Realtime Methods for Superfluid Dynamics

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Outline

• Unitary Fermi gas and the SLDA/ASLDA
  Describe SLDA/ASLDA and connection to mean-field theory
  Fits to box data, parameters
  Maybe remind of phases and of LOFF from Aurel's talk

• Dynamics
  TDDFT, hydrodynamics, GPE, two fluid model
  Realtime Techniques
  Directly probe dynamics
  Efficient simulation (Quantum Friction state prep., extract pinning interaction)

• Applications
  MIT soliton experiment
  Vortex Pinning and Pulsar Glitches
  Vortex-Pinning and Vortex-Vortex interactions (Fermionic DFTs)
  Quantum Turbulence in vortex networks (superfluid hydrodynamics)
    emphasize scaling of computations
  Fission in nuclei, Excitations (GDR), Reactions

• From Cold Atoms to Nuclei and Neutron Stars
  Validated Methods
  DFT, Vortex pinning, Glitches, Quantum Turbulence

---

FIG. 1 (color online). Deflection of a vortex in the ETF model of trapped dilute neutron matter as a UFG by a repulsive (left panel) and attractive (right panel) pinning potential.
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• From Cold Atoms to Nuclei and Neutron Stars
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Fermionic Superfluids

Neutron Matter
- $k_F \sim \text{fm}^{-1}$
- $a_{nn} = -19 \text{ fm}$
- $r_{nn} = 2 \text{ fm}$

Unitary Fermi Gas
- $a = \infty$
- $r_e = 0$

Cold Atoms
- $k_F \sim \mu \text{m}^{-1}$
- Tuneable $a$
- $r_{nn} \sim 0.1 \text{ nm}$
- Many systems
  - different species
  - dipole interactions
  - optical lattices
  - quantum simulators

Other Superfluids
- Superconductors (charged + phonons)
- Quarks (gluon interactions, Dark Matter?)
- $^3\text{He}$ (p-wave)

Nuclei
- neutrons
- protons

Wednesday, April 15, 15
Fermionic Superfluids

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Nuclei
neutrons and protons

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Unitary Fermi Gas (uFG)

\[ \hat{H} = \int \left( \hat{a}^{\dagger} \hat{a} E_a + \hat{b}^{\dagger} \hat{b} E_b \right) - \int V \hat{n}_a \hat{n}_b \]

\[ E_{a,b} = \frac{p^2}{2m} - \mu_{a,b}, \quad \mu_{\pm} = \frac{\mu_a \pm \mu_b}{2} \]

• Characterize interactions by single number:
  • S-wave scattering length \( a \)
    Gas is dilute so we can ignore small-scale structure

• Tune interactions with magnetic field
  Feshbach Resonance
Unitary Fermi Gas (uFG)

\[ \hat{\mathcal{H}} = \int \left( \hat{a}^{\dagger} \hat{a} E_a + \hat{b}^{\dagger} \hat{b} E_b \right) - \int V \hat{n}_a \hat{n}_b \]

\[ E_{a,b} = \frac{p^2}{2m} - \mu_{a,b}, \quad \mu_\pm = \frac{\mu_a \pm \mu_b}{2} \]

• Unitary limit \( a=\infty \): No interaction length scale!

• Universal physics:
  • \( \mathcal{E}(\rho) = \xi \mathcal{E}_{\text{FG}}(\rho) \propto \rho^{5/3}, \quad \xi=0.370(5) \)

• Simplest non-trivial model (dimensional analysis)
Unitary Fermi Gas (uFG)

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• Universal physics:
  • \( \mathcal{E}(\rho) = \xi \mathcal{E}_{FG}(\rho) \propto \rho^{5/3}, \quad \xi = 0.370(5) \)

• Simple, but hard to calculate!
  
Bertsch Many Body X-challenge
Unitary Equation of State

- Only scales: $T$ and $N$
- One convex dimensionless function $\hbar T(\mu/T)$

$$ P = \left[ T h_T \left( \frac{\mu}{T} \right) \right]^{5/2} $$

- Measured to percent level:
  - $\xi_{exp} = 0.370(5)(8)$

Figure from Drut, Lähde, Wlazłowski, and Magierski, PRA (2012)
Experiment: Ku, Sommer, Cheuk, and Zwierlein, Science (2012)
Zürn, Lompe, Wenz, Jochim, Julienne, and Hutson PRL (2013) corrected resonance
BEC-bcs Crossover
Phase Diagram (T=0)

Grand canonical
What happens in middle?
Still need precision measurements for asymmetric systems

P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)
Symmetric Matter

P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)
Symmetric BCS state

Fully Polarized (One Species) Fermi Gas

P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)
Symmetric Unitary Gas

Fully Polarized (One Species) Fermi Gas

Zero momentum pairs

BEC

BCS

P_1

P_2

\frac{\delta \mu}{\Delta} = \frac{1}{k_{Fa}}

P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)


p = p_a + p_b = 0

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Symmetric BEC state

\[ \frac{\delta \mu}{\Delta_0} \]

Tightly bound pairs

\[ \mathbf{a} \quad \mathbf{b} \]

Fully Polarized (One Species) Fermi Gas

\[ \mathbf{P}_1 \quad \mathbf{P}_2 \]

BCS

P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)
Asymmetric?

Unequal Fermi surfaces

• Frustrates pairing

P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)
Asymmetric P-wave pairs

P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)
Asymmetric P-wave BEC

BEC and P-wave superfluids coexist homogeneously

Fully Polarized (One Species) Fermi Gas

P-wave states by A. Bulgac, M.M. Forbes, A. Schwenk (PRL 2006)
Asymmetric Gapless superfluid

Pairing promotes particles?

“Breach” in pairing

Still induced P-wave

May need large mass ratio or structured interactions (not likely at weak coupling in cold atoms)

P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)
Asymmetric FFLO

Pairs have momenta $p_1 + p_2 \neq 0$

Fully Polarized (One Species) Fermi Gas

BEC

BCS

State (LO) is crystal (supersolid)


$P$-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)
DFT predicts (FF)LO at Unitarity: Supersolid!

