

Realtime Methods for Superfluid Dynamics

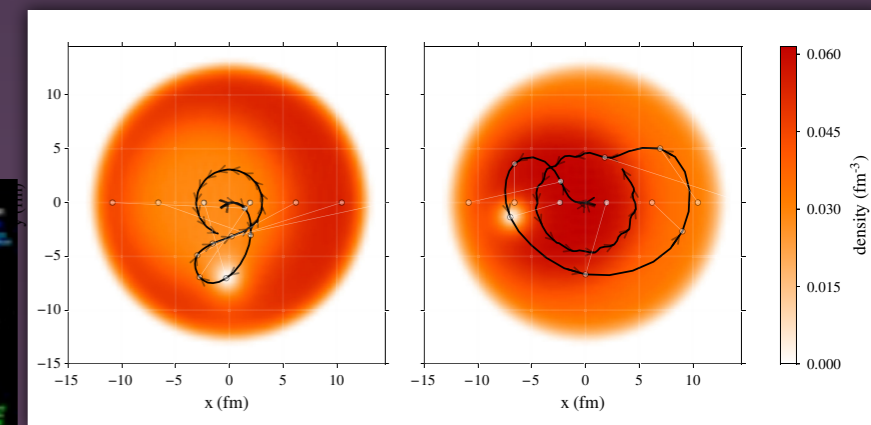
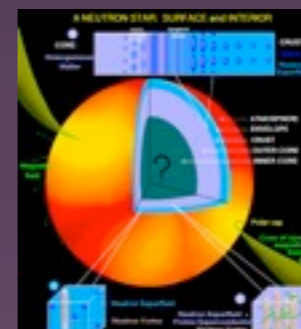
Michael McNeil Forbes

Washington State University, Pullman

University of Washington, Seattle

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



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

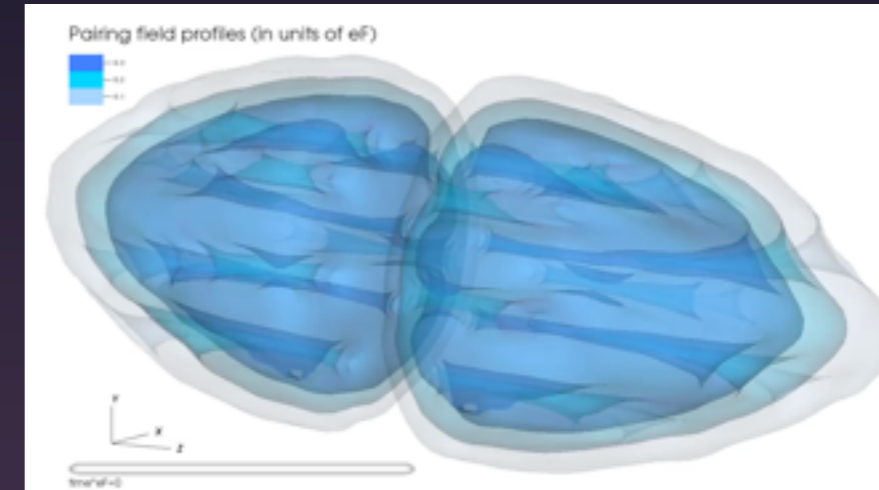
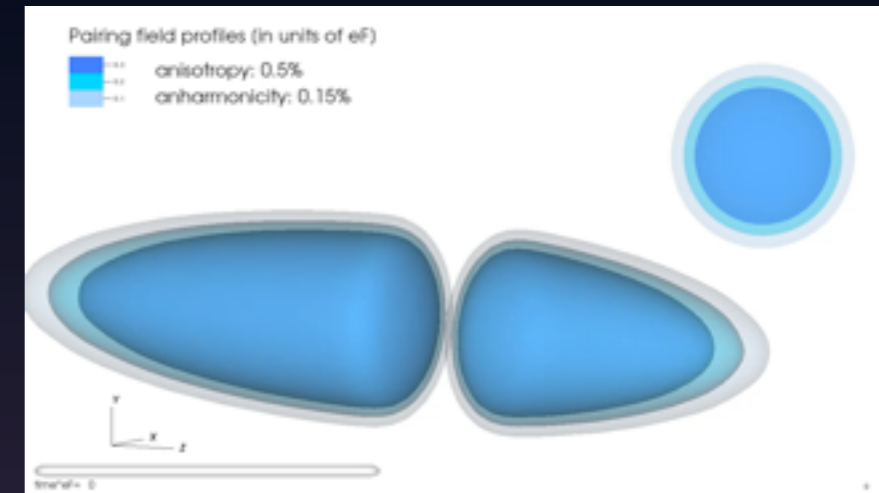
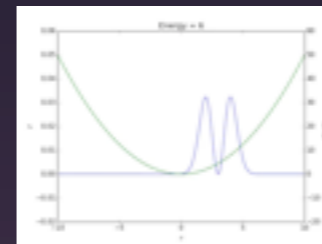
- Dynamics

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)

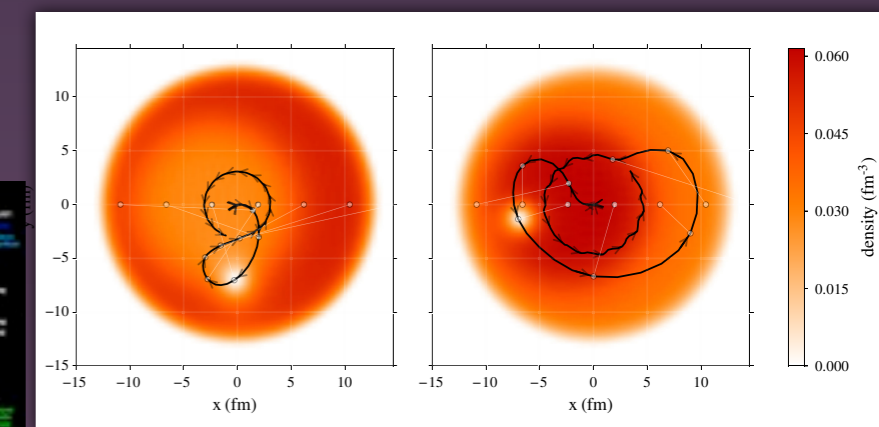
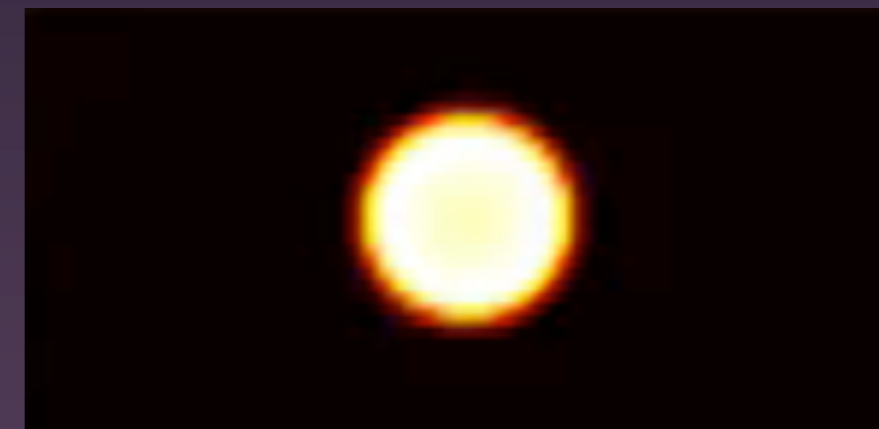
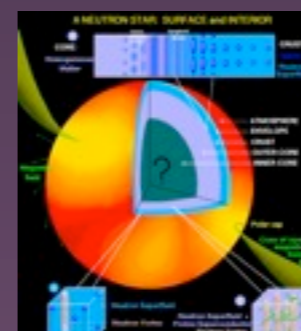
emphasize scaling of computations

