Real-time Methods for Cooling and Simulating Macroscopic Fermi Systems

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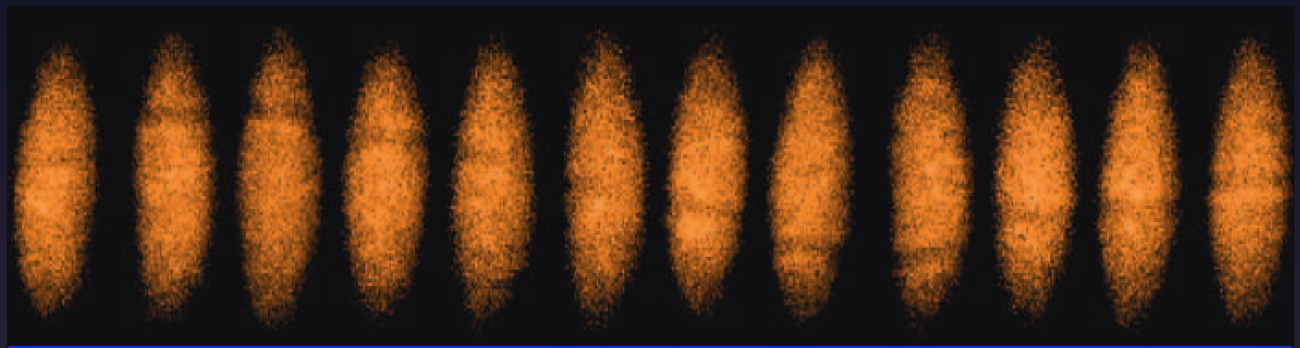
Goal: Simulate Large Fermi Systems

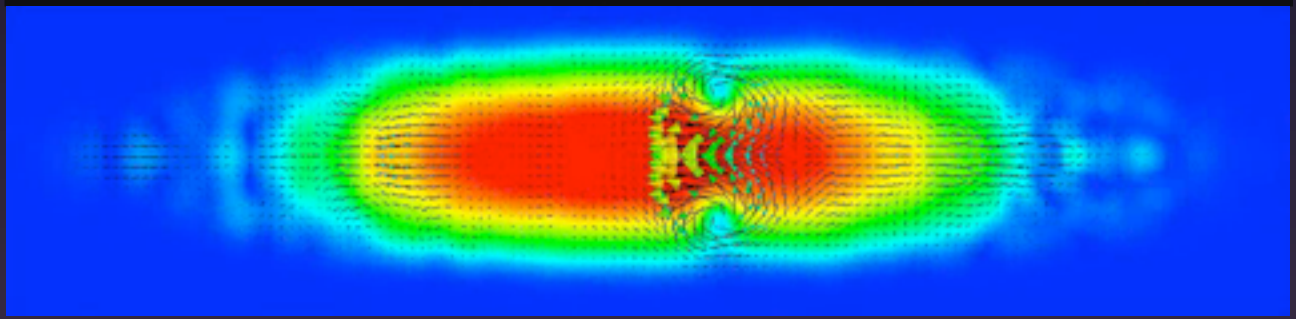
- Neutron stars
  - Glitching (thousands of vortices pinning on nuclei)
  - Macroscopic dynamic properties
- 10^6 cold atoms in traps
  - Preparation
  - Imaging
- Quantum turbulence, vortex tangles

Problem: Fermions are Expensive

- Even Fermionic DFTs too costly:
  - How to find ground state?
  - Limited to few thousand particles
- How to scale up to study macroscopic systems?

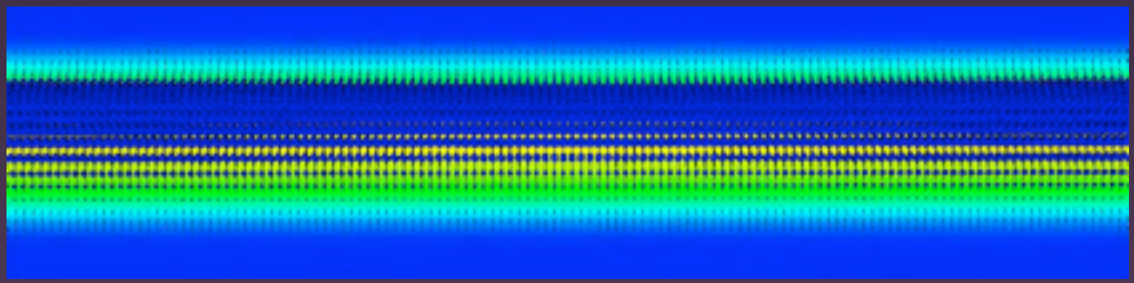
Outline





- Resolving a Mystery: MIT Heavy Solitons = Vortex Rings

  Fermionic DFT for small systems validates bosonic model for realistic systems



- Fermionic DFTS
  - Real-time State Preparation

    Adiabatic Switching + Quantum Friction
  - Real-time extraction of forces
- Modelling Fermions with Bosons
  - ETF model (like GPE)

Fermionic Superfluids Universality

Fermionic Superfluids

Neutron Matter

$k_F \sim \text{fm}^{-1}$

$a_{nn} = -19$ fm

$r_{nn} = 2$ fm

Nuclei

neutrons and protons

Unitary Fermi Gas

$a = \infty$

$r_e = 0$

Cold Atoms

$k_F \sim \mu\text{m}^{-1}$

Tuneable a

$r_{nn} \sim 0.1$ nm

Many systems

- different species
- dipole interactions
- optical lattices
- quantum simulators

Other Superfluids

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

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Unitary Fermi Gas (UFG)

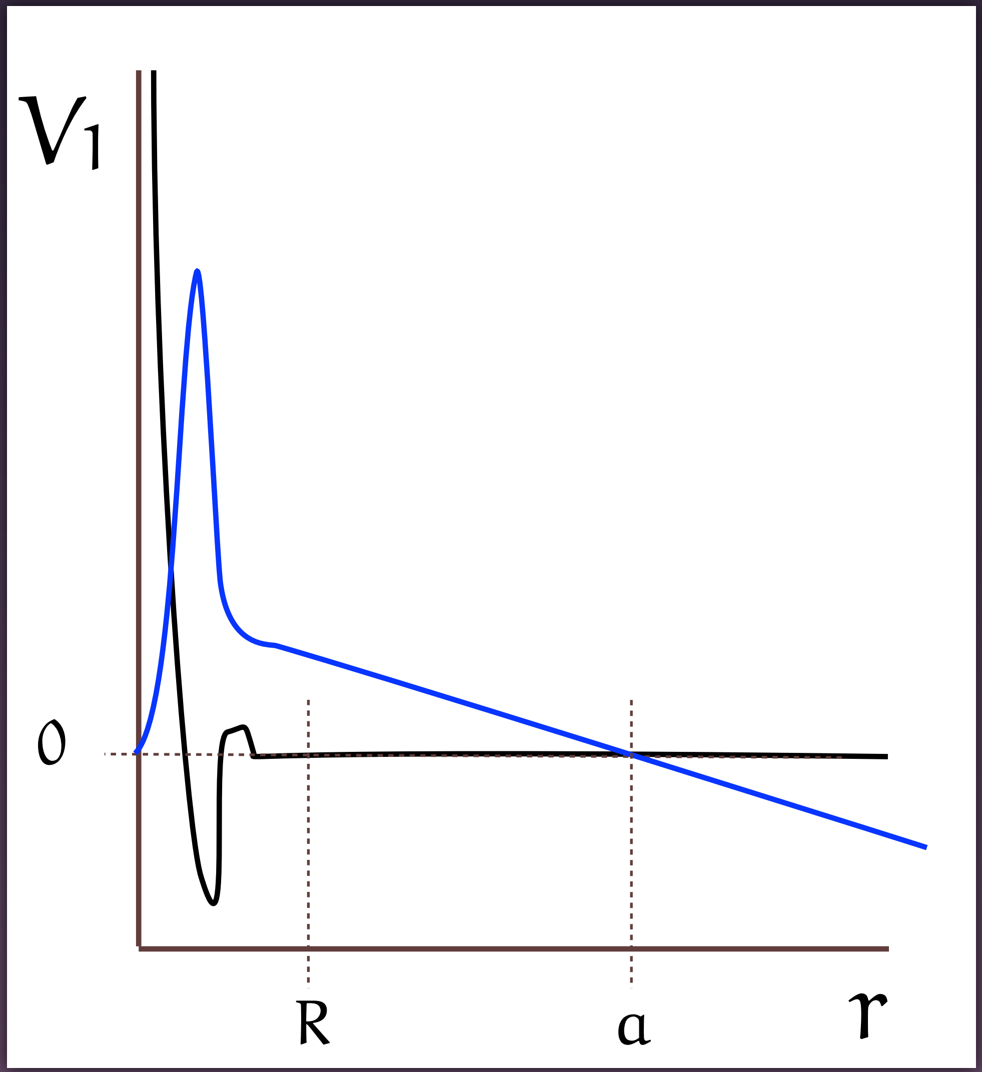
$$\widehat{\mathcal{H}} = \int \left(\widehat{a}^\dagger \widehat{a} E_a + \widehat{b}^\dagger \widehat{b} E_b\right) - \int V \widehat{a}^\dagger \widehat{b}^\dagger \widehat{b} \widehat{a}$$

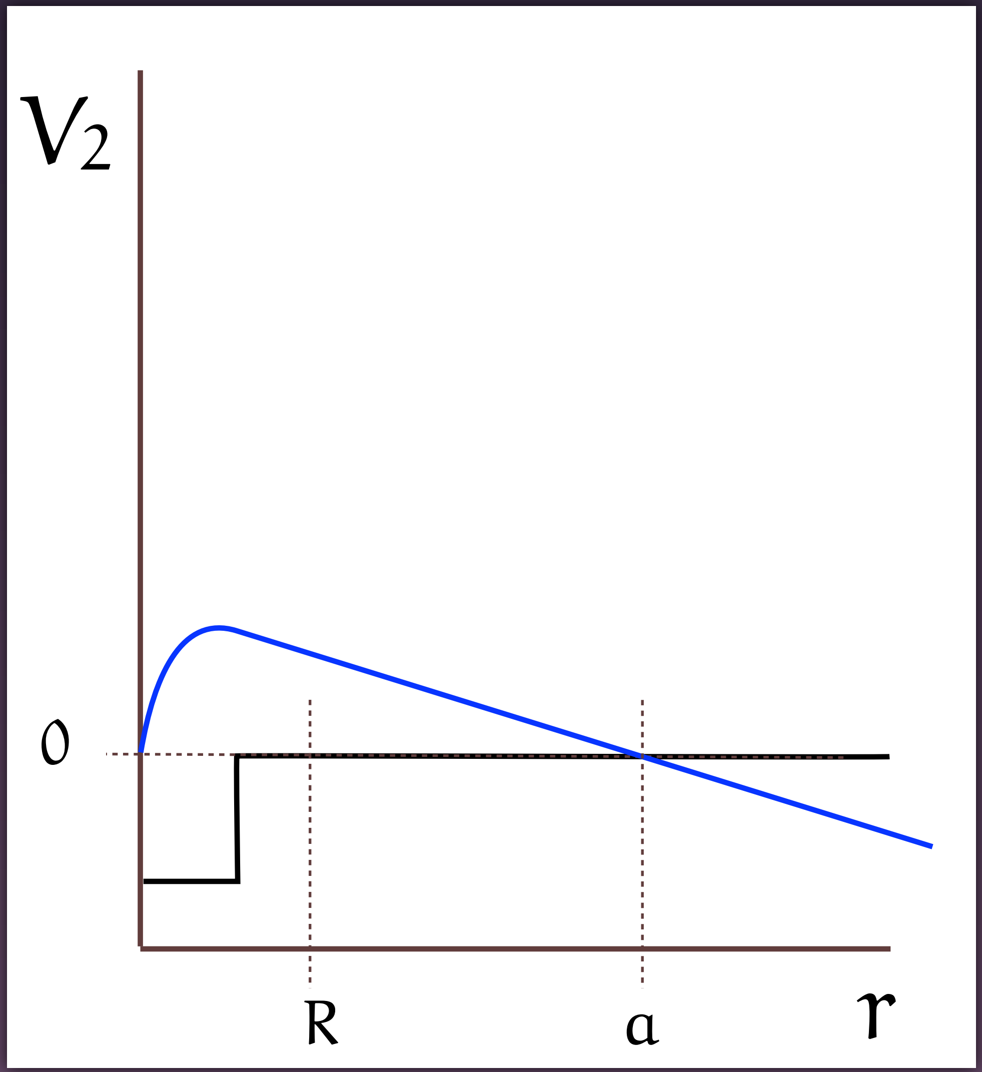
$$E_{a,b} = \frac{p^2}{2m} - \mu_{a,b}, \quad \mu_\pm = \frac{\mu_a \pm \mu_b}{2}$$

- Take regulator $\lambda \to \infty$ and coupling $g \to 0$ to fix s-wave scattering length $a^{-1} \propto (\lambda - g^{-1}) = 0$ (unitary limit)

Universality

- Short distance irrelevant:
  - At long distance $(r>R)$ potentials equivalent $V_1 \equiv V_2$
  - Characterized by scattering length a





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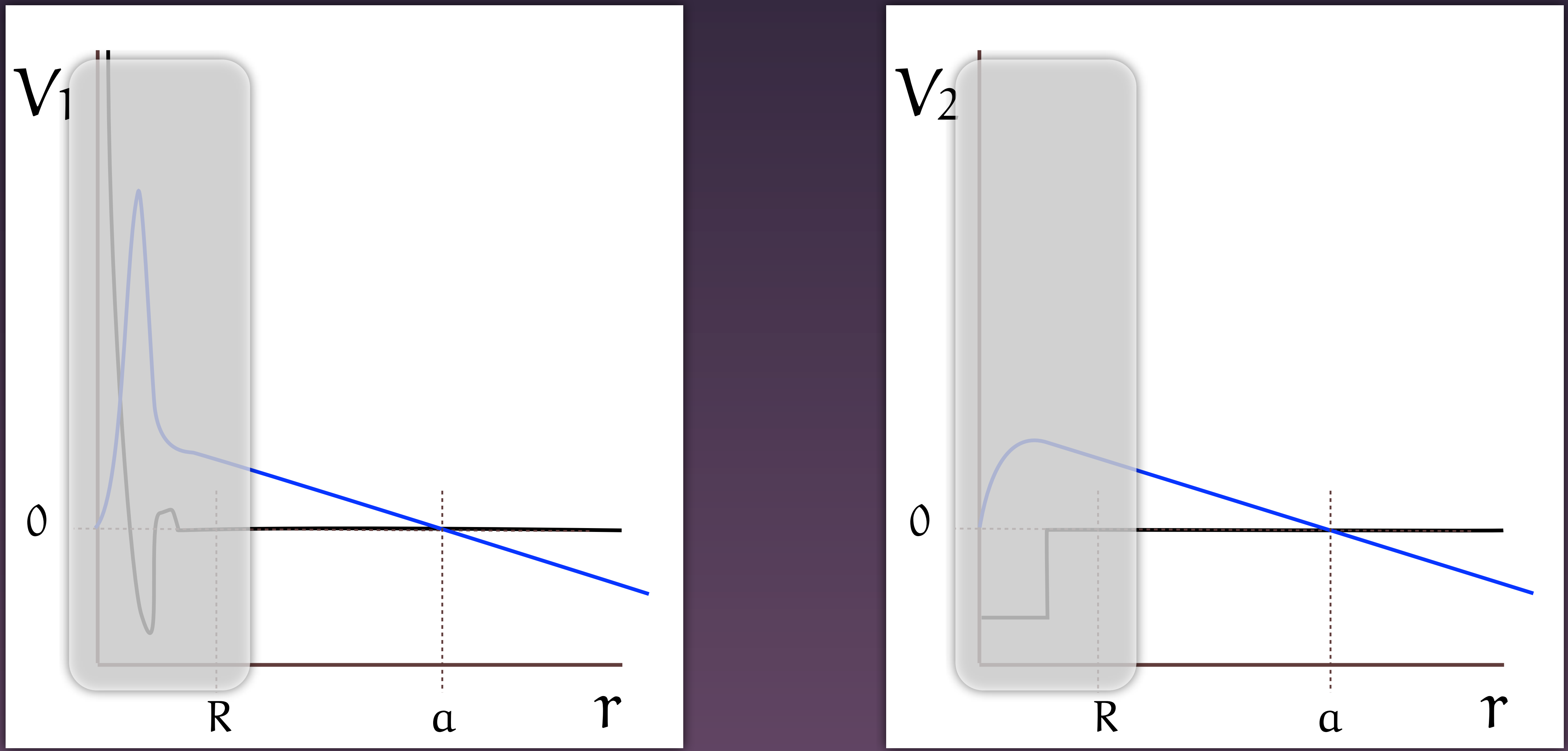

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- Unitary limit $a=\infty$: No interaction length scale!
- Universal physics:
  - $\mathcal{E}(\rho) = \xi \mathcal{E}_{FG}(\rho) \propto \rho^{5/3}$, $\xi_{exp} = 0.370(5)(8)$
- Simple, but hard to calculate!

  Bertsch Many Body X-challenge

Unitary Fermi Gas (UFG)

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- Unitary limit $a=\infty$: No interaction length scale!
- Universal physics:
  - $\mathcal{E}(\rho) = \xi \mathcal{E}_{FG}(\rho) \propto \rho^{5/3}$, $\xi=0.376(5)$
- Lithium 6 (^{6}Li)
- Dilute neutron matter in neutron stars
  - $a_{nn} = -19$ fm

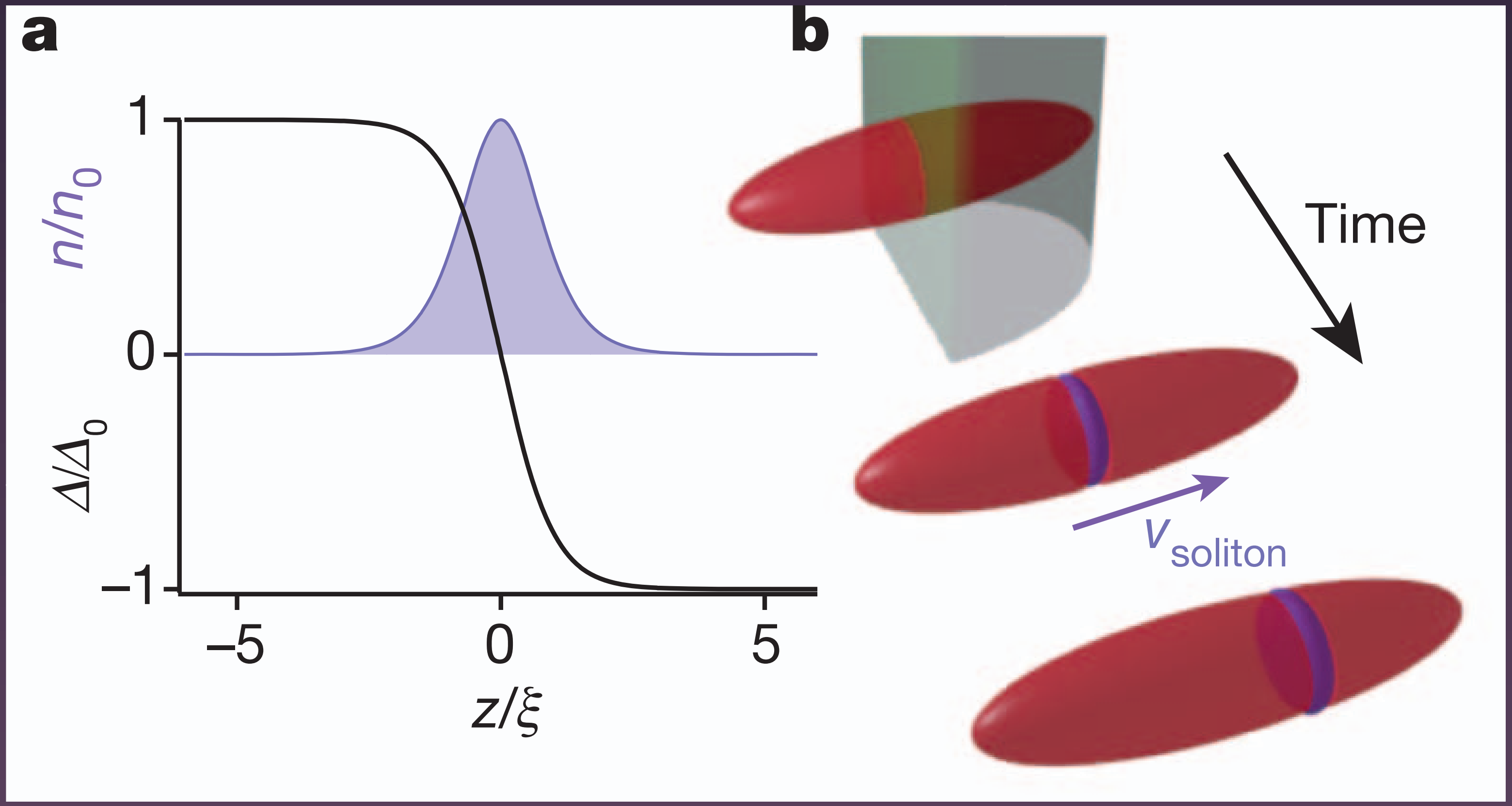
MIT Experiment

- ^{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 $T \approx 12 T_z$
  - Bosonic solitons (BECs) oscillate with $T \approx \sqrt{2} T_z \approx 1.4 T_z$
  - Fermionic solitons (BdG) oscillate with $T \approx 1.7 T_z$
  - Interpret as "Heavy Solitons"

Yefsah et al. Nature 499 (426) 2013 [arXiv:1302.4736]

MIT Experiment

$$\hbar\partial_t(\delta\varphi) = \delta V$$



Imprint soliton

Step potential phases evolve to π phase shift

Flat domain wall (dark/grey soliton)

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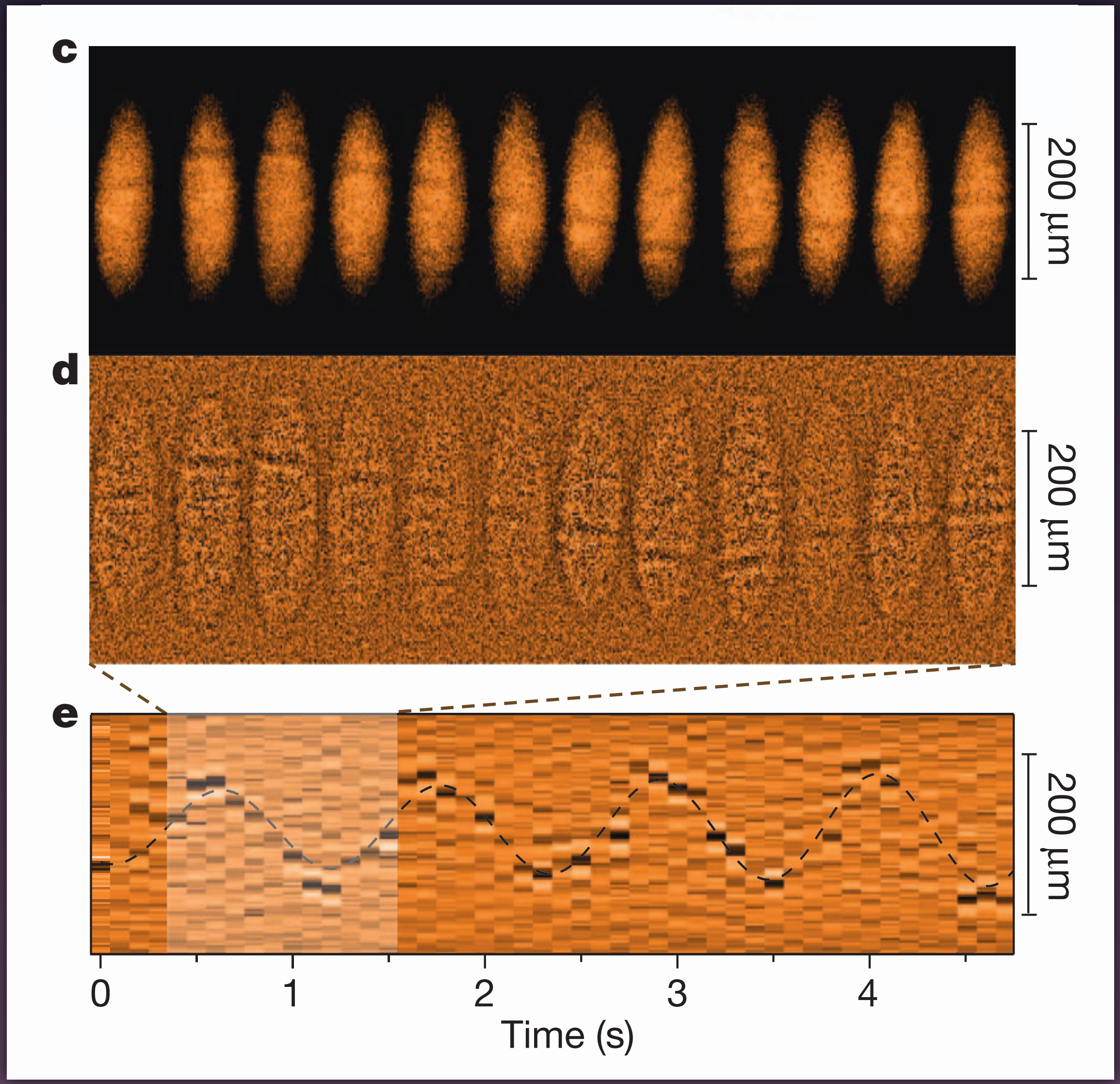
MIT Experiment

(each image is a different run)



Soliton oscillates back and forth

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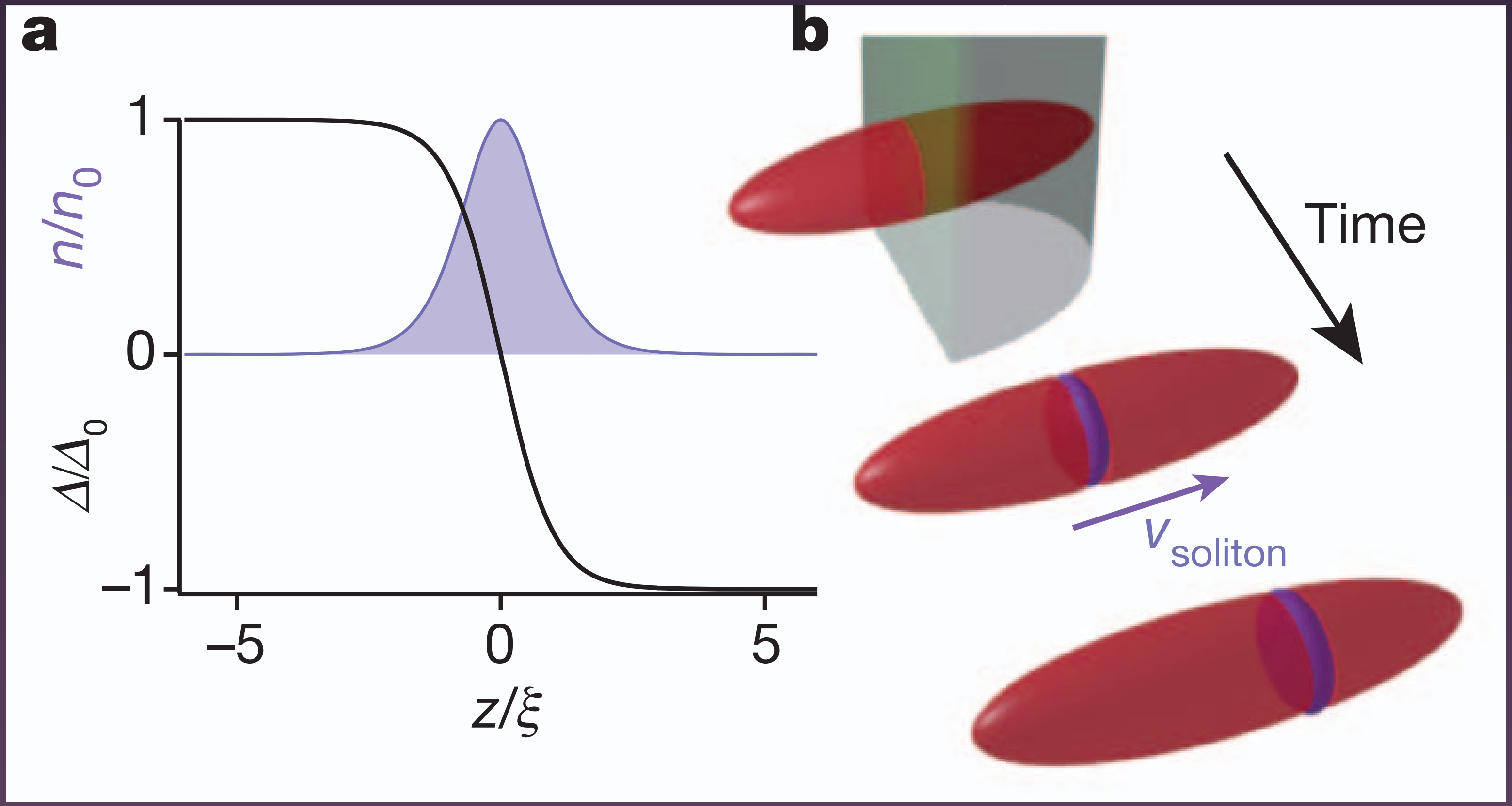

