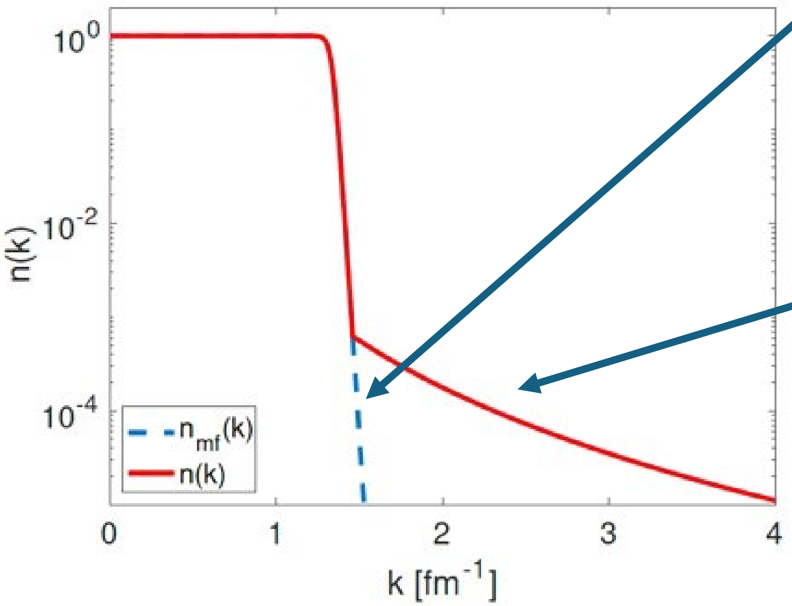
- Textbook expression of the equilibrium single-particle occupation probability,

Methods of QFT in statistical physics, Abrikosov, Gorkov, and Dzyaloshinski (1963)

$$n_{\rm mf}(k) = \frac{1}{1+\exp\beta[\epsilon(k)-\mu]}$$

← This is often not true!

Short Range Correlations (SRC): Levinger (1951), Sartor and Mahaux (1980), Frankfurt and Strikman (1981), Shina Tan (2008), …….., Hen (2017), …… and many others.
This is a result now firmly established in both theory and experiments.



Maxwellian distribution

$n(k) \propto \frac{C}{k^4}$

Typical quantum equilibrium occupation probability in the presence of short-range correlations and valid in a wide range of momenta.

Extending the formalism to Time-Dependent Phenomena and Superfluidity

"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."

Time-Dependent Superfluid Local Density Approximation (TDSLDA) equations
By construction, they resemble mean field equations, similar to
Hartree-Fock-Bogoliubov equations for quasiparticle wave functions.

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

Δ → Andreev reflection

Hole states ("Dirac sea")

Particle states

$$\int d\zeta\, n(\xi,\zeta)\phi_k(\zeta) = n_k\phi_k(\xi), \quad 0 \leqslant n_k \leqslant 1, \quad n(\xi,\zeta) = \langle\Phi|\psi^\dagger(\zeta)\psi(\xi)|\Phi\rangle.$$

$$\sum\!\!\!\!\!\!\int_\xi \phi_k^*(\xi)\phi_l(\xi) = \delta_{kl},$$

$$N = \sum\!\!\!\!\!\!\int_k n_k,$$

Canonical wave functions/natural orbitals

$$\tilde{u}_{l,\tau}(\xi) = \sqrt{1-n_l}\,\phi_{l,-\tau}(\xi),$$

$$\tilde{v}_{l,\tau}(\xi) = \tau\sqrt{n_l},\, \phi^*_{l,\tau}(\xi),$$

Let me stir UFG in an infinite circular cylinder with a subsonic velocity stirrer.

In this case the system is driven.
By the end, the system is in a steady state.

Sound velocity $v_s = v_F \sqrt{\frac{\xi}{3}} \approx 0.35\, v_F$

Free Fermi gas velocity

From the supplemental material in Bulgac, et al, Science 332, 1288 (2011)
Videos available at http://faculty.washington.edu/bulgac//UFG/

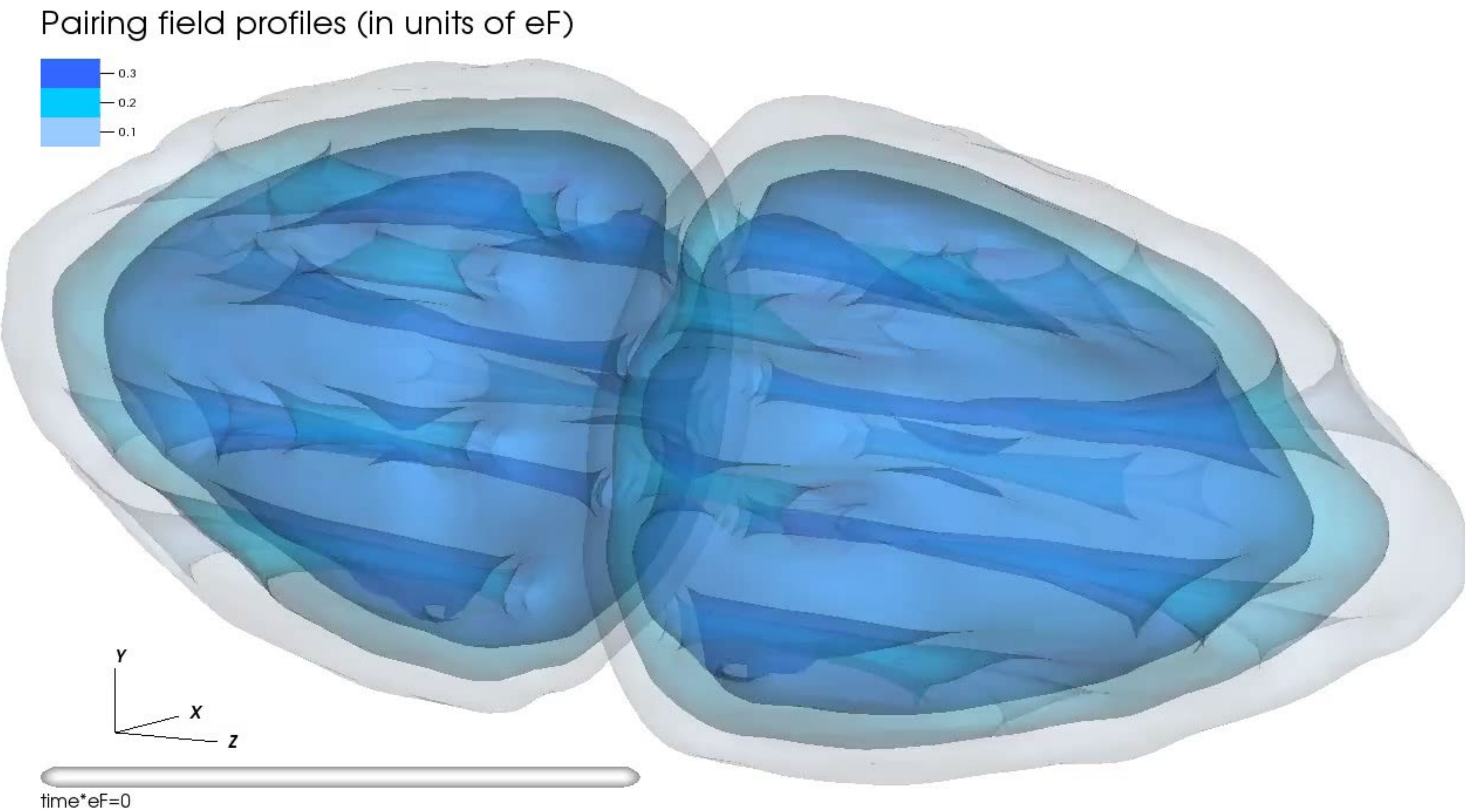
Let me stir UFG in an infinite circular cylinder with a supersonic velocity stirrer.

In this case the system is continuously driven.
By the end, the system is in a steady state.
Will the superfluidity survive?

$$v_S = v_F \sqrt{\frac{\xi}{3}}$$

From the supplemental material in Bulgac, et al, Science 332, 1288 (2011)
Videos available at http://faculty.washington.edu/bulgac//UFG/

The first ab initio simulation of quantum turbulence in a compressible fermionic superfluid.



Approximately 1270 fermions on a 48x48x128 spatial lattice, ≈ 260,000 complex PDEs, ≈ 309,000 time-steps, 2048 GPUs on Titan, 27.25 hours of wall time (initial code).

Wlazłowski et al, Phys. Rev. A 91, 031602(R) (2015)

The Unitary Fermi gas (UFG) is a unique system in many respects, but one aspect is unique to UFG, not known for any other physical system and UFG is extremely important for quantum many-body theory.

UFG is characterized by a single physical dimensional parameter.

1) The Schrödinger equation for the UFG can be solved for infinite homogeneous systems with various number of spin-up and spin-down fermions. The **3 coupling constants** defining the energy density functional needed in Density Functional Theory (DFT) are known from Quantum Monte Carlo (QMC) results for homogeneous systems at zero temperature and from experiment. These aspects allow to confirm the equivalence of Schrödinger and DFT descriptions at 1-body level.