Fission in nuclei, Excitations (GDR), Reactions

- From Cold Atoms to Nuclei and Neutron Stars

Validated Methods

DFT, Vortex pinning, Glitches, Quantum Turbulence



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

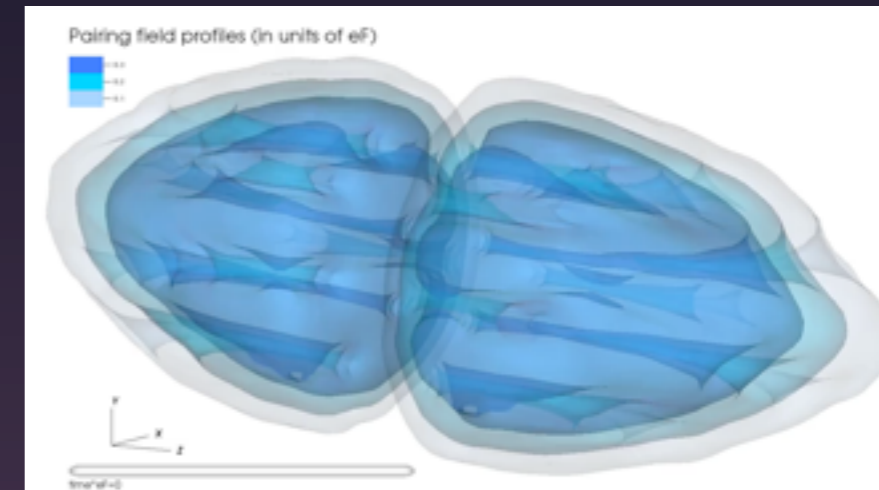
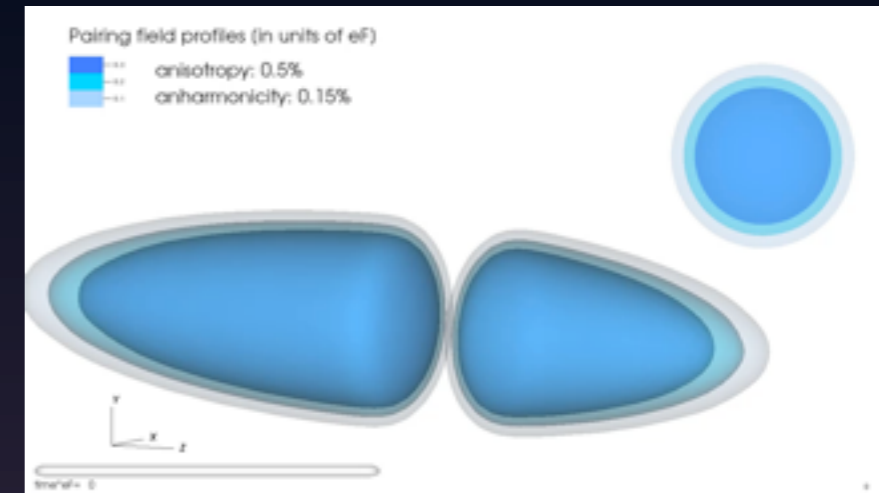
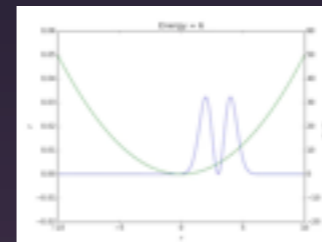
- Dynamics

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)

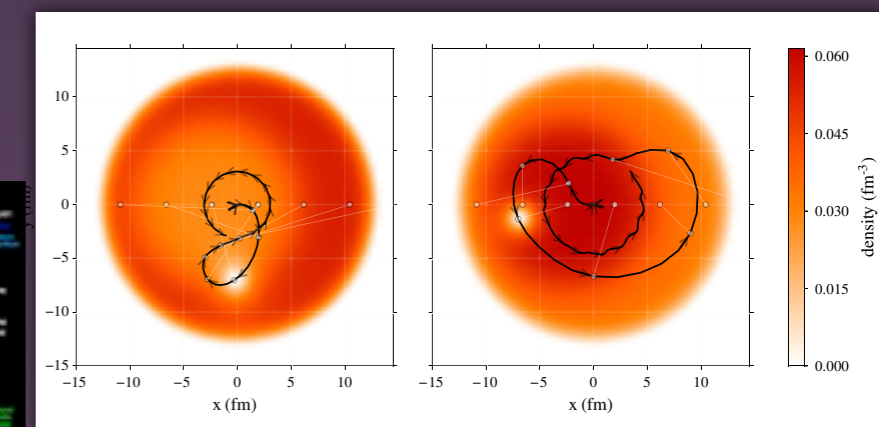
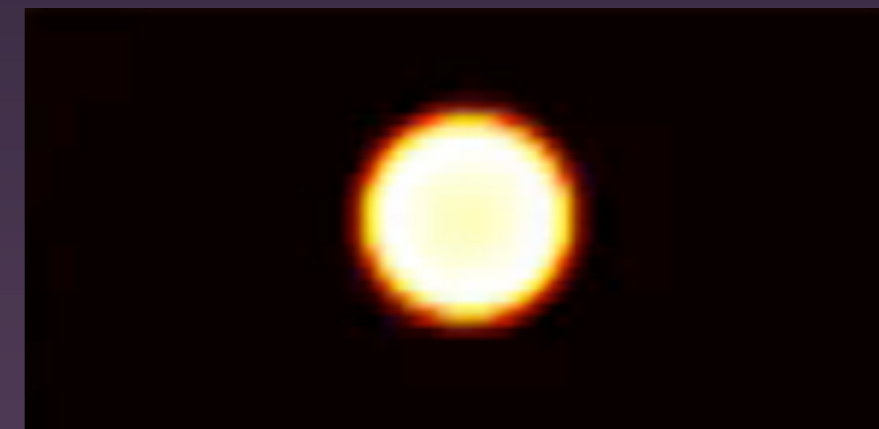
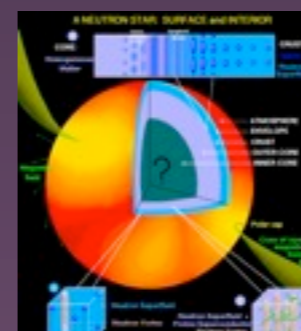
emphasize scaling of computations

Fission in nuclei, Excitations (GDR), Reactions

- From Cold Atoms to Nuclei and Neutron Stars

Validated Methods

DFT, Vortex pinning, Glitches, Quantum Turbulence



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

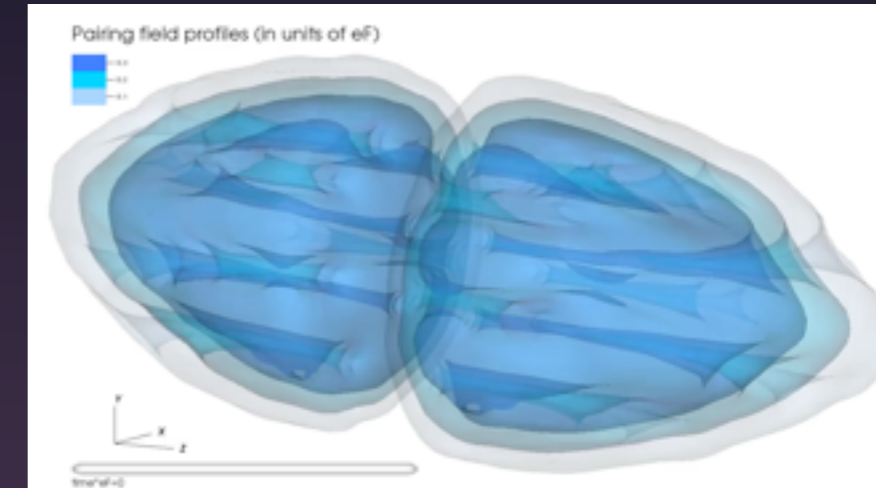
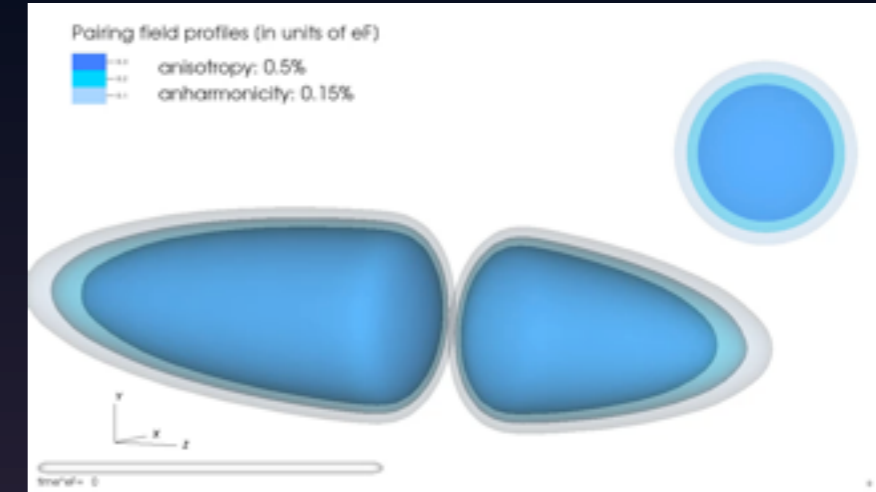
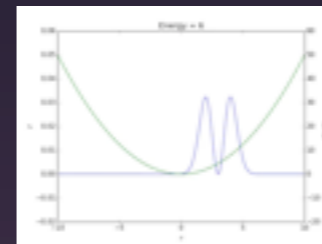
- Dynamics