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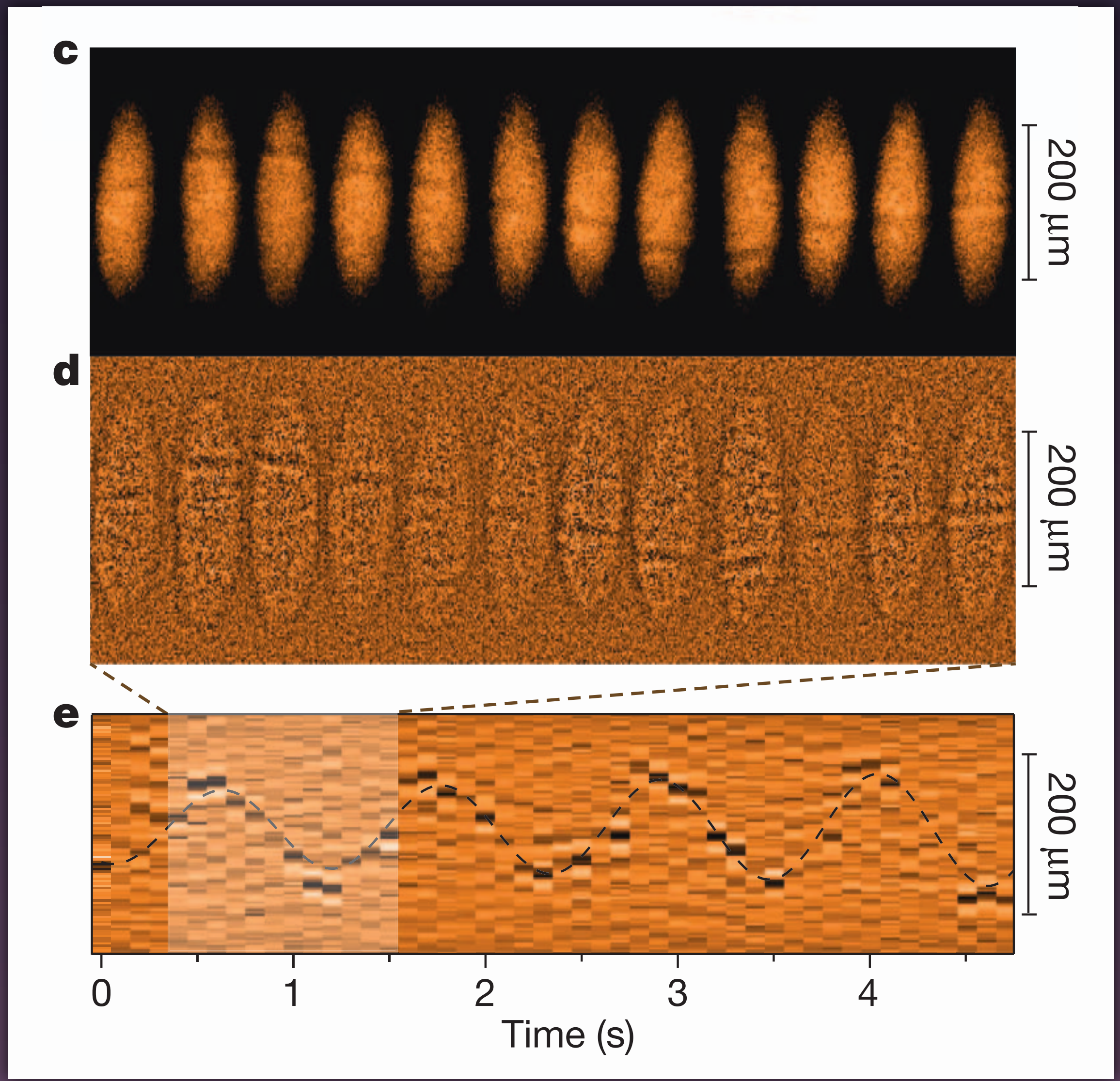

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Soliton oscillates back and forth

Trapped Domain Walls

- Bosonic solitons (GPE) have $T \approx \sqrt{2} T_z \approx 1.4 T_z$

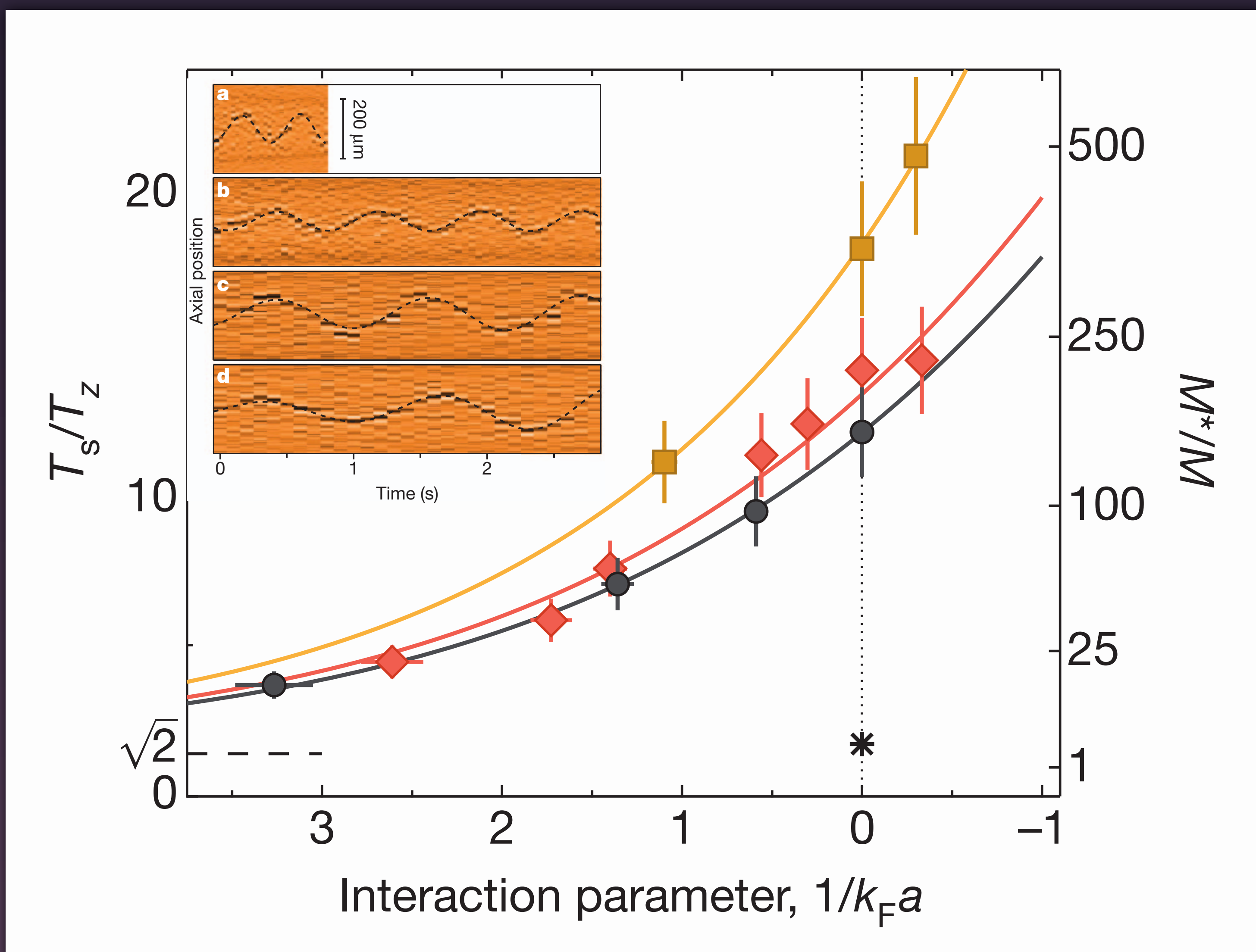
  Busch and Anglin (2000)

- Fermionic solitons (BdG) have $T \approx \sqrt{3} T_z \approx 1.7 T_z$

  Liao, Brand (2011); Scott, Dalfovo, Pitaevskii, Stringari (2011)

- Experiment sees $T \approx 10 T_z - 20 T_z$
  - Order of magnitude larger than theory!

MIT Experiment



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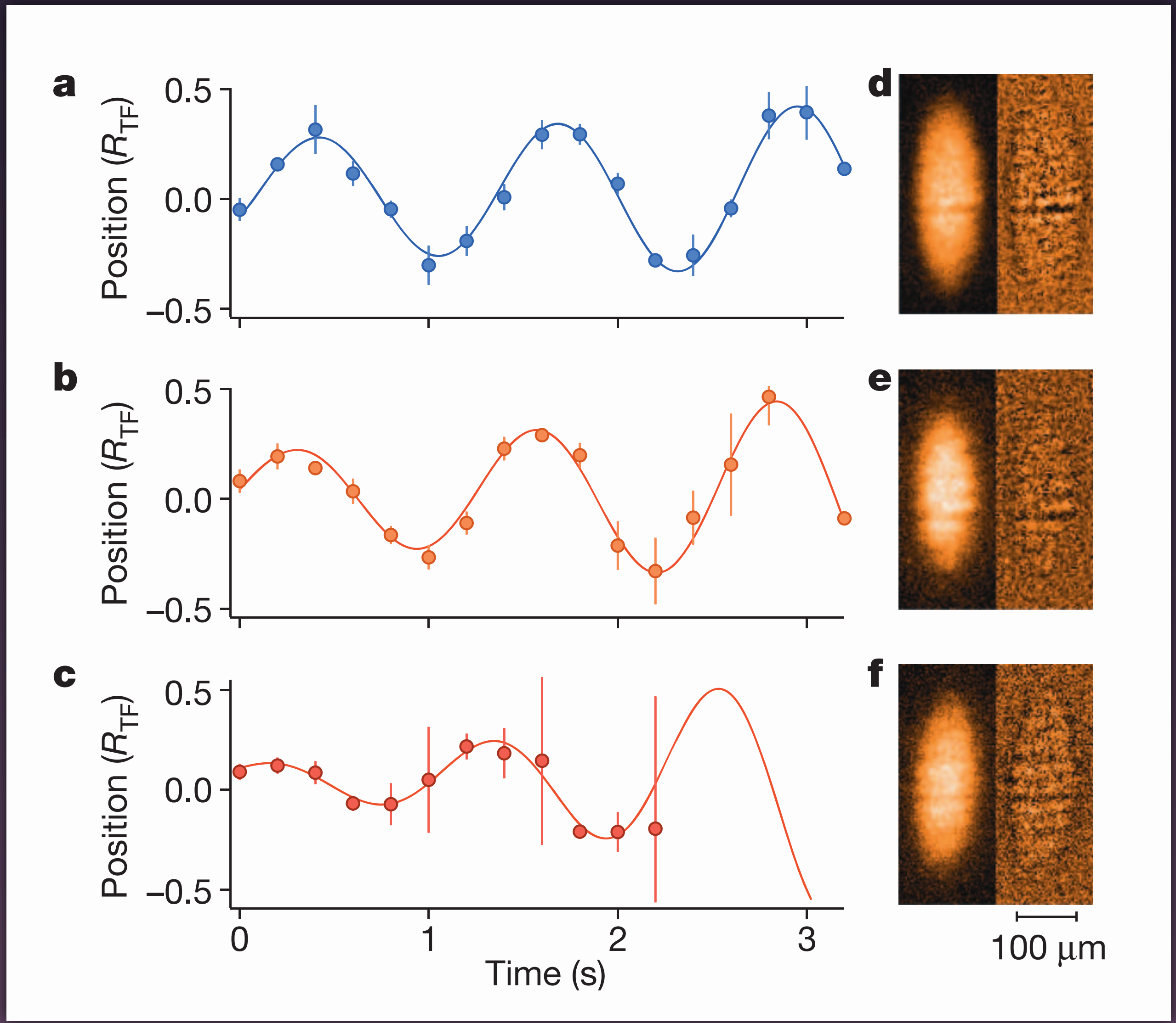
Period depends on:

- Aspect ratio $\lambda \in \{3.3, 6.2, 12\}$
- Interaction

Much longer than predicted for domain walls

MIT Experiment



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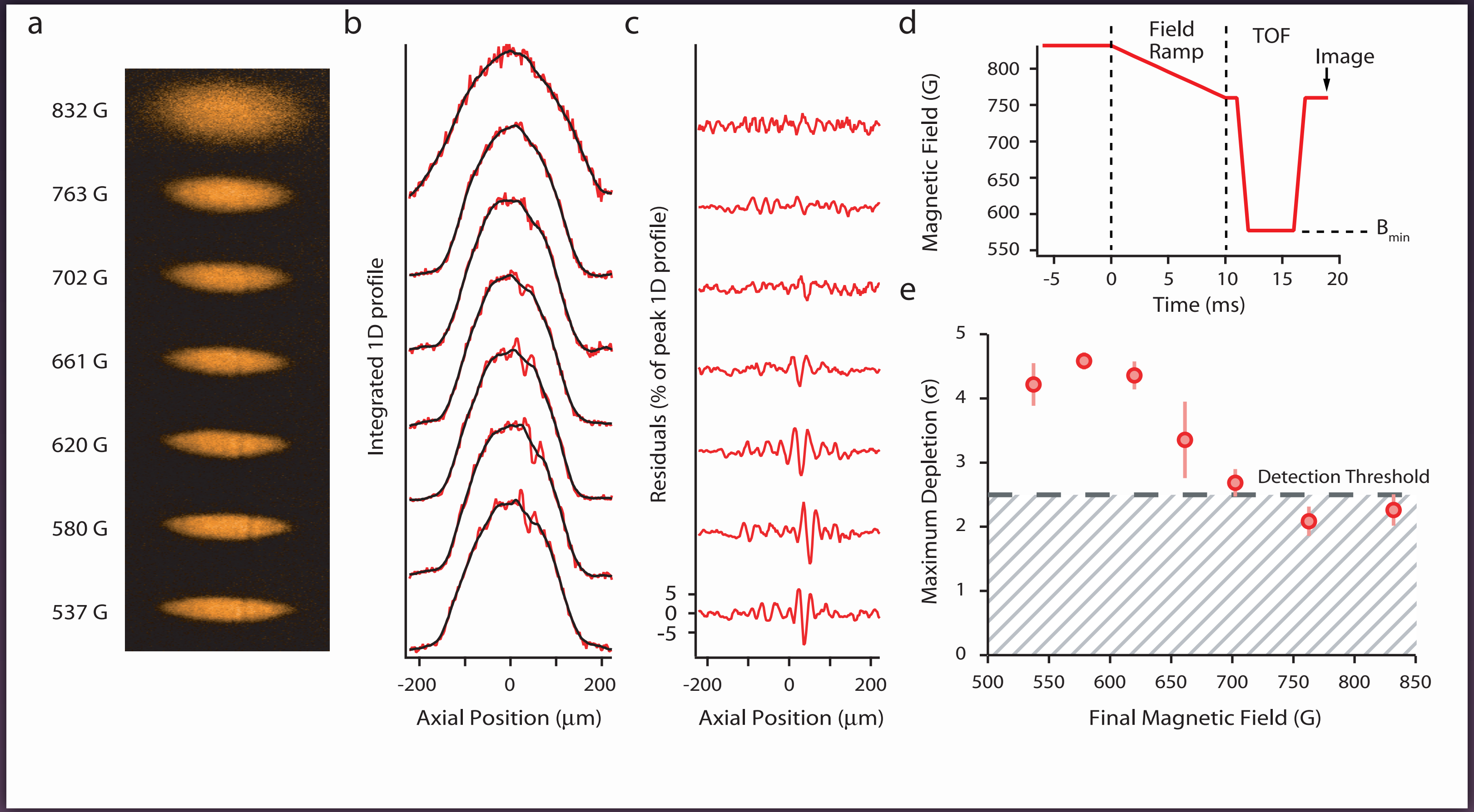
Finite temperature:

- Anti-decay
- (Negative mass)

MIT Experiment



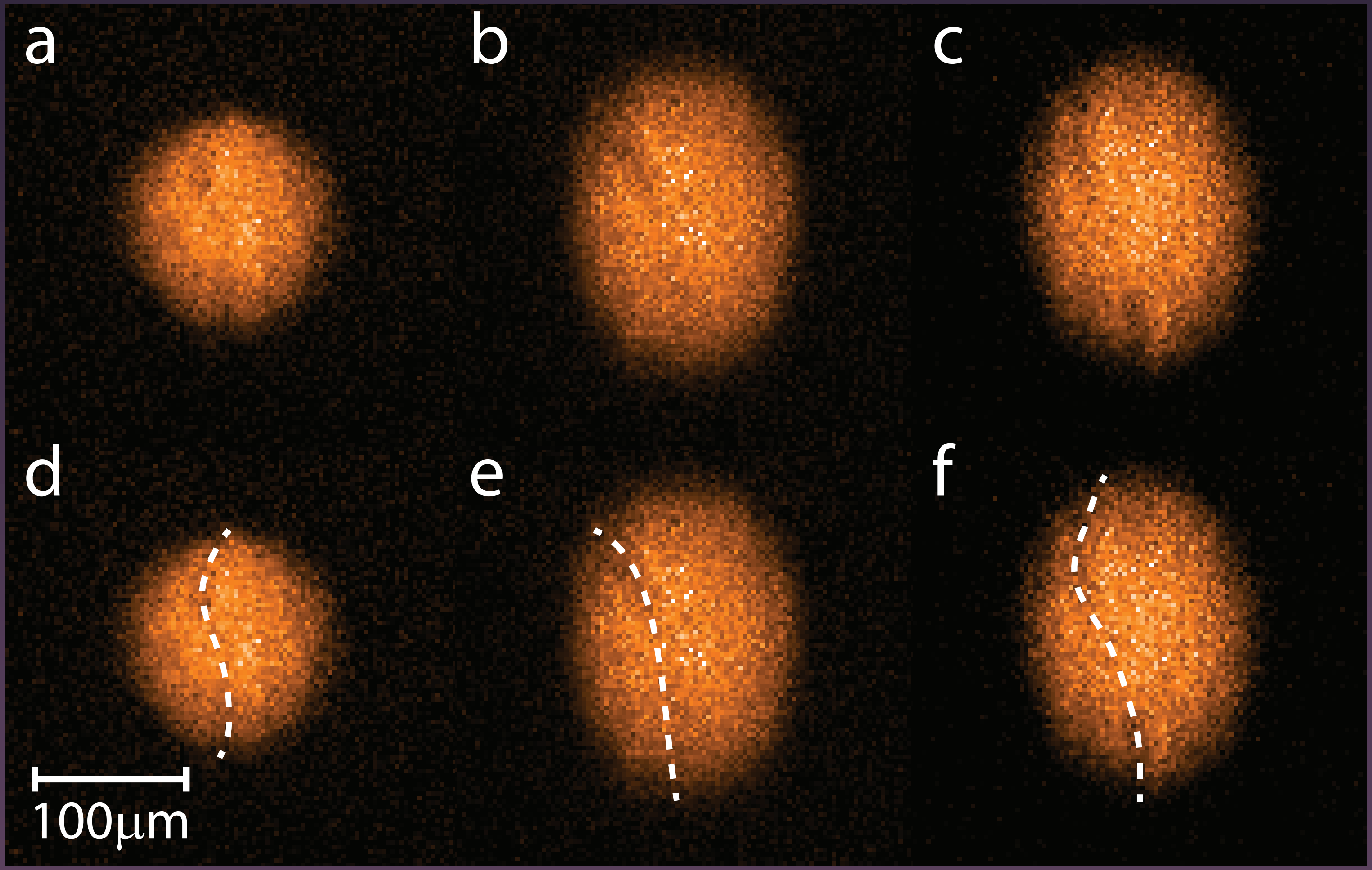
Subtle imaging:

- Need expansion (turn off trap)
- Must ramp to B<700G
- ~10% depletion

Yefsah et al. Nature 499 (426) 2013 [arXiv:1302.4736]

Friday, October 18, 13

MIT Experiment



Domain walls should have snake instability

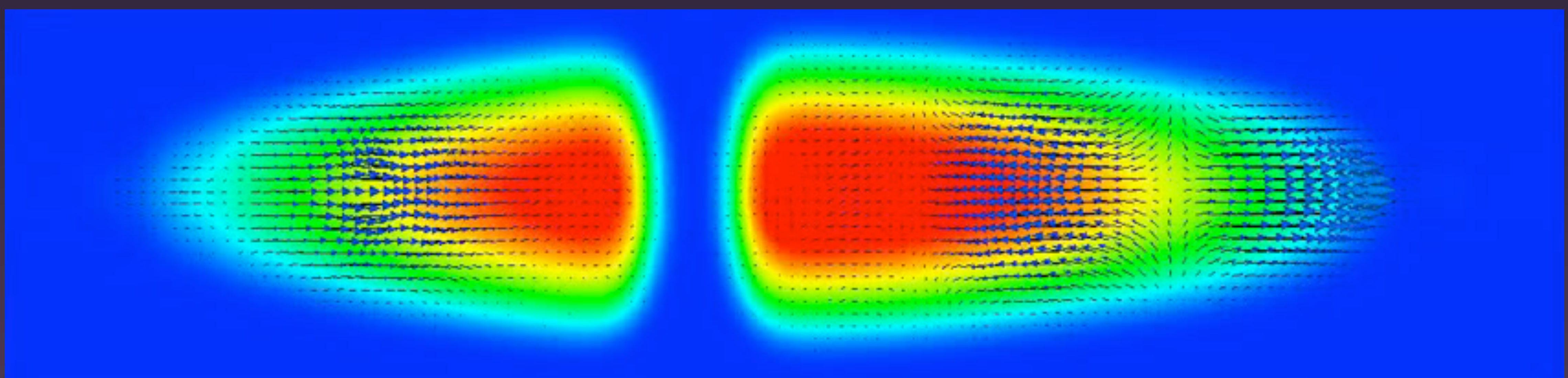
- They observe something for small aspect ratios

Yefsah et al. Nature 499 (426) 2013 [arXiv:1302.4736]

MIT Experiment Interpretation

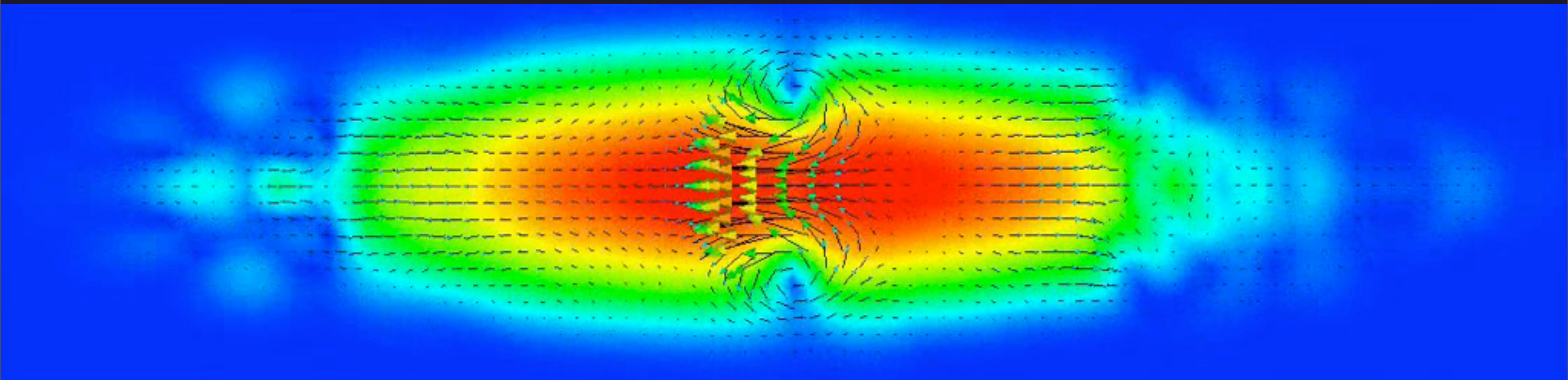
- “Heavy solitons”
  - Effective mass larger by orders of magnitude
  - Extremely stable (thick) filled domain walls
  - Interpreted as a new quantum phenomenon not described by current theories
- What do fully 3D simulations see?

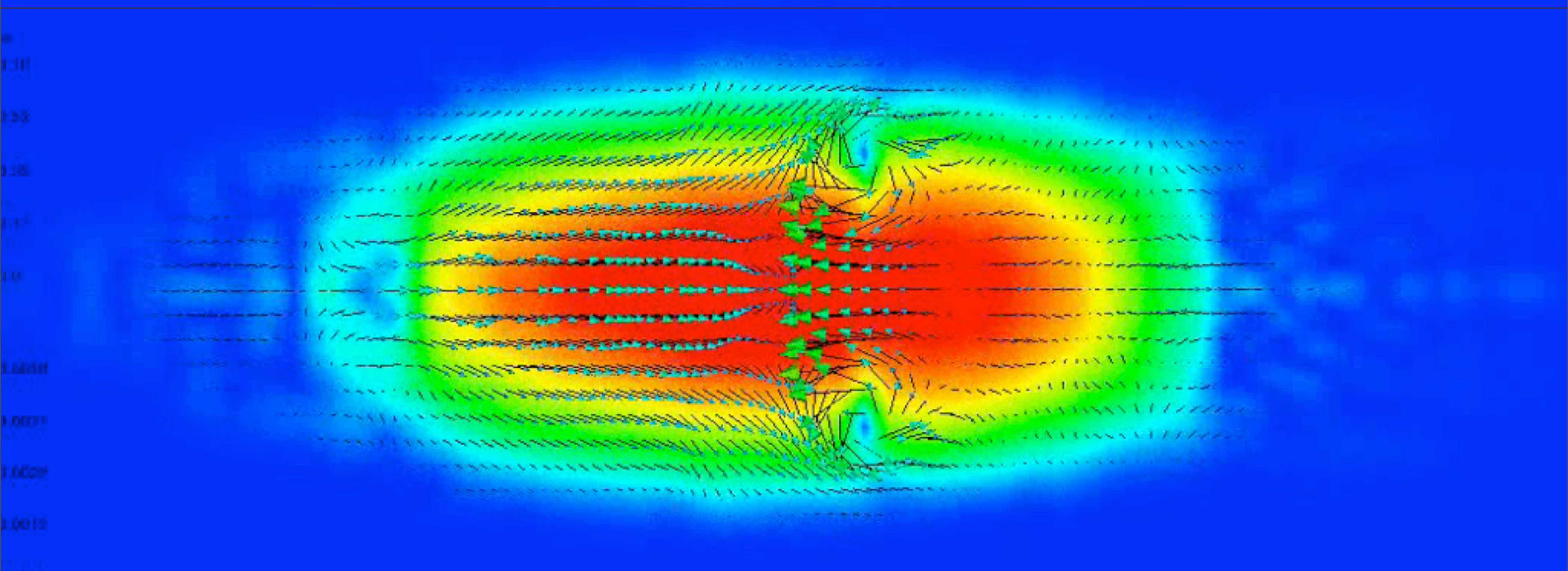
SLDA Simulations



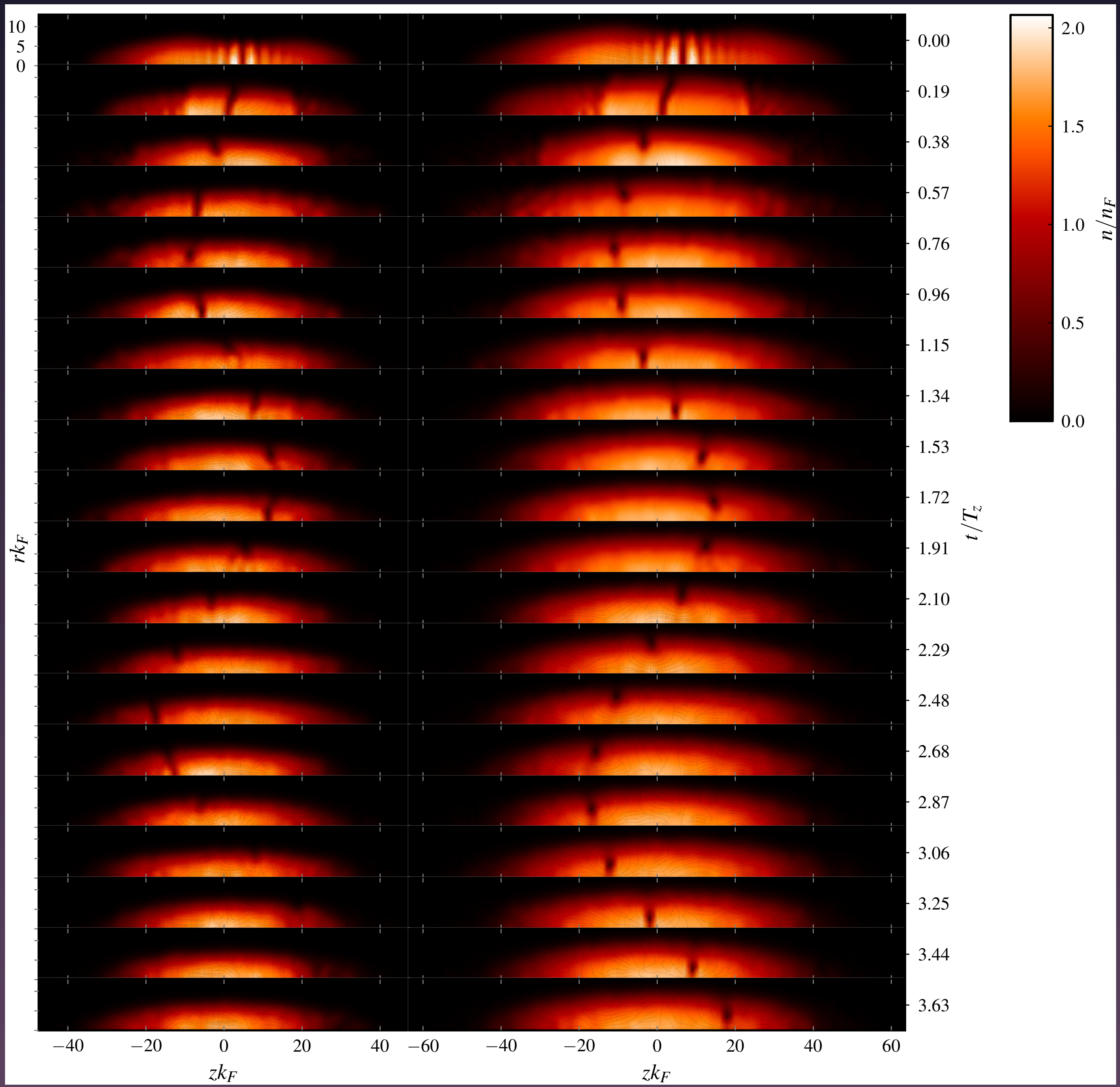
Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]: 32x32x128