Large density contrast (factor of 2)

Similar to contrast of vortex core

Observations: Nothing?

Paired core
Polarized wings
Maybe there are no interesting polarized superfluid phases?

MIT Experimental data from Shin et. al (2008)
DFT predicts (FF)LO at Unitarity: Supersolid!

Large density contrast (factor of 2)

Similar to contrast of vortex core

Observations: Inconclusive

• Need detailed structure or novel signature

MIT Experimental data from Shin et. al (2008)
Why FFLO not seen?

• It is not there:
  • Other homogenous phases might be better.
  • $T$ might be too high (fluctuations kill 1D FFLO).
  • Trap frustrates formation (traps are not flat enough).

• It is not seen:
  • Noise washes out signature.
  • Small physical volume for FFLO.

• Need a nice flat trap: Large physical volume of FFLO

see idea of Ozawa, Recati, Delehaye, Chevy, and Stringari PRA 90 (2014) 043608
Asymmetric Exotica?

Need IR structure
Sign problem
Please benchmark!
Computational Costs

Classical: $6N N_t$

Quantum: $N x^3 N N_t$

Fermionic dft: $N N x^3 N_t$

Bosonic dft: $N x^3 N_t$
Bosons are "easy"

\[
E[\Psi] = \int d^3\vec{x} \left( \frac{\hbar^2 |\nabla \Psi(\vec{x})|^2}{2m_B} + V_F(\vec{x})\rho_F + g\frac{|\Psi|^4}{2} \right)
\]

\[
i\partial_t \Psi = \left( -\frac{\nabla^2}{2m_B} + [V + g|\Psi|^2] \right) \Psi
\]

- Gross-Pitaevskii Equation (GPE)
- (all) bosons in single ground state
  - Include interactions through mean field
- Non-linear Schrödinger equation
- Only one wave function \( \rho = |\Psi|^2 \)
Misses “shell” effects

Forbes, Gandolfi, Gezerlis [PRA 86 (2012) 053603]
Fermions are harder

\[ i \partial_t \Psi_n = H[\Psi] \Psi_n = \left( \begin{array}{c} -\frac{\alpha \nabla^2}{2m} - \mu + U \\ \Delta \end{array} \right) \begin{pmatrix} \Delta^\dagger \\ \frac{\alpha \nabla^2}{2m} + \mu - U \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} \]

- Pauli Exclusion (blocking)
- Particles in different states
- Must track \( N \) wavefunctions
  - Non-linear Schrödinger equation for each wavefunction
  - Hartree-Fock–Bogoliubov (HFB), Bogoliubov de-Gennes (BdG)
- Must use symmetries or supercomputers

\( (N) N x^3 N_t \)
Fermions are harder

\[ \imath \partial_t \Psi_n = H[\Psi] \Psi_n = \left( \frac{-\alpha \nabla^2}{2m} - \mu + U \right) \Delta \left( \frac{-\alpha \nabla^2}{2m} + \mu - U \right) \begin{pmatrix} \Delta^\dagger \\ \Delta \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} \]

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Fermi Surface

\[ k_{Fa} \quad k_{Fb} \]

\[ a \quad b \]

\[ (N) N x^3 N_t \]
Fermions are harder

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• Evolution: \( (N) N_x^3 N_t \)
  Scales reasonably well

• Ground state
  Need repeated diagonalization!

\[ (NN_x^3)^3 \]

(or does it...)

Fermi Surface

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Correct “shell” effects

Forbes, Gandolfi, Gezerlis [PRA 86 (2012) 053603]
SLDA: Superfluid Local Density Approximation

\[ \mathcal{E}(n, \tau, \nu) = \alpha \frac{\tau}{m} + \beta \frac{(3\pi^2 n)^{5/3}}{10m\pi^2} + g_{\text{eff}} \nu^\dagger \nu \]

- Three densities:
  \( n \approx \langle a^\dagger a \rangle, \tau \approx \langle \nabla a^\dagger \nabla a \rangle, \nu \approx \langle ab \rangle \)

- Three parameters:
  - Effective mass \((m/\alpha)\)
  - Hartree \((\beta)\), Pairing \((g)\)

Forbes, Gandolfi, Gezerlis [PRA 2012]
BdG: contained in SLDA

\[ \langle \hat{\nabla}^\dagger \hat{\nabla} \rangle + \langle \hat{\nabla}^\dagger \hat{\nabla} \rangle \]
\[ \mathcal{E}(n, \tau, \nu) = \alpha \frac{\tau}{m} + \beta \frac{(3\pi^2 n)^{5/3}}{10m \pi^2} + g_{\text{eff}} \nu^\dagger \nu \]

• Variational: \( \mathcal{E} = \langle H \rangle \) (minimize over Gaussian states)

• Bogoliubov-de Gennes (BdG) contained in SLDA

• Unit mass \( (\alpha = 1) \)

• No Hartree term \( (\beta = 0) \)
  • (No polaron properties)
**SLDA: Superfluid Local Density Approximation**

\[ \mathcal{E}(n, \tau, \nu) = \alpha \frac{\tau}{m} + \beta \frac{(3\pi^2 n)^{5/3}}{10m\pi^2} + g_{\text{eff}} \nu^\dagger \nu \]

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Forbes, Gandolfi, Gezerlis (2012)
SLDA: Superfluid Local

Three densities:
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- Effective mass \((m/\alpha)\)
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- Pairing \((g)\)

Forbes, Gandolfi, Gezerlis (2012)
Unbiased sLDA fit at $r_{\text{eff}} = 0$

Fit “unbiased” results

- $\xi = 0.3742(5)$
- $\Delta = 0.65(1)$
- $\alpha = 1.104(8)$
- $\chi^2 = 0.3$

Forbes, Gandolfi, Gezerlis (2012)
**Works in traps (ASLDA)**

<table>
<thead>
<tr>
<th>Normal State</th>
<th>Superfluid State</th>
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Within few % except for smallest systems

Can add gradients

Forbes [arXiv:1211.3779]