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)

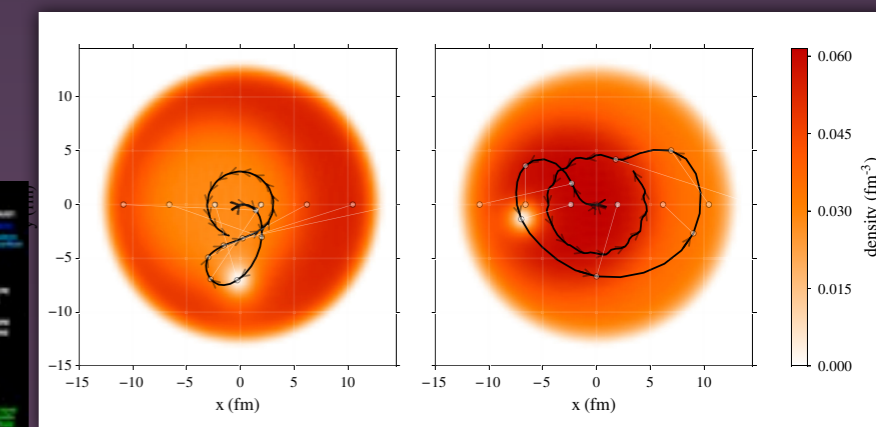
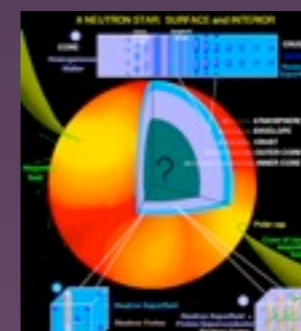
emphasize scaling of computations

Fission in nuclei, Excitations (GDR), Reactions

- From Cold Atoms to Nuclei and Neutron Stars

Validated Methods

DFT, Vortex pinning, Glitches, Quantum Turbulence



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)

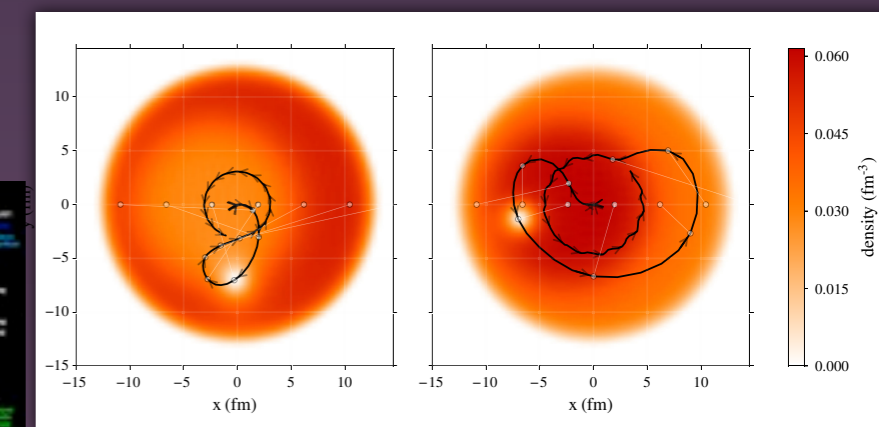
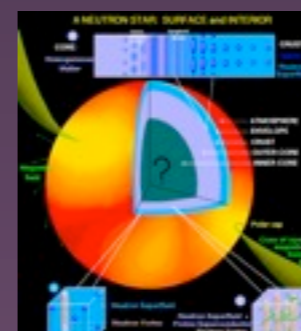
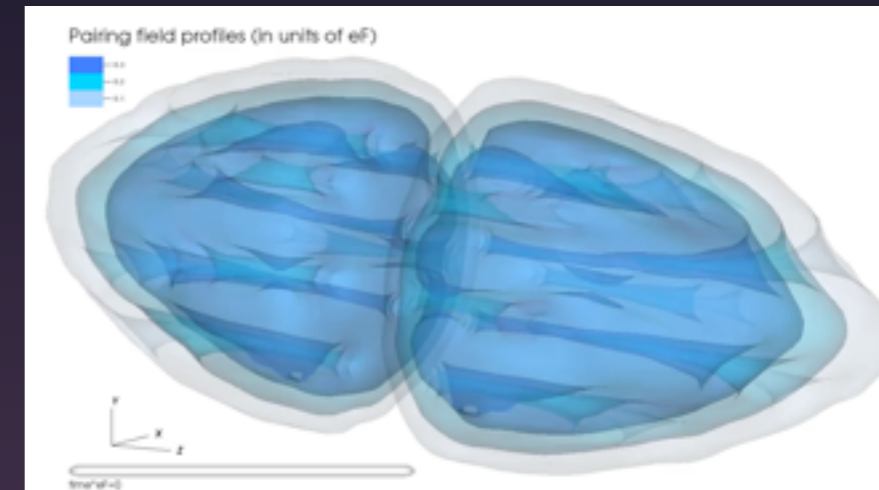
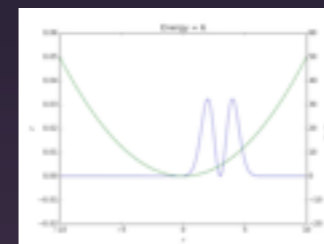
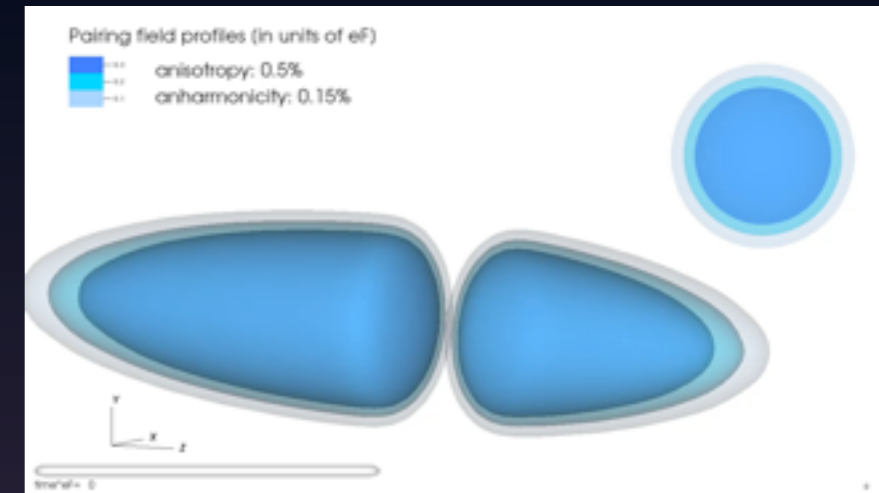
emphasize scaling of computations

Fission in nuclei, Excitations (GDR), Reactions

- From Cold Atoms to Nuclei and Neutron Stars

Validated Methods

DFT, Vortex pinning, Glitches, Quantum Turbulence



Fermionic Superfluids

Universality

Fermionic Superfluids

Neutron Matter

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

$$a_{nn} = -19 \text{ fm}$$

$$r_{nn} = 2 \text{ fm}$$

Nuclei

neutrons
and protons

Unitary Fermi Gas

$$a = \infty$$

$$r_e = 0$$

Cold Atoms

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

Tuneable a

$$r_{nn} \sim 0.1 \text{ nm}$$

Many systems

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

Other Superfluids

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

Fermionic Superfluids

Universality

Fermionic Superfluids

Neutron Matter

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

$$a_{nn} = -19 \text{ fm}$$

$$r_{nn} = 2 \text{ fm}$$

Nuclei
neutrons
and protons

Unitary Fermi Gas

$$a = \infty$$

$$r_e = 0$$

Cold Atoms

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

Tuneable a

$$r_{nn} \sim 0.1 \text{ nm}$$

Many systems

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

Other Superfluids

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

Unitary Fermi Gas (UFG)