SLDA Simulations





Vortex Ring Oscillation



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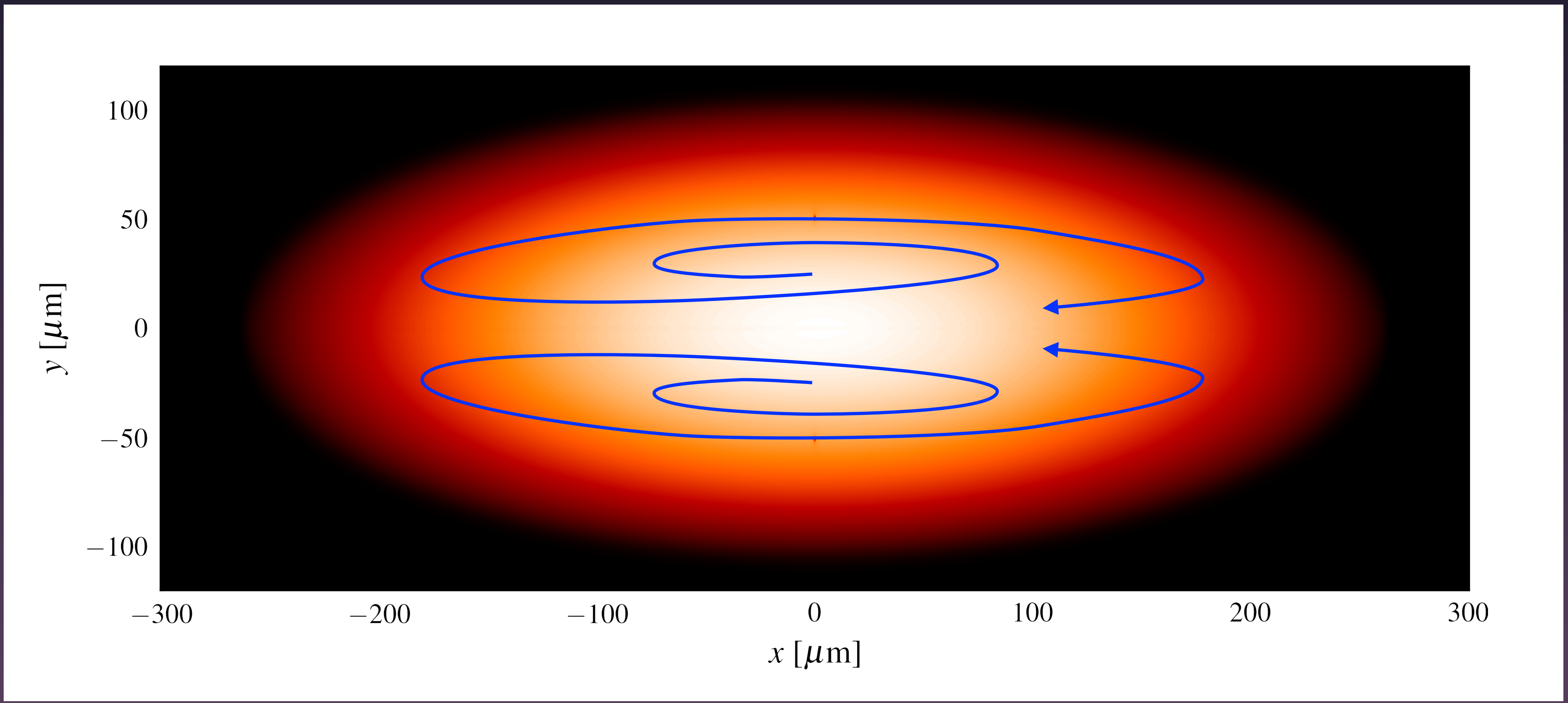
Vortex Rings

$$E \sim \frac{mn\kappa^2}{2} R \ln \frac{R}{l_{coh}}, \qquad v = \frac{dE}{dp} \sim \frac{\kappa}{4\pi}\frac{1}{R}\ln\frac{R}{l_{coh}}$$

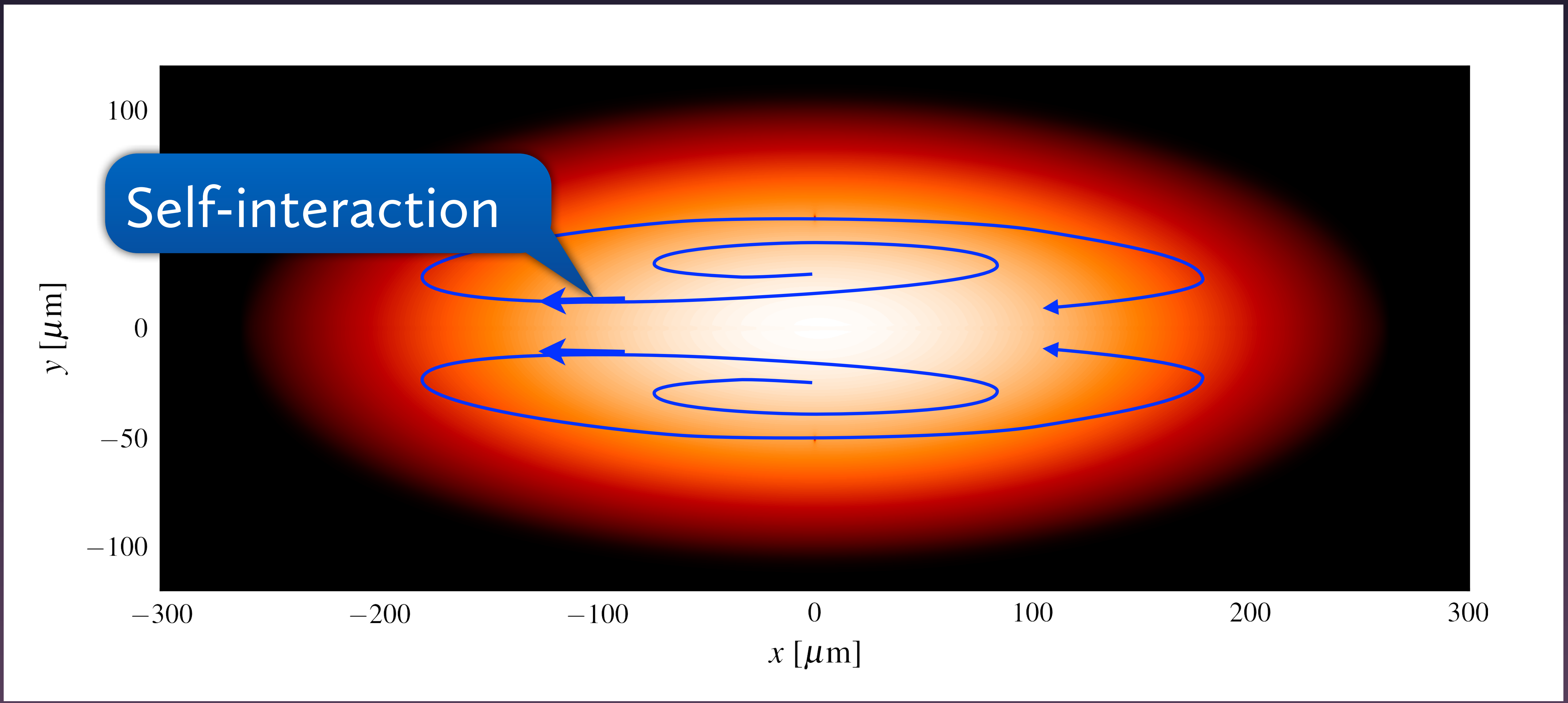
- Thin vortex approximation in infinite matter
  (follows essentially from Biot-Savart law)
- Approximately valid for rings near core
  (but not too near)

Vortex Ring Motion



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

Vortex Ring Motion



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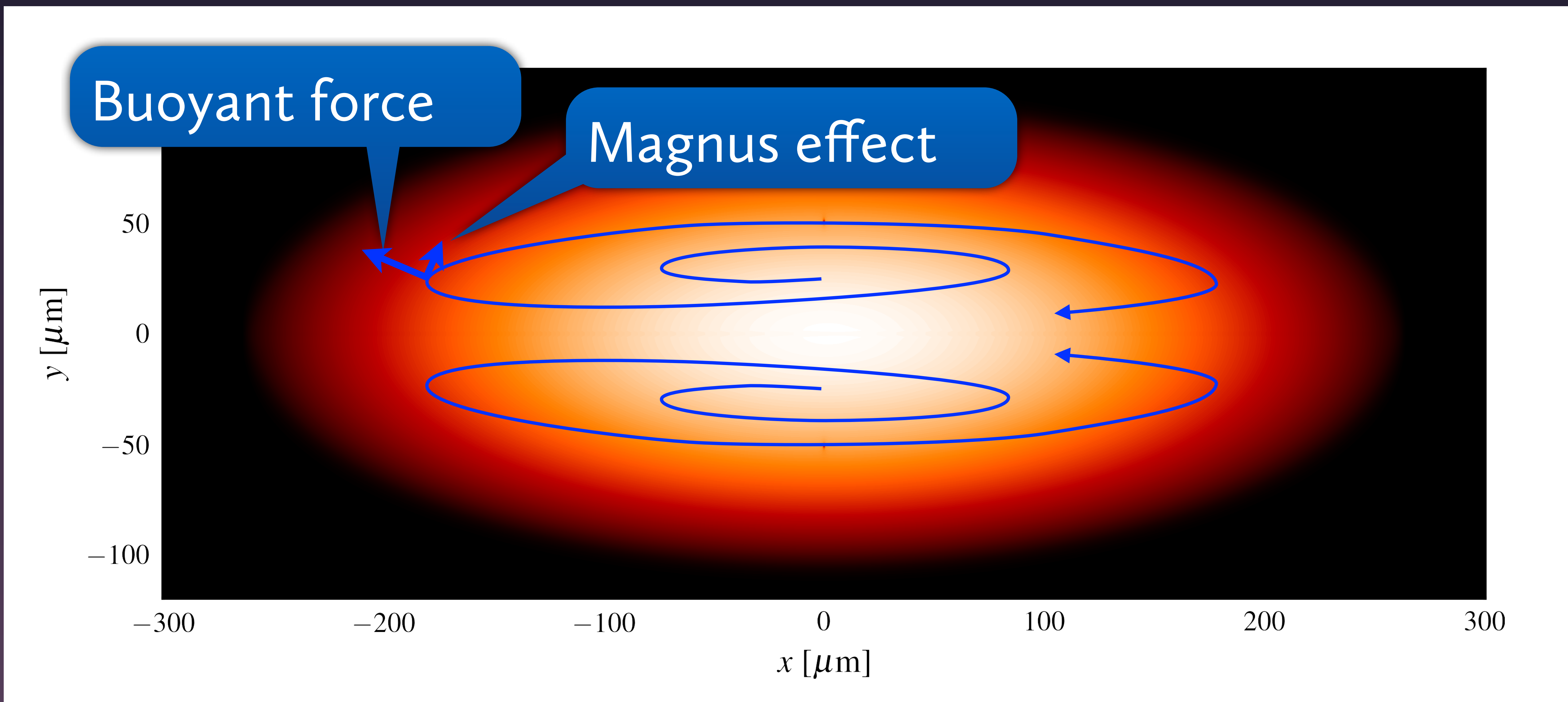

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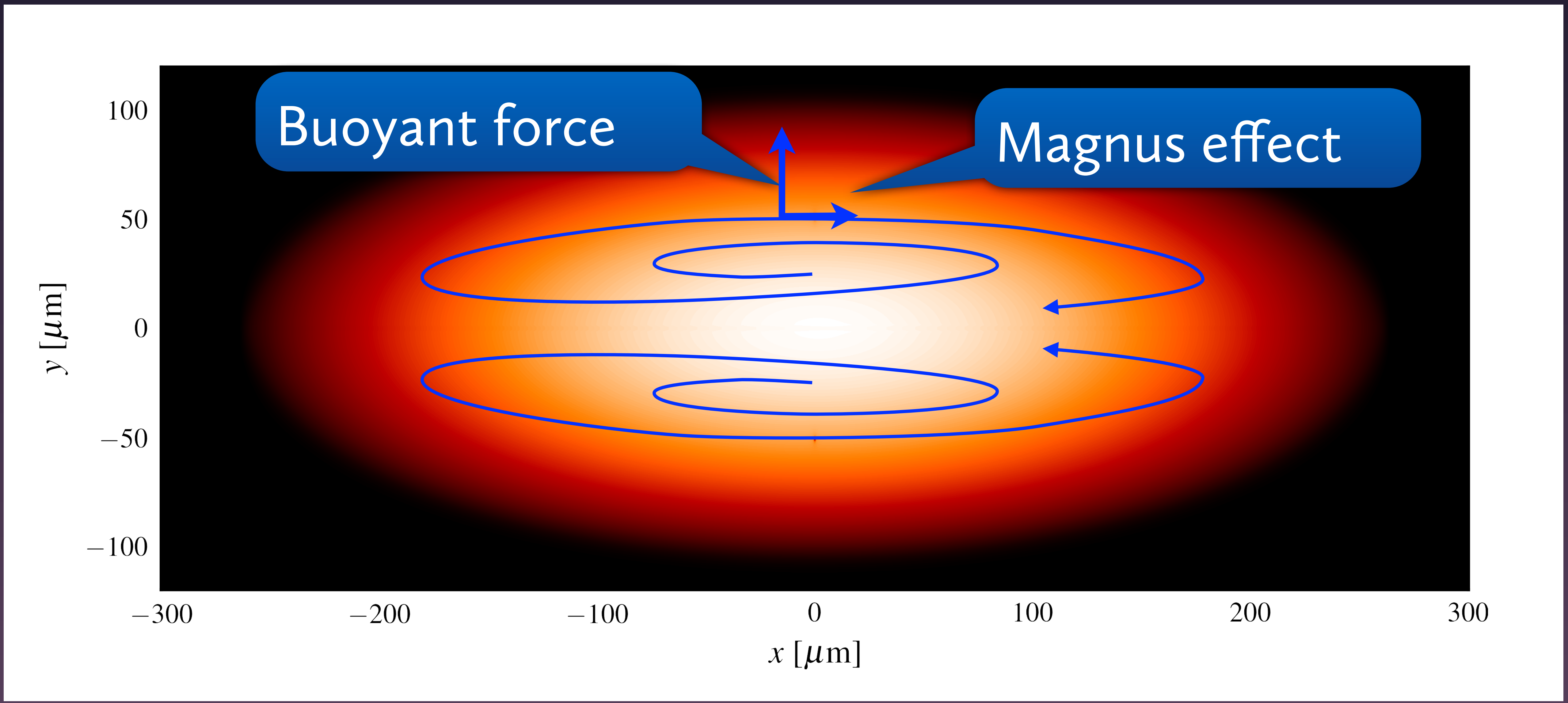

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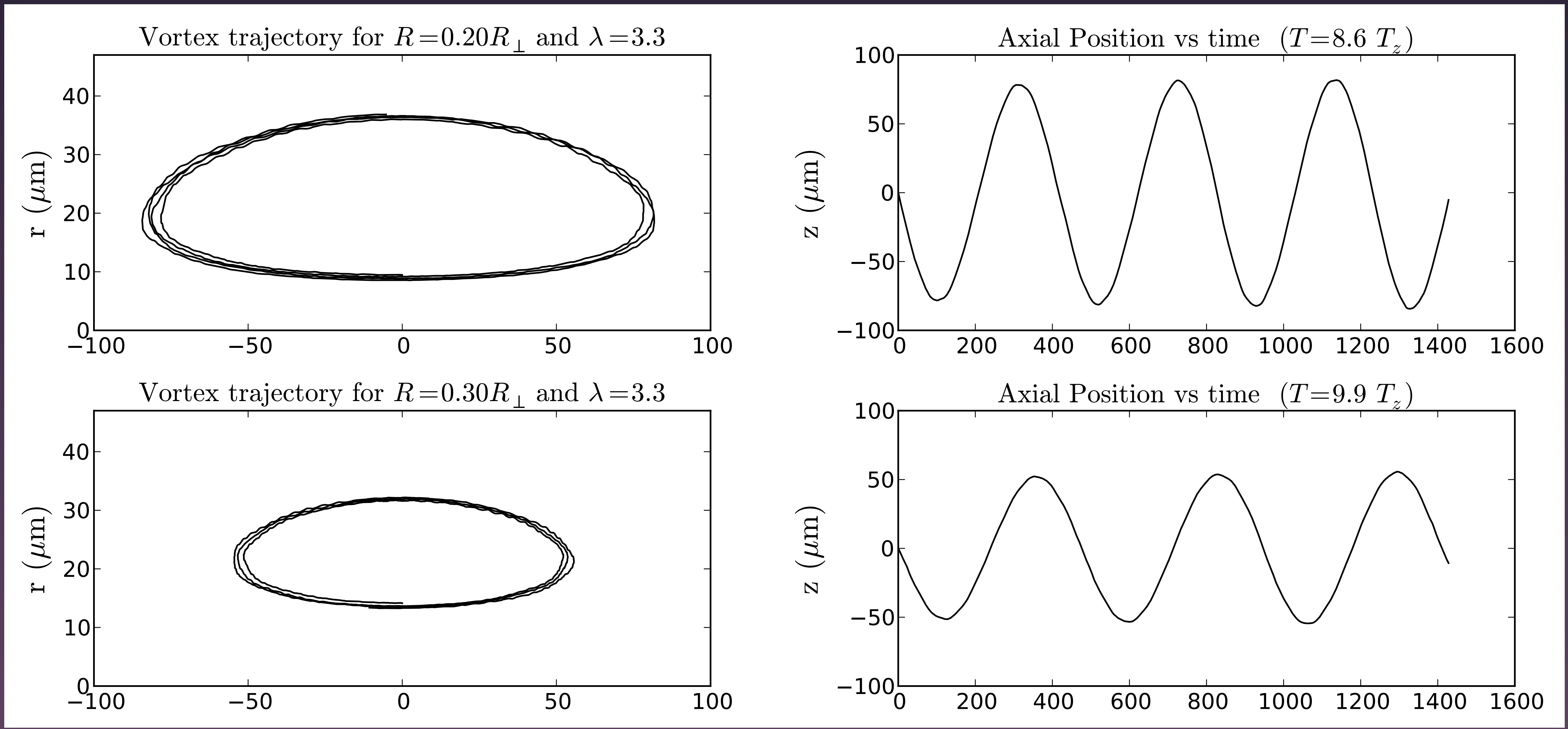
Near-Harmonic Motion



Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]

Vortex Rings in a Trap

$$M_{\mathrm{I}} = \frac{F}{\dot{v}} \sim 8\pi^2 mnR^3 \left(\ln \frac{R}{l_{\mathrm{coh}}}\right)^{-1}$$

$$M_{VR} = mN_{\mathrm{VR}} \sim mn\, 2\pi R\, \pi l_{\mathrm{coh}}^2$$

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

$$\frac{T}{T_z} \sim \sqrt{\frac{M_{\mathrm{I}}}{M_{\mathrm{VR}}}} \sim \frac{2R/l_{\mathrm{coh}}}{\sqrt{\ln(R/l_{\mathrm{coh}})}}$$

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 Rings in a Trap

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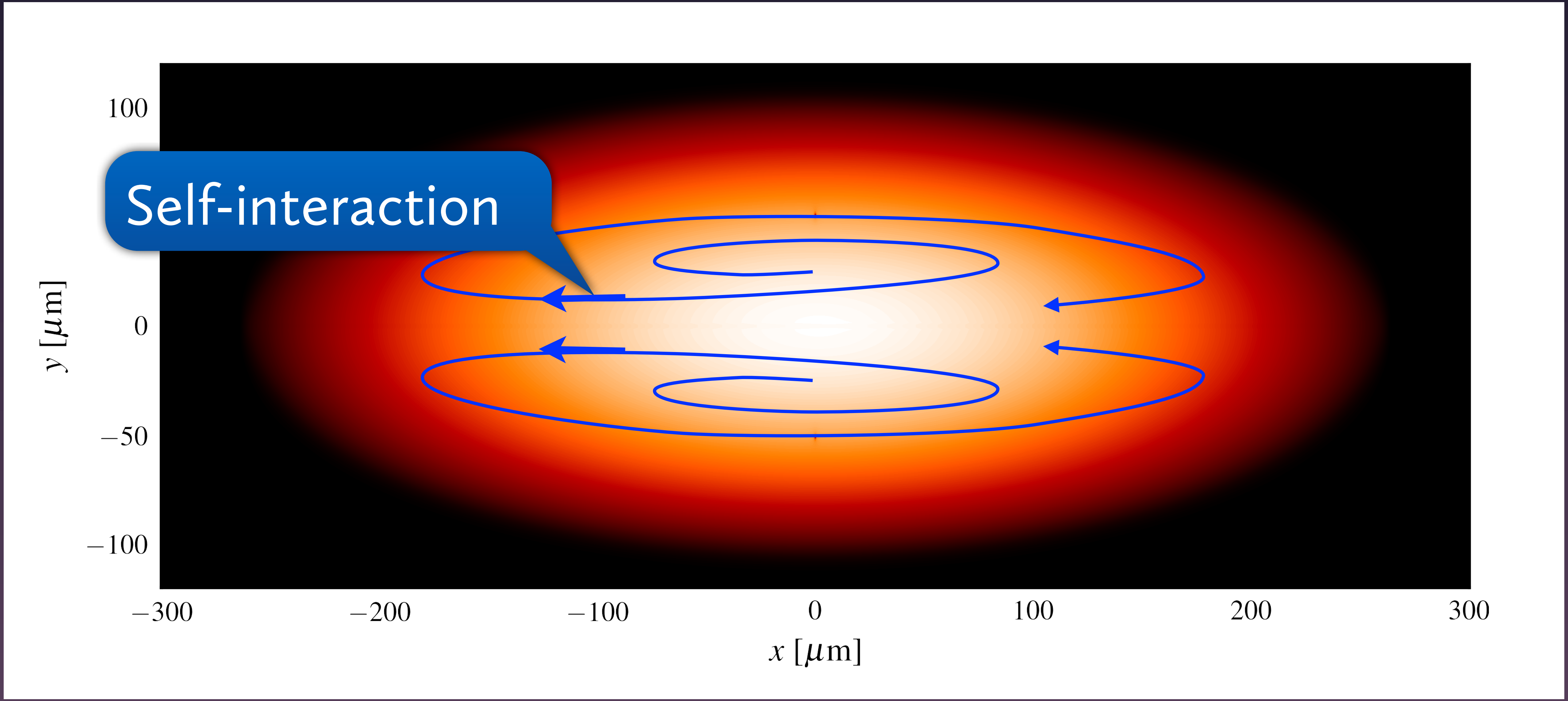
Vortex Ring Motion

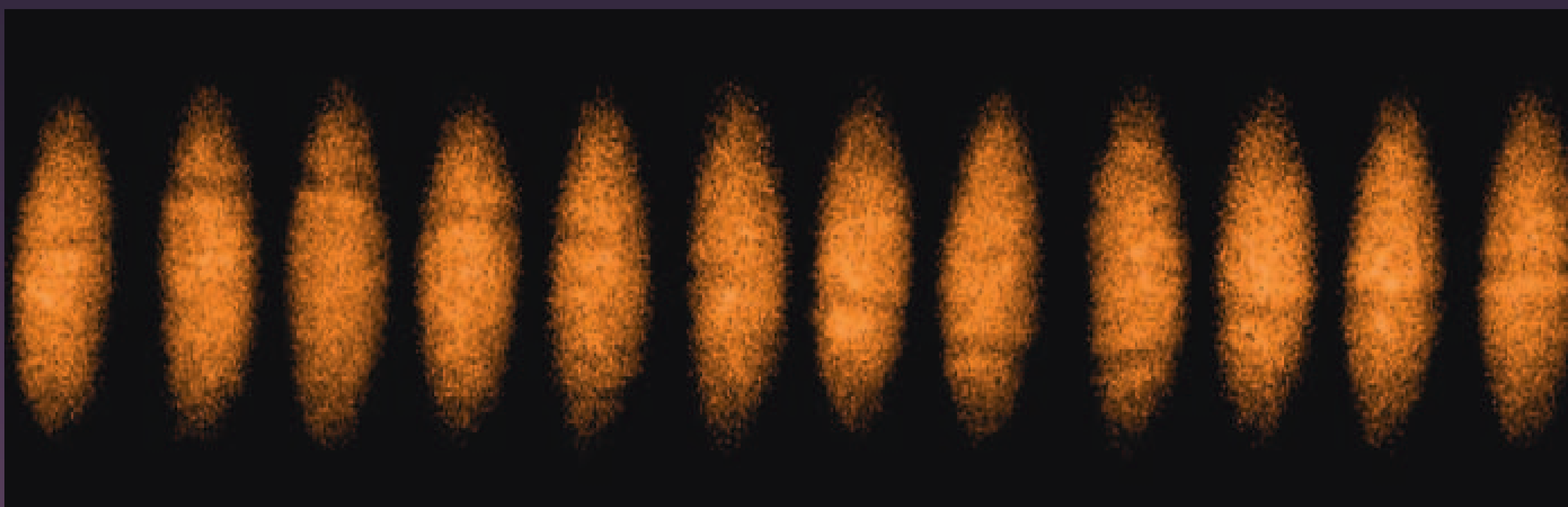


Vortex ring motion (here in the presence of “thermal” noise, hence the inverse decay)

Does MIT measure vortex rings?