What about Dynamics?
Realtime Evolution

\[ i \partial_t \Psi_n = H[\Psi] \Psi_n = \left( \begin{array}{ccc} -\frac{\alpha \nabla^2}{2m} & -\mu + U & \Delta^\dagger \\ \Delta & \frac{\alpha \nabla^2}{2m} + \mu - U \end{array} \right) \begin{pmatrix} u_n \\ v_n \end{pmatrix} \]

• No diagonalization needed for evolution
  Just apply Hamiltonian
  Use FFT for kinetic term

• Efficient realtime evolution the scales well
  Distribute wavefunctions over nodes
  Utilize GPUs

• Split Operator or ABM evolution
DFT: Fermion still hard

\[ i\partial_t \Psi_n = \hat{H}[\Psi] \Psi_n = \left( \begin{array}{cc} -\frac{\alpha \nabla^2}{2m} & \Delta \\ \Delta^\dagger & \frac{\alpha \nabla^2}{2m} + \mu - U \end{array} \right) \left( \begin{array}{c} u_n \\ v_n \end{array} \right) \]

- 48x48x128 lattice
- 131 629 two-component wavefunctions
- 1TB per state

Wlazłowski, Bulgac, Forbes, and Roche PRA(R) (2015)
Scaling Properties

- **SLDA realtime code**
  - Both Weak and Strong scaling

- **Fully utilizes GPUs**
  (GPUs provide 90% of TITAN’s compute power)
State Preparation?

• How to find initial (ground) state?

• Root-finders repeatedly diagonalize s.p. Hamiltonian
  Slow and does not scale well

• Imaginary time evolution?
  Non-unitary: spoils orthogonality of wavefunctions
  Re-orthogonalization unfeasible (communication)
Quantum Friction

\[ V_t \propto -\frac{\hbar \vec{\nabla} \cdot \vec{j}_t}{\rho_t} = \frac{\hbar \dot{\rho}_t}{\rho_t} \propto -\mathcal{I}(\psi^\dagger_t \nabla^2 \psi_t) \]

• Unitary evolution (preserves orthonormality)

• Easy to compute: local time-dependent potential
  Acts to remove local currents

• Couple with quasi-adiabatic state preparation
  Bulgac, Forbes, Roche, and Wlazłowski (2013) [arXiv:1305.6891]
Quantum Friction

\[ V_t \propto -\frac{\hbar \nabla \cdot \vec{j}_t}{\rho_t} = \frac{\hbar \dot{\rho}_t}{\rho_t} \propto -\mathcal{I}(\psi_t^\dagger \nabla^2 \psi_t) \rho_t \]

• Consider evolution with potential \( H + V_t \):

\[ \partial_t E = -i \text{ Tr } ([H, \rho] \cdot V_t) \]

• Therefore \( V_t = i[H, \rho] \dagger \) guarantees \( \partial_t E \leq 0 \)

Non-local potential equivalent to “complex time” evolution
Not suitable for fermionic problem

• Diagonal version is a local potential: \( V_t = \text{ diag}(i[H, \rho] \dagger) \)
Quantum Friction

Potential counteracts currents

Use with dynamics to minimize energy

Harmonic oscillator with an excited state
Quantum Friction

Potential counteracts currents
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Quantum Friction

Potential counteracts currents
Use with dynamics to minimize energy

Harmonic oscillator with an excited state
State Preparation

Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]:
32x32x128
Quantum Friction

$V_t \propto -\frac{\hbar \nabla \cdot \vec{j}_t}{\rho_t} = \frac{\hbar \dot{\rho}_t}{\rho_t} \propto -\mathcal{I}(\psi_t^\dagger \nabla^2 \psi_t)$

• General method: (works for many problems)
  Needs a good initial state to ensure reasonable occupation numbers

• Easy to compute: local time-dependent potential
  Acts to remove local currents

• Couple with quasi-adiabatic state preparation
  Bulgac, Forbes, Roche, and Włazłowski (2013) [arXiv:1305.6891]
Bosons are “easy”

\[
E[\Psi] = \int d^3 \vec{x} \left( \frac{\hbar^2 |\nabla \Psi(\vec{x})|^2}{2m_B} + V_F(\vec{x}) \rho_F + g \frac{|\Psi|^4}{2} \right)
\]

\[i \partial_t \Psi = \left( -\frac{\nabla^2}{2m_B} + [V + g|\Psi|^2] \right) \Psi\]

- Gross-Pitaevskii Equation (GPE)
- (all) bosons in single ground state
  Include interactions through mean field
- Non-linear Schrödinger equation
- Only one wave function \( \rho = |\Psi|^2 \)
  Or a few if modelling coupled fluids
GPE model for ufg?

\[ E[\Psi] = \int d^3 \vec{x} \left( \frac{|\nabla \Psi(\vec{x})|^2}{4m_F} + V_F(\vec{x})\rho_F + \xi \mathcal{E}(\rho_F, \{\nabla \rho_F\}) \right) \]

\[ i\partial_t \Psi = \left( -\frac{\nabla^2}{4m_F} + 2[V_F + \xi \epsilon(\rho_F, \{\nabla \rho_F\})] \right) \Psi \]

• Think:
  • Boson = Fermion pair (dimer) \[ \rho_F = 2|\Psi|^2 \]
  • Galilean Covariant (fixes mass) \[ \mathcal{E}_{FG} \propto \rho_F^{5/2} \]
  • Match Unitary Equation of State \[ \epsilon_F = \mathcal{E}'_{FG}(\rho_F) \propto \rho_F^{3/2} \]
  • “Extended Thomas-Fermi” (ETF) model
Comparison

Fermions
SLDA TDDFT

Gross Pitaevskii model

Bulgac et al. (Science 2011)
Fermions:
- Simulation hard!
- Evolve $10^4$–$10^6$ wavefunctions
- Requires supercomputers

GPE:
- Simulation much easier!
- Evolve 1 wavefunction
- Use supercomputers to study large volumes
Matching Theories: The Good

- Galilean Covariance (fixes mass/density relationship)
- Equation of State
- Hydrodynamics
  - speed of sound (exact)
  - phonon dispersion (to order $q^3$)
  - static response (to order $q^2$)

Forbes and Sharma (PRA 2014)
What is missing?