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

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

- 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)

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

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

- Unitary limit $a \rightarrow \infty$: No interaction length scale!
- Universal physics:
 - $\mathcal{E}(\rho) = \xi \mathcal{E}_{\text{FG}}(\rho) \propto \rho^{5/3}$, $\xi = 0.370(5)$
- Simplest non-trivial model (dimensional analysis)

Unitary Fermi Gas (UFG)

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

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

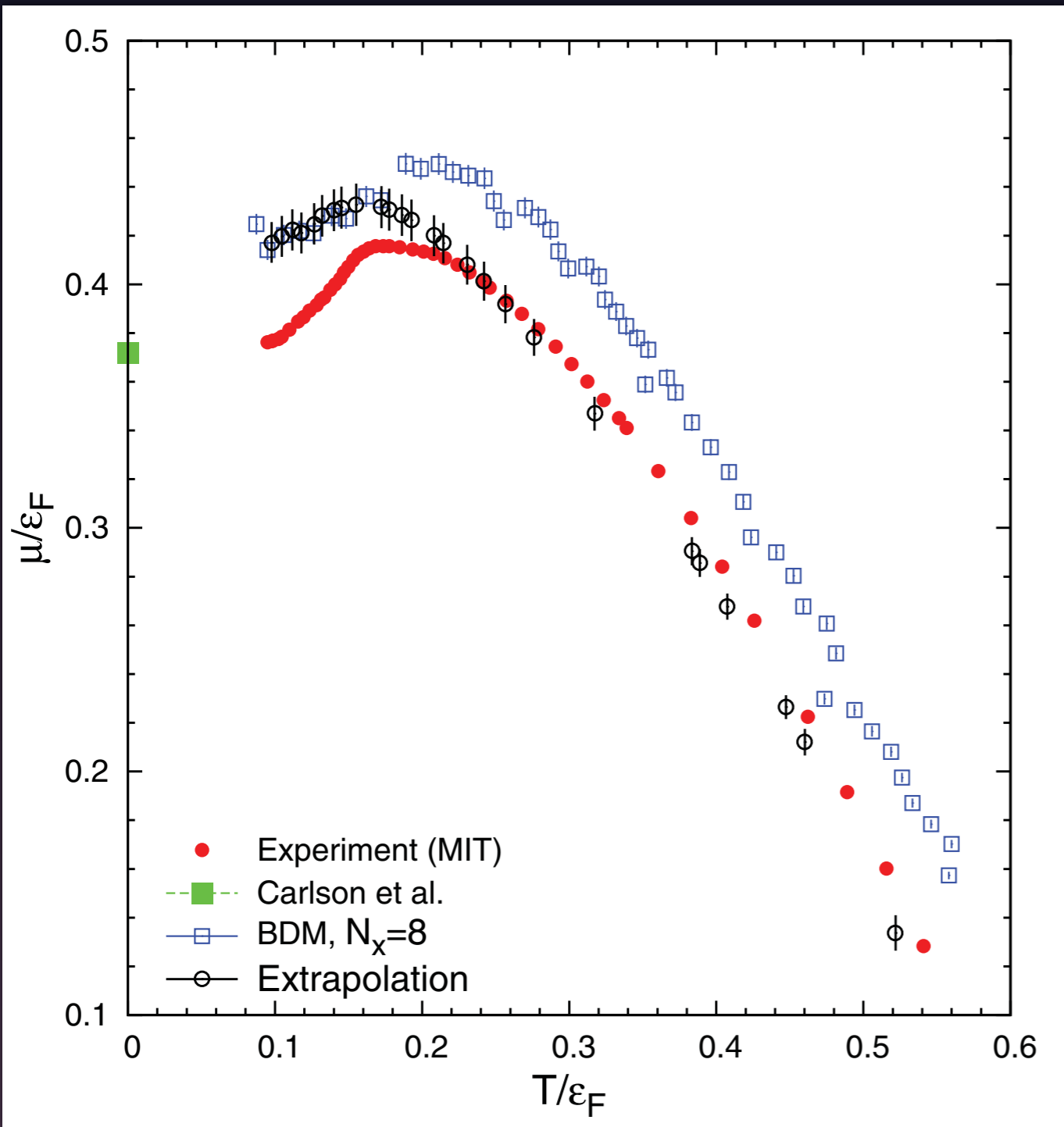
- Universal physics:

- $\mathcal{E}(\rho) = \xi \mathcal{E}_{\text{FG}}(\rho) \propto \rho^{5/3}$, $\xi = 0.370(5)$

- Simple, but hard to calculate!

Bertsch Many Body X-challenge

Unitary Equation of State



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

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

- Measured to percent level:

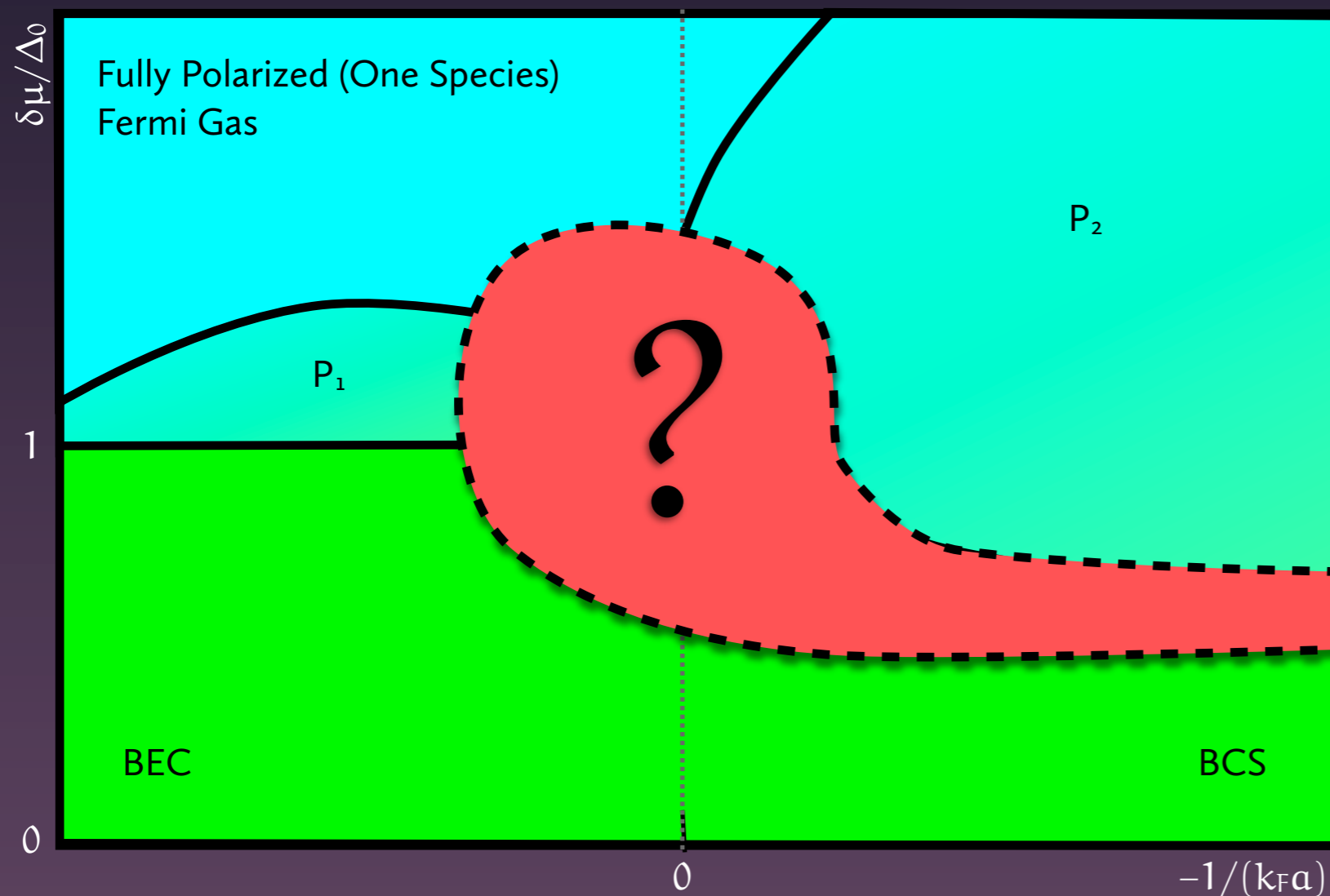
$$\bullet \xi_{\text{exp}} = 0.370(5)(8)$$