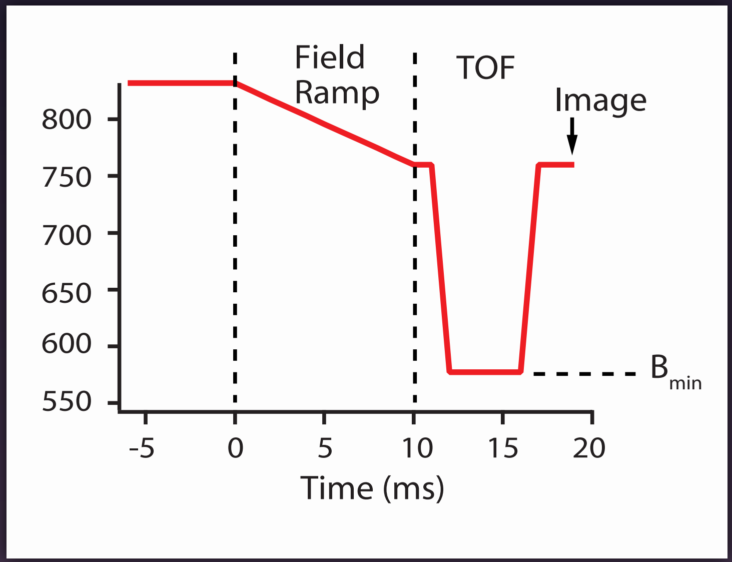
- Reproduces all qualitative dependences:
  - ✓Long periods
  - ✓Anti-decay at "finite temperature"
  - ✓Dependence on aspect ratio and interaction strength

But MIT sees domain walls, not rings



Yefsah et al. Nature 499 (426) 2013 [arXiv:1302.4736]

Imaging Vortex Rings (small ring)



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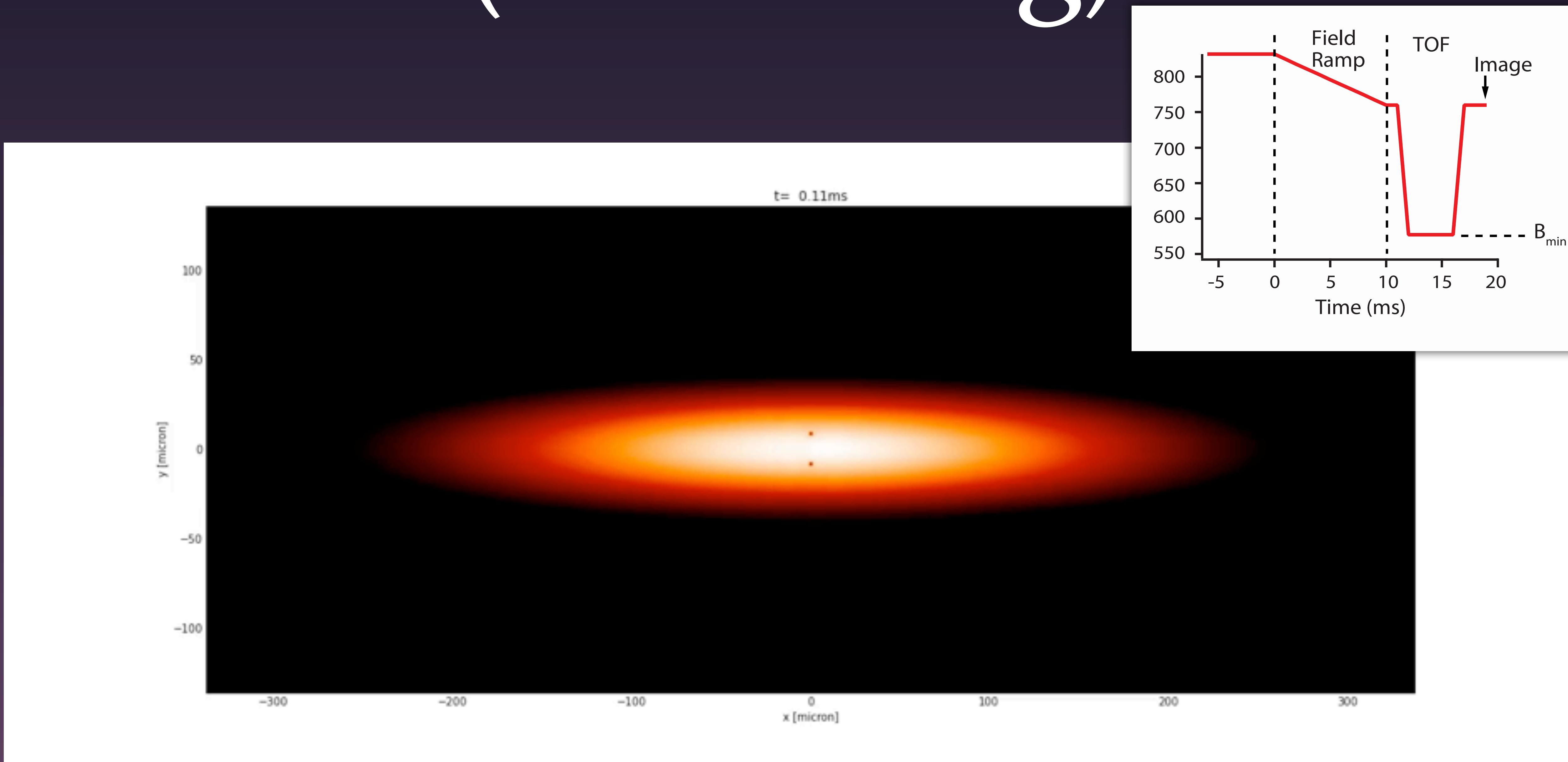

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Image after expansion (integrated average)

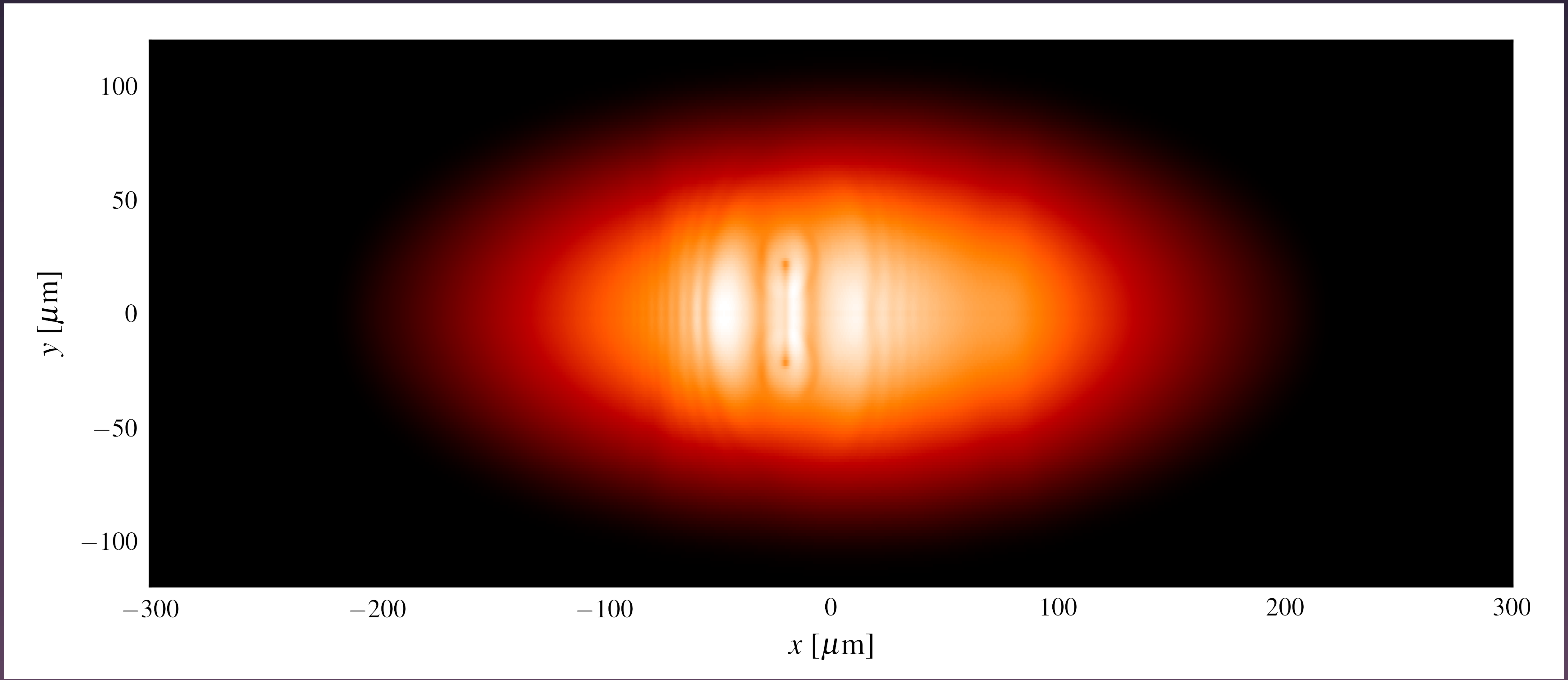

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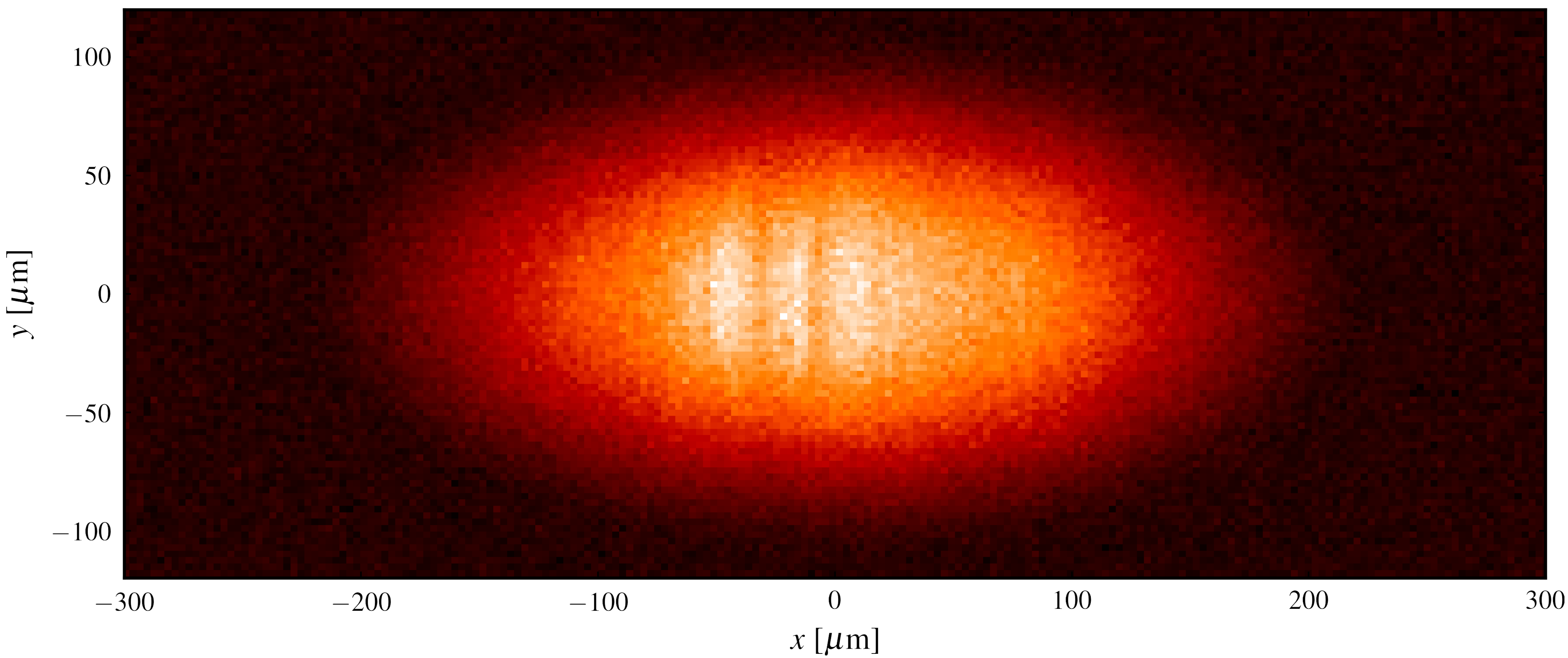
Image after expansion (simulate noise)



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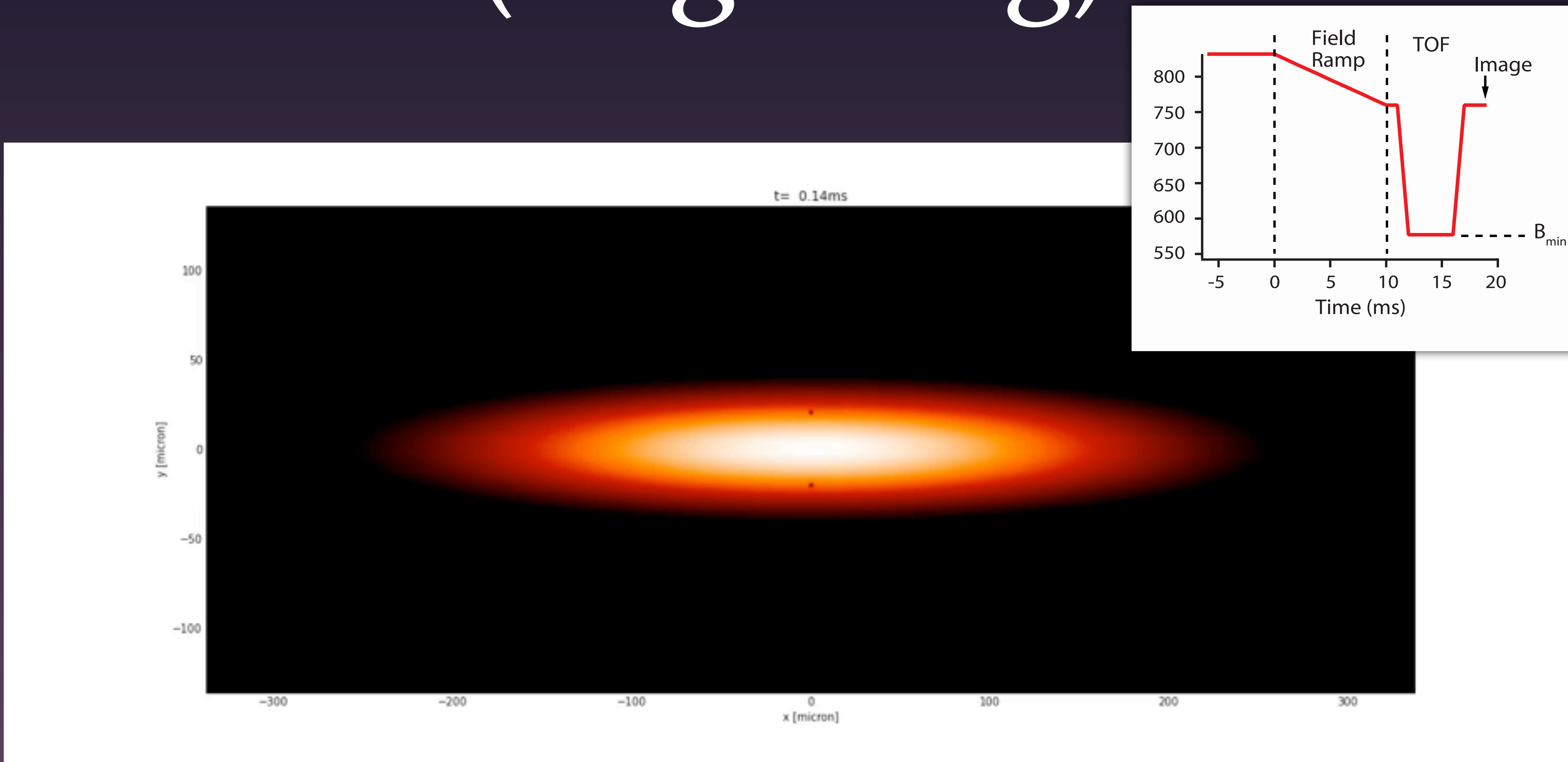
Imaging Vortex Rings (large ring)



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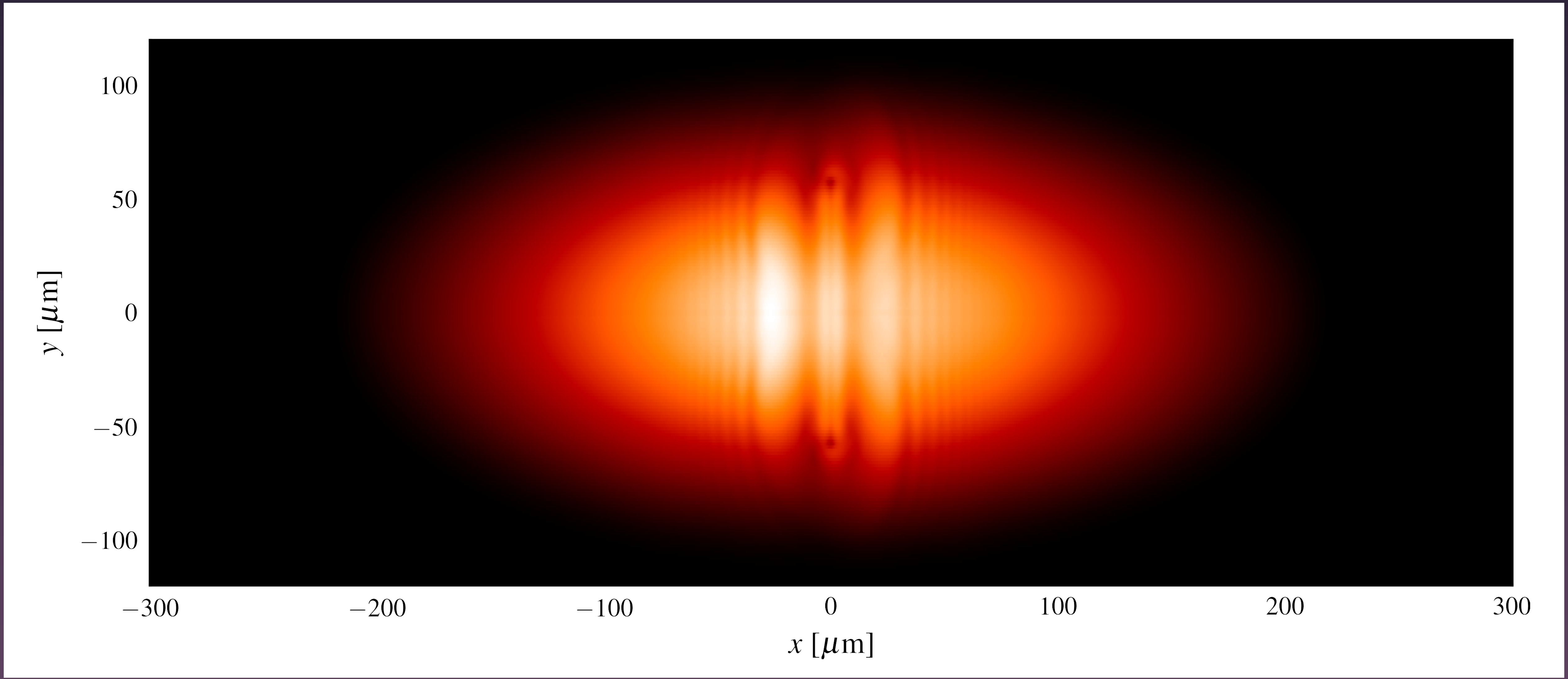

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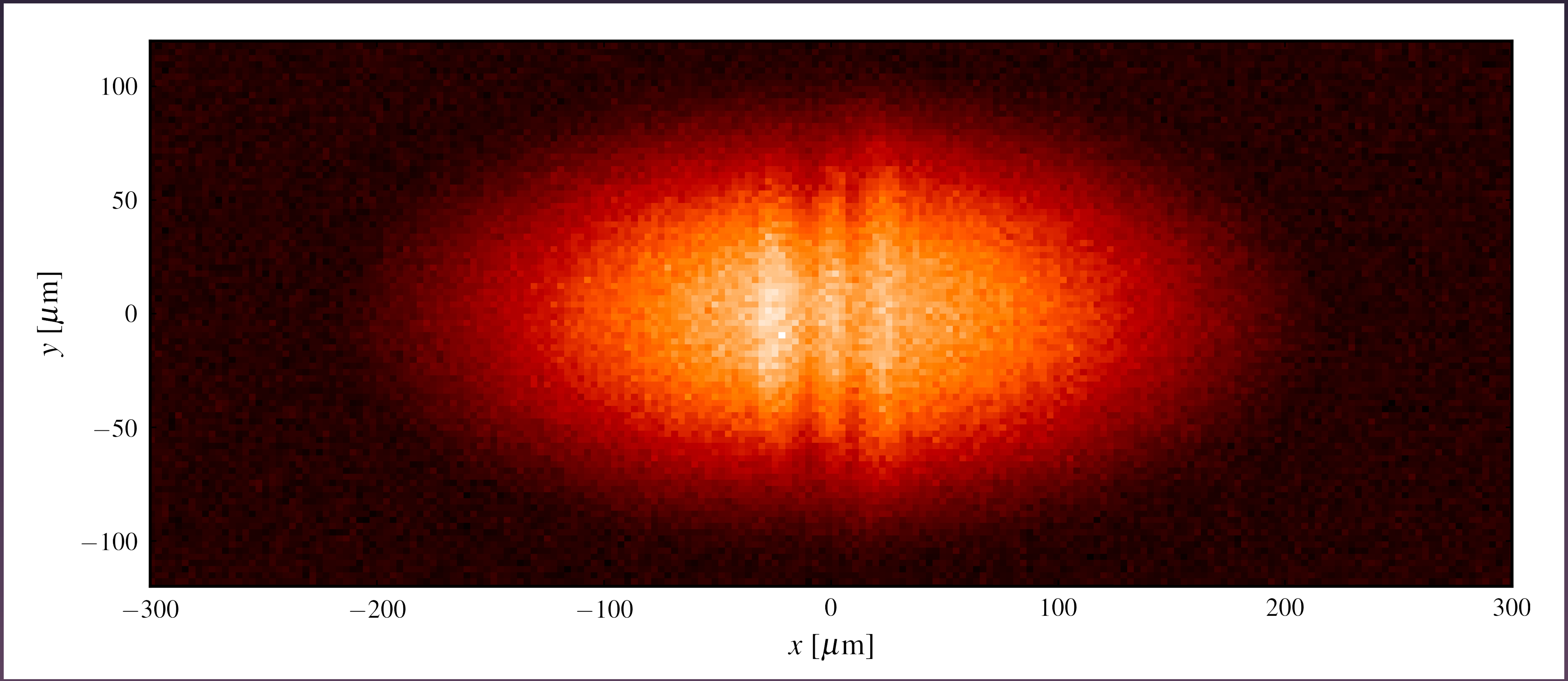

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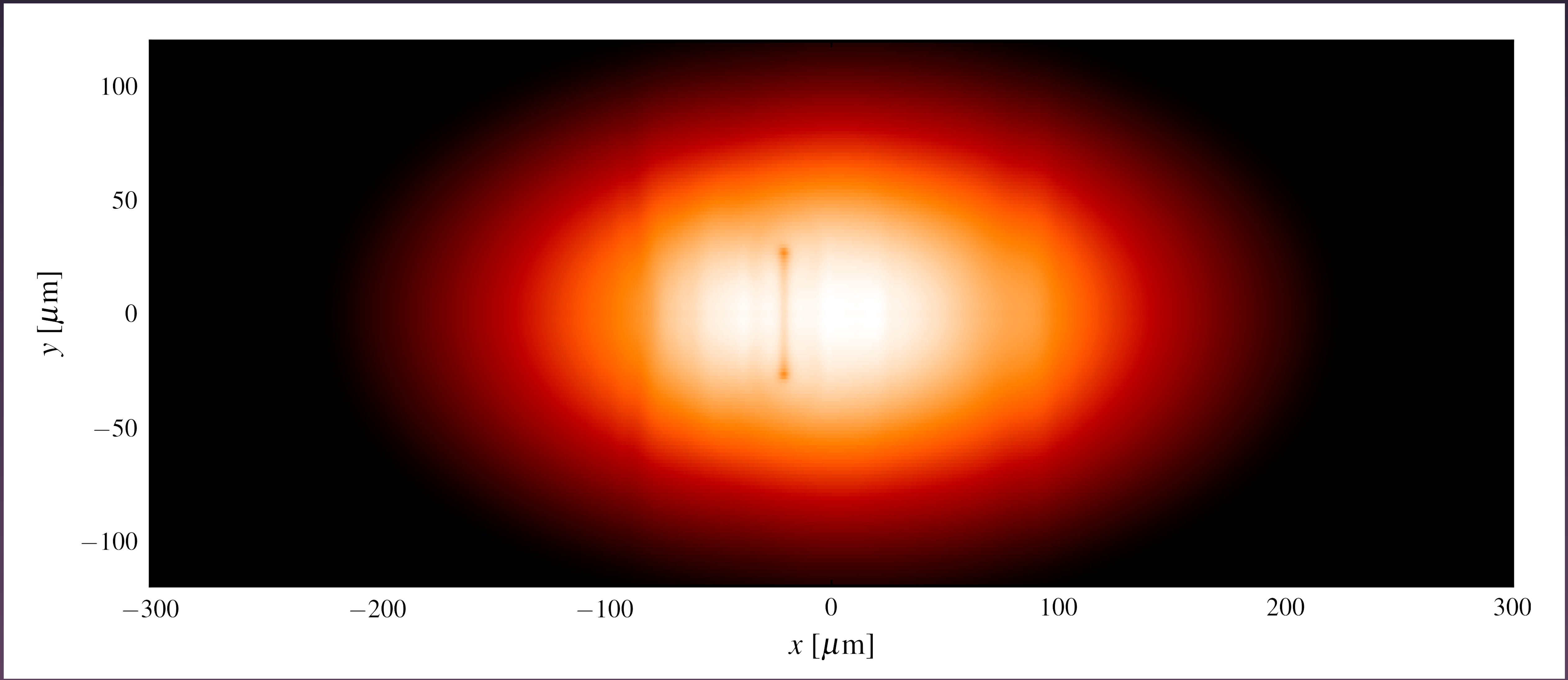
Image after expansion borderline B_{min}=702G



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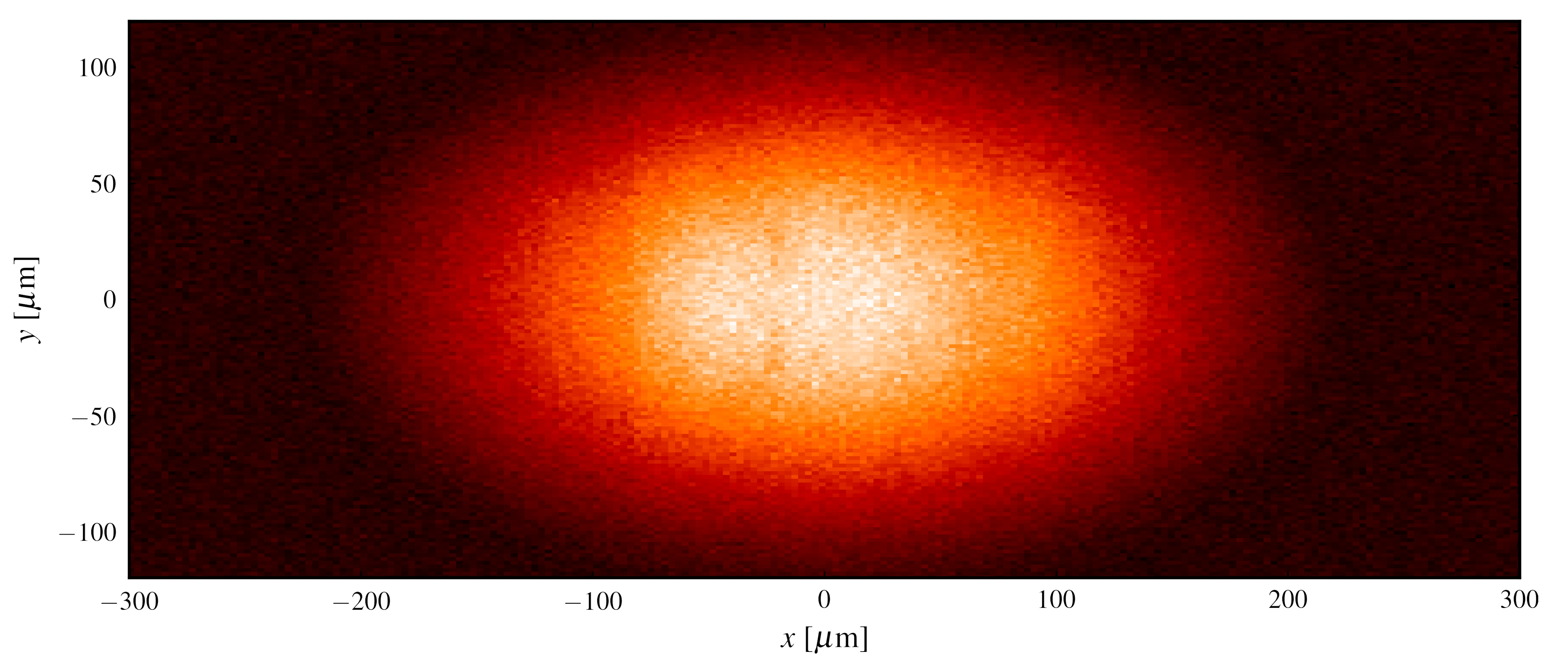