- Excessive phonon noise
- Short-wavelength dissipation
- Vortex lattice doesn’t crystallize
- Incorrect vortex mass
- Vortices move too slowly
Matching Theories: The Bad

- $G\rho = 2|\Psi|^2$
- Density vanishes in core of vortex
- Implies $\int |\Psi|^2$ conserved
  - (Approximate conservation $\int |\Psi|^2$ in Fermi simulations provides measure of applicability)
- No “normal state”
- Two fluid model needed?
- Coarse graining (transfer to “normal” component)

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Vortex Structure (empty core)
Linear Response

Michael Forbes and Rishi Sharma PRA 90 (2014) 043638
Low energy Phonons

Michael Forbes and Rishi Sharma PRA 90 (2014) 043638
Missing Pair-breaking

Michael Forbes and Rishi Sharma PRA 90 (2014) 043638
Data from Joseph, Thomas, Kulkarni, and Abanov
PRL (2011)
Ancilotto, L. Salasnich, and F. Toigo (2012)

GPE vs. Experiment

Fig. 4

1D density profiles at different times $t$ showing the collision of two strongly interacting Fermi clouds.

Left part: our calculations

Right part: experimental data from Ref.

We simulated the whole procedure by using the Runge-Kutta-Gill fourth-order method to propagate in time the solutions of the following non-linear Schrödinger equation (NLSE):

$$i\hbar \frac{\partial}{\partial t} \Psi = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \frac{2}{\alpha} U(\mathbf{r}) + \frac{\hbar^2}{2m} \left( \frac{3\pi^2}{2} \right)^{\frac{2}{3}} \xi |\Psi|^4 + \left( 1 - \frac{4\lambda}{\hbar^2} \right) \frac{\hbar^2}{4m} \nabla^2 |\Psi|^2 \right] \Psi$$

(31)

which is strictly equivalent to Eqs. (17) and (18), with $E(n, \nabla n)$ given by Eq. (4), and

$$\Psi(\mathbf{r},t) = \sqrt{n(\mathbf{r},t)} e^{i\theta(\mathbf{r},t)}$$

(32)

Since the confining potential used in the experiments is cigar-shaped, we have exploited the resulting cylindrical symmetry of the system by representing the solution of our NLSE on a 2-dimensional $(r, z)$ grid. During the time evolution of our system, when the two clouds start to overlap, many ripples whose wavelength is comparable to the interparticle distance are produced in the region of overlapping densities. In order to properly compare our results with the experimental data of resonant fermions...
FIG. 8. (Color online) Conservation of the integrated squared pairing gap (squared smoothed $\psi$) for the simulations for $v_{\text{stir}} = 0.1v_F$ ($v_{\text{stir}} = 0.11v_F$), $v_{\text{stir}} = 0.2v_F$ ($v_{\text{stir}} = 0.197v_F$), and $v_{\text{stir}} = 0.25v_F$ ($v_{\text{stir}} = 0.242v_F$) for SLDA (ETF). The wave function was smoothed by convolving with a two-dimensional Gaussian smearing function of spatial width $0.75/k_F$. Note that the scales of the three plots are different: The $v_{\text{stir}} \sim 0.1v_F$ integral is essentially unchanged, while the $v_{\text{stir}} \sim 0.25v_F$ integral decreases by about 25%.

**Conjecture**

Resolve with:

Two-fluid hydrodynamics
Normal + Superfluid

Conversion via coarse-graining/condensation
Provide dissipation - mocks pair-breaking

Normal fluid will fill vortices

Michael Forbes and Rishi Sharma PRA 90 (2014) 043638
Applications

Heavy Solitons are Vortex Rings/Lines
Quantum Turbulence
Glitches in Neutron Stars
Nuclear Fission
Vortices: an application

- Resolving a Mystery: MIT Heavy Solitons = Vortex Rings & Vortices
  Fermionic DFT for small systems validates bosonic model for realistic systems

- Vortex Reconnection

- Quantum Turbulence
  New arena:
  Strong interactions (unlike BECs)
  Experiments
  Reliable theory (unlike He)
MIT Experiment

- $^6$Li atoms ($N \approx 10^6$) cooled in harmonic trap
- Step potential used to imprint a soliton
- Let system evolve
- Image after ramping magnetic field $B$ and expanding
- Observe an oscillating soliton with long period $T \approx 12T_z$
  - Bosonic solitons (BECs) oscillate with $T \approx \sqrt{2}T_z \approx 1.4T_z$
  - Fermionic solitons (BdG) oscillate with $T \approx 1.7T_z$
- Interpret as “Heavy Solitons”
- Later resolved as vortex rings and vortices

Ku et al. PRL 113 (2014) 065301
MIT Experiment

\[ \hbar \delta_t(\delta \varphi) = \delta V \]  (phase difference on either side of trap)

Imprint soliton

Step potential phases evolve to \( \pi \) phase shift

Flat domain wall (dark/grey soliton)

Ku et al. PRL 113 (2014) 065301
MIT Experiment

Thick solitons
• 10 × coherence length

Slowly moving
T ≈ 12Tz

Theory (Walls):
T ≈ 1.2–1.4Tz

Is theory wrong?