F. Dyson, Nature, 427, 6972 (2004), reminiscing on a conversation between J. von Neumann and E. Fermi,
with J. von Neumann saying: ***With four parameters I can fit an elephant, with five I can make him wiggle his trunk.***

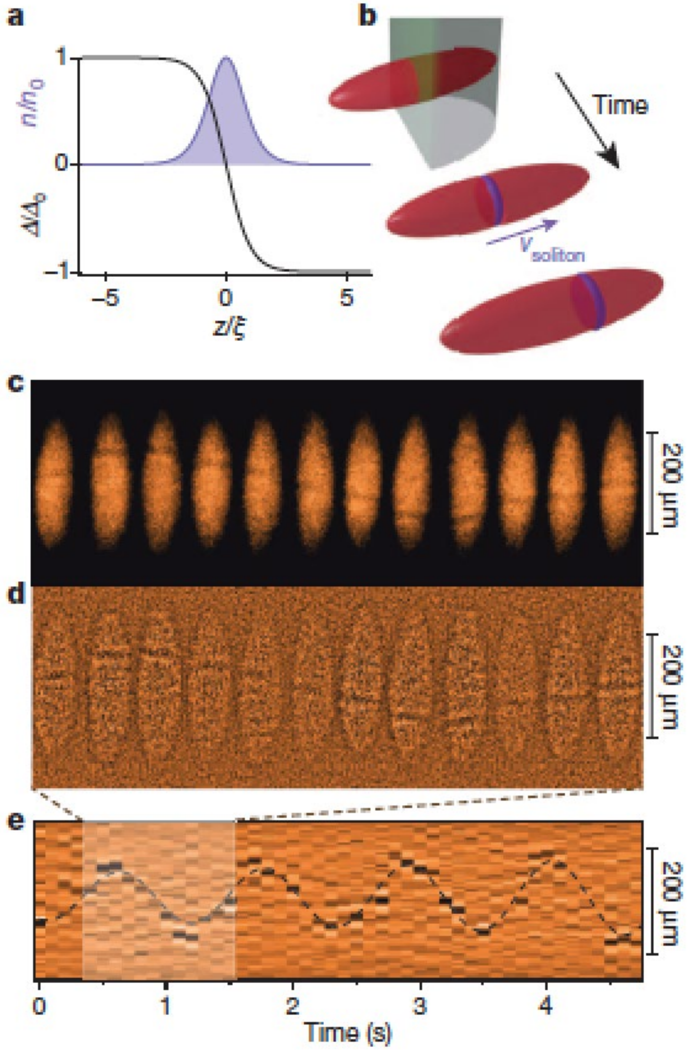
2) The Schrödinger equation for the UFG can be solved for systems with varying number of spin-up and spin-down fermions in external fields using QMC techniques. At this point one can confront the Schrödinger solutions to the Density Functional Theory static solutions for many superfluid and normal systems, for various number of particles in various external potentials and even make predictions, not postdictions.

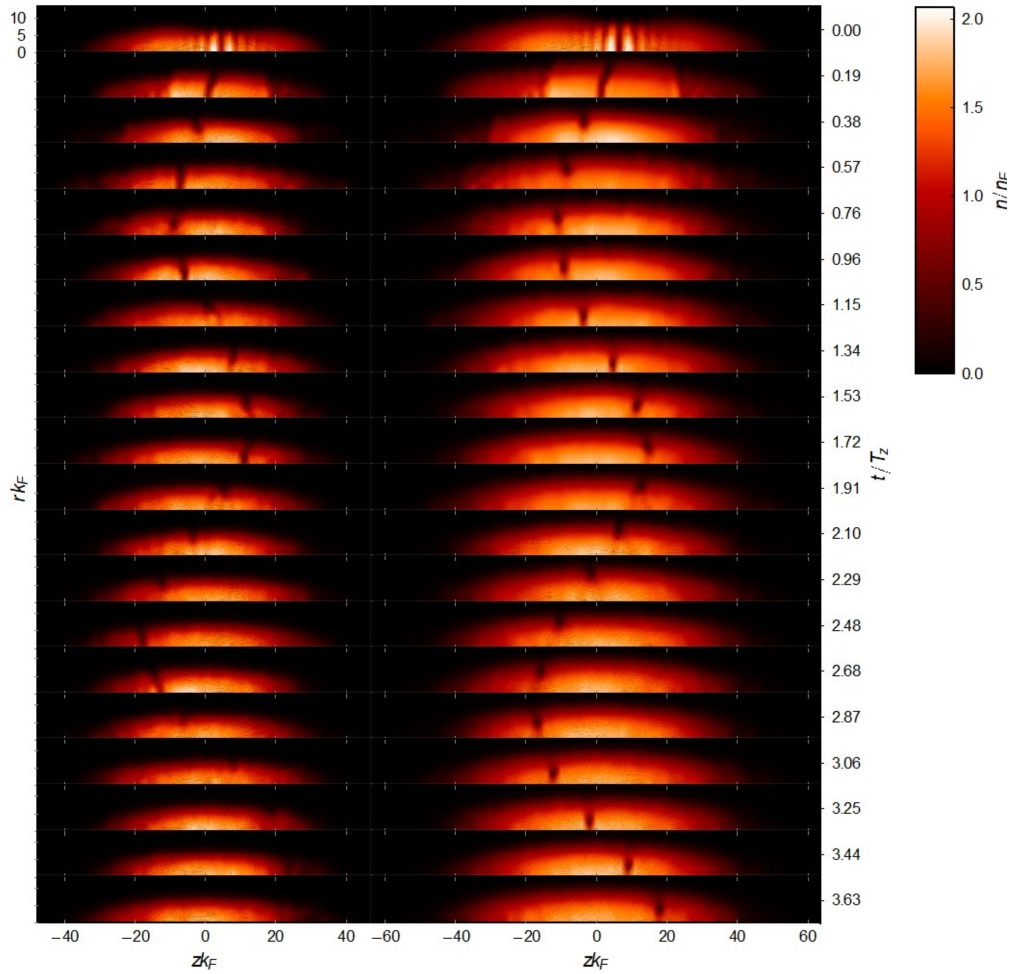
3) Extension of DFT to time-dependent phenomena is trivial, one needs to enforce only the Galilean invariance.

4) The time-dependent DFT solutions can be tested against known experimental results, in the case of highly non-equilibrium processes, for which solutions of the many-body Schrödinger equation are unavailable, e.g. quantum turbulence, dynamics of vortices in neutron star crusts, etc.

UFG within TDSLDA manages to wiggle its "tail" with 3 parameters only!

A great example on how TDSLDA helped clarify a great puzzle and give a correct interpretation to an experimental result. <u>The “heavy soliton” proved to be a vortex ring.</u>





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]

Nature, 429, 426-430 (2013)
Submitted on 2/19/2013, published on 7/17/2013

PRL **112,** 025301 (2014) PHYSICAL REVIEW LETTERS week ending 17 JANUARY 2014

Quantized Superfluid Vortex Rings in the Unitary Fermi Gas

Aurel Bulgac,[1] Michael McNeil Forbes,[2,1,3] Michelle M. Kelley,[4] Kenneth J. Roche,[5,1] and Gabriel Wlazłowski[6,1]

Received on 6/20/2013

We were a bit late, since GPUs on Titan became available only in May, 2013.

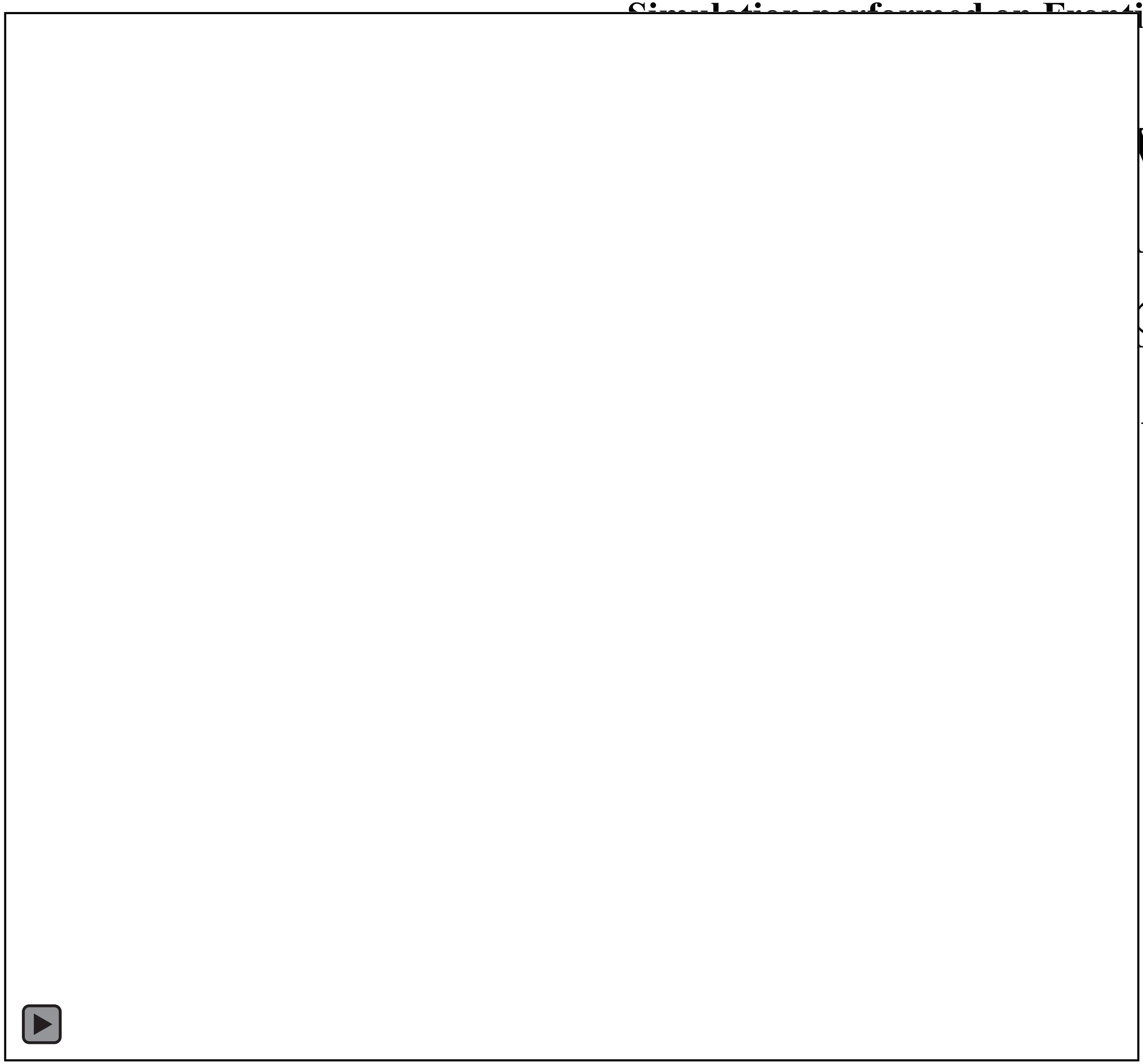
Rigol, Srednicki, Phys. Rev. Lett. 108, 110601 (2012)