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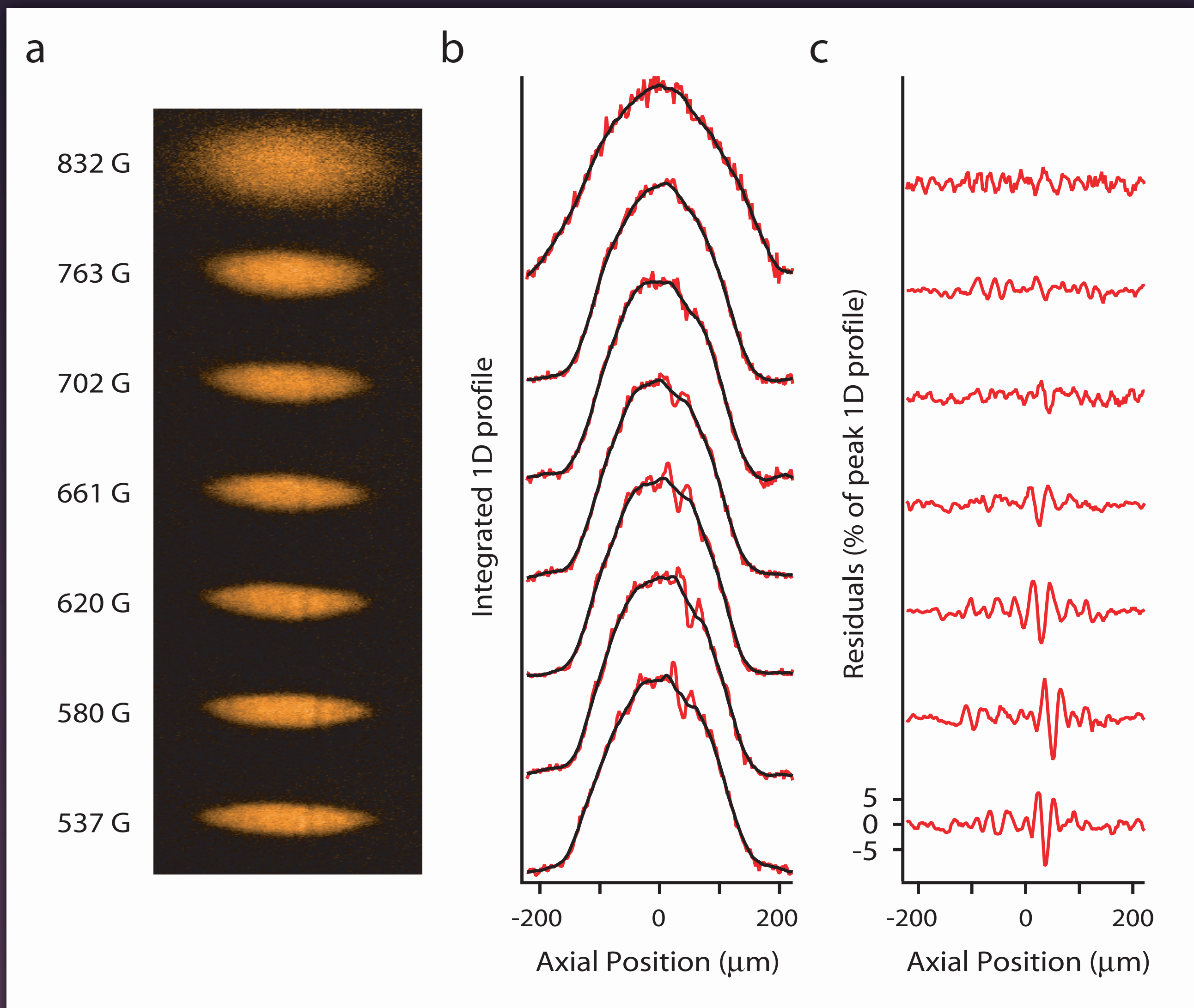
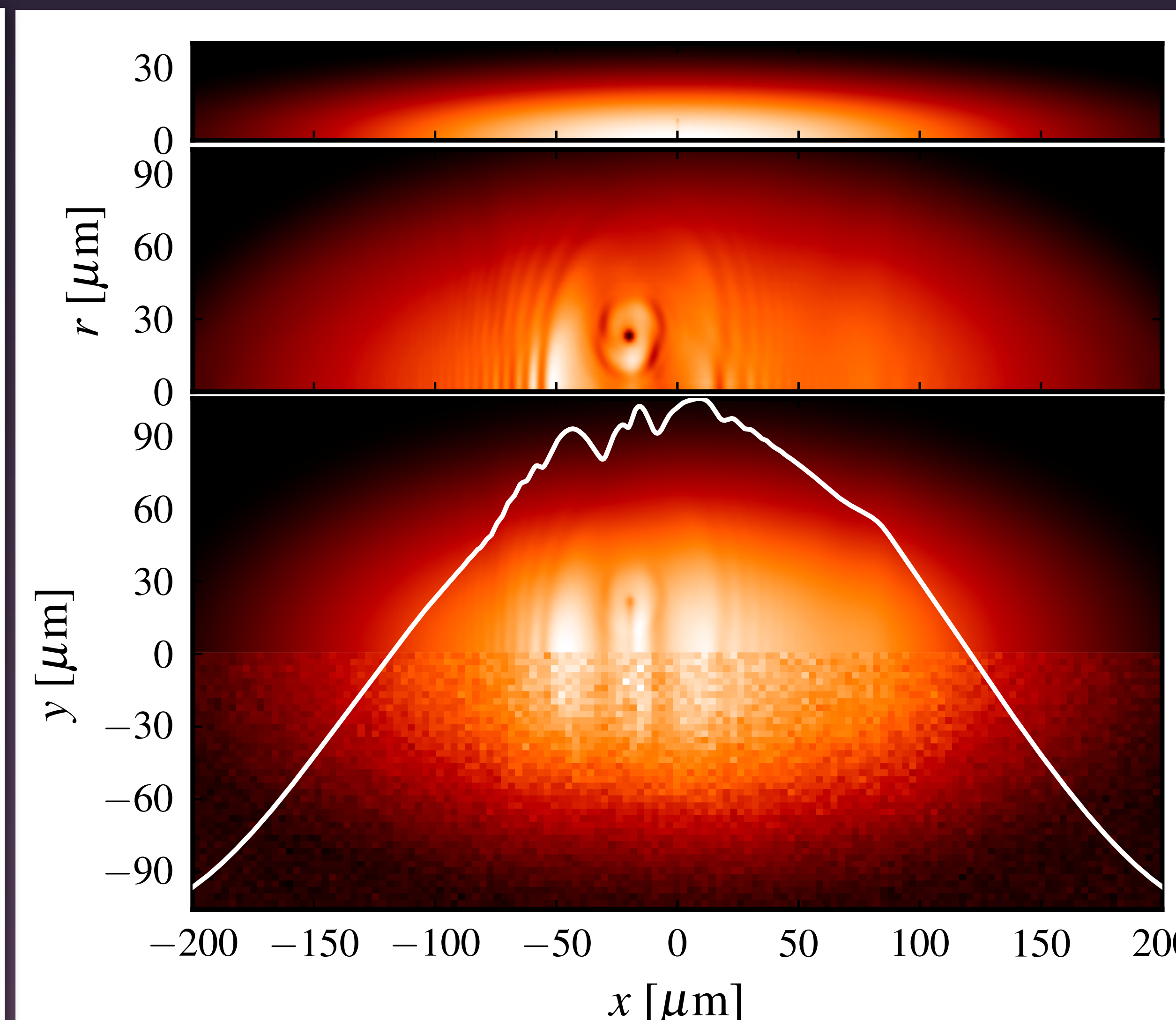
Explains Dependence on B_{min}





Yefsah et al. Nature 499 (426) 2013

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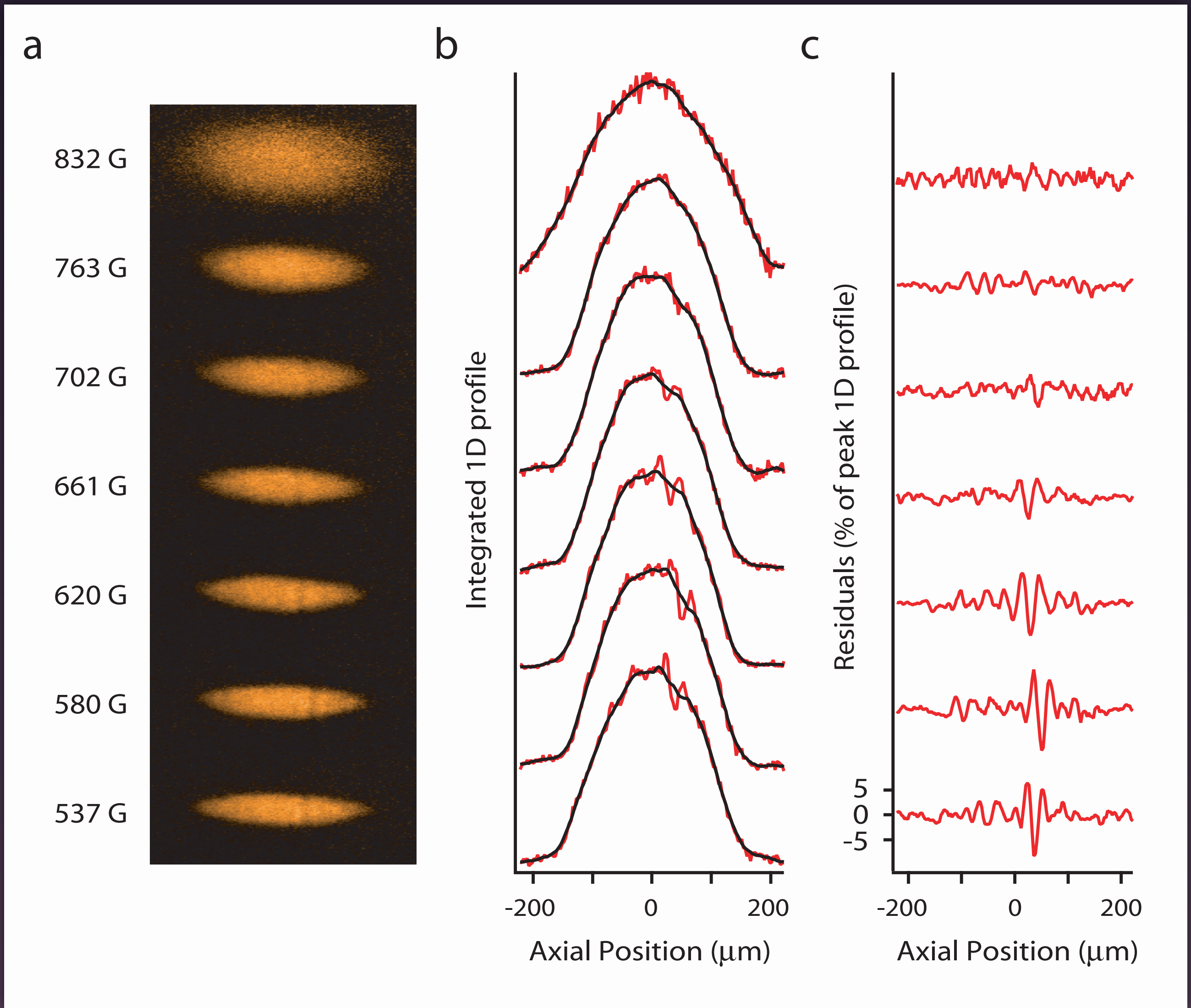

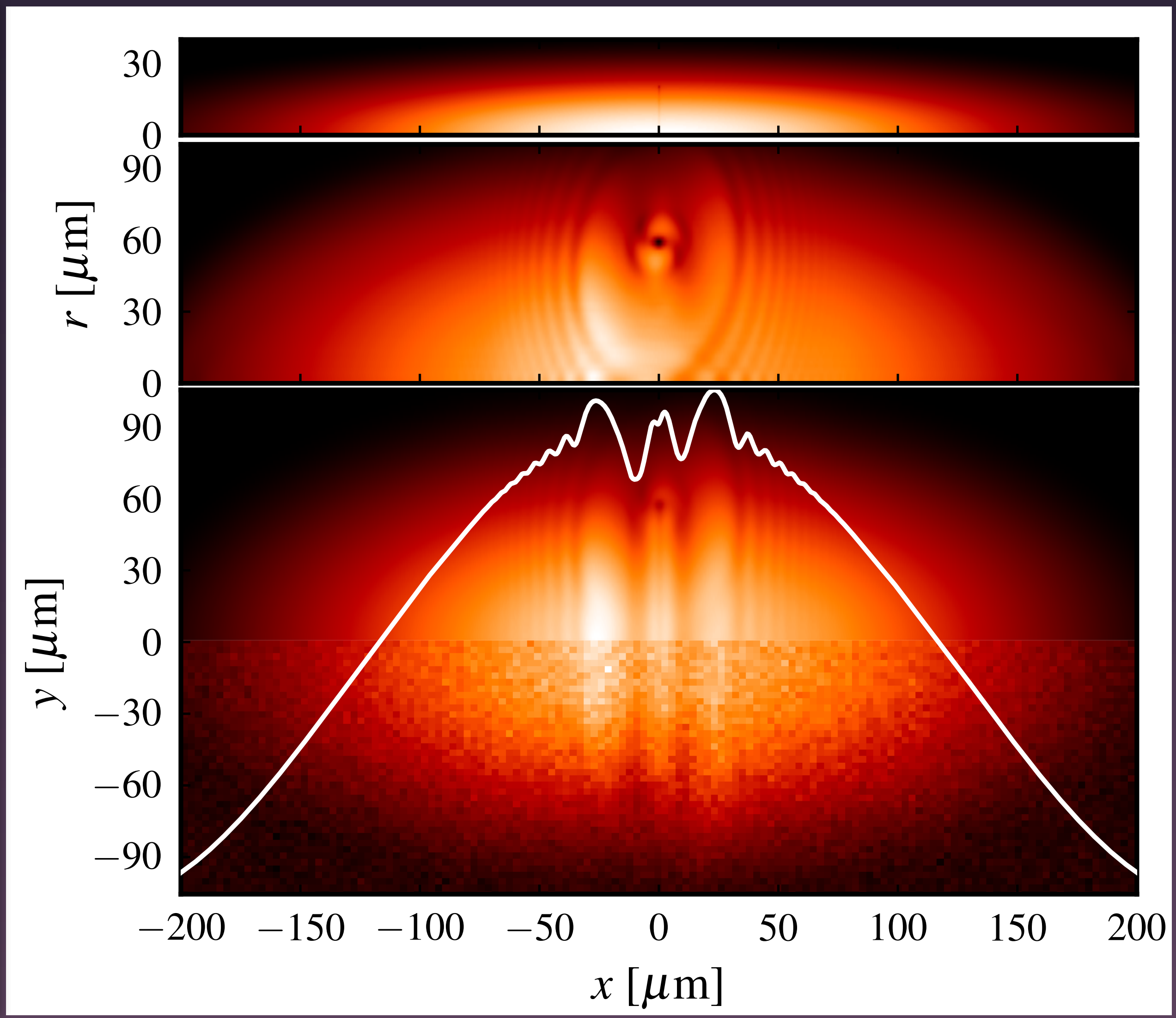

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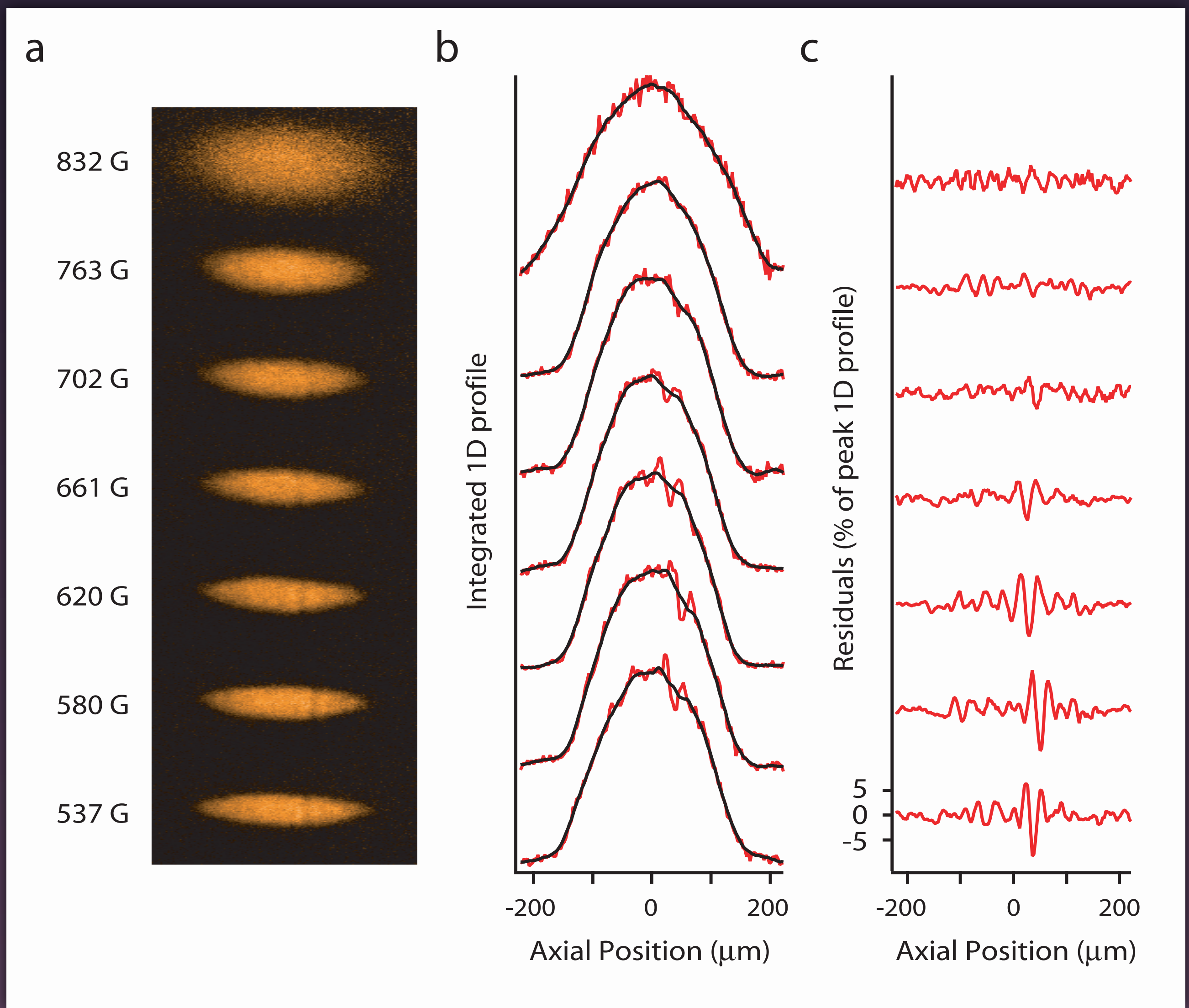

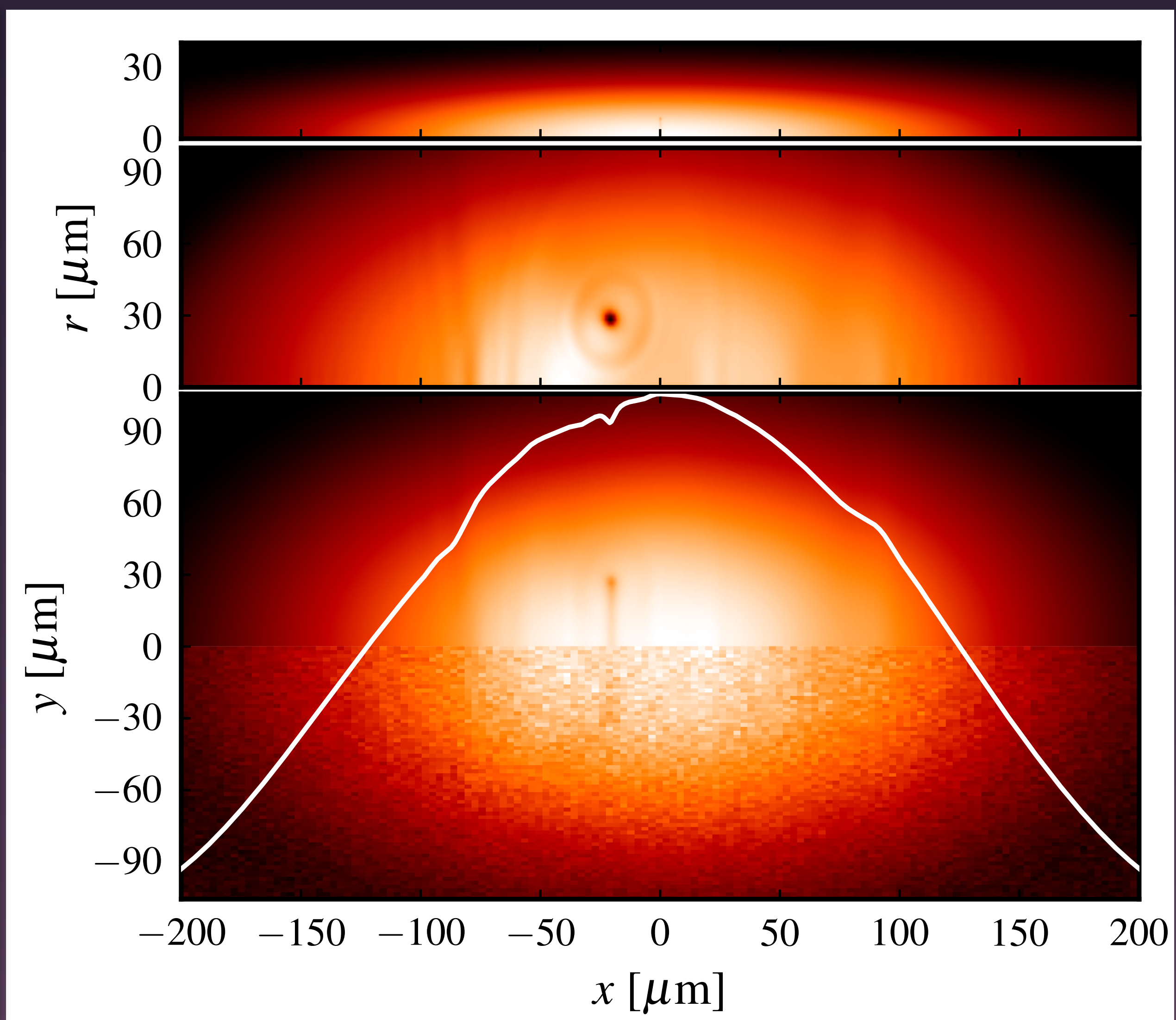

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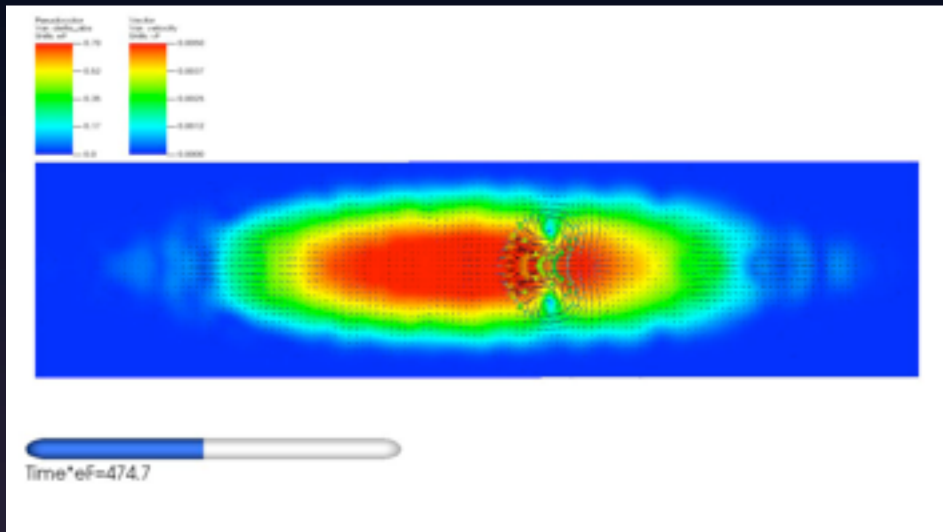
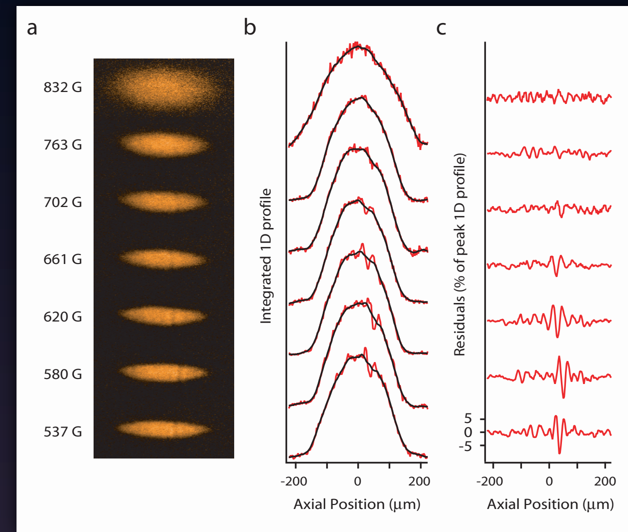
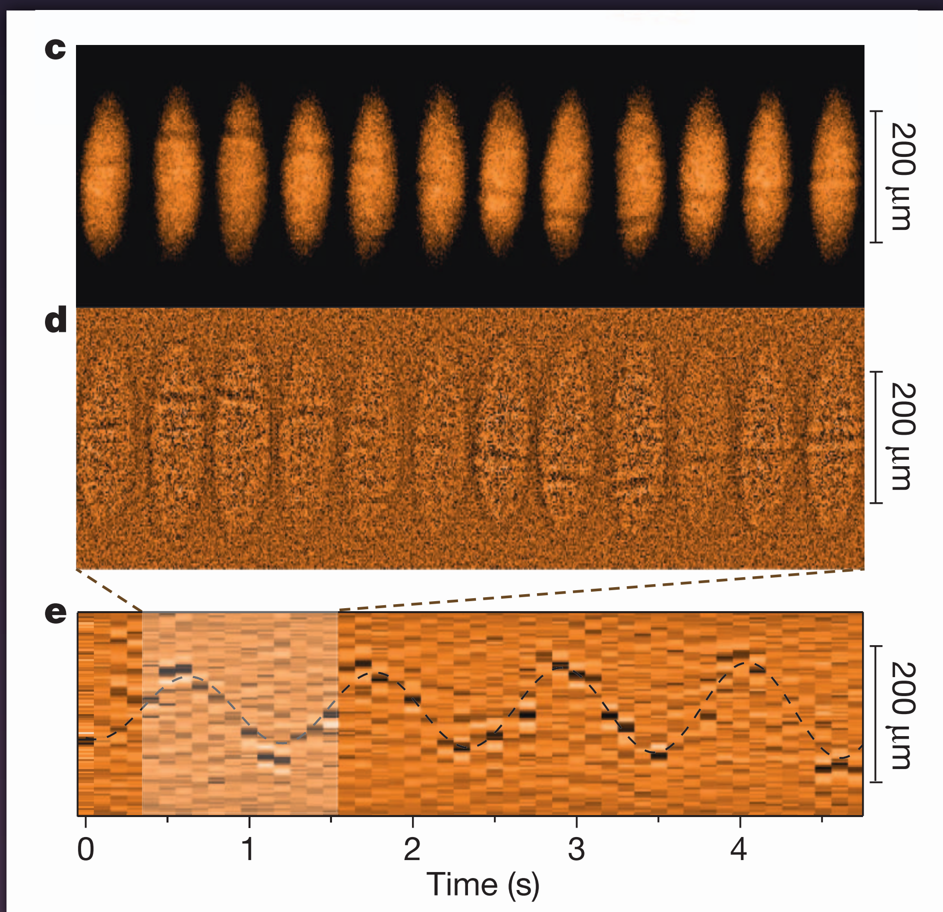
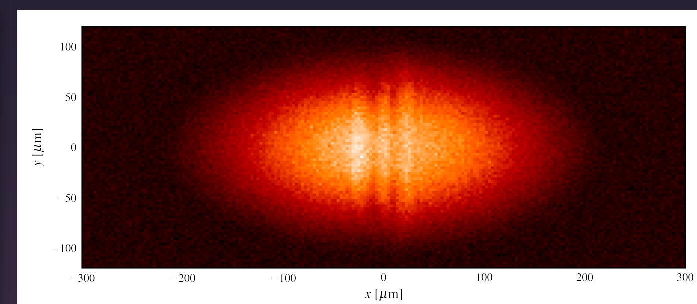
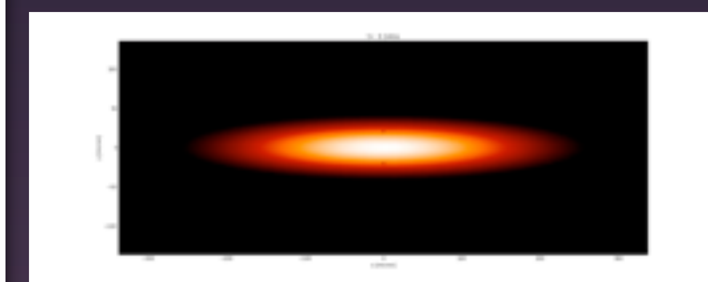


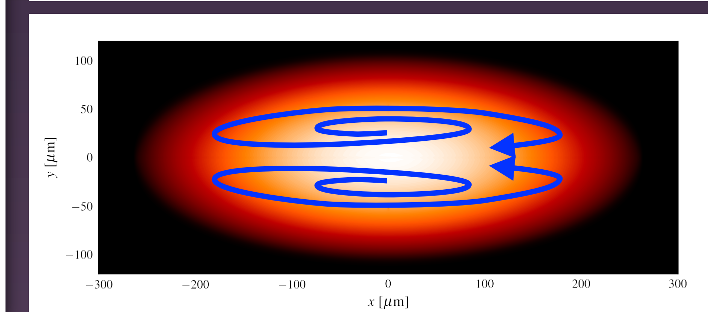


Solitions? Rings!