Objects are Vortices

Better tomographic imaging reveals vortex

Gravity breaks trap asymmetry

Only imaged in one direction

Width consistent with a vortex core $\sim l_{\text{coh}}$

Ku et al. PRL 113 (2014) 065301
Wall, Ring, Vortex

Wlazłowski, Bulgac, Forbes, and Roche [arXiv:1404.1038]
MIT Experiment

Period depends on:
• Aspect ratio
  \( \lambda \in \{3.3, 6.2, 12\} \)
• Interaction

Much longer than predicted for domain walls

MIT Experiment

Finite temperature:
• Anti-decay
• (Negative mass)

Density Functional Theory (DFT)

- Superfluid Local Density Approximation (SLDA)
  - Well tested for statical properties
  - Can we also use for dynamics
  - Expensive
    (one of the largest supercomputing calculations to date)

- Effective Thomas-Fermi (ETF) model
- “Bosonic model” (GPE with correct EOS)
- Not as reliable, but can be scaled up
State Preparation

Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]:
32x32x128
State Preparation

Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]: 32x32x128
State Preparation

Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]:
32x32x128
FIG. 4. (color online) Oscillations of a vortex ring in a harmonic trap on a $24 \times 24 \times 96$ lattice (left) and a $32 \times 32 \times 128$ lattice (right). We start with a cylindrical cloud (not shown, see Ref. [30, 38]) with central density $n = k_F^3/\pi^2$ where the Fermi wavevector $k_F = 1/\sqrt{\pi x} = 1/\sqrt{1}$. The harmonic trapping potential along $z$ is then increased slowly while applying the quantum cooling algorithm described in [38] to cool the system to a state with two separate clouds. These are the phases imprinted with $\phi = \pi$ and the knife edge is removed, allowing the soliton to evolve as shown. Movies, including a case for a $48 \times 48 \times 128$ lattice, may be found in [30]. This ring then oscillates along the axis of the trap. In the smaller simulation, the ring does not fully form, and it collapses in on itself, re-forming as a dark-soliton near the turning points. This behavior mirrors that seen in BEC [25], but is demonstrated here for the first time in a fermionic system. This new domain wall exhibits the same initial instability, and a vortex ring of the opposite circulation and similar size forms and moves back along the trap in the opposite direction. This oscillation is at the limit of the fermionic equivalent of the domain-wall branch of these types of excitations [26]. Note that [26] also discusses collision of these excitations, which are elastic at low energies. Reducing the width of the trap, one will continuously approach the quasi-1D situation of oscillating domain walls. Note that the period $T = T_z/\pi$ in this case approximately agrees with other the quasi-1D simulations [14, 17, 18].
Vortex Rings

\[ E \sim \frac{m n \kappa^2}{2} R \ln \frac{R}{l_{\text{coh}}}, \quad \nu = \frac{dE}{dp} \sim \frac{\kappa}{4\pi} \frac{1}{R} \ln \frac{R}{l_{\text{coh}}} \]

• Thin vortex approximation in infinite matter
  (follows essentially from Biot-Savart law)

• Approximately valid for rings near core
  (but not too near)

• Logarithmic + Thomas Fermi approx. in trap:
  Pitaevskii arXiv:1311.4693
Vortex Rings in a Trap

\[ M_I = \frac{F}{\dot{v}} \sim 8\pi^2 mnR^3 \left( \ln \frac{R}{l_{coh}} \right)^{-1} \]

\[ M_{VR} = mN_{VR} \sim mn 2\pi R \pi l_{coh}^2 \]

- **\( M_I \): Inertial (kinetic mass) differs significantly from
- **\( M_{VR} \): Mass depletion
- **Long periods

\[ \frac{T}{T_z} \sim \sqrt{\frac{M_I}{M_{VR}}} \sim \frac{2R/l_{coh}}{\sqrt{\ln(R/l_{coh})}} \]
Vortex Rings in a Trap

• Behaviour depends on $T \sim R/l_{coh} \sim k_F R$

• Large traps have long periods ($k_F R \sim 20$ for experiment)

• Small (narrow) approach domain wall $T \approx \sqrt{2} T_z$
  Formula does not apply

• Depends on $l_{coh}$
  Characterizes dependence on scattering length
Vortex ring motion (here in the presence of “thermal” noise, hence the inverse decay)
Vortex Ring Motion

Vortex ring motion (here in the presence of “thermal” noise, hence the inverse decay)
Vortex Ring Motion

Vortex ring motion (here in the presence of “thermal” noise, hence the inverse decay)
Near-Harmonic Motion

Bulgac, Forbes, Kelley, Roche, Włazłowski (2013) [arXiv:1306.4266]
Vortex Motion

Buoyant force

Magnus effect

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“Too Thick” for Vortex Rings?

MIT Experiment

Subtle imaging:
- Need expansion (turn off trap)
- Must ramp to $B < 700$ G
- $\sim 10\%$ depletion

Imaging Vortex Rings

Imaging Vortex Rings

Imaging Vortex Rings

Imaging Vortex Rings

Explains Dependence on $B_{\text{min}}$

Yefsah et al. Nature 499 (426) 2013

Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013)
Explains Dependence on $B_{\text{min}}$

Yefsah et al. Nature 499 (426) 2013

Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013)
Explains Dependence on $B_{\text{min}}$

Yefsah et al. Nature 499 (426) 2013

Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013)
We Assumed Axial Symmetry

- 2013 MIT paper claimed cylindrical symmetry
- Scherpelz et al.
  - Trapped rings unstable: decay to vortex (arXiv:1401.8267)
- Rings and vortices move in the same way:
  - Buoyant force, Magnus effect, and speed
  - Imaging process
  - Small quantitative differences
Asymmetric Rings Decay to Vortices

Reconnection
• Quantum turbulence

See online supplemental material to Bulgac, Luo, Magierski, Roche, and Yu, Science, 332, 1288 (2011)
Asymmetric Rings
Decay to Vortices

Reconnection
• Quantum turbulence

See online supplemental material to Bulgac, Luo, Magierski, Roche, and Yu, Science, 332, 1288 (2011)
Evolution of a Vortex

Paired field profiles (in units of eF)

- Anisotropy: 9%
- Anharmonicity: 0%

Wlazłowski, Bulgac, Forbes, and Roche [arXiv:1404.1038]
Consistent Alignment?