Lattice 1D boson or fermion systems

Theoretical study of ETH in 1D lattice systems of fermions or bosons

- **Time evolution of quantum turbulence in an Unitary Fermi Gas (UFG)**

Bulgac, Kafker, Abdurrahman, and Wlazlwoski, Phys. Rev. Research, 108, L051303 (2024)



Simulation performed on Frontier #1 on Top500 supercomputers list

$$V = L^3=(32\ l)^3$$

$$l = 1$$

$$p_{max} = \pi / l = \pi$$

$$V_{phase\ space}= 32^3$$

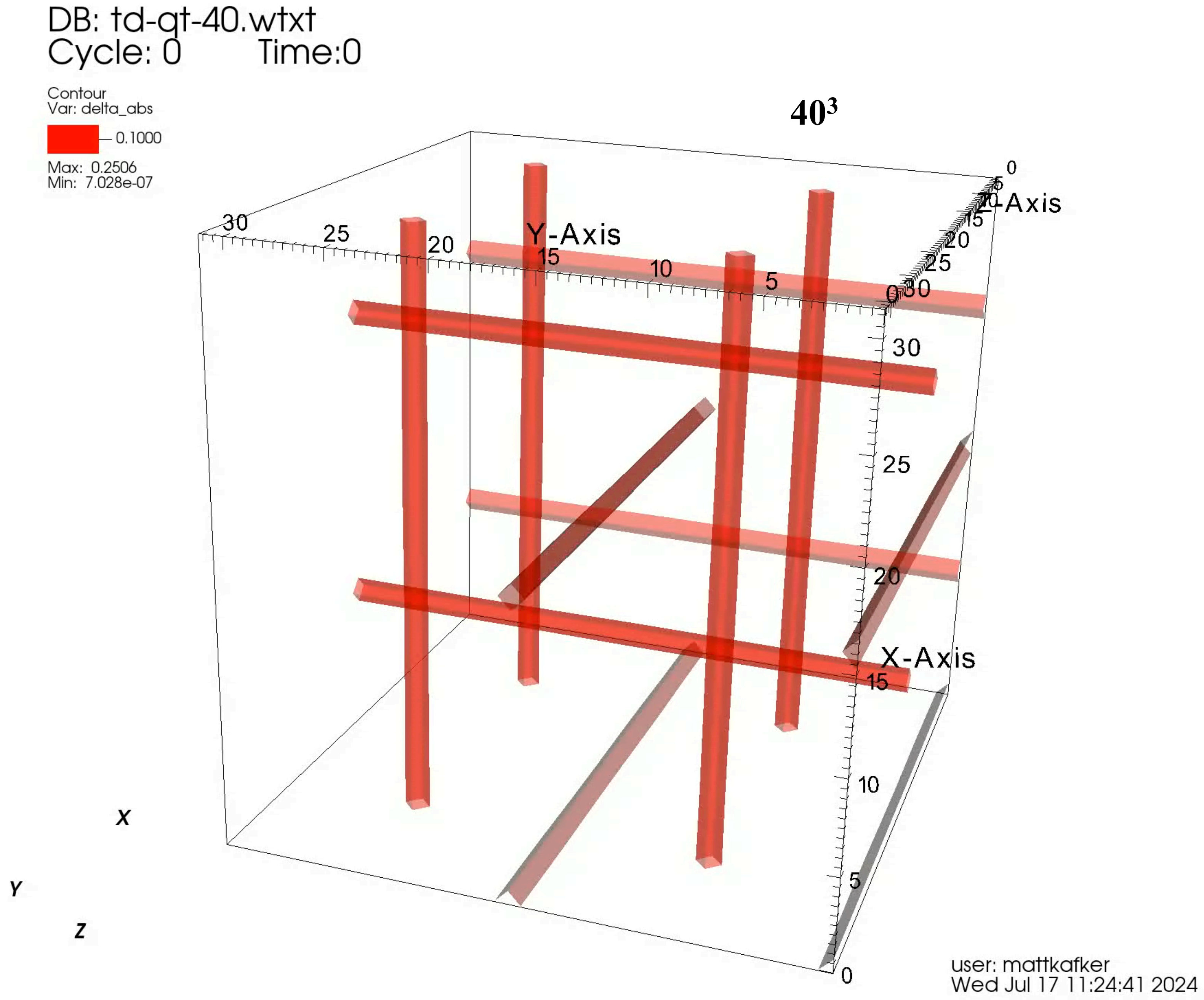
For Unitary Fermi Gas

$\hbar = m = 1$

About 1000 particle

$k_F \approx 0.66$

n = $\frac{N}{V} \approx 0.03$



$V = L^3 = (40\ l)^3$

$l = 0.8$

$p_{max} = \pi / l = 5\pi / 4$

$V_{phase\ space} = 40^3$

For Unitary Fermi Gas

$\hbar = m = 1$

About 1000 particle

Does TDSLDA include correlations or particle collisions?
Since this is mean field approximation.
Naïve answer NO!   Reality is more nuanced though.

TDSLDA is similar to BN/BUU equation, which includes correlations, and also mathematically identical to time-dependent Gorkov equations describing non-equilibrium superconductors.

Equation devised by Nordheim (BN-1928) and Uehling and Uhlenbeck (BUU-1933) and widely used approach in relativistic and non-relativistic heavy-ion collisions

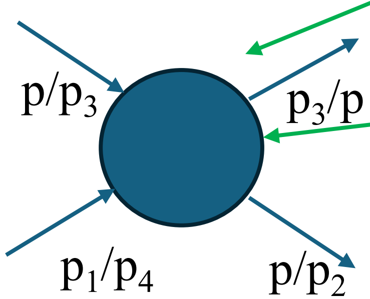
$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m} \cdot \frac{\partial f}{\partial \boldsymbol{q}} + \boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{p}} = I_{\rm coll}(\boldsymbol{p}, t), \qquad (3)$$

$$\begin{aligned} I_{\rm coll}(\boldsymbol{r}, \boldsymbol{p}, t) = -\frac{1}{(2\pi\hbar)^3} \int d\Omega \int d\boldsymbol{p}_2 \int d\boldsymbol{p}_4\, v \frac{d\sigma(q, \Omega)}{d\Omega} \\ \times \{f(\boldsymbol{r}, \boldsymbol{p}, t) f(\boldsymbol{r}, \boldsymbol{p}_2, t)[1 + \theta f(\boldsymbol{r}, \boldsymbol{p}_3, t)] \\ \times [1 + \theta f(\boldsymbol{r}, \boldsymbol{p}_4, t)] \\ - f(\boldsymbol{r}, \boldsymbol{p}_3, t) f(\boldsymbol{r}, \boldsymbol{p}_4, t)[1 + \theta f(\boldsymbol{r}, \boldsymbol{p}, t)] \\ \times [1 + \theta f(\boldsymbol{r}, \boldsymbol{p}_2, t)]\} \\ \times \delta(\boldsymbol{p} + \boldsymbol{p}_2 - \boldsymbol{p}_3 - \boldsymbol{p}_4), \end{aligned} \qquad (4)$$

loss (first bracketed term)

gain (second bracketed term)

$$mv = q = |\boldsymbol{p} - \boldsymbol{p}_2|. \qquad (5)$$



- BN/BUU is a semiclassical equation for the one-body number density also f(**r**,**p**,t).
- TDSLDA is however a quantum equation for the one-body number densities!

Phys. Rev. C 105, L021601 (2022)

$I_{\rm coll}$ (v,v ⇄ u,u)

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

gain ($u_{k\uparrow}, u_{k\downarrow}$)

loss ($v_{k\uparrow}, v_{k\downarrow}$)

- TDSLDA uses amplitudes for transitions, thus capable of describing interference and entanglement and thus fully quantum.