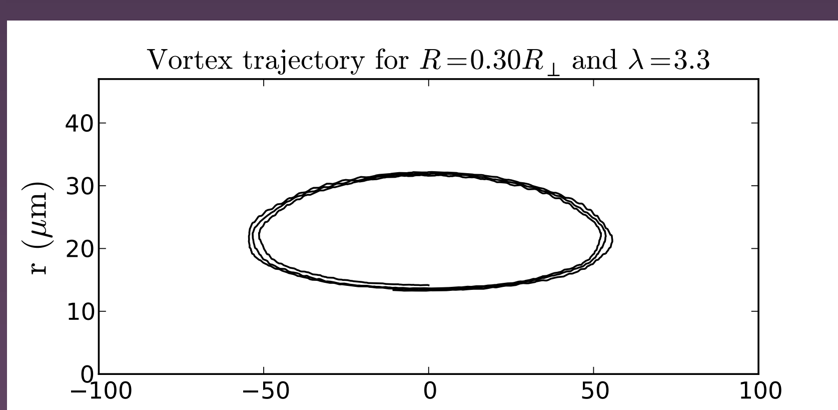


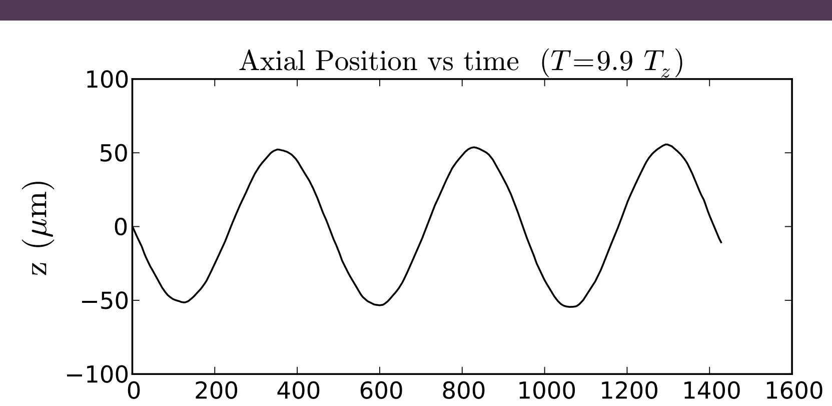




Vortex rings explain MIT experiment

- Long periods
- Dependence on aspect ratio and interaction
- Imaging limitations
- Validates DFT

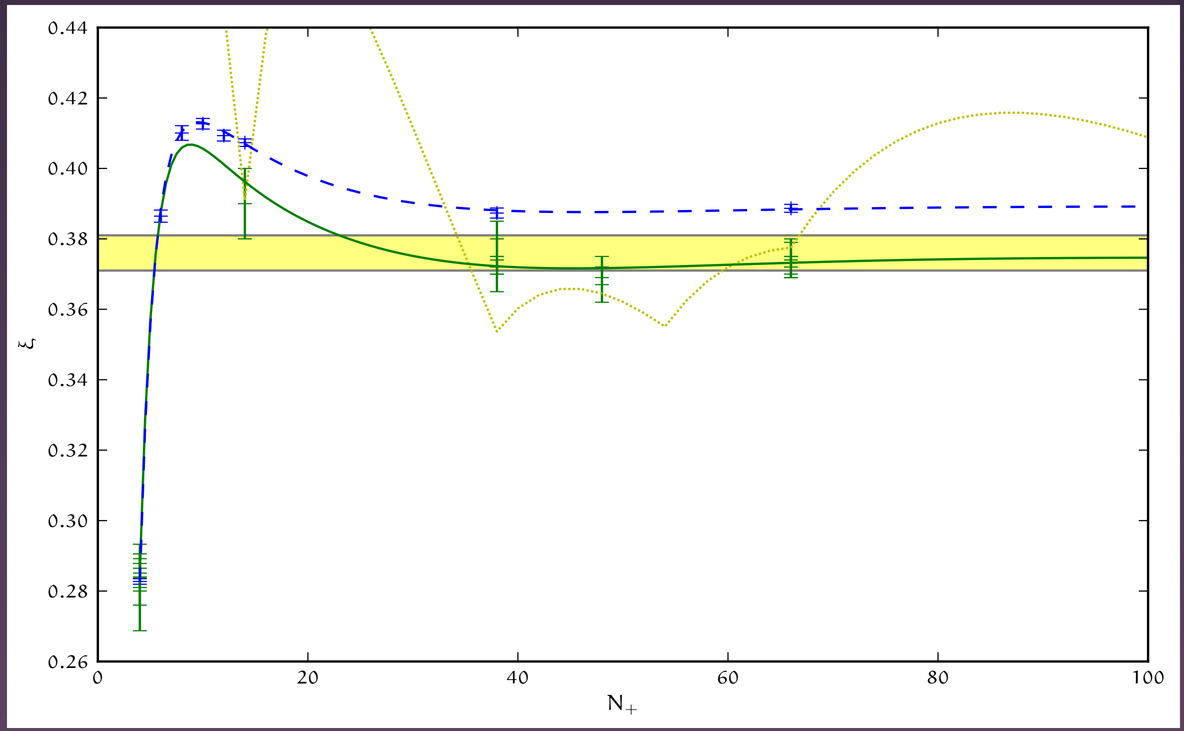




SLDA: Superfluid Local Density Approximation

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

- 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/α)
  - Hartree (β), Pairing (g)



Forbes, Gandolfi, Gezerlis (2012)

BdG: contained in SLDA

$$\langle\nabla\hat{a}^\dagger\nabla\hat{a}\rangle + \langle\nabla\hat{b}^\dagger\nabla\hat{b}\rangle \qquad \langle\hat{a}^\dagger\hat{b}^\dagger\rangle\,\langle\hat{b}\hat{a}\rangle$$

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

- 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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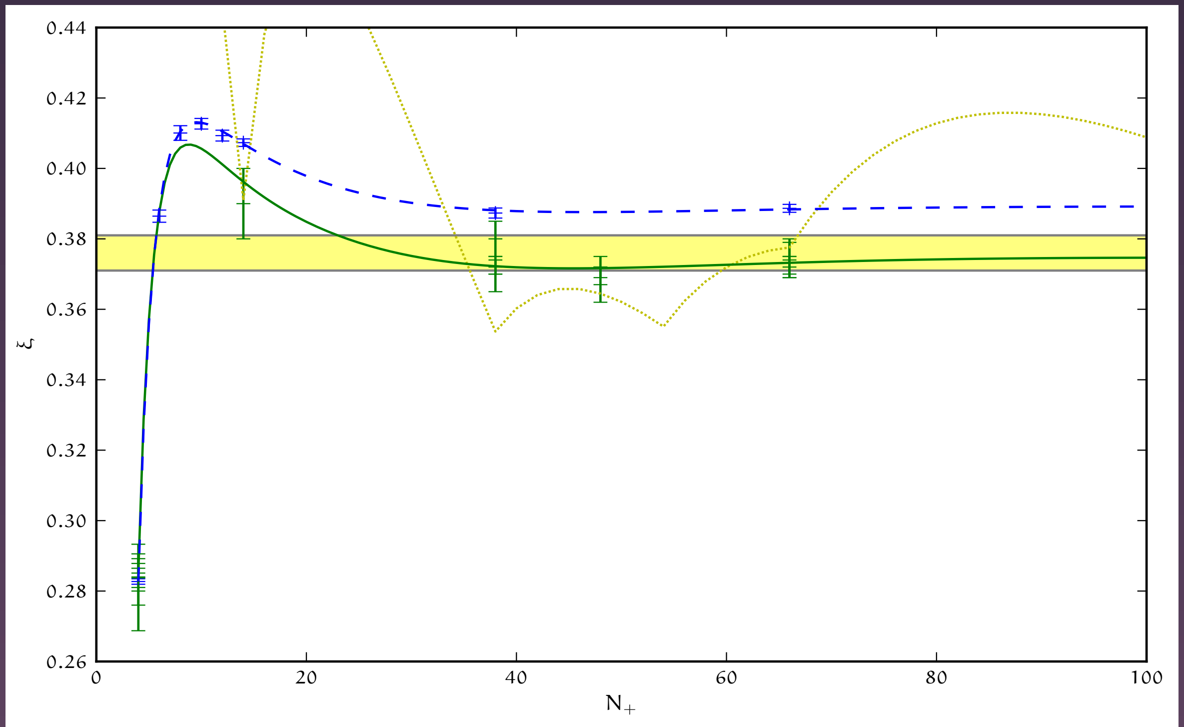
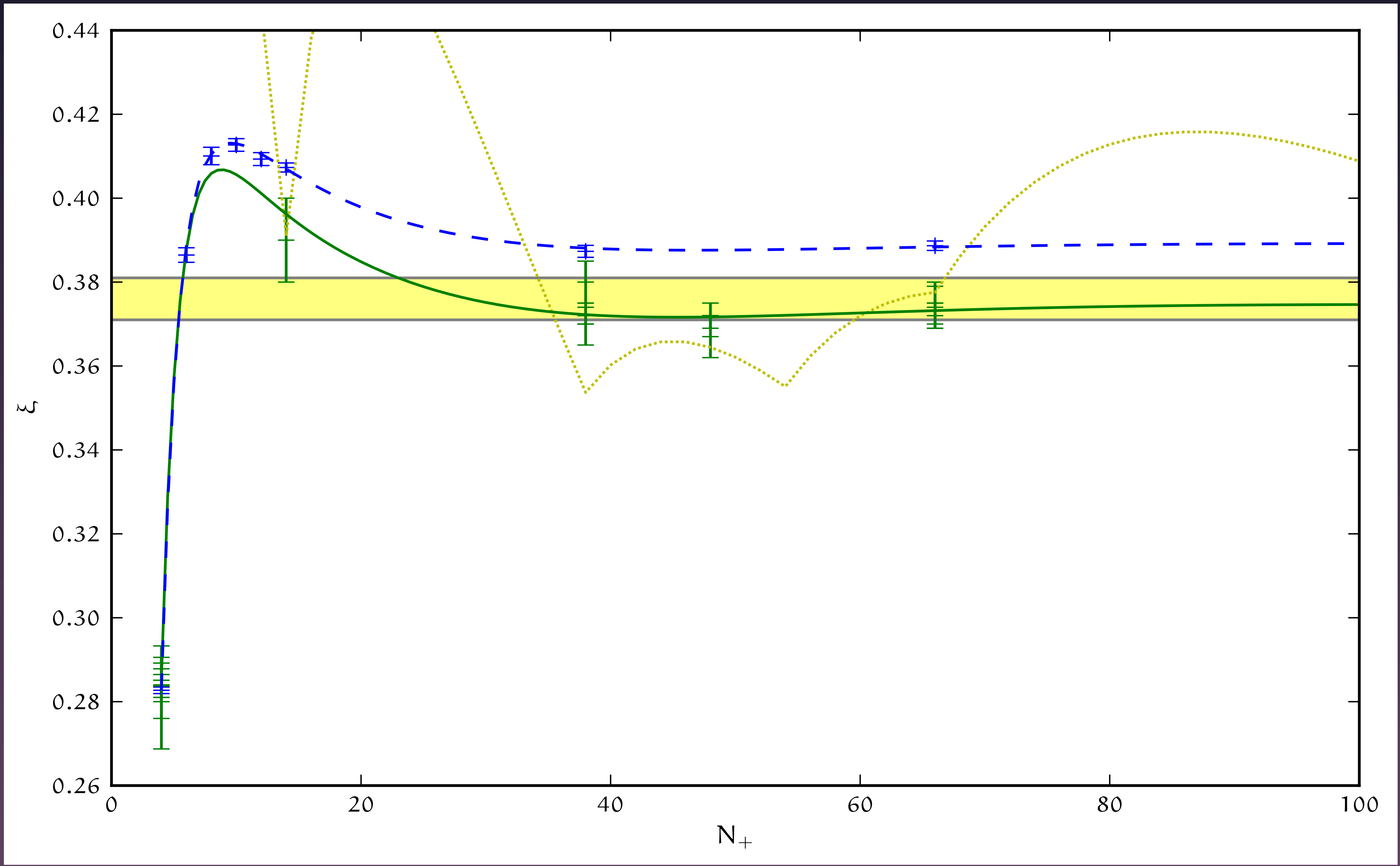


Forbes, Gandolfi, Gezerlis (2012)

Slda: Superfluid Local



Forbes, Gandolfi, Gezerlis (2012)

TDDFT (TDSLDA)

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

- No diagonalization needed for evolution
  - Just apply Hamiltonian
  - Use FFT for kinetic term
- Efficient real-time evolution the scales well
  - Distribute wavefunctions over nodes
  - Utilize GPUs

TDDFT (TDSLDA)

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

- Computational challenge: Finding initial (ground) state?

  Root-finders requires repeated diagonalization of s.p. Hamiltonian

  Slow and does not scale well

  Only suitable for small problems or if symmetries can be used

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

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

- 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

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

- Consider evolution with potential $H+V_t$:

$$\partial_t E = -i \, \mathrm{Tr}\left([H,\rho] \cdot V_t\right)$$

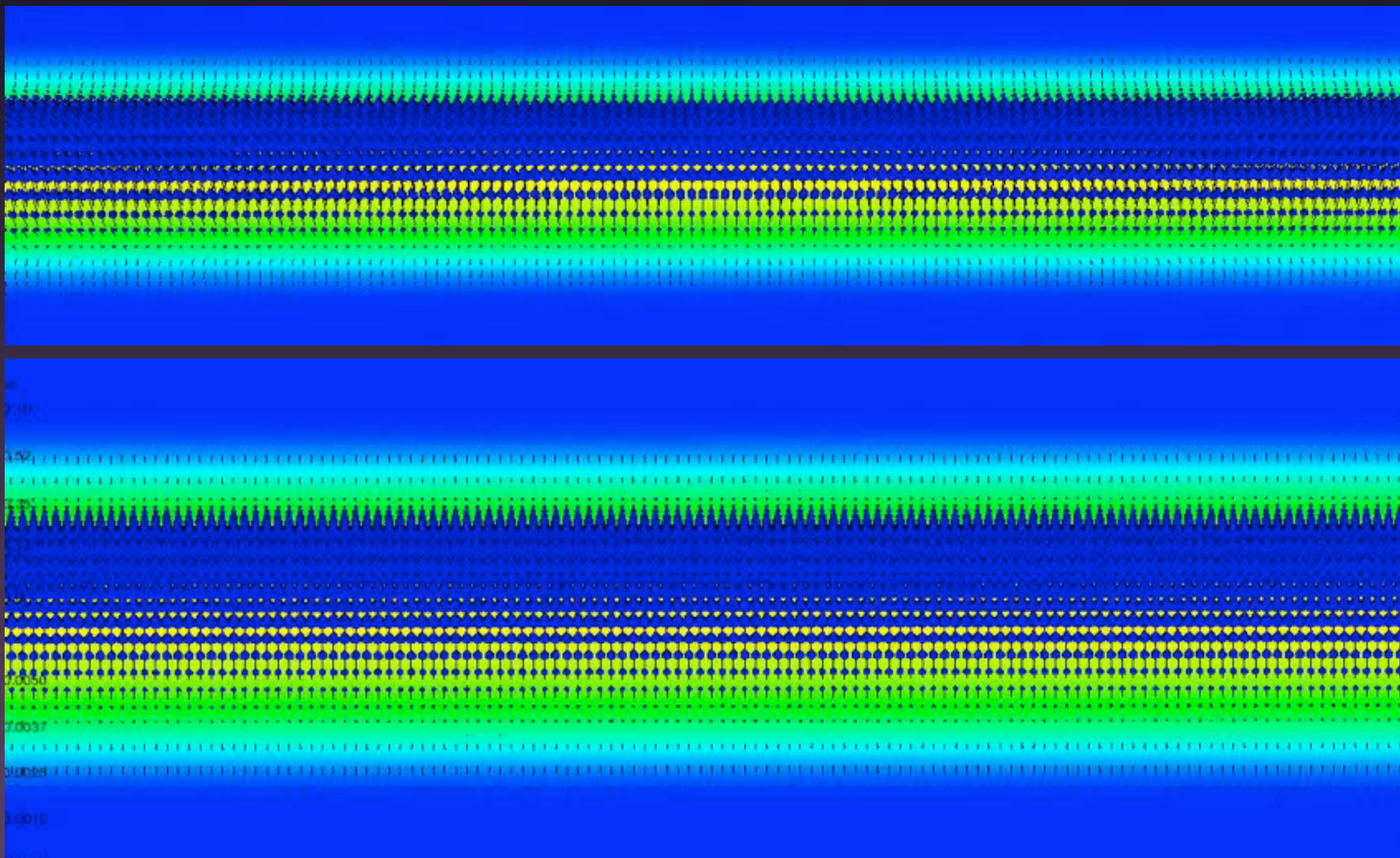
- Therefore $V_t = i[H,\rho]^\dagger$ guarantees $\partial_t E \leqslant 0$

  Non-local potential equivalent to “complex time” evolution

  Not suitable for fermionic problem

- Diagonal version is a local potential: $V_t = \mathrm{diag}(i[H,\rho]^\dagger)$

State Preparation



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

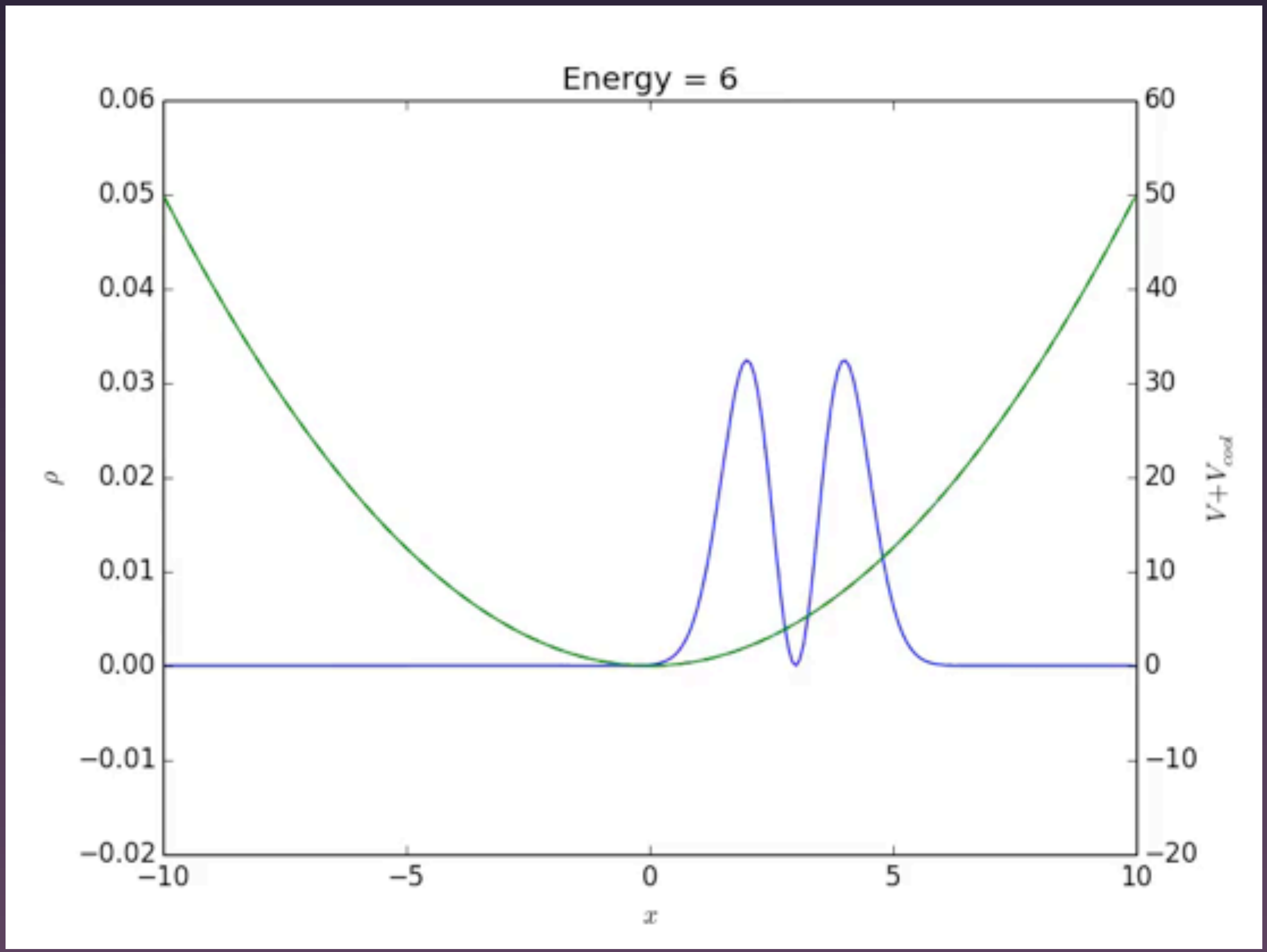
Quantum Friction

Potential counteracts currents

Use with dynamics to minimize energy

Harmonic oscillator with an excited state

Quantum Friction



Harmonic oscillator with an excited state

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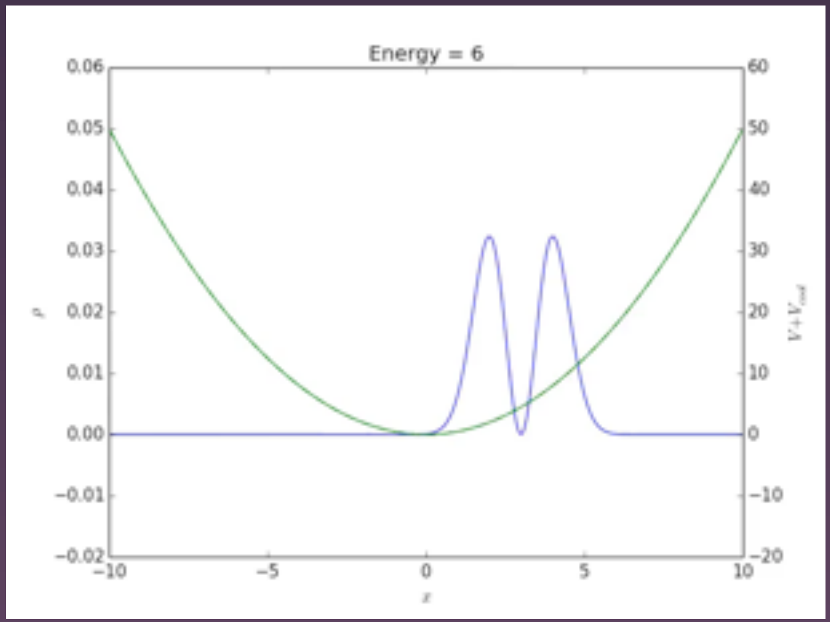

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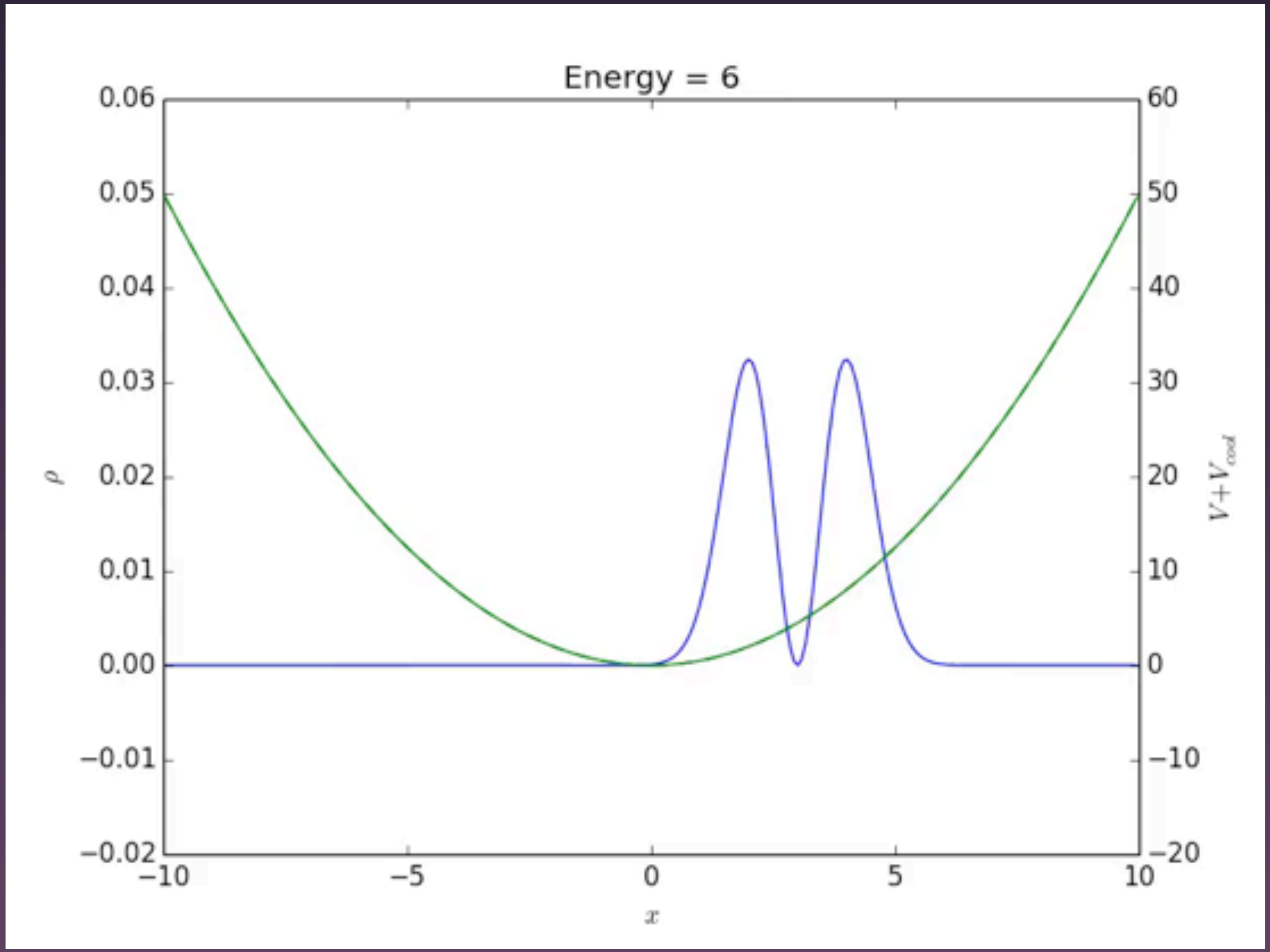

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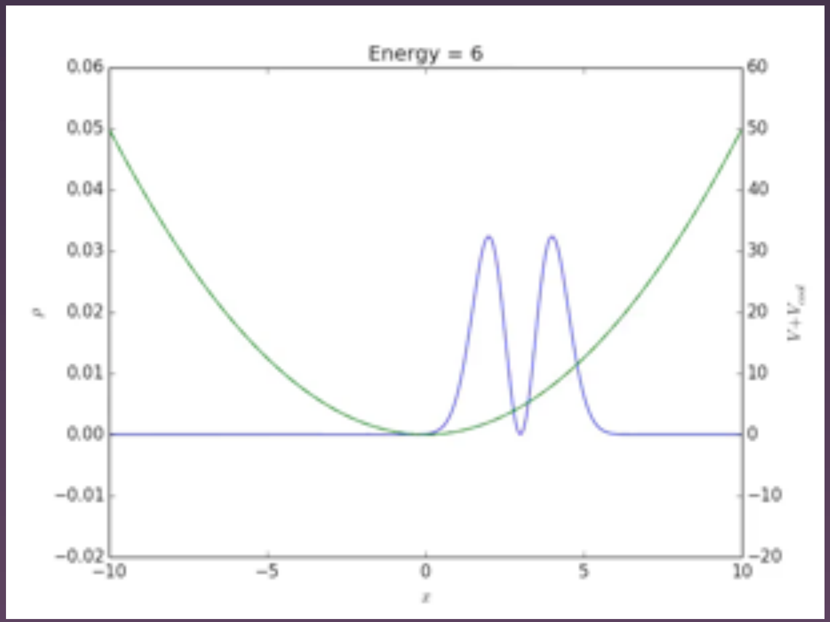


Quantum Friction

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

- 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 Wlazłowski (2013) [arXiv:1305.6891]

TDDFT (TDSLDA)

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

- Still Computationally expensive:

  Need to evolve each hundreds of thousands of wavefunctions

- Possible for moderate systems (nuclei) using supercomputers, resonances, induced fission etc.

  Maybe cold atoms (if axially symmetric etc.)