Short vortex = lower E
No vortex = lowest E!
Depends on geometry?
This vortex is along long axis

Wlazłowski, Bulgac, Forbes, and Roche [arXiv:1404.1038]
Alignment

Tilt to imprint vortex
N. Parker Ph.D. thesis 2004

Oblique vortex rotates
Alignment needs dissipation

Wlazłowski, Bulgac, Forbes, and Roche [arXiv:1404.1038]
Vortex Reconnection
Quantum Turbulence

• Vortex reconnection: the origin of quantum turbulence
  • Feynman 1955
  • Very few experimental realizations

Paoletti, Fisher, Sreenivasan, and Lathrop,
PRL 101, 154501 (2008)
Quantum Turbulence with Fermions

Wlazłowski, Bułgac, Forbes, and Roche [arXiv:1404.1038]
Neutron Star Glitches

• Rapid increase in pulsation rate

• Anderson and Itoh (1975) suggested pinned superfluid vortices

Pulsar Astronomy by Andrew G. Lyne and Francis Graham-Smith
Understanding Pinning

• Calculate vortex pinning forces and vortex interactions
  Probably requires fermionic DFTs (i.e. Skyrme, HFB) with shell effects, etc.

• Calculate dynamics of vortex networks
  Probably requires large numbers of vortices: tangles, knock-on, knock-off, turbulence, 3D dynamics, etc.
  Needs efficient superfluid hydrodynamics

• Can’t use the same tool for both
  Use hybrid approach: fermionic DFT → hydrodynamics → filament models
Pinning from Statics

Energy calculations

Must diagonalize to high precision
(subtraction involved)

How to extract $F(r)$?

Pinning: Dynamics

Extract force with dynamical methods

Scales well numerical:
No diagonalization

Extract force at any separation

Still needs fermion DFT

Aurel Bulgac, Michael Forbes, and Rishi Sharma: PRL 110 (2013) 241102
Pinning: Dynamics

Extract force with dynamical methods

Scales well numerical:
No diagonalization

Extract force at any separation

Multiscale analysis:
• Microscopic DFT
• Mesoscopic GPE
• Macroscopic hydro

Aurel Bulgac, Michael Forbes, and Rishi Sharma: PRL 110 (2013) 241102
Application to Nuclei

• Hydrodynamic DFT for nuclei
  Much simpler/faster than HFB, Skyrme, etc.

• Fits to nuclear masses and charge radii

• Giant Dipole Resonances (GDR)

• $^{238}$U Fission

• Collaboration with
  • Aurel Bulgac and Shi Jin
    University of Washington
  • Piotr Magierski
    Warsaw University of Technology, University of Washington
Density Functional

\[
E = \int d^3x \left( \mathcal{E}(\rho_n, \rho_p) + \mathcal{E}_\nabla(\nabla \rho_n, \nabla \rho_p, \cdots) \right) + E_C(\rho_n, \rho_p)
\]

- Extended Thomas-Fermi (ETF) form
  - \( \mathcal{E}(\rho_n, \rho_p) \)
    Equation of state. Saturation and symmetry properties: 4 parameters
  - \( \mathcal{E}_\nabla(\nabla \rho_n, \nabla \rho_p, \cdots) \)
    Gradients: Weisäcker term and higher order: 1-4 parameters
- \( E_C(\rho_n, \rho_p) \)
  Coulomb (includes nucleon charge form-factors)
- Pairing (by hand)
Equation of State

\[ \mathcal{E}(\rho_n, \rho_p) = \frac{3}{5} \frac{\hbar^2 (3\pi^2 \rho_n)^{2/3}}{2m_n} + \frac{3}{5} \frac{\hbar^2 (3\pi^2 \rho_p)^{2/3}}{2m_p} + \]

\[ + \left( a_0 \rho_+^{2/3} + a_1 \rho_+ + a_2 \rho_+^{4/3} + \cdots \right) \rho_+ + \]

\[ + \left( b_0 \rho_+^{2/3} + b_1 \rho_+ + b_2 \rho_+^{4/3} + \cdots \right) \rho_+ \left( \frac{\rho_n - \rho_p}{\rho_+} \right)^2 \]

• Thomas-Fermi (TF) non-interacting
Equation of State

\[ \mathcal{E}(\rho_n, \rho_p) = \frac{3}{5} \frac{\hbar^2 (3\pi^2 \rho_n)^{2/3}}{2m_n} + \frac{3}{5} \frac{\hbar^2 (3\pi^2 \rho_p)^{2/3}}{2m_p} + \]

\[ + \left( a_0 \rho_+^{2/3} + a_1 \rho_+ + a_2 \rho_+^{4/3} + \cdots \right) \rho_+ \]

\[ + \left( b_0 \rho_+^{2/3} + b_1 \rho_+ + b_2 \rho_+^{4/3} + \cdots \right) \rho_+ \left( \frac{\rho_n - \rho_p}{\rho_+} \right)^2 \]

• Symmetric nuclear matter
• Exchange for saturation properties:
Equation of State

\[ \mathcal{E}(\rho_n, \rho_p) = \frac{3}{5} \frac{\hbar^2 (3\pi^2 \rho_n)^{2/3}}{2m_n} + \frac{3}{5} \frac{\hbar^2 (3\pi^2 \rho_p)^{2/3}}{2m_p} + \]

\[ + \left( a_0 \rho_+^{2/3} + a_1 \rho_+ + a_2 \rho_+^{4/3} + \cdots \right) \rho_+ + \]

\[ + \left( b_0 \rho_+^{2/3} + b_1 \rho_+ + b_2 \rho_+^{4/3} + \cdots \right) \rho_+ \left( \frac{\rho_n - \rho_p}{\rho_+} \right)^2 \]

• Symmetry Energy
Equation of State

\[ E(\rho_n, p) = \frac{3}{5} \frac{\hbar^2 (3\pi^2 \rho_n)^{2/3}}{2m_n} + \frac{3}{5} \frac{\hbar^2 (3\pi^2 \rho_p)^{2/3}}{2m_p} + \]

\[ + \left( a_0 \rho_+^{2/3} + a_1 \rho_+ + a_2 \rho_+^{4/3} + \cdots \right) \rho_+ + \]

\[ + \left( b_0 \rho_+^{2/3} + b_1 \rho_+ + b_2 \rho_+^{4/3} + \cdots \right) \rho_+ \left( \frac{\rho_n - \rho_p}{\rho_+} \right)^2 \]

• \(a_0\) and \(b_2\) small (neglect)
  