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

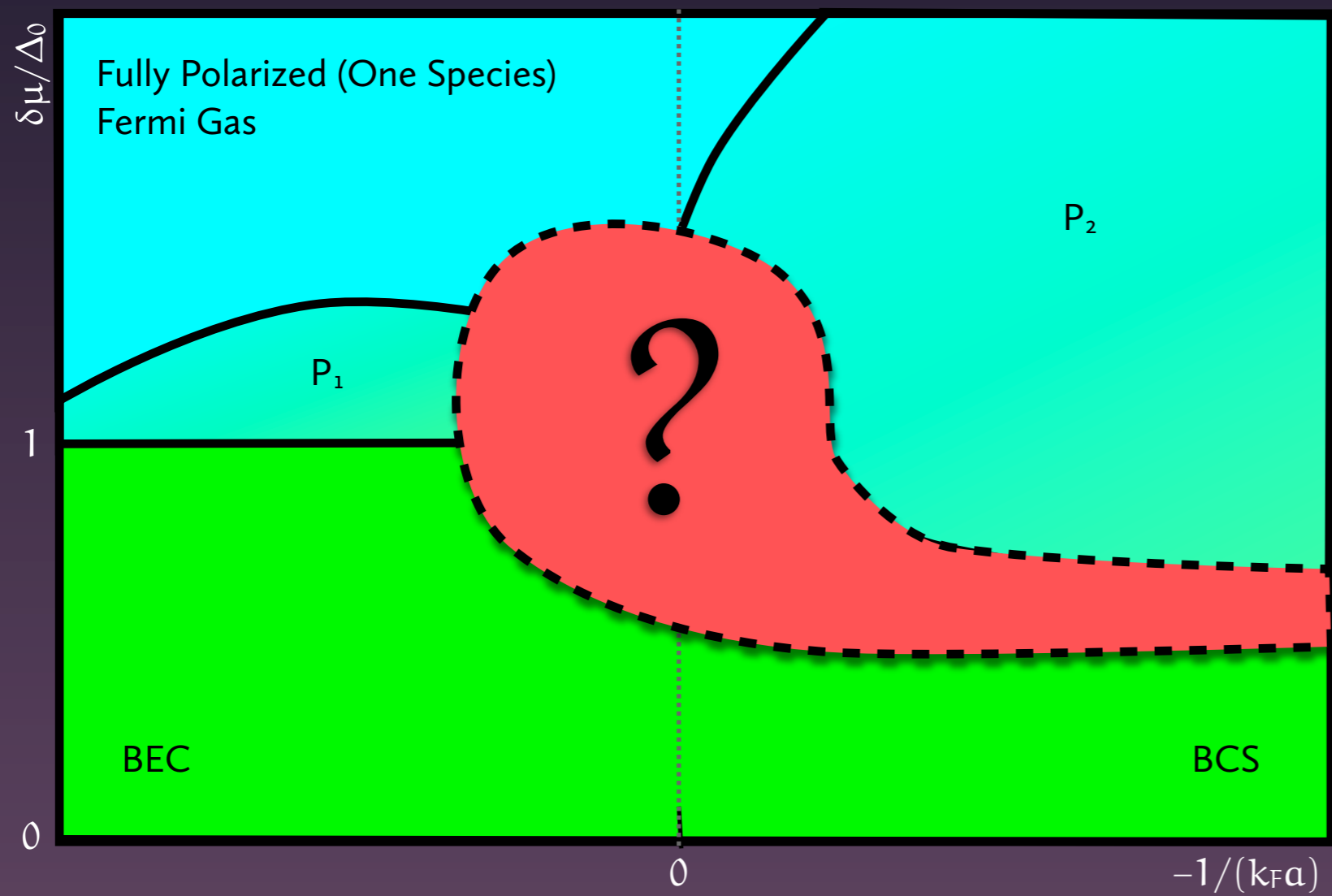
What happens in
middle?

Still need precision
measurements for
asymmetric systems

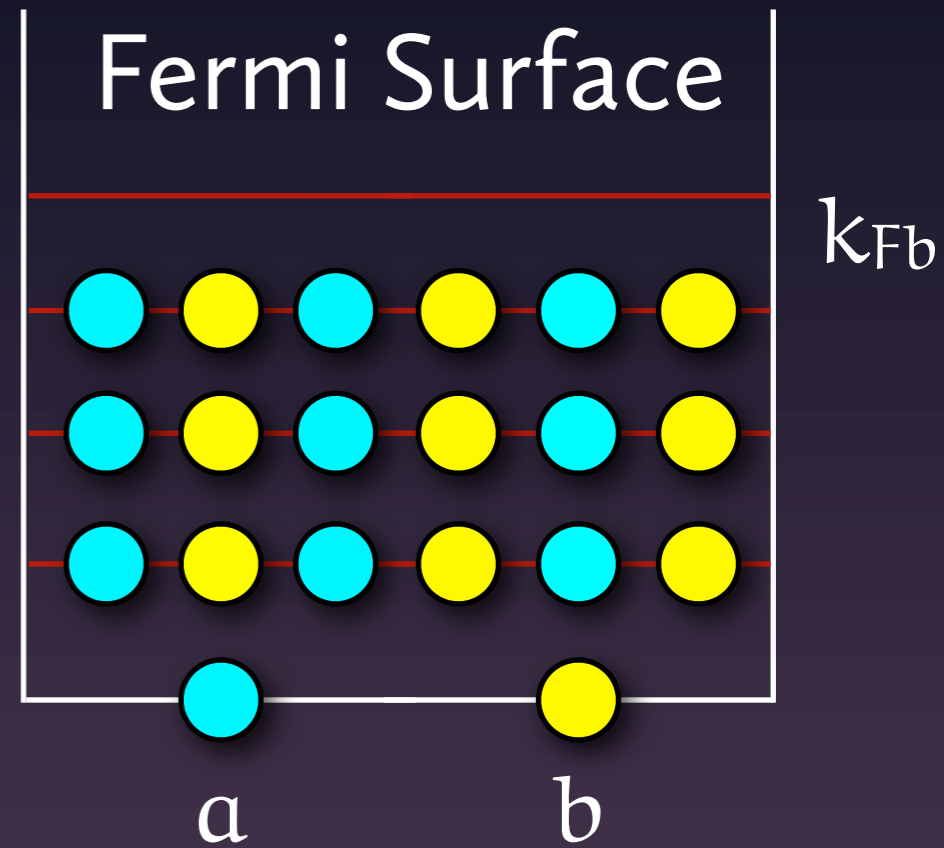
D.T. Son and M. Stephanov (2005)