  Probably not for neutron stars (glitching dynamics)

A Tale of Two Simulations

- ETF: (Effective Thomas Fermi model)
  - "Bosonic" DFT simulation of dimers

    Gross-Pitaevskii equation (GPE) tuned to model the unitary Fermi gas (UFG)

    Quantum hydrodynamics
  - Easy to compute
- SLDA: (Superfluid Local Density Approximation)
  - Fermionic Kohn-Sham DFT

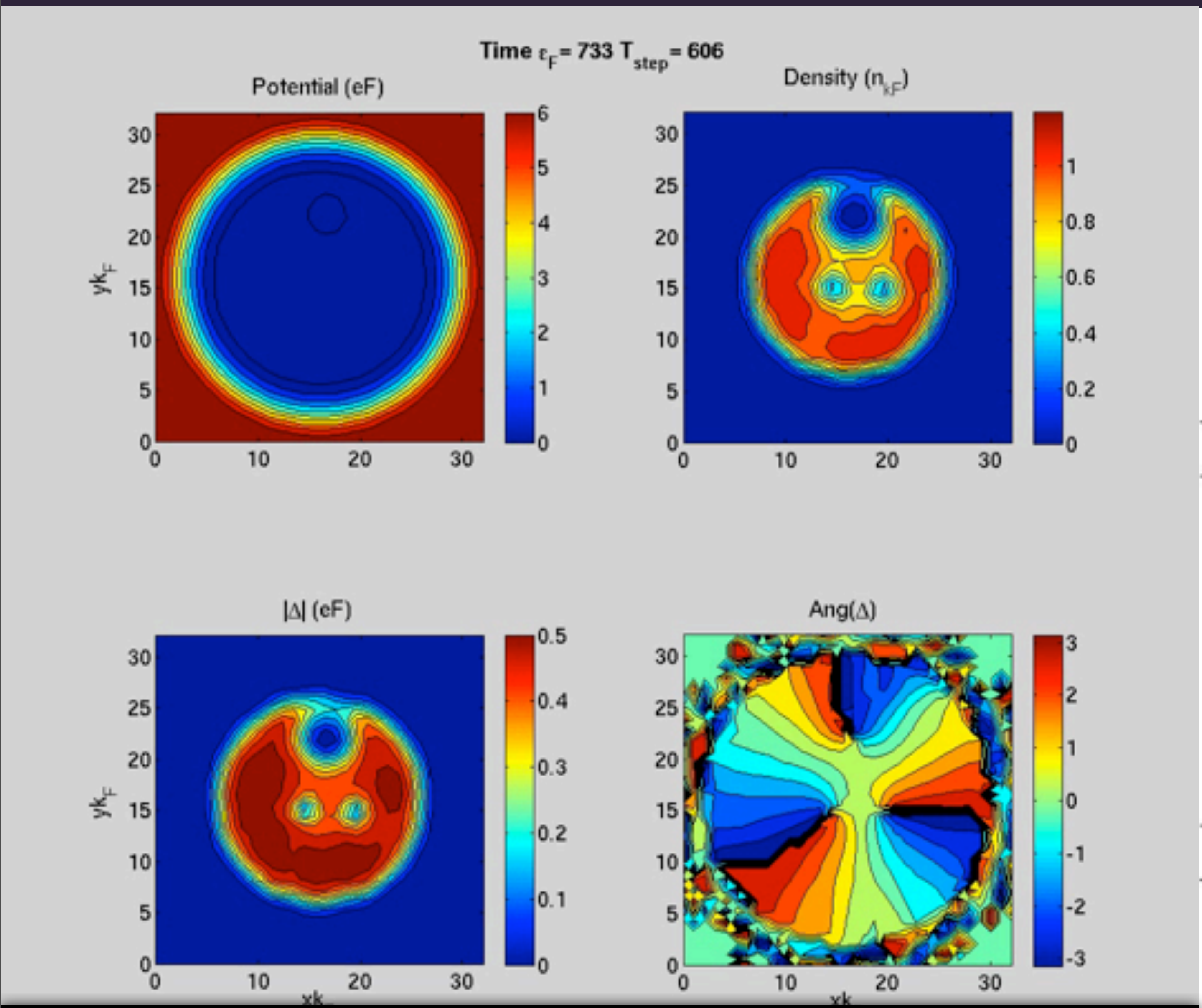
    Like HFB or BdG mean-field theory with tuned parameters
  - Hard to compute, but more accurate

Comparison

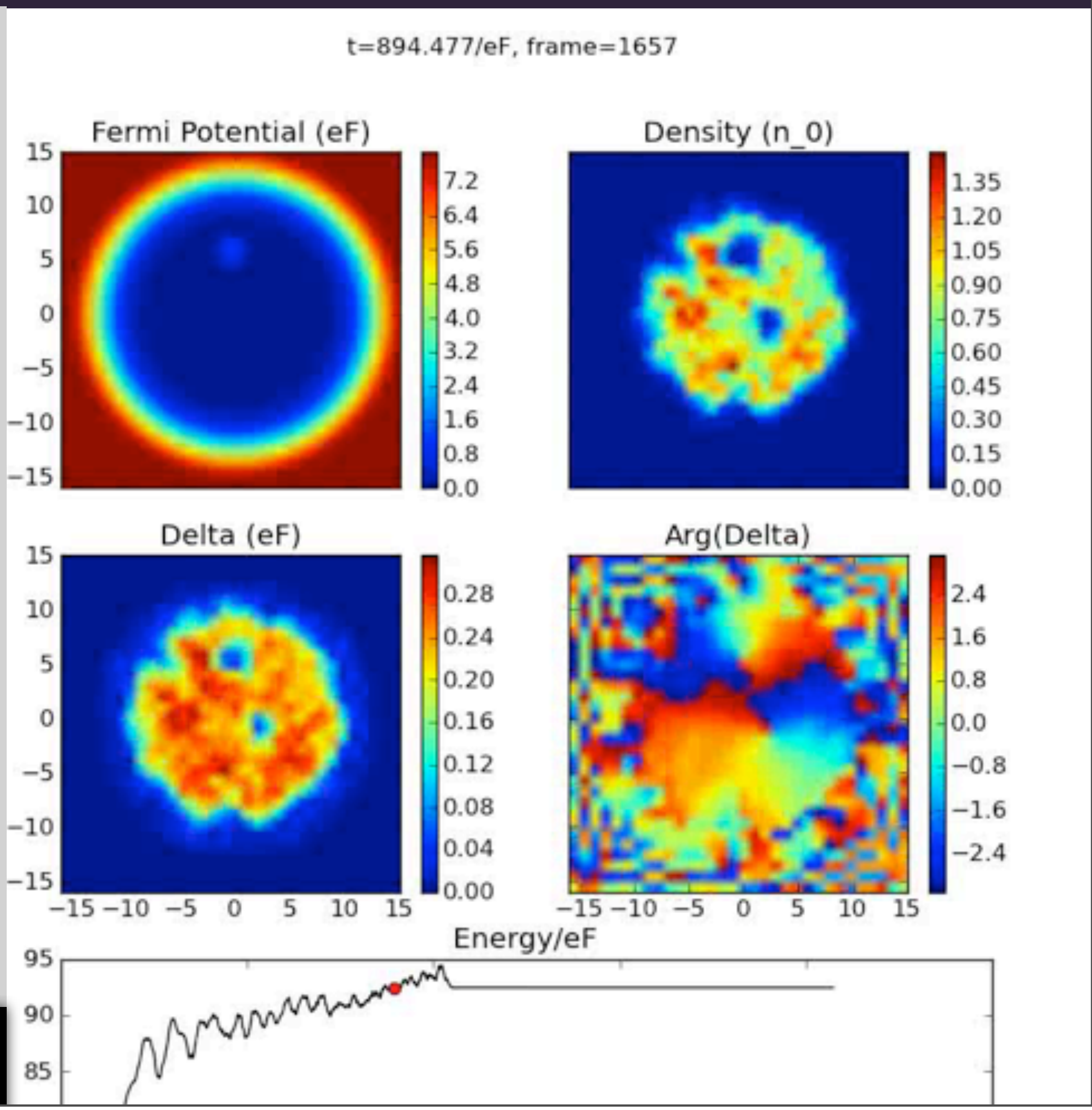
With Rishi Sharma [arXiv:1308.4387]

Fermions
SLDA TDDFT

Gross Pitaevskii
model

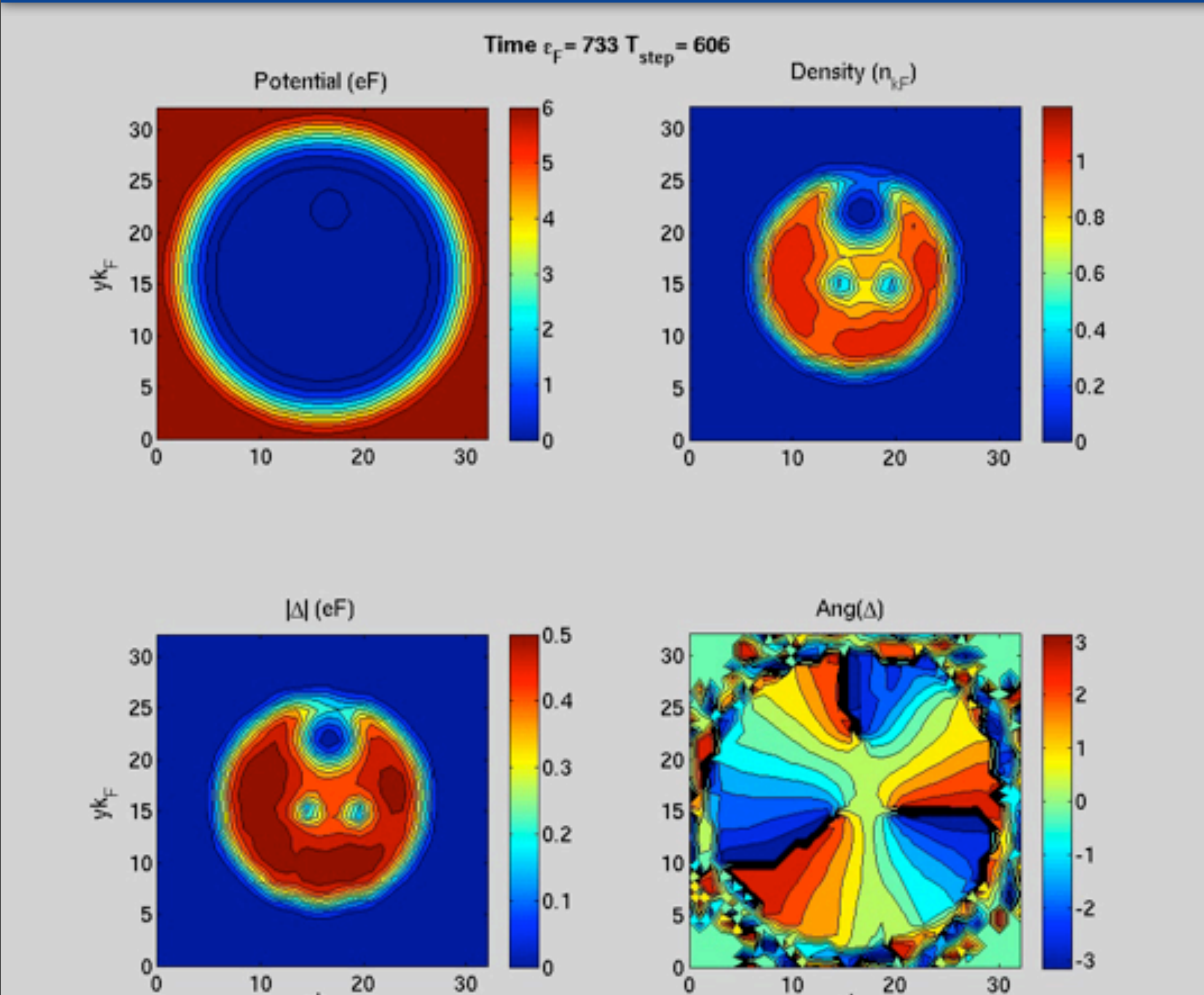


Bulgac et al. (Science 2011)



- Fermions:
  - Simulation hard!
  - Evolve 10^4–10^6 wavefunctions
  - Requires supercomputers

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



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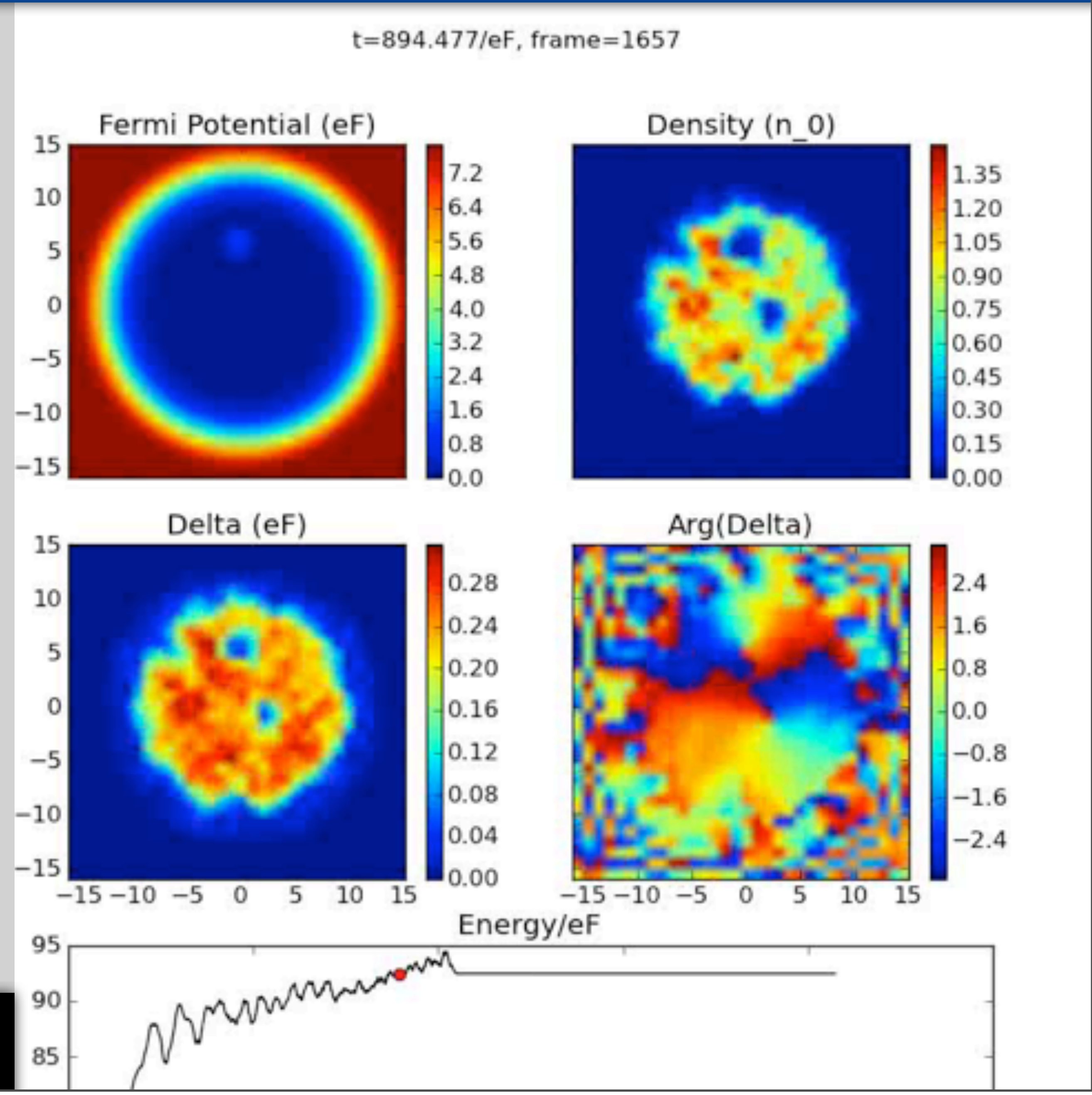


GPE model for UFG

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

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

- Think:
  - Boson = Fermion pair (dimer)
- Galilean Covariant (fixes mass)
- Match Unitary Equation of State

$$\rho_F = 2|\Psi|^2$$

$$\mathcal{E}_{FG} \propto \rho_F^{5/2}$$

$$\epsilon_F = \mathcal{E}'_{FG}(\rho_F) \propto \rho_F^{3/2}$$

GPE model = Extended Thomas Fermi (ETF)

$$E[\Psi] = \int d^3\vec{x} \left(\frac{|\nabla\sqrt{\rho_F}|^2}{8m_F} + V_F(\vec{x})\rho_F + \xi\mathcal{E}_{FG}(\rho_F) \right)$$

- Vortices etc. appear as kinks in $\sqrt{\rho_F}$

GPE model for UFG

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

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

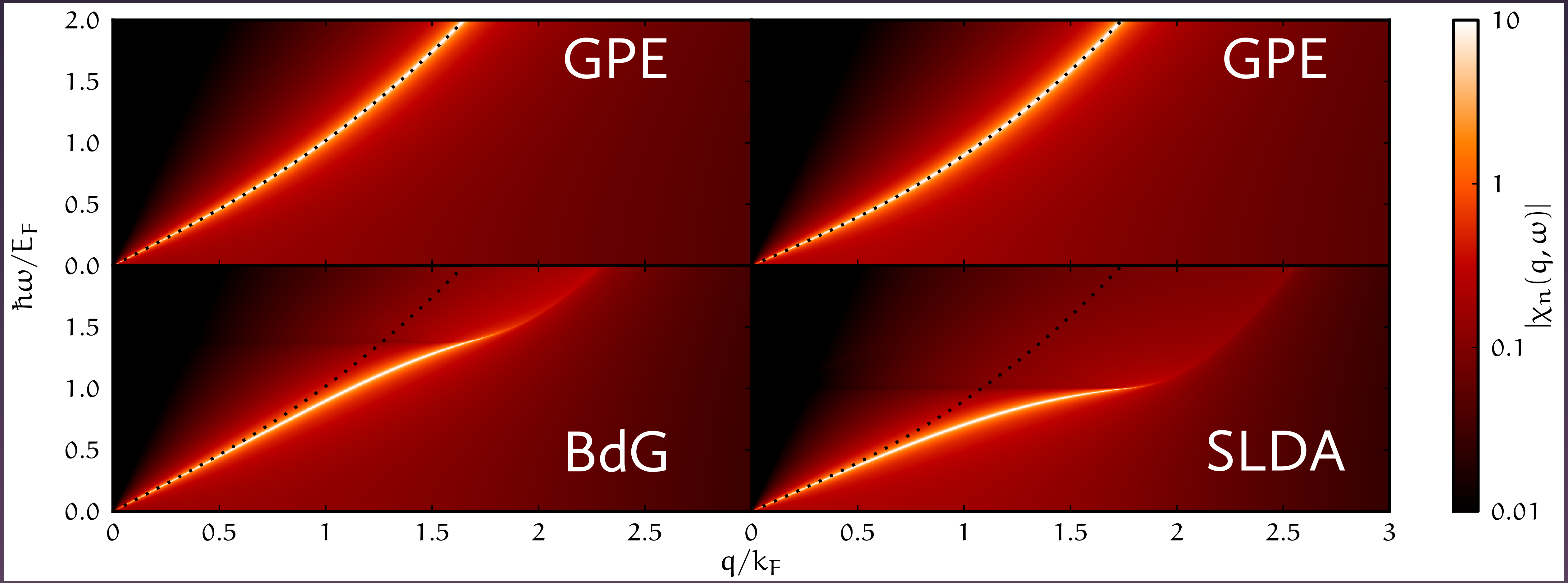
- Dynamics are much easier than SLDA
  - Only one wavefunction to evolve
- Contains superfluid hydrodynamic equations
- Match to low-energy physics

Matching Theories: The Good

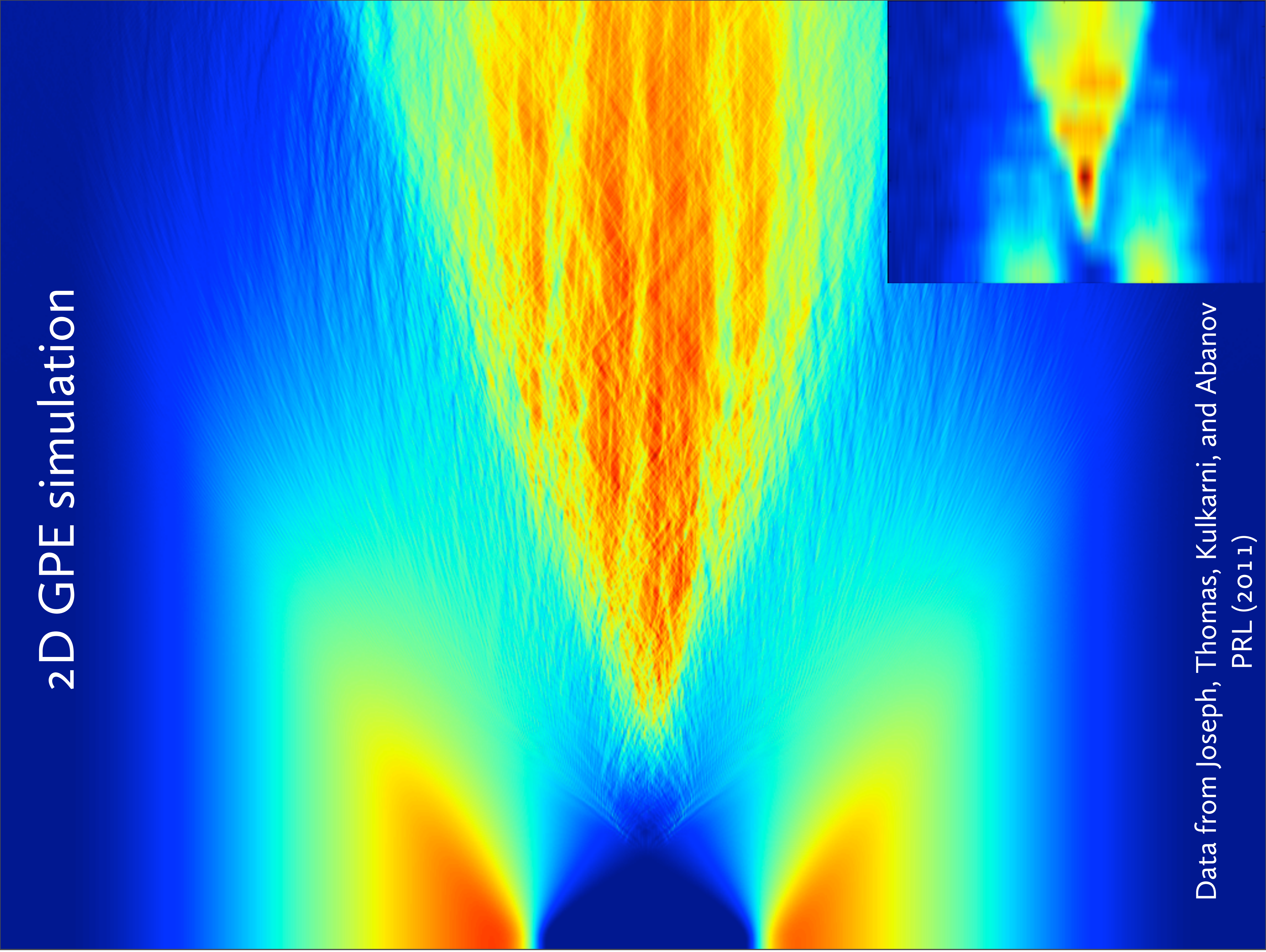
- Galilean Covariance (fixes mass/density relationship)
- Equation of State
- Hydrodynamics
  - speed of sound (exact)
  - phonon dispersion (to order q^3)
  - static response (to order q^2)

With Rishi Sharma [arXiv:1308.4387]

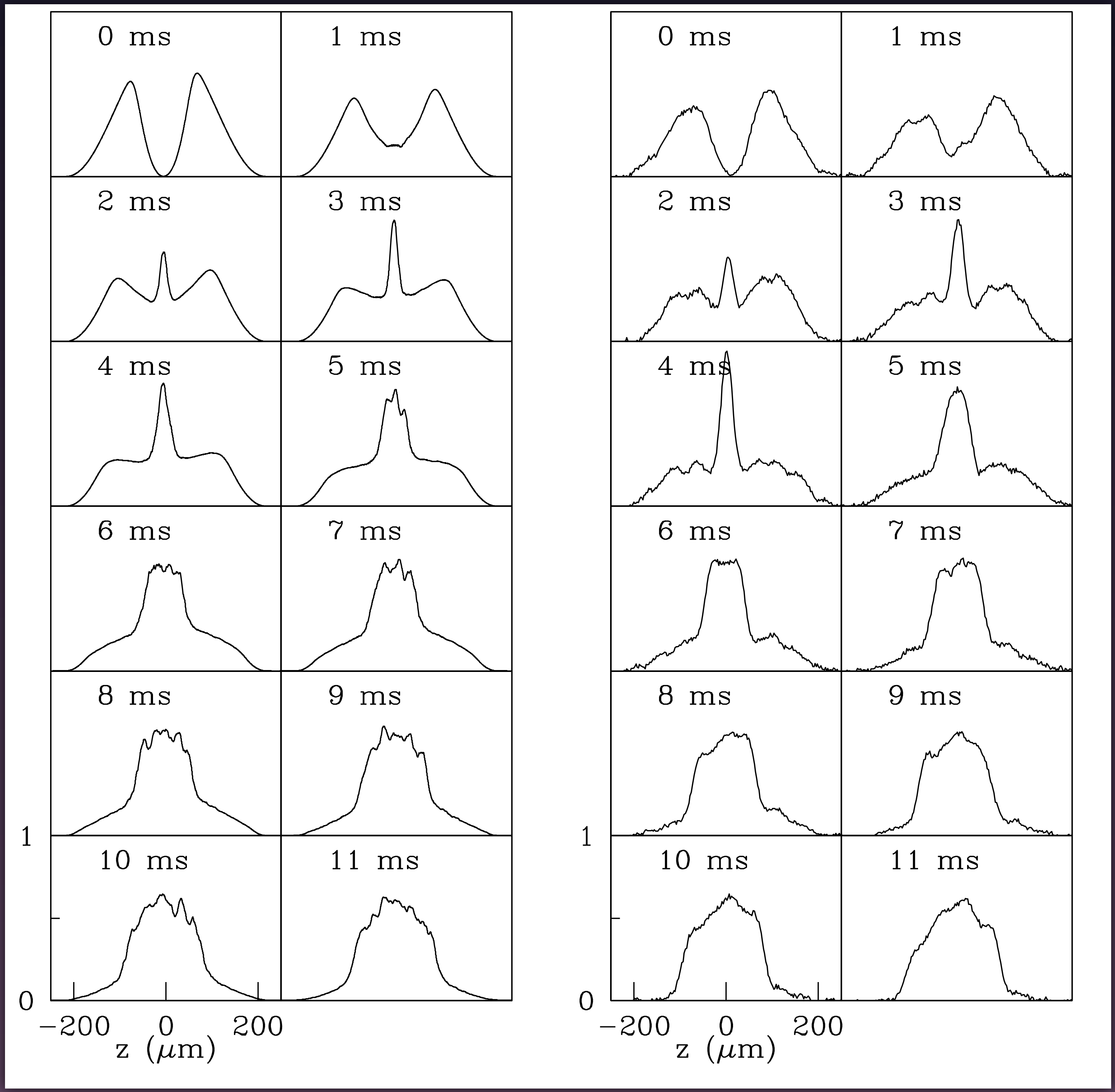
Linear Response



With Rishi Sharma [arXiv:1308.4387]


2D GPE simulation
Data from Joseph, Thomas, Kulkarni, and Abanov
PRL (2011)

GPE vs. Experiment

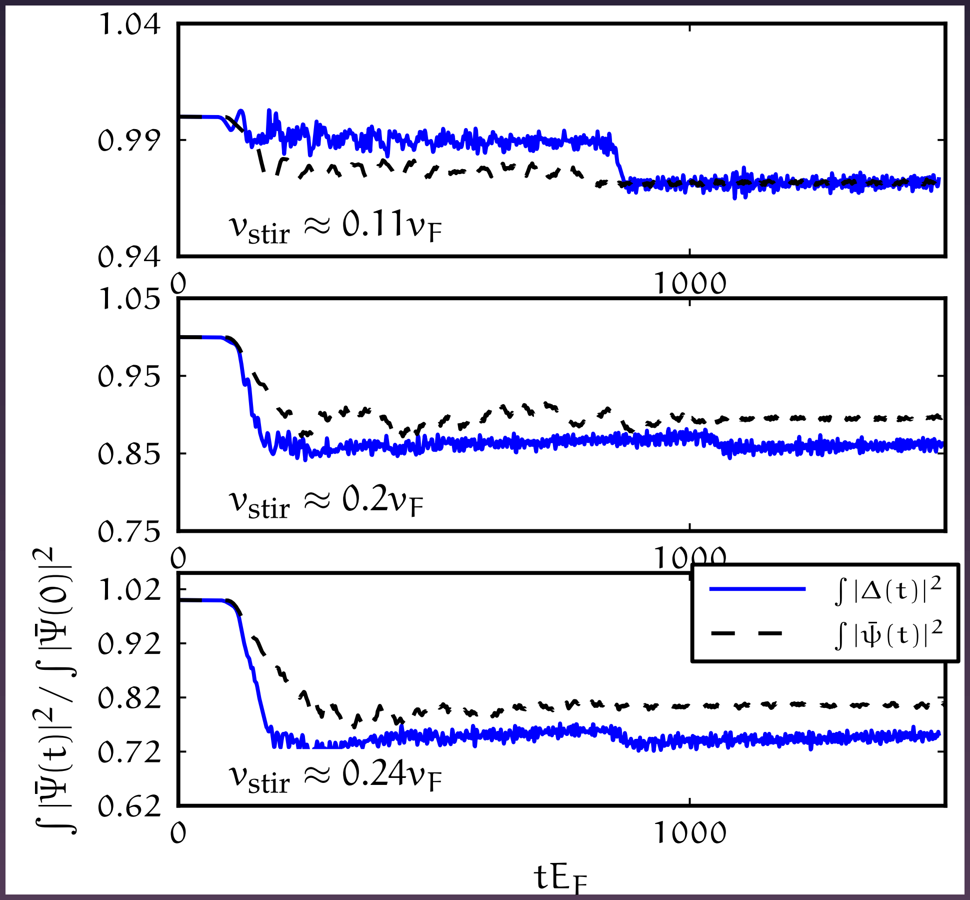


Ancilotto, L. Salasnich, and F. Toigo (2012)

Matching Theories: The Bad

- ETF has $\rho = 2|\Psi|^2$
  - Density vanishes in core of vortex
  - Implies $\int|\Psi|^2$ conserved

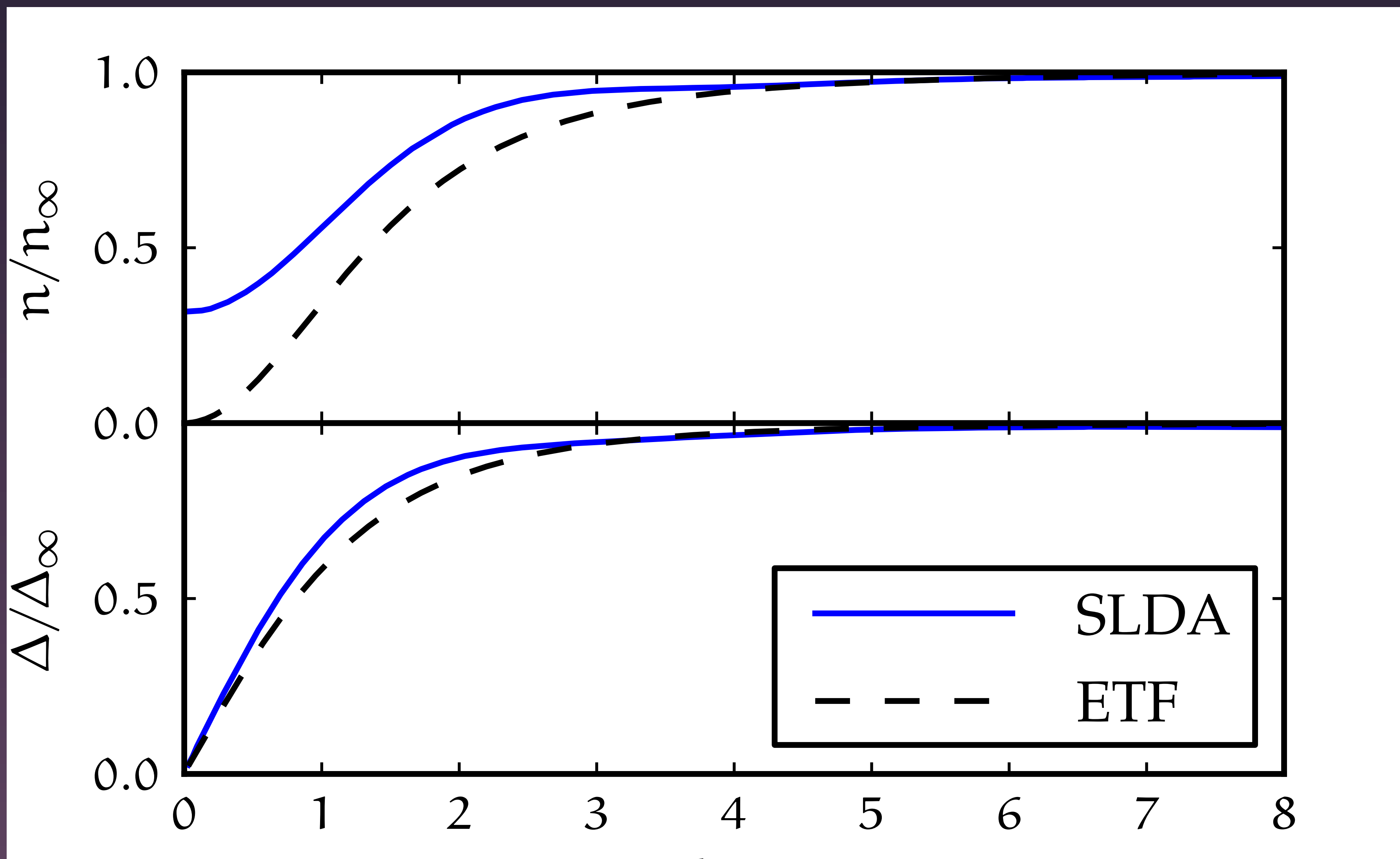
  (Conservation of coarse-grained $\int|\Psi|^2$ provides a measure of validity)



- No "normal state"
  - Two fluid model needed?
  - Coarse graining (transfer to "normal" component)

With Rishi Sharma [arXiv:1308.4387]

Vortex Structure



With Rishi Sharma [arXiv:1308.4387]

Defect motion

- Like GPE, the ETF has $T \approx \sqrt{2} T_z \approx 1.4 T_z$ for domain walls
  - Fermionic theories (SLDA, BdG) have $T \approx 1.7 T_z$
  - Consistent with occupation of fermionic cores (fermionic walls are heavy)
- ETF vortex rings have period 1.8 shorter than experiment. Consistent when compared with SLDA.