- BN/BUU uses probabilities for transitions and is thus semiclassical in spirit.

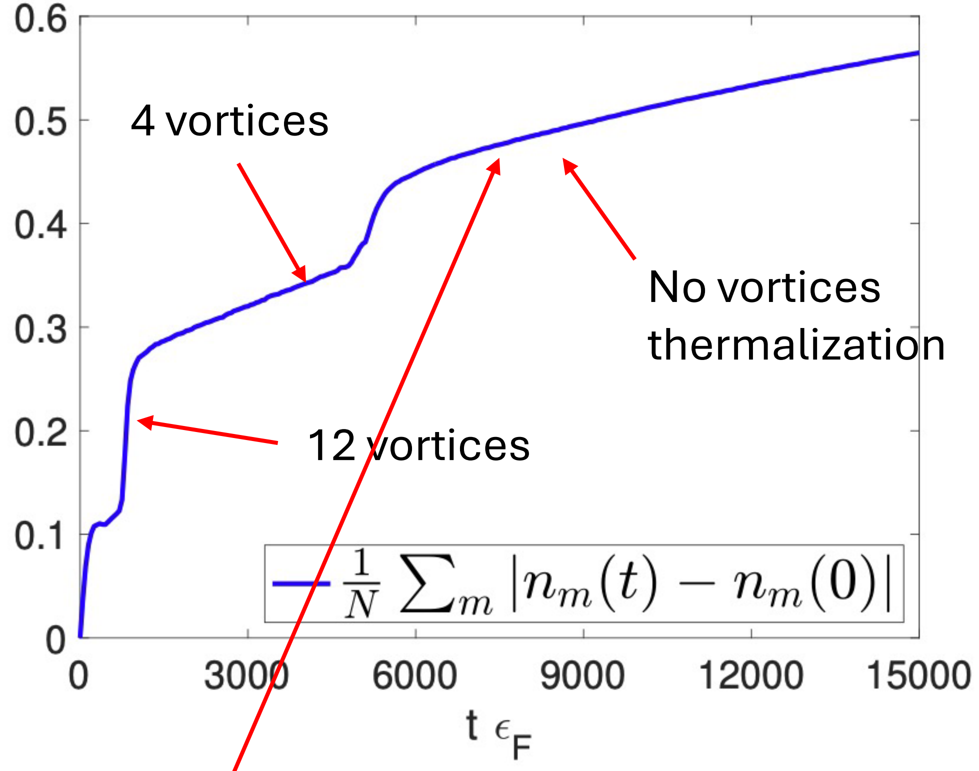


FIG. 1. The fractional sum $0 \leq \sigma_1(t) \leq 2$ of the absolute differences between single-particle occupation probabilities $n_m(t)$ at the initial time and at the final time t.

In pure mean field (HF):

- $n_m(t) \equiv 0$ or 1
- There is no thermalization

32^3

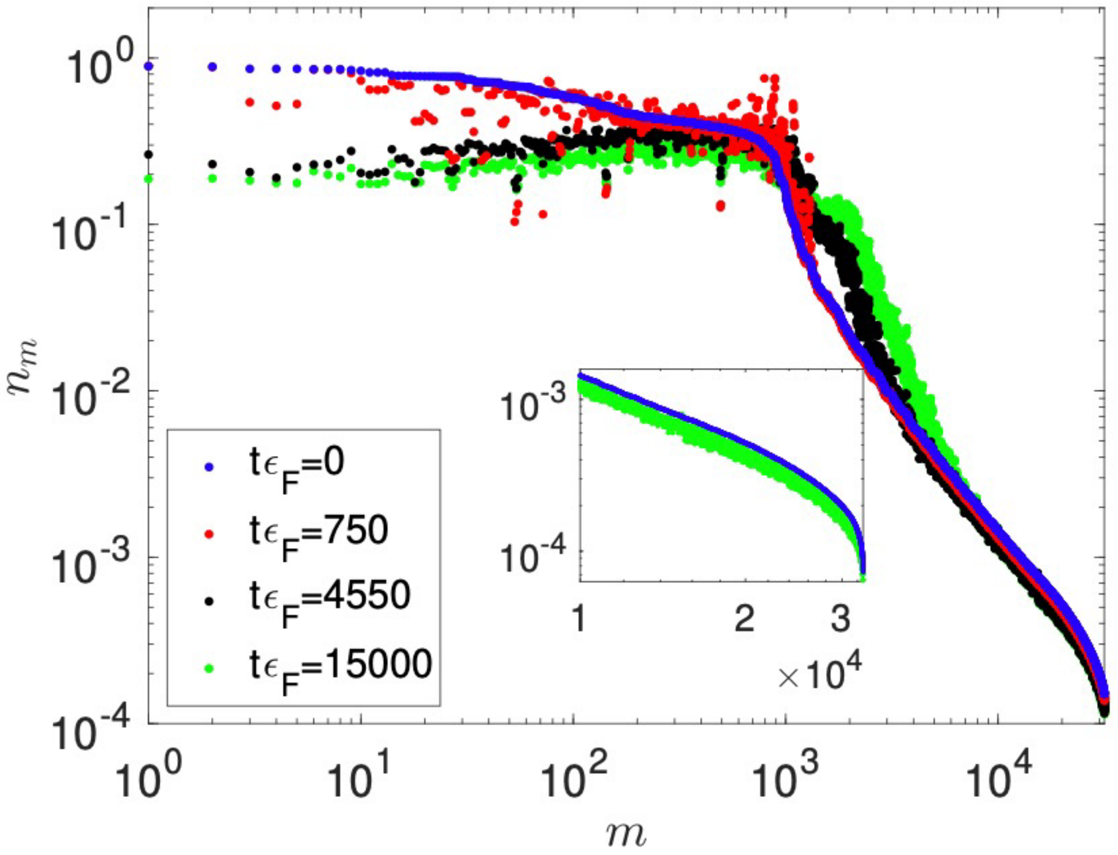
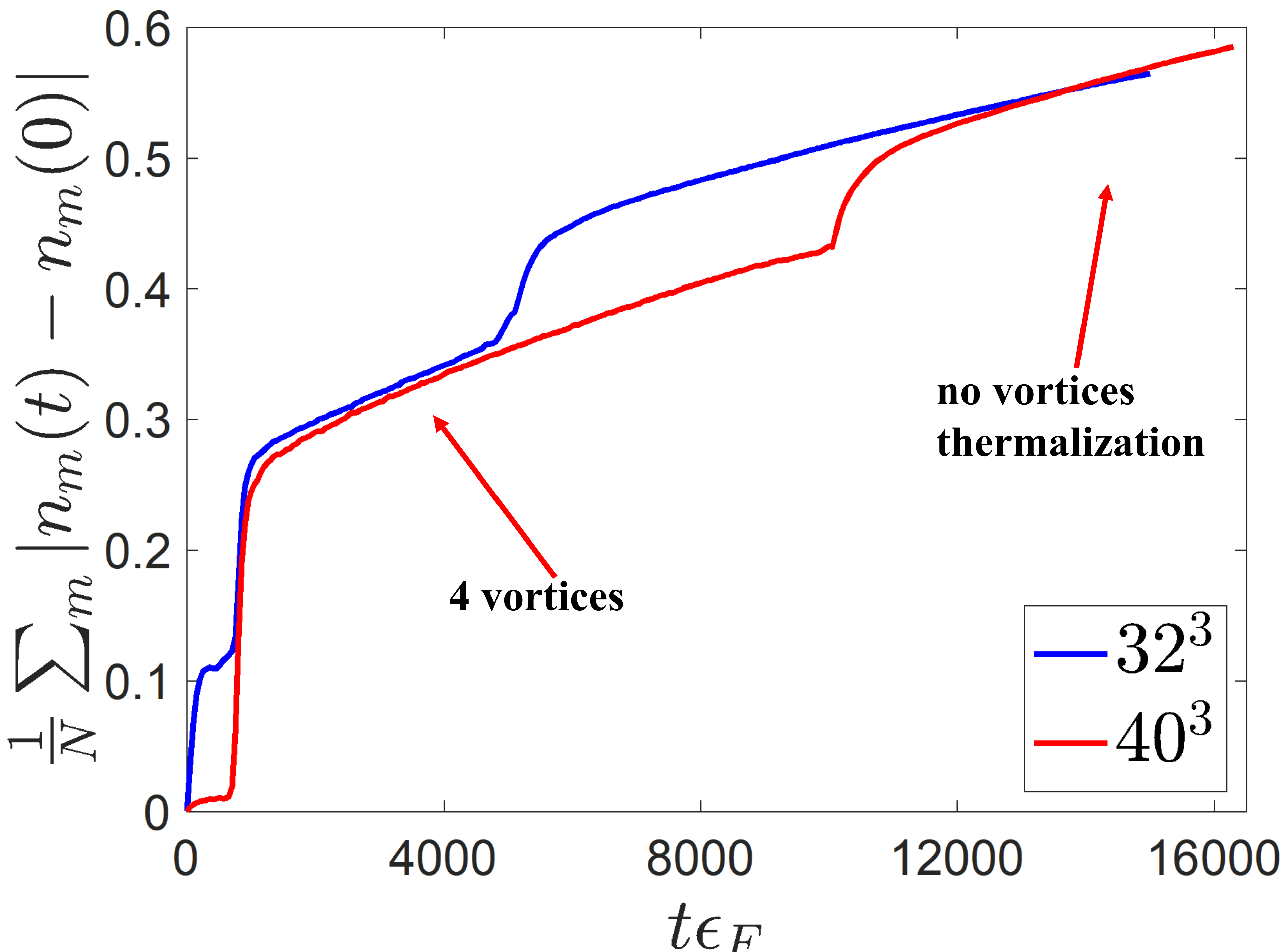


FIG. 2. The time-dependent occupation probabilities $n_m(t)$ at several times during the evolution. Due to the s-wave collisions the single-particle occupation probabilities in the final "thermalized" state are drastically redistributed. The states are ordered in decreasing order of the initial occupation probability $n_m(0)$. Since $\sum_m n_m(t) = N_\uparrow = N_\downarrow$ the initial high occupation probability quasiparticle states are depopulated at the expense of quasiparticle states with higher energies, but smaller than the upper cutoff energy $\epsilon_{cut} \approx \mathcal{O}(\pi^2/2l^2)$, see inset.