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

Symmetric Matter



k_{Fa}

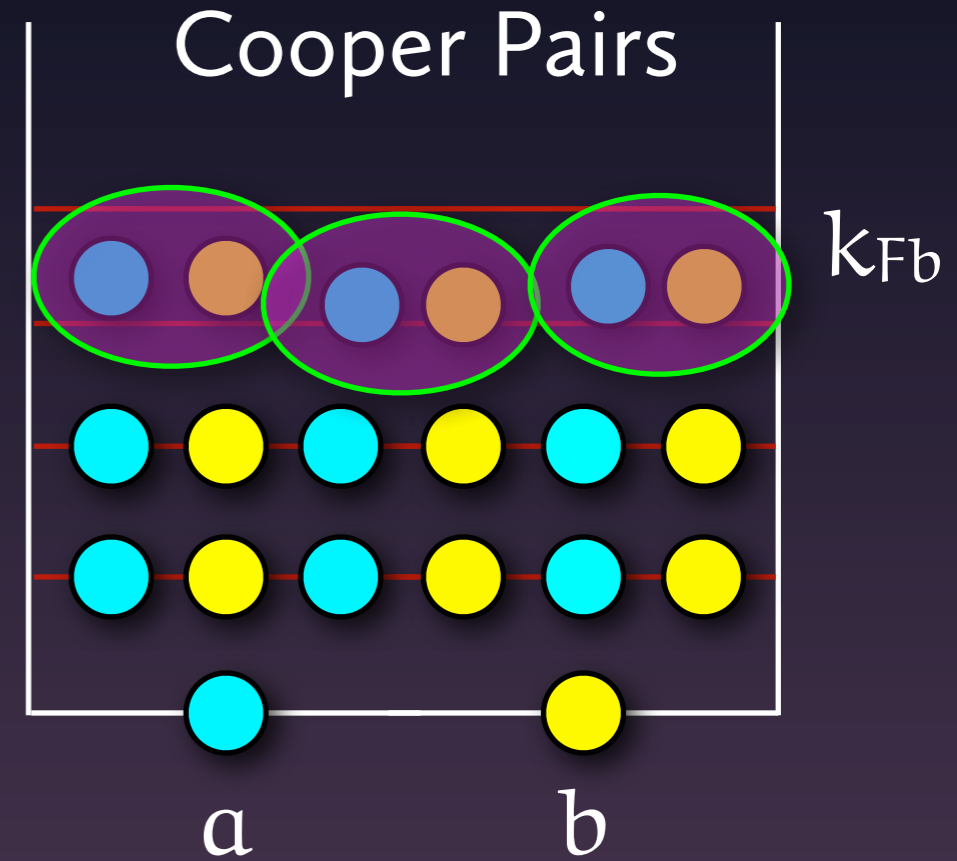
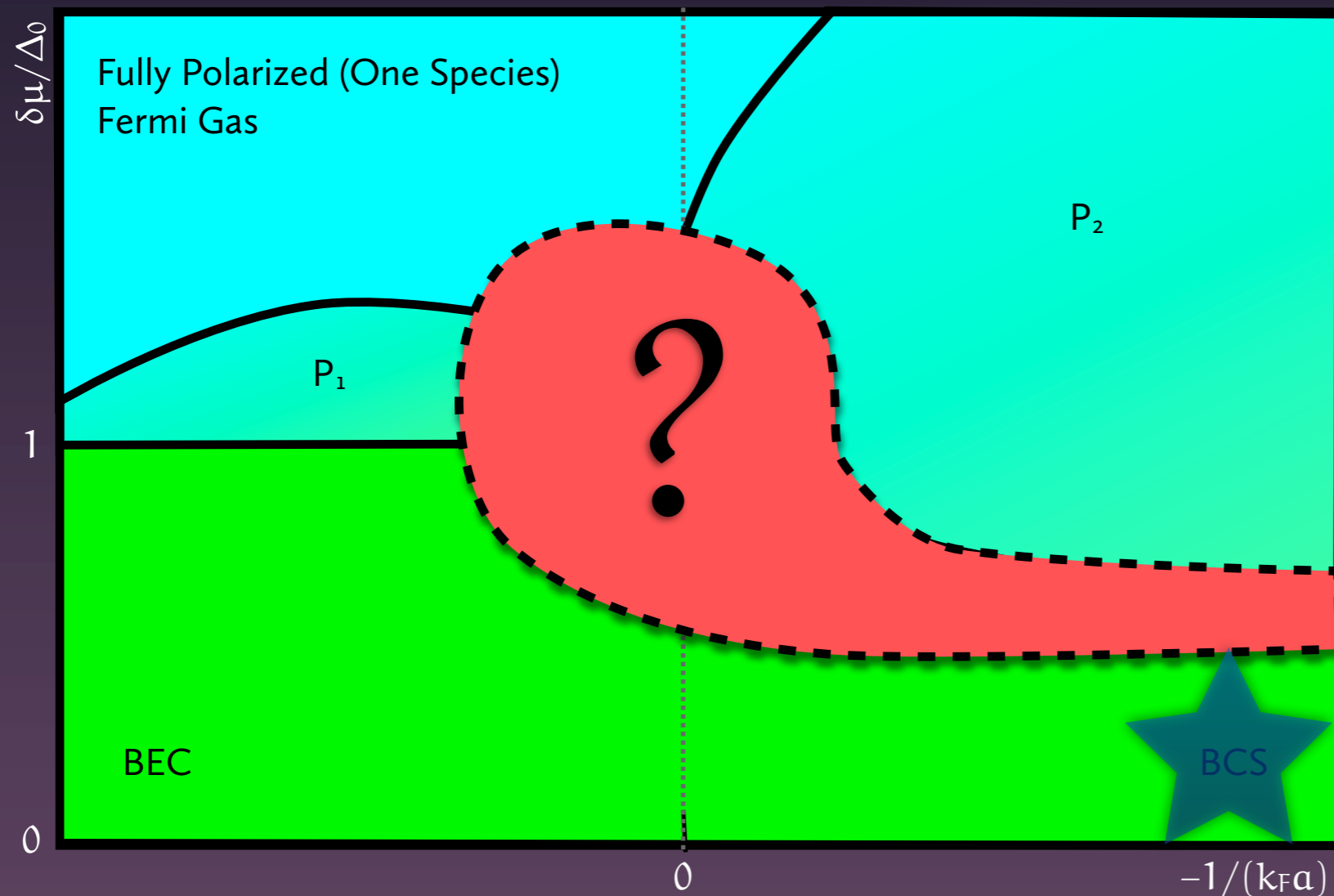


Equal Fermi surfaces

D.T. Son and M. Stephanov (2005)

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

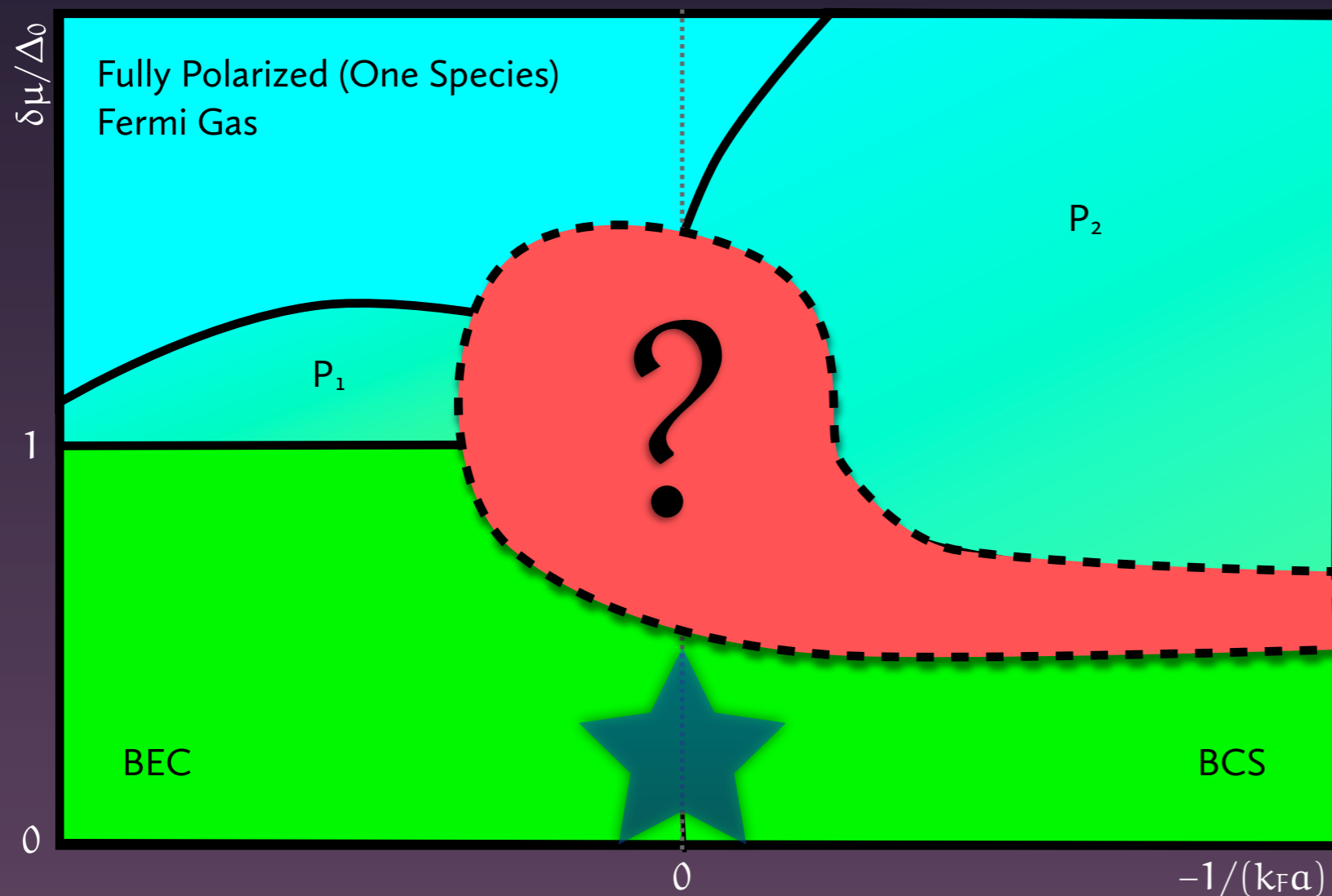
Symmetric BCS state



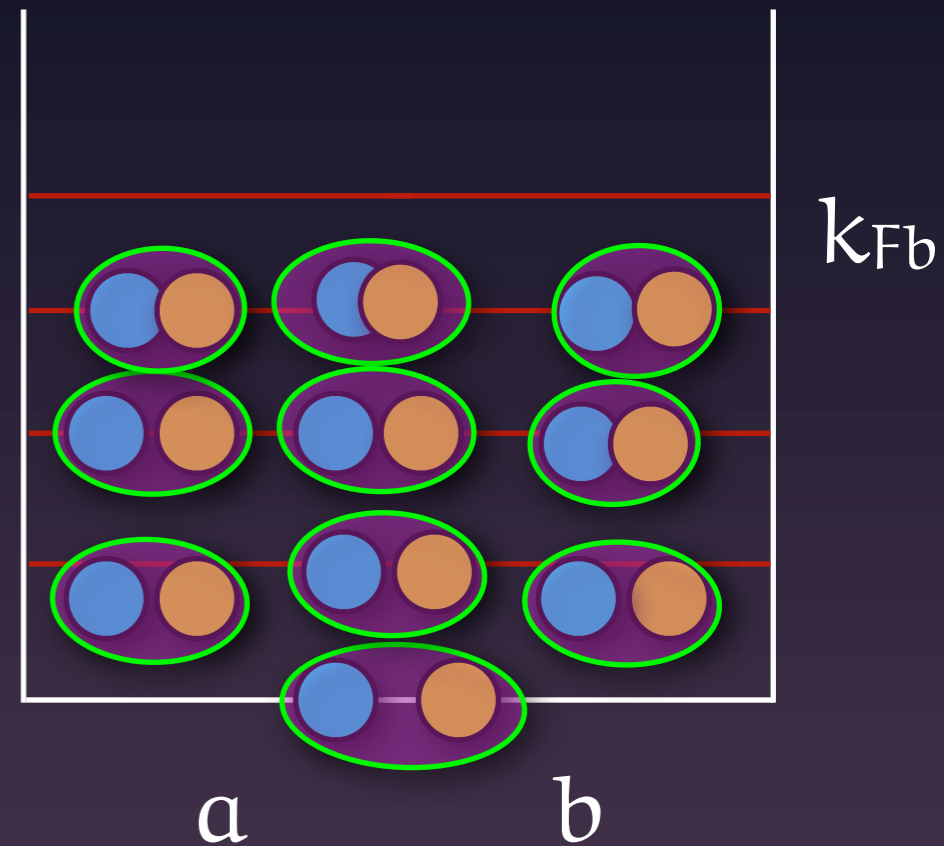
D.T. Son and M. Stephanov (2005)

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

Symmetric Unitary Gas



k_{Fa}



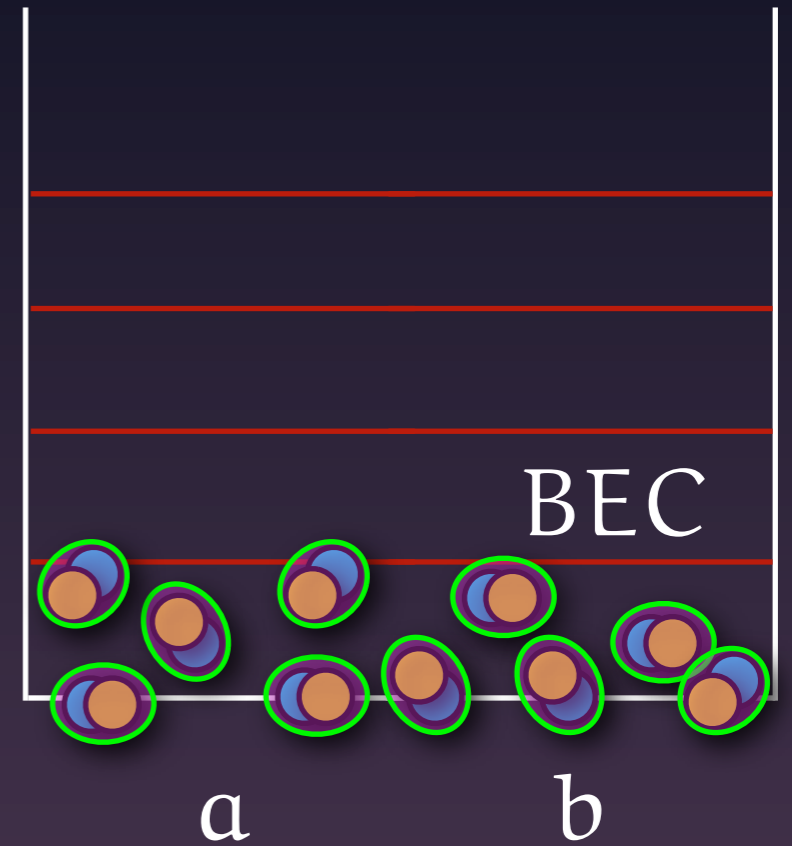
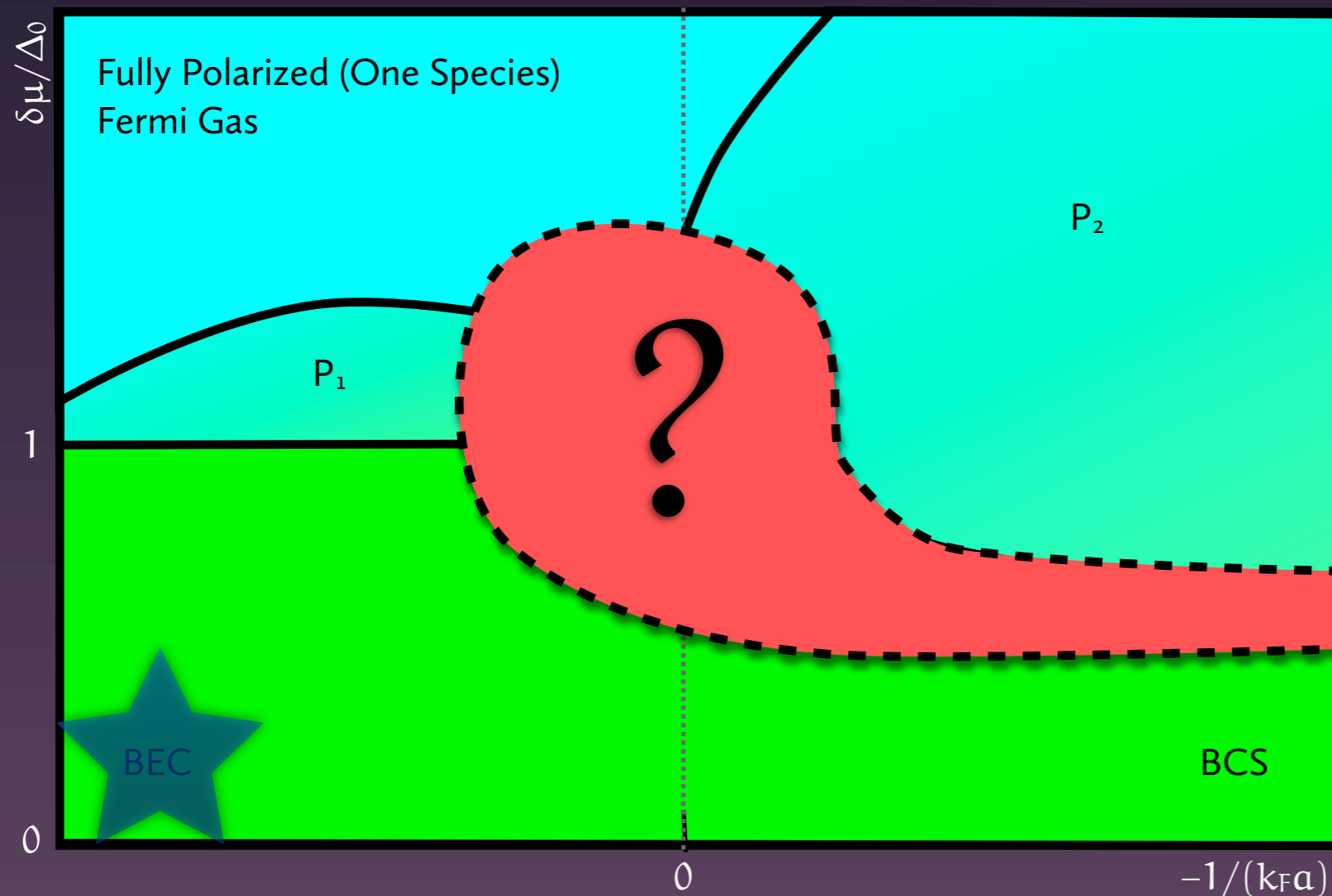
Zero momentum pairs