TABLE II. Benchmark of the ETF periods to the SLDA periods for sizes $24 \times 24 \times 96$, $32 \times 32 \times 128$, and $48 \times 48 \times 128$.

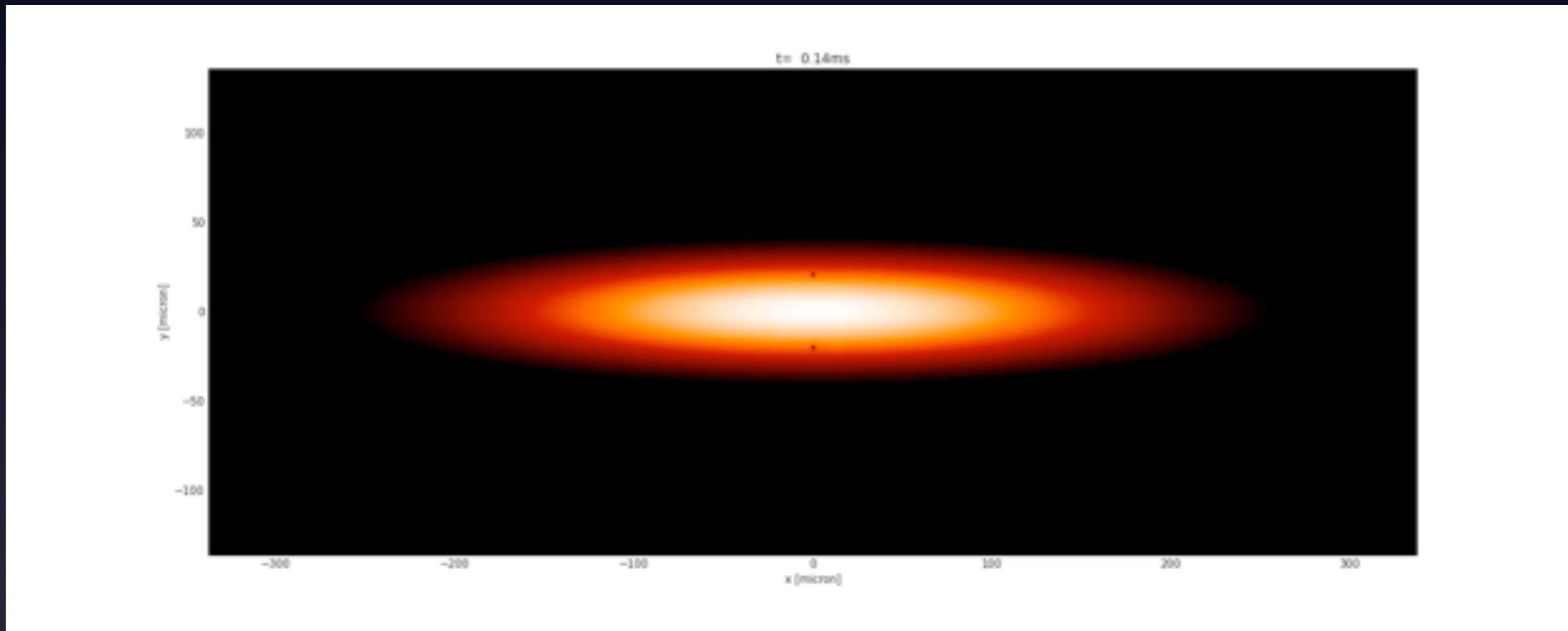
Size	T_{ETF}	T_{SLDA}	$T_{\mathrm{SLDA}}/T_{\mathrm{ETF}}$
$24 \times 24 \times 96$	$1.4T_z$	$1.7T_z$	1.2
$32 \times 32 \times 128$	$1.6T_z$	$1.9T_z$	1.2
$48 \times 48 \times 128$	$1.9T_z$	$2.6T_z$	1.4

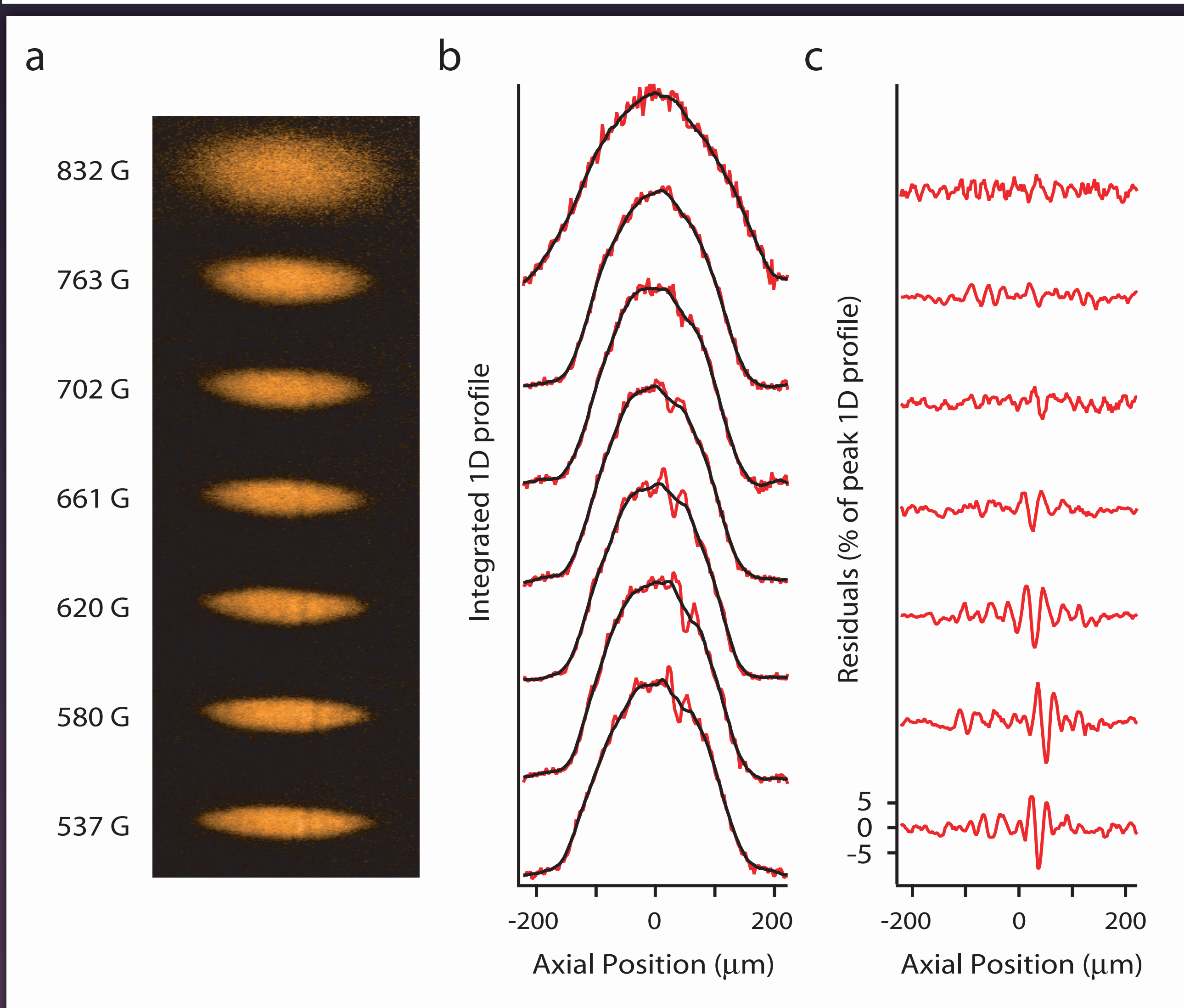
Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]

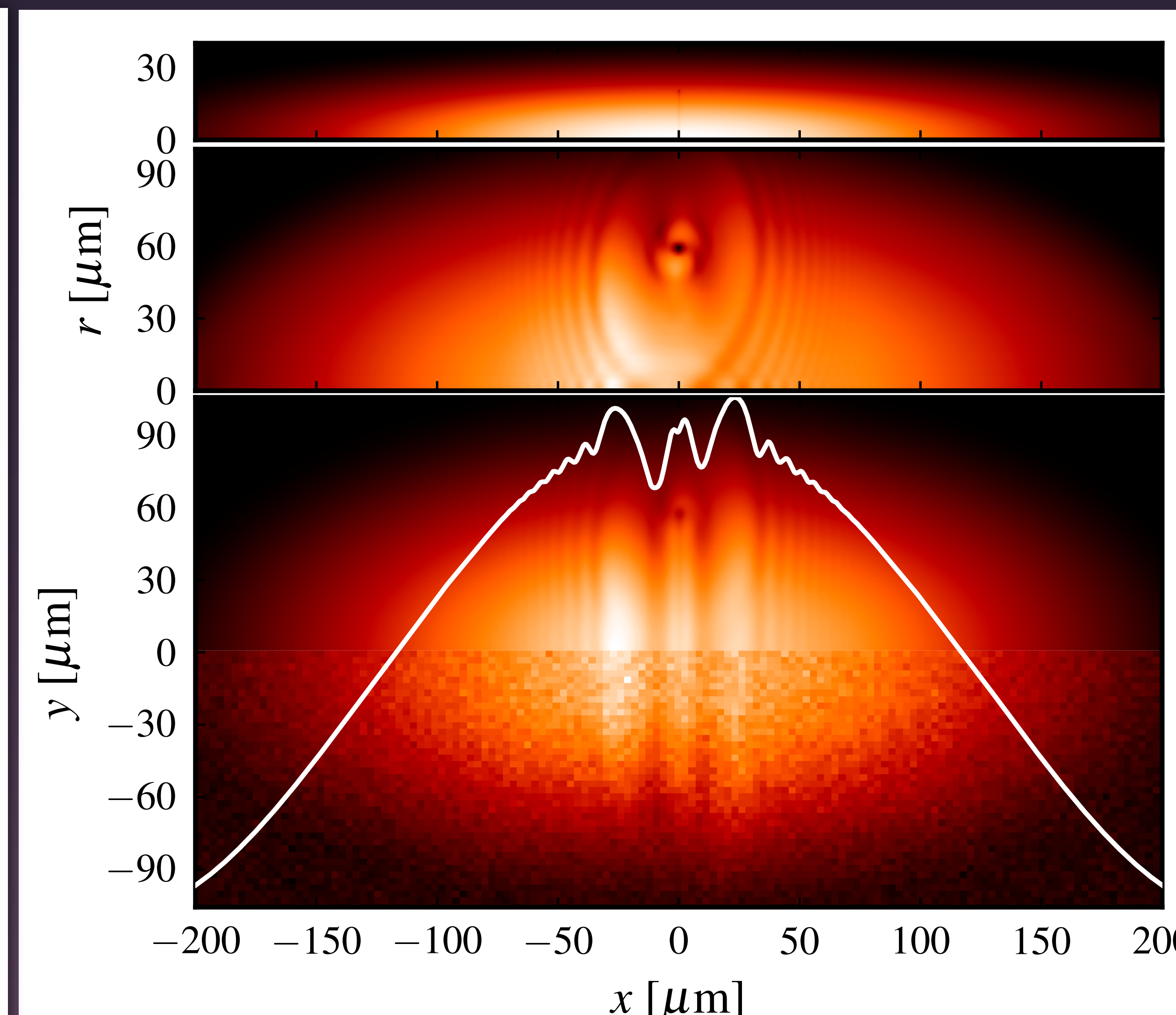
Disagreement with MIT experiment?

- Periods slightly underestimated
  - Will probably be resolved with full SLDA simulation
- Fringe pattern does not exactly match
  - Again, likely resolved by full SLDA

Fringe Pattern







Yefsah et al. Nature 499 (426) 2013

Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013)

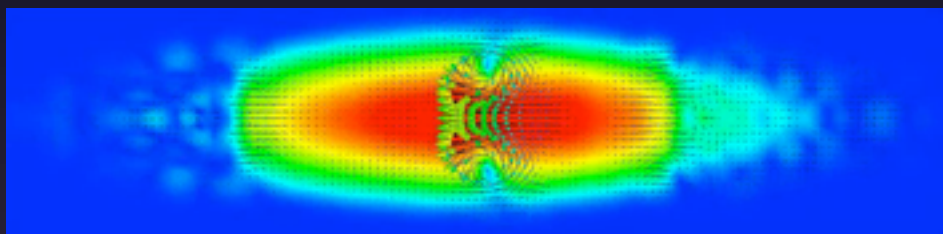
Conclusion

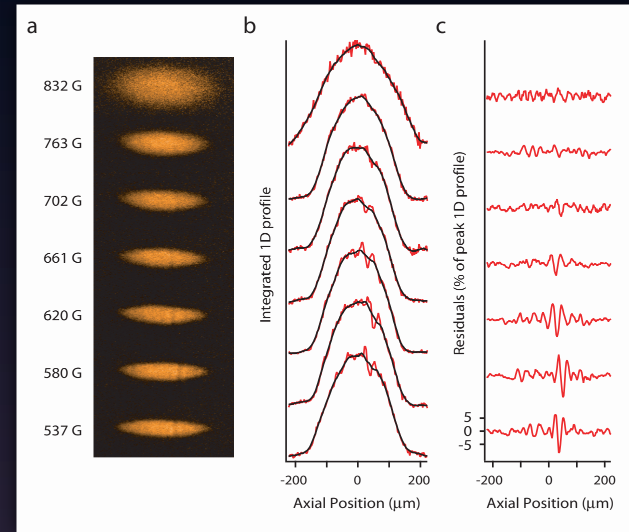
- Virtually all aspects of the MIT experiment are explained by vortex rings:

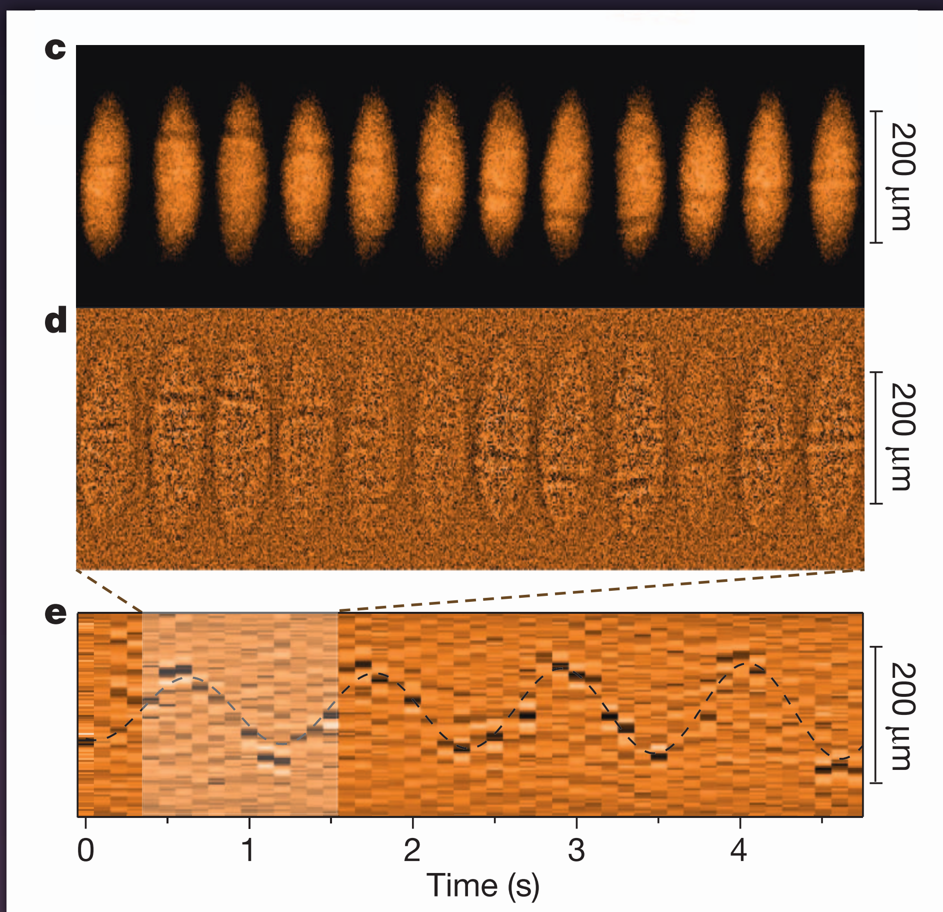
  Long periods, dependence on aspect ratio and interaction strength, anti-decay at finite temperature, imaging after expansion and dependence on B_{min}

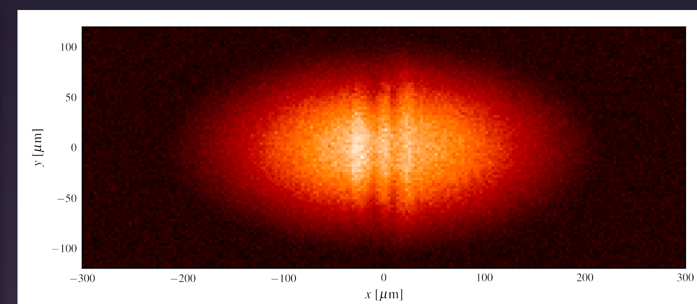
Image Credit

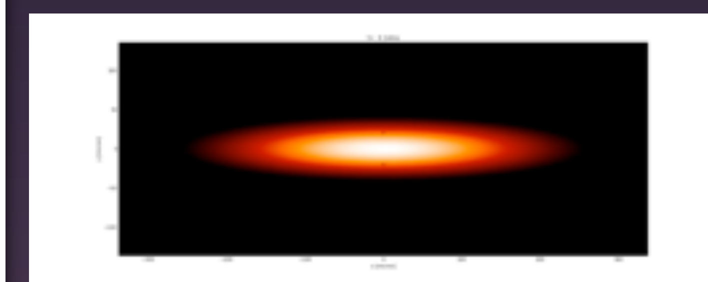
Solitions? Rings!

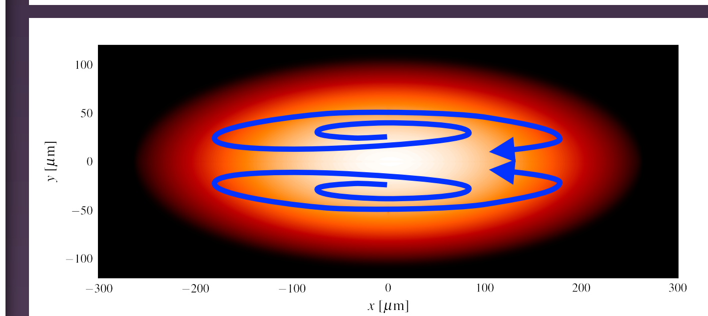


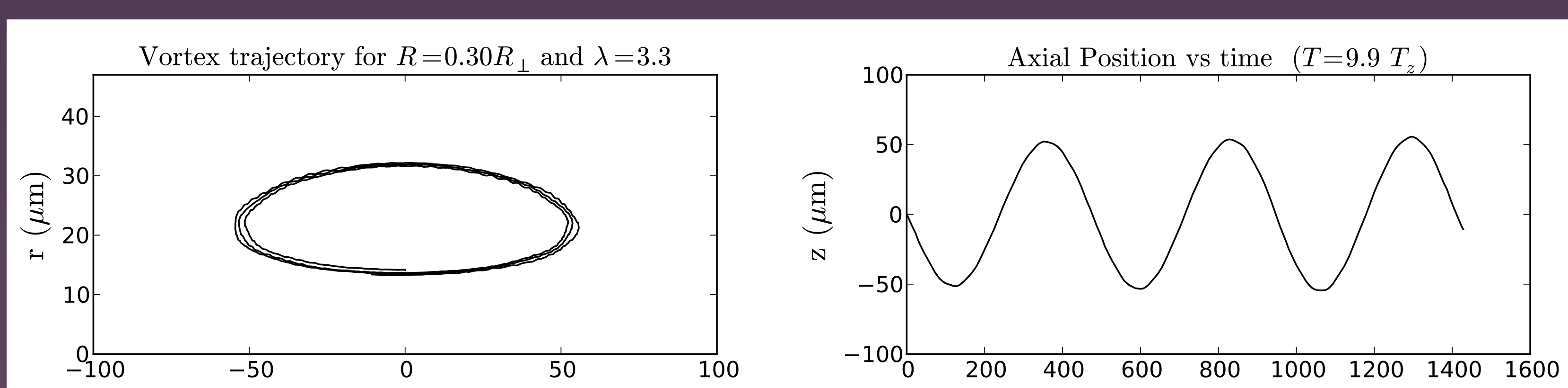












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- Dependence on aspect ratio and interaction
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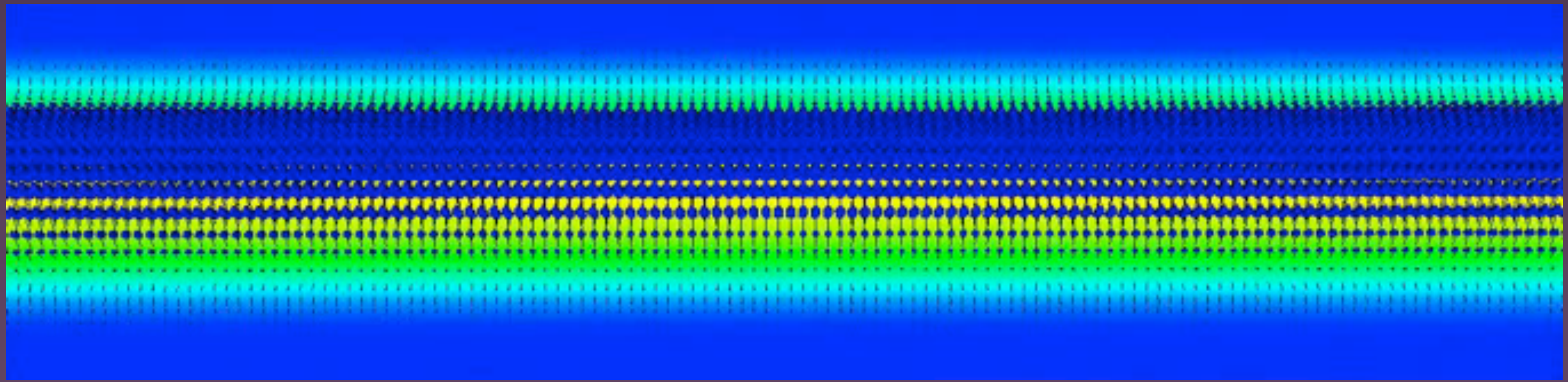
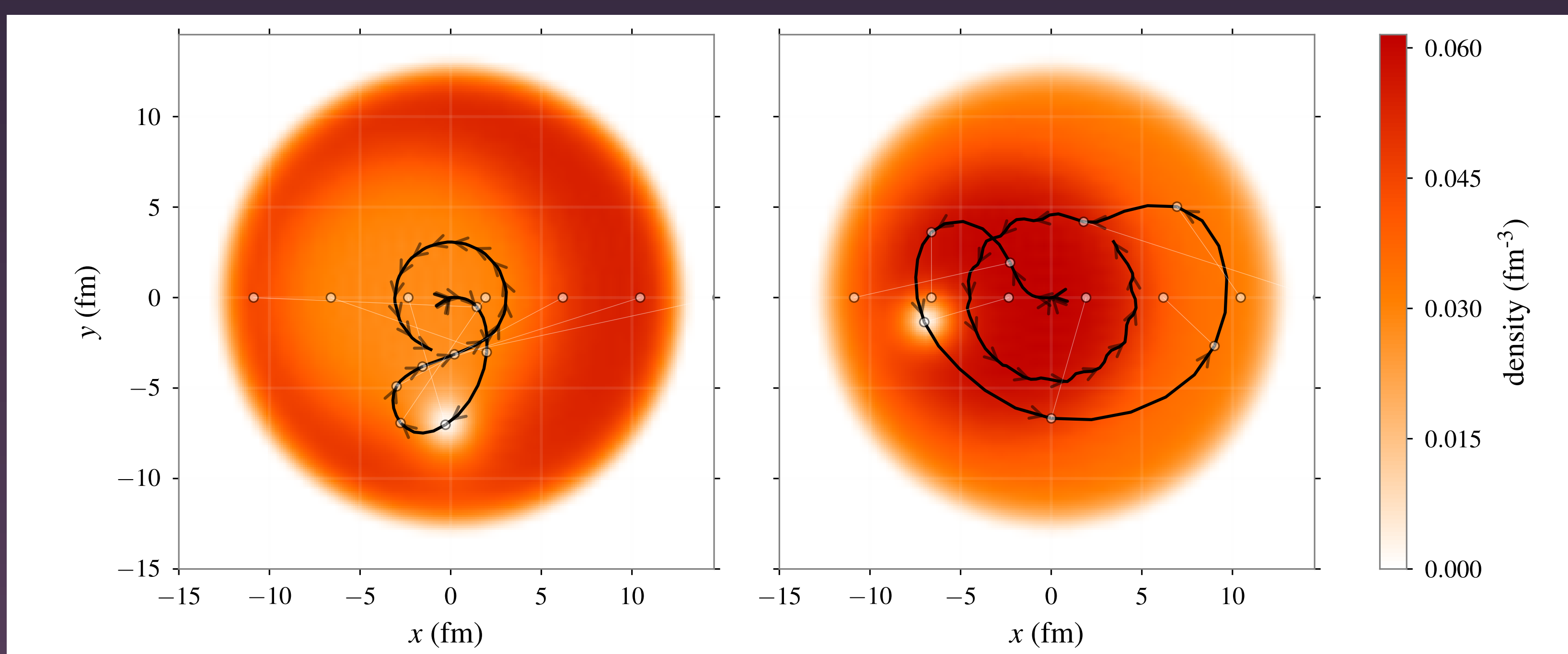
- Combined approach:
  - ETF for large systems validated with SLDA
  - Efficient realtime methods for cooling, analyzing
    - Quantum Friction



Pinning Force

$$\frac{dE}{dt} = -\vec{v}\cdot\vec{F}$$



Thermodynamics

- Well defined: (unlike vortex mass)
- Accessible from dynamic simulations
- Extract from stirring simulations

Bulgac, Forbes, Sharma PRL 110 (2013) 241102 [arXiv: 1302.2172]

Conclusion

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- Combined approach:
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- Details validate reliability of DFTs for dynamical simulations of defects etc. in neutron stars.