0.6
0.5
0.4
0.3
0.2
0.1
0
$\frac{1}{N}\sum_m |n_m(t) - n_m(0)|$
0
4000
8000
12000
16000
$t\epsilon_F$
no vortices
thermalization
4 vortices
32^3
40^3

32^3

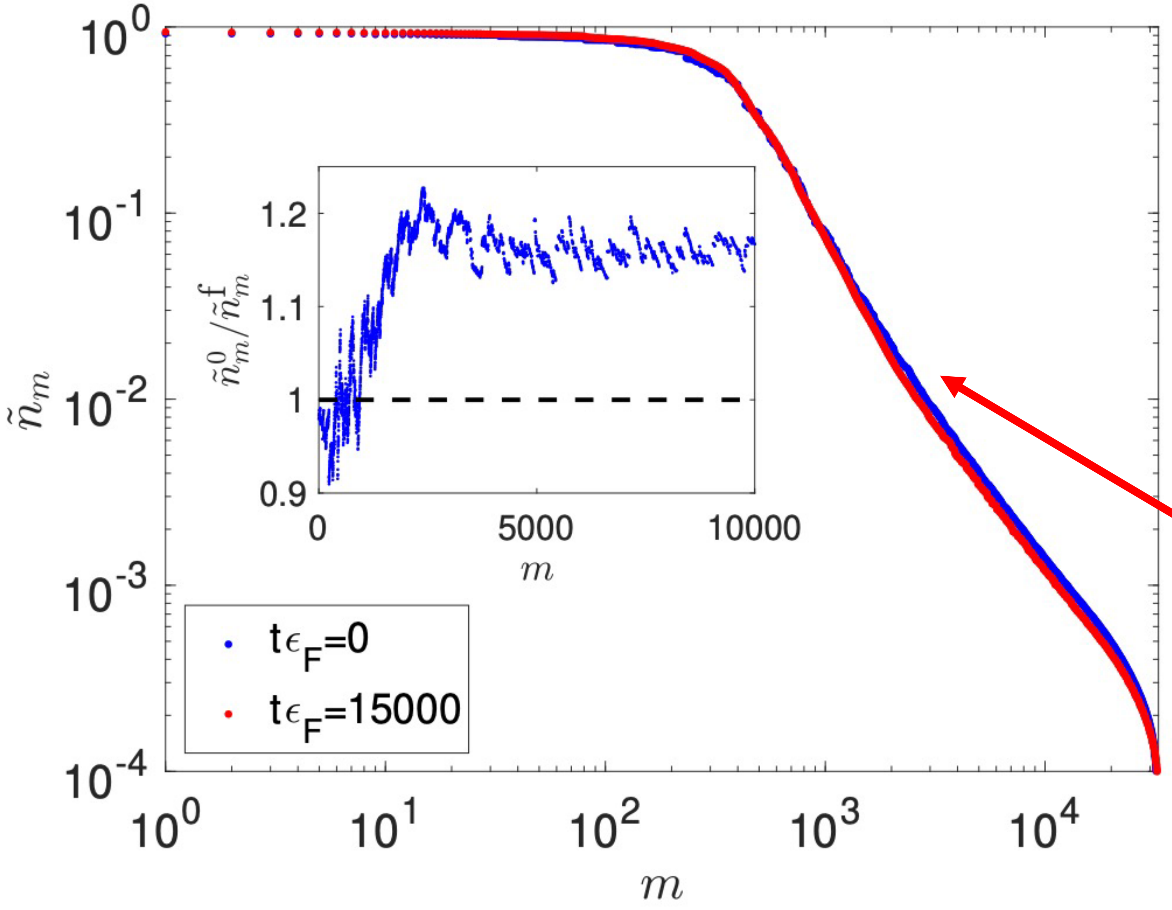


FIG. 3. The initial and final canonical occupation probabilities $\tilde{n}_m(t) = v_m^2(t)$, ordered by magnitude, which are the eigenvalues of the correspond instantaneous one-body density matrix, see Ref. [30, 53]. In the inset we show the ratio of the initial over final canonical occupation probabilities $\tilde{n}^0_m/\tilde{n}^f_m$. Since canonical occupation probabilities change with time there is no one-to-one correlation between their subscripts m.

Notice: Canonical occupation probabilities for the initial and final states are almost indistinguishable.

In the initial state the system had 12 “empty’ tubes, thus it has a higher average number density.

- Final state is for an almost equilibrium homogeneous state of a superfluid UFG
- Asymptotic power law behavior of the momentum distribution C/k^4.

$$n(\xi,\zeta) = \langle\Phi|\psi^\dagger(\zeta)\psi(\xi)|\Phi\rangle.$$

$$\int d\zeta\, n(\xi,\zeta)\phi_k(\zeta) = n_k\phi_k(\xi), \quad 0 \leqslant n_k \leqslant 1,$$

$$\sum\!\!\!\!\!\!\int_\xi \phi_k^*(\xi)\phi_l(\xi) = \delta_{kl},$$

$$N = \sum\!\!\!\!\!\!\int_k n_k,$$

12 vortices

no vortices

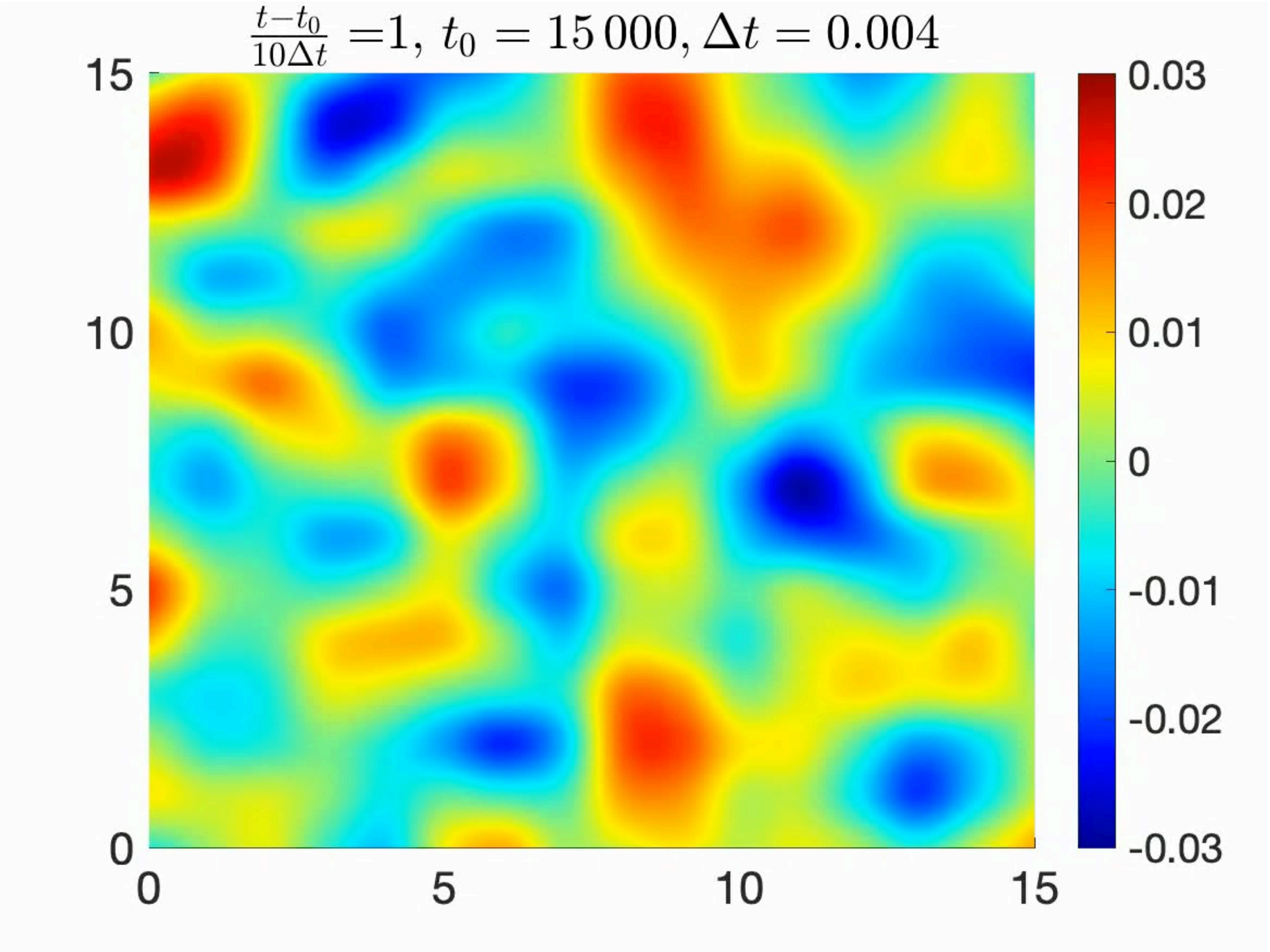
4 vortices

Eigenstate Thermalization Hypothesis (ETH)