  E.g. fit \(a \rho_+^{\gamma+1}\) finding \(\gamma = 4/3\)
  
  Think expansion in \(k_f = (3\pi^2 \rho)^{1/3}\)

• New term in symmetry energy: \(b_0 \rho_+^{5/3}\)
  
  Introduced by Tondeur (1978) to fit P. Siemens nuclear matter calculations
  
  Not in Skyrme functionals, but important for fits! (needed in unitary gas limit)
Saturation Properties

\[ \varepsilon \approx (\varepsilon_0 + \frac{1}{2} K_0 \delta^2) + \left( S_0 - L \delta + \frac{1}{2} K_S \delta^2 \right) \left( \frac{\rho_n - \rho_p}{\rho} \right)^2 \]

\[ \delta = \frac{\rho_0 - \rho}{3\rho_0} \]

• Trade \( a_0, a_1, a_2 \) for saturation properties: \( \rho_0, \varepsilon_0, K_0 \)

• Trade \( b_0, b_1, b_2 \) for symmetry properties: \( S_0, L, K_S \)
Coulomb Energy

\[ E_C(\rho_n, \rho_p) = e^2 \left( \int d^3\vec{x} \, d^3\vec{y} \frac{Q(\vec{x})Q(\vec{y})}{2\|\vec{x} - \vec{y}\|} - \frac{3}{4} \left( \frac{3}{\pi} \right)^{1/3} \rho_p^{4/3} \right) \]

\[ Q = G_E^p \ast \rho_p + G_E^n \ast \rho_n \]

• No new fit parameters

• Fixed proton and neutron form factors \( G_E \)

• Last term - the Coulomb exchange term - minor role
  Omitting does not significantly alter fits, but it helps somewhat
  Fitting finds coefficient close to unity
Semiclassical Expansion of Kinetic Energy

\[ \frac{\hbar^2}{2m} \left( c_0 \rho^{5/3} + c_2 (\nabla \sqrt{\rho})^2 + c_4 n^{1/3} \left[ \left( \frac{\nabla^2 \rho}{\rho} \right)^2 - \frac{9}{8} \left( \frac{\nabla^2 \rho}{\rho} \right) \left( \frac{\nabla \rho}{\rho} \right)^2 + \frac{1}{3} \left( \frac{\nabla \rho}{\rho} \right)^4 \right] + \cdots \right) \]

• \( c_2 = 1/9 \) (non-interacting)

• Suggests form for gradient terms

See e.g. Brack and Bhaduri “Semiclassical physics” (1997) or Dreizler and Gross “Density Functional Theory: An Approach to the Quantum Many-Body Problem” (1990)
Figure 4.1: Tests of the kinetic energy functional $\tau_{ETF}[\rho]$. Left: Woods-Saxon potential with $N = 126$ nucleons with typical deformations for nuclear fission (see the $c, h$ shapes shown in Fig. 8.2), taken along $h = 0$. Right: Axially symmetric harmonic-oscillator potential with frequency ratio $q$ with $N = 112$ particles. (After Refs. [35, 36].)
Functional

\[ \mathcal{E} = \mathcal{E}_{TF}(\rho_n, \rho_p) + a_1 \rho^2 + a_2 \rho^{7/3} + \left( b_0 \rho^{5/3} + b_1 \rho^2 \right) \left( \frac{\rho_n - \rho_p}{\rho} \right)^2 \]

\[ + \eta \frac{\hbar^2}{2} \left( \frac{(\nabla \sqrt{\rho_n})^2}{m_n} + \frac{(\nabla \sqrt{\rho_p})^2}{m_p} \right) + c_4 \text{ terms} + \text{Coulomb} \]

- Original form due to von Weizsäcker (1935)
  - \( \eta = 1 \)
    Valid in the limit of a rapidly fluctuating (but weak) external potential

- Semiclassical expansion (non-interacting)
  - \( \eta = 1/9 \)
    Valid in the limit of a small gradients

- Fit: \( \eta = 1/2 \)
  \( \eta = 1/4 \) looks like dimers
Liquid Drop Formula

\[ a_{\text{vol}} A + a_{\text{surf}} A^{2/3} + a_{\text{Coul}} \frac{Z^2}{A^{1/3}} + a_{\text{sym}} \frac{(Z - N)^2}{A} + a_{\text{pair}} \frac{(Z \mod 2) + (N \mod 2)}{A^{1/2}} \]
\[ + a_{\text{CoulS}} \frac{Z^2}{A^{2/3}} + a_{\text{symS}} \frac{(Z - N)^2}{A^{4/3}} \]

- 5 parameter fit to 2249 nuclei
  - \( \chi_r = 2.95 \) MeV
- 7-parameters fit to 2249 nuclei
  - \( \chi_r = 2.49 \) MeV

Fit to Audi (2012) data with errors < 200keV
No charge form-factors

\[ \mathcal{E}_{TF} + a_1 \rho^2 + a_2 \rho^{7/3} + \left( b_0 \rho^{5/3} + b_1 \rho^2 \right) \left( \frac{\rho_n - \rho_p}{\rho} \right)^2 + \frac{\hbar^2}{2m} (\nabla \sqrt{\rho})^2 + \ldots \]

Just fit masses

Close agreement with liquid drop model (red) (but fewer parameters!)

Missing shell effects

Masses:
  Audi (2012) - 2236 nuclei
  Angeli (2013) - 879 radii
No charge form-factors

\[ \mathcal{E}_{\text{TF}} + a_1 \rho^2 + a_2 \rho^{7/3} + \left( b_0 \rho^{5/3} + b_1 \rho^2 \right) \left( \frac{\rho_n - \rho_p}{\rho} \right)^2 + \frac{\hbar^2}{2m} (\nabla \sqrt{\rho})^2 + \ldots \]

Just fit masses

Close agreement with liquid drop model (red) (but fewer parameters!)