$$p = p_a + p_b = 0$$

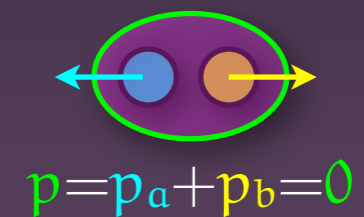
D.T. Son and M. Stephanov (2005)

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

Symmetric BEC state



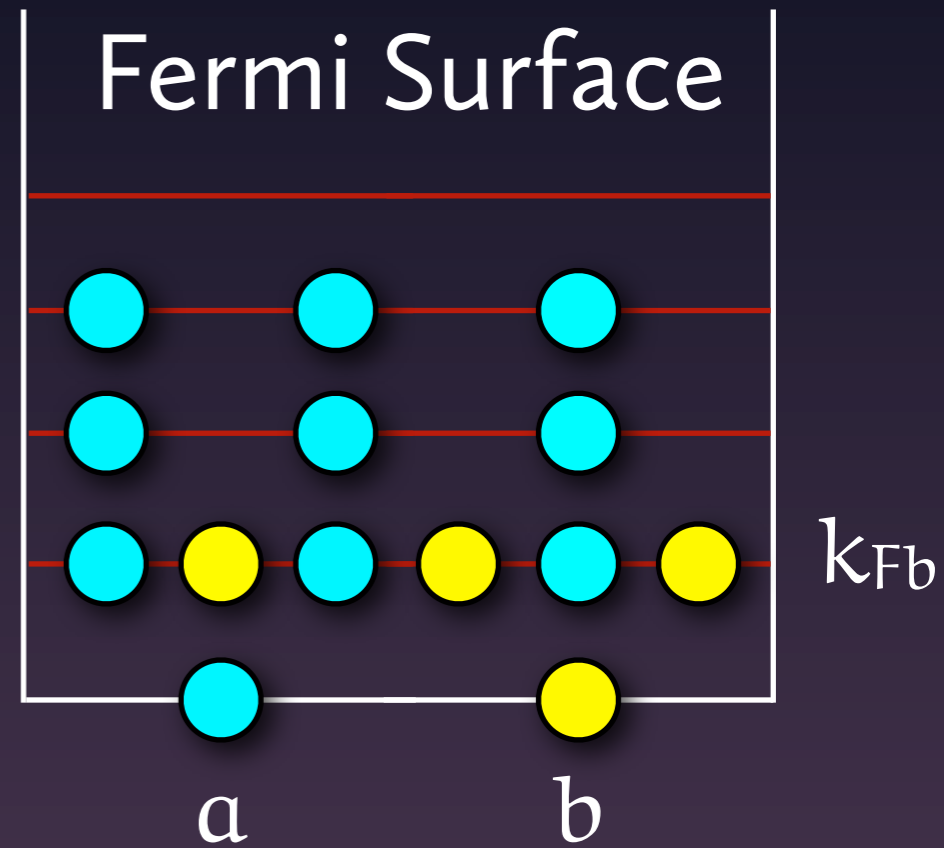
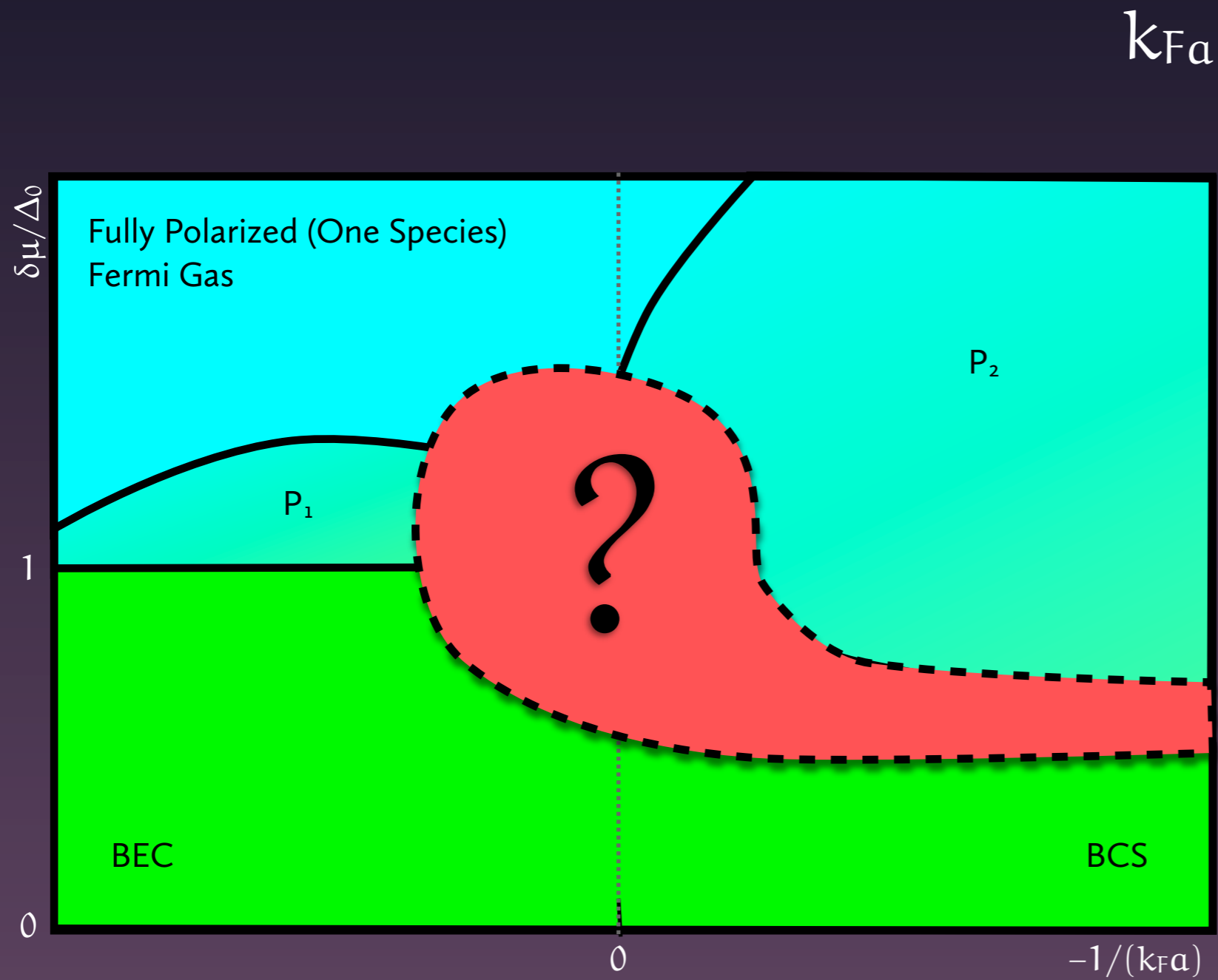
Tightly bound pairs



D.T. Son and M. Stephanov (2005)

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

Asymmetric?