Time dependent thermal fluctuations

John von Neumann (1929)
Michael Berry (1977)
Mark Srednicki (1994)

Time-dependent density fluctuations in a superfluid system in equilibrium at finite temperature



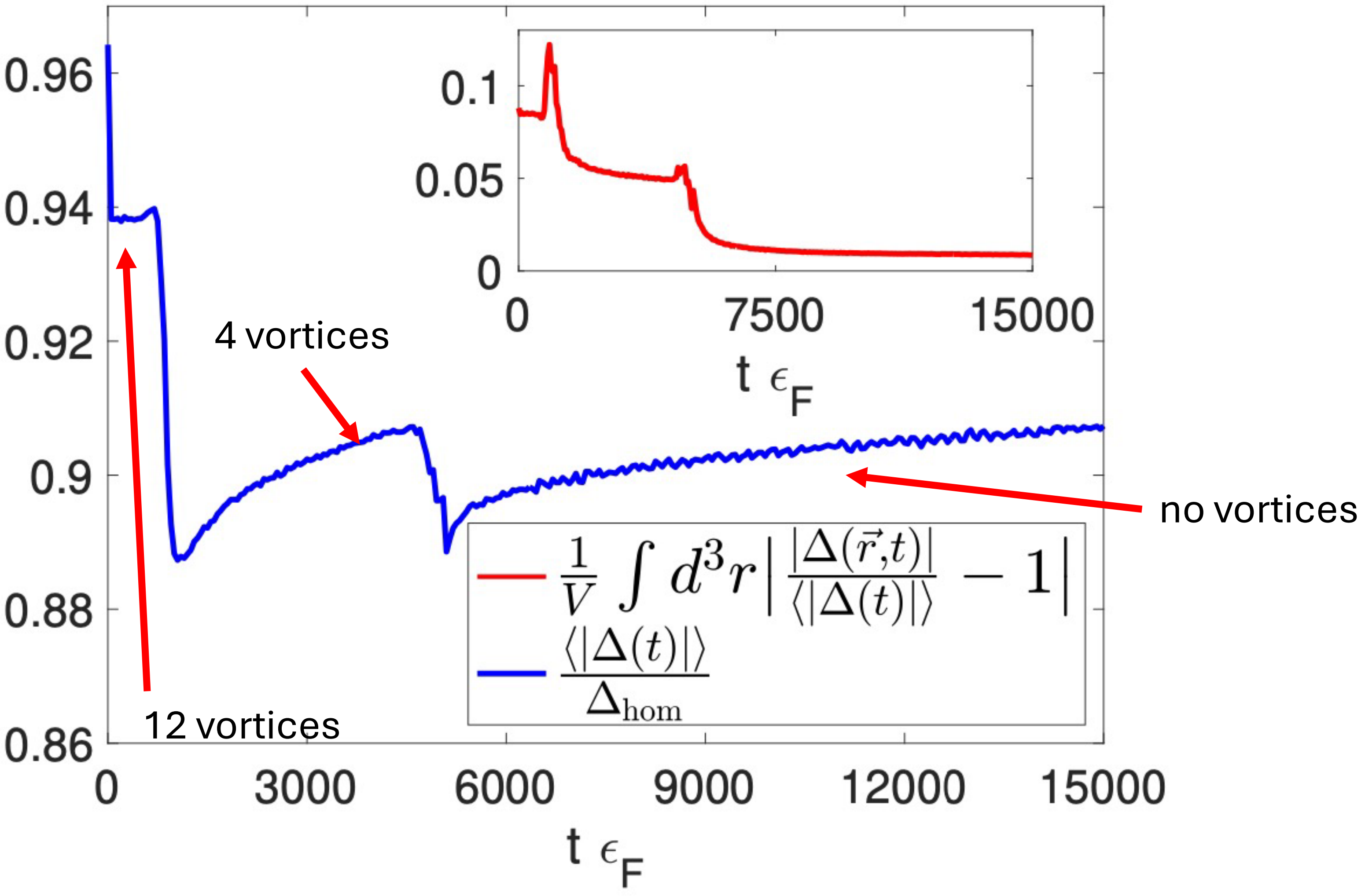


FIG. 5. The time evolution of the average of absolute value of the pairing gap, divided by its value in the homogeneous UFG at the same number density. The inset shows the average fluctuation of this quantity.

UFG within TDSLDA manages to wiggle its “tail” with 3 parameters only!

Chapter II: Nuclear systems

- **Vortex – impurity interaction**
- **Induced nuclear fission**

Nuclear systems are much more complicated, even though some aspects resemble UFG.

To solve the Schrödinger equation for a many-nucleon system one needs the 2-, 3-, and 4-body nucleon interactions. The average separation between nucleons is comparable with the nucleon-nucleon interaction range and the sum of their nucleon radii. (Basically cannon balls or atoms in a liquid or in a solid.)

- 2-nucleon interaction are extracted experimentally from scattering data.
- Inverse scattering problem, no unique solution and insufficient experimental data.
- NN-online, phase-shifts, about 4,000 data.
- 2-nucleon effective field theory (EFT) potentials, depend on 21 parameters.
- On top one also needs also 3- and 4-nucleon interactions.

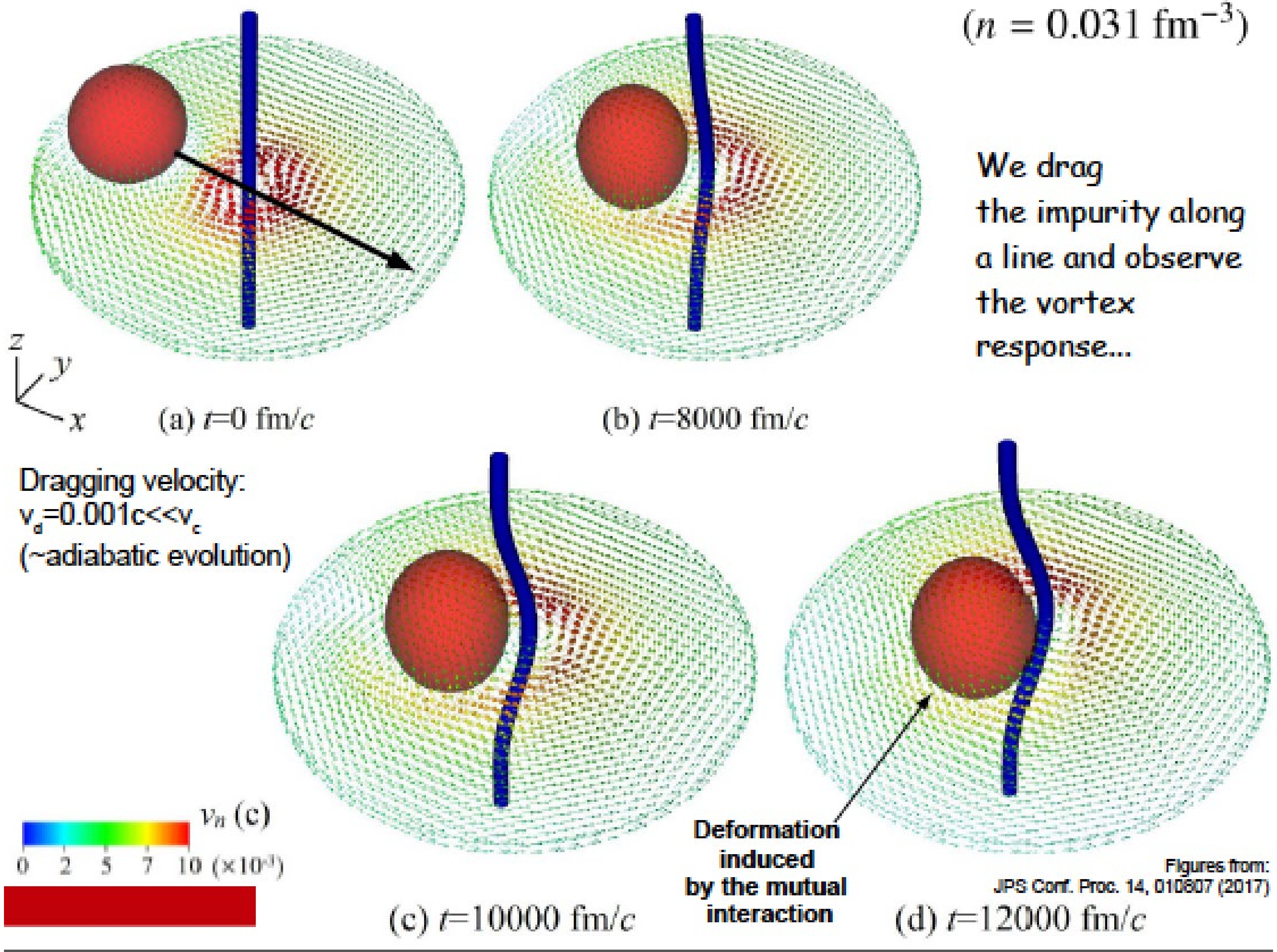
Density Functional Theory (DFT) is mathematically equivalent to many-body Schrödinger equation at 1-body level .

- Non-optimized energy density functional depends on only 7 very well-known parameters + proton charge + average nucleon mass, and QMC for neutron matter with chiral EFT interactions (2- and 3-body).
- Absolute energy rms 1.74 MeV, or about 0.1% in c ase of heavy nuclei, for 606 even-even nuclei, charge radii for
- 345 even-even nuclei rms 0.038 fm.
- A related quantum liquid drop model for 2375 nuclei has an absolute energy rms 2.86 MeV (better than Bethe-Weizsäcker liquid drop formula) and for charge radii of 883 nuclei of 0.041 fm (new element to quantum liquid drop formula), with only 4 parameters.

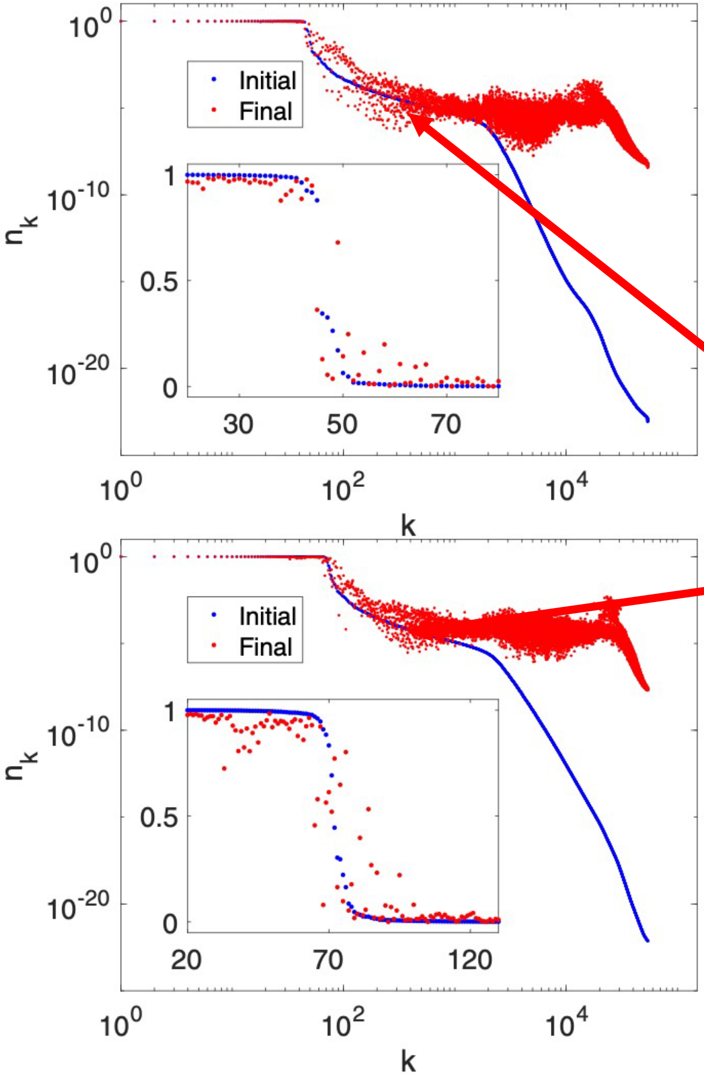
- TDDFT for vortices in neutron star crust, heavy-ion collisions, fission studies put in evidence already a significant number of aspects unknown until recently, either theoretically or experimentally.

The vortex pinning in neutron star crust was a theoretical puzzle for more than 4 decades, since Anderson and Itoh, Nature (1975), with theoretical models predicting either attraction or repulsion, under identical conditions and with varying degrees of strength.

These results from Wlazlowski, Sekizawa, Magierski, Bulgac, Forbes, Phys. Rev. Lett. 117, 232701 (2016).



- **Induced nuclear fission $^{235}U(n_{therm},f)$**



^{239}Pu(n,f)

Low energy neutron incident on ^{239}Pu induces fission

$$\propto \frac{1}{k^4}$$

$$\sum_k^{\infty} n_k(t) = 240$$

FIG. 1. In the upper and lower panels we show the initial and final proton and neutron single-particle occupation probabilities, evaluated performing a fission simulation of ^{236}U with the NEDF SeaLL1, starting near the top of the outer fission barrier, with the full set of initial quasiparticle wave functions, see Table III, until the FFs are partially fully separated. Since the occupation probabilities are double degenerate, we display only 1/2 of their spectrum, in this case only $\Omega = 54\,000$. The results presented in this figure were obtained with $Q_{20} = 140.02$ b and $Q_{30} = 14.63\text{b}^{3/2}$ set of initial conditions.

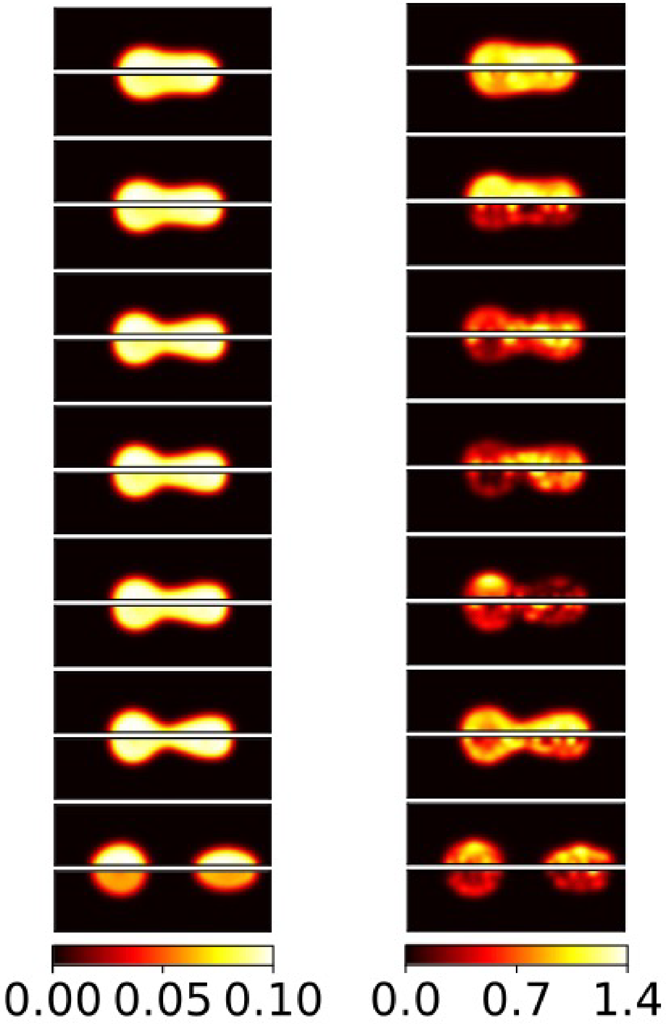


FIG. 4. Time frames illustrating the profiles of the neutron (top) and proton number densities (first column) and the absolute value so the pairing gap (second column), separated in time by about 500 fm/c. The last row are for colorbars for the densities in units of fm^{-3} and MeV for the pairing gaps. The initial state was the same as in Fig. 1.

Similar behavior in case of fission!

Bulgac et al, Phys. Rev. C 109, 064617 (2024)

Nuclear systems are also superfluid and much more complex, neutrons and protons (charged), much more complex interactions.

Neck formation

Scision

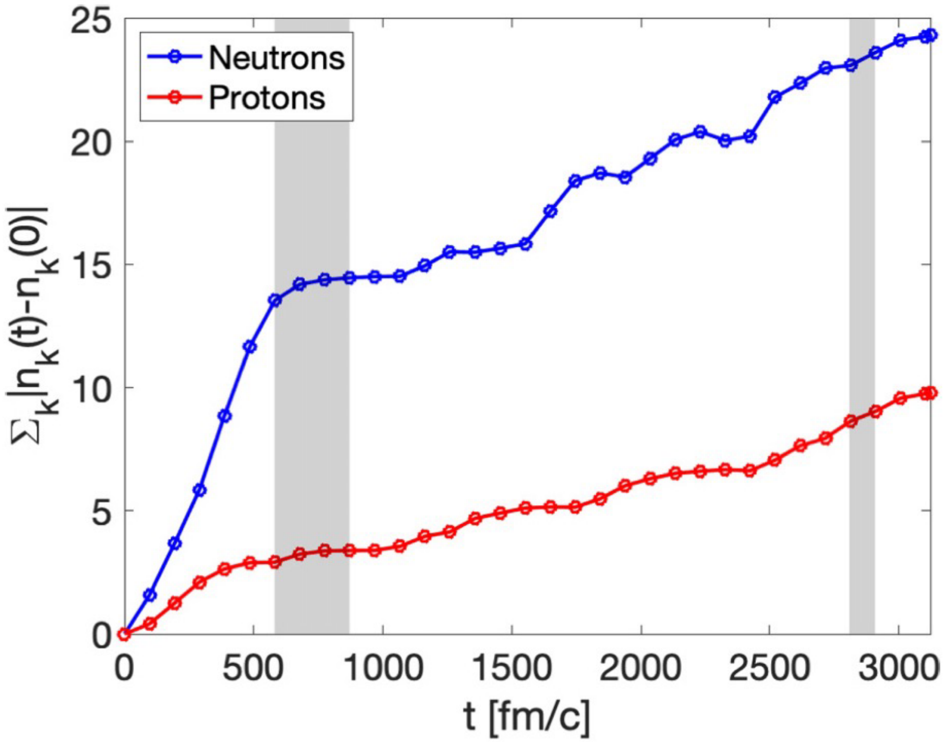
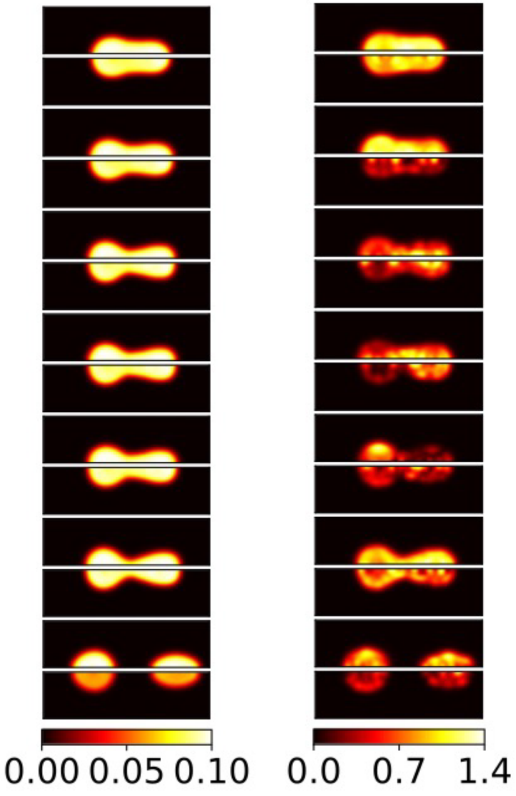


FIG. 3. The sum of the absolute differences between the single-particle occupation probabilities at the initial time and at time t. Initial conditions are the same as in Fig. 1.

^{239}Pu(n,f)

Low energy neutron incident on ^{239}Pu induces fission

$$\sum_k^{\infty} n_k(t) = 240$$



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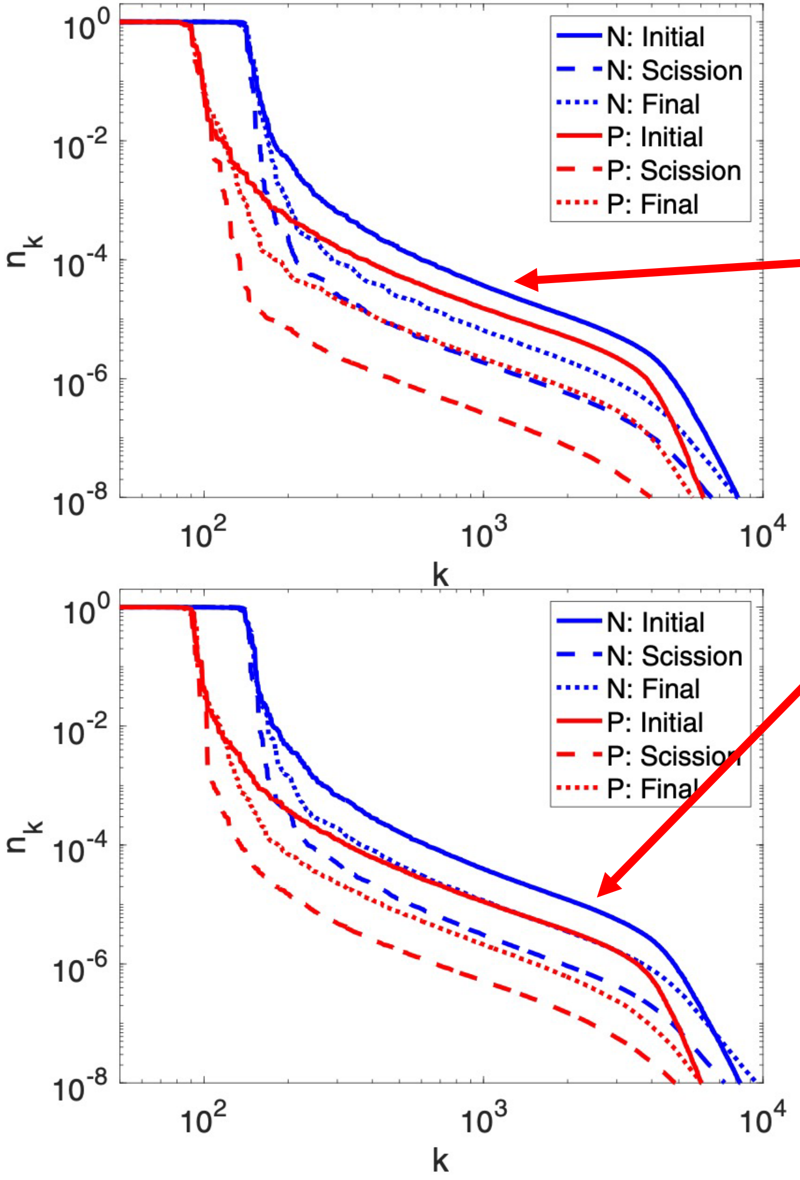

FIG. 12. The time evolution of the canonical occupation probabilities for neutron and proton levels at the initial time, scission, and the final time for the same data presented in Fig. 11. The upper panel correspond the trajectory shown with dashed limes, while the lower panel corresponds to the trajectory shown with solid lines in Fig. 11.

$\propto \frac{1}{k^4}$

$^{239}Pu(n,f)$

Low energy neutron incident on ^{239}Pu induces fission

$$\sum_{k}^{\infty} n_k(t) = 240$$

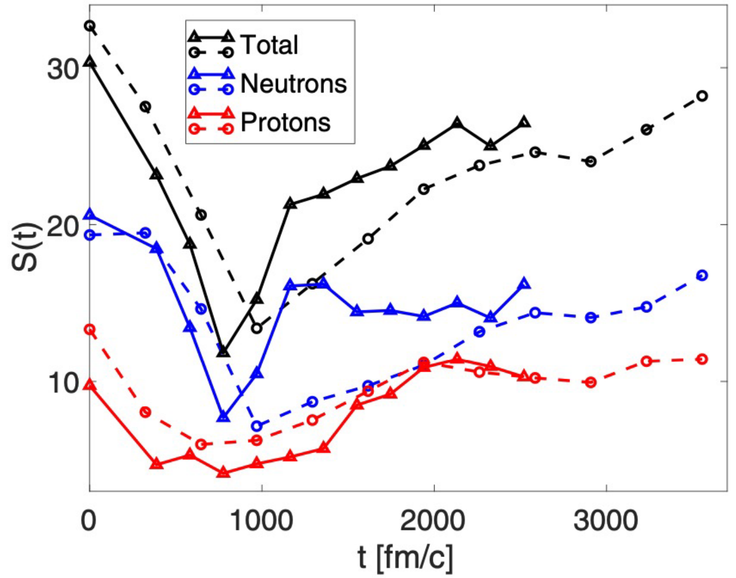

FIG. 11. The orbital entropy $S(t)$ as a function for time for fission of ^{236}U in a large simulation box $48^2 \times 120$ fm^3 for two of the simulations reported in Ref. [144], for two different set of initial conditions. The initial deformations of the fissioning nuclei were $Q_{20} = 159.64$ b and $Q_{30} = 17.80$ b$^{3/2}$ for one trajectory (solid lines) and $Q_{20} = 135.25$ b and $Q_{30} = 12.44$ b$^{3/2}$ for the other trajectory (dashed lines), near the top of the outer barrier. The entropy is plotted separately for proton and neutron subsystems and for the entire fissioning system. For more details concerning these simulations see Ref. [144].

$$S(t) = -g\sum_k n_k(t)\ln n_k(t) - g\sum_k [1 - n_k(t)]\ln[1 - n_k(t)]$$

Orbital entanglement entropy is a measure of the complexity of the many-body wave function.

Conclusions

- I introduced a formalism capable to describe the time-dependent evolution of an isolated quantum system in non-equilibrium, a system of pure quantum kinetic equations.

- Unlike the semiclassical BN/BUU extension of the classical Boltzmann equation (valid only for very dilute systems) this new approach is based fully on quantum mechanics.

- This framework allows for the presence of quantized vortices, interference phenomena, and entanglement.

- I have demonstrated how quantum turbulence eventually thermalizes, the role of the energy cascade from large to small scales quantized vortices decay fully into phonons and the system evolves into a thermal state with time-dependent quantum fluctuations.
Significantly slower (by 2-3 orders of magnitude) than suggested by ETH.

- The dynamics of a strongly interacting quantum many-body system in non-equilibrium was shown have a clear non-Markovian behavior.

- Collisions are not isolated in either space or time (unlike in the Boltzmann eq.), the system is dense.
Strong correlations/entanglement ?!