Missing shell effects

Masses:
- Audi (2012) - 2236 nuclei
- Angeli (2013) - 879 radii
Add Charge form factors

\[ \varepsilon_{TF} + a_1 \rho^2 + a_2 \rho^{7/3} + \left( b_0 \rho^{5/3} + b_1 \rho^2 \right) \left( \frac{\rho_n - \rho_p}{\rho} \right)^2 + \eta \frac{\hbar^2}{2m} (\nabla \sqrt{\rho})^2 + \cdots \]

\[ \chi_E = 2.55 \text{ MeV}, \chi_{LD} = 0.36 \text{ MeV}, \chi_R = 0.1278 \text{ fm} \]
\[ \eta = 0.47, a_1 = -738, a_2 = 934, b_0 = 137, b_1 = -160 \]
\[ \rho_0 = 0.14, \varepsilon_0 = -15.2, S = 26, L = 29, K = 222 \]
Fit Charge Radii too

\[ \xi_{TF} + a_1 \rho^2 + a_2 \rho^{7/3} + \left( b_0 \rho^{5/3} + b_1 \rho^2 \right) \left( \frac{\rho_n - \rho_p}{\rho} \right)^2 + \eta \frac{\hbar^2}{2m} (\nabla \sqrt{\rho})^2 + \ldots \]

\[ \chi_E = 2.66 \text{ MeV}, \chi_{LD} = 0.81 \text{ MeV}, \chi_R = 0.0557 \text{ fm} \]
\[ \eta = 0.48, a_1 = -706, a_2 = 868, b_0 = 136, b_1 = -157 \]
\[ \rho_0 = 0.15, \epsilon_0 = -15.5, S = 26, L = 30, K = 227 \]

Charge radii from Angeli (2013)
Fit individual $c_4$ terms

$$\varepsilon_{TF} + a_1 \rho^2 + a_2 \rho^{7/3} + \left( b_0 \rho^{5/3} + b_1 \rho^2 \right) \left( \frac{\rho_n - \rho_p}{\rho} \right)^2 + \eta \frac{\hbar^2}{2m} (\nabla \sqrt{\rho})^2 + \cdots$$

$\chi_E = 2.59$ MeV, $\chi_{LD} = 0.60$ MeV, $\chi_R = 0.0583$ fm

$\eta = 0.47$, $a_1 = -712$, $a_2 = 881$, $b_0 = 137$, $b_1 = -160$

$\rho_0 = 0.14$, $\varepsilon_0 = -15.4$, $S = 26$, $L = 29$, $K = 226$
Missing Shell Effects

\[ \chi_E = 2.55 \text{ MeV}, \chi_{LD} = 0.51 \text{ MeV}, \chi_R = 0.0583 \text{ fm} \]
\[ \eta = 0.47, a_1 = -712, a_2 = 881, b_0 = 137, b_1 = -160 \]
\[ \rho_0 = 0.14, \epsilon_0 = -15.4, S = 26, L = 29, K = 226 \]
• Coupled equations for protons and neutrons
  Follow from varying the functional while imposing Galilean covariance

• Pure superfluid hydrodynamics
  Irrotational implies
  Could extend with viscosity etc.
  Implement as a non-linear Schrödinger equation

\[
\begin{align*}
\partial_t \rho + \vec{\nabla} \cdot (\rho \vec{v}) &= 0 \\
m \left( \partial_t + \vec{v} \cdot \vec{\nabla} \right) \vec{v} + \vec{\nabla} \left( \frac{\delta \mathcal{E}(\rho, \nabla \rho, \cdots)}{\delta \rho} \right) &= 0
\end{align*}
\]
Implement as NLSEQ

\[
\mathcal{L}(\rho, \dot{\rho}, \phi, \dot{\phi}) = -\rho \left( \dot{\phi} + \frac{1}{2m} (\nabla \phi)^2 \right) - \mathcal{E}(\eta) - \eta \frac{\hbar^2}{2m} (\nabla \sqrt{\rho})^2,
\]

\[
\mathcal{L}(\psi, \dot{\psi}) = \psi^\dagger \left( -i\hbar \partial_t - \frac{\hbar^2 \nabla^2}{2m} \right) \psi - \mathcal{E}(\rho), \quad \hbar = \hbar \sqrt{\eta}
\]

• Numerically stable and efficient (same code as before)
  (Some tricks with Coulomb)

• Artificial “quantization”
  but \(\eta=1/4\) looks like dimers...
Giant Dipole Resonance

Preliminary results

\[ E_{\text{GDR}} \approx 31.2A^{-1/3} + 20.6A^{-1/6} \]

Calculation by Piotr Magierski
Empirical formula from Berman and Fultz (1975)

\[ \sim 30\% \text{ too low} \]
Entrainment

\[ \frac{m_n \nu_n^2}{2} + \frac{m_p \nu_p^2}{2} + \alpha \frac{m \rho_n \rho_p}{2 \rho_0} |\vec{v}_n - \vec{v}_p|^2 \]

Galilean invariant

Best fit: \( \alpha = -0.3 \)

30% to effective mass

Time-dependent Skyrme functionals do not have this term...
Entrainment does not spoil mass fits

\[
\frac{m_n v_n^2}{2} + \frac{m_p v_p^2}{2} + \alpha \frac{m \rho_n \rho_p}{2 \rho_0} |\vec{v}_n - \vec{v}_p|^2
\]

\( \chi_E = 2.65 \text{ MeV}, \chi_{LD} = 0.80 \text{ MeV}, \chi_R = 0.0537 \text{ fm} \)
\( \eta = 0.48, a_1 = -706, a_2 = 868, b_0 = 136, b_1 = -157 \)
\( \rho_0 = 0.15, \varepsilon_0 = -15.5, S = 26, L = 29, K = 227 \)
$^{238}\text{U}$ Fission

$^{238}\text{U}$ ground state $\rho_{n,p}$

Quadrupole $\nu$ added

Fully 3D simulation
20 min on laptop

$32 \times 32 \times 64$ (dx=1 fm)

(Preliminary results)
Can you simulate nuclei?

Boselets, Fermilets, ...
Realtime Methods

• Efficient

• DFT + Hydro.
  • Validated with cold atoms, nuclei

• New arena to study Quantum Turbulence and neutron star phenomenology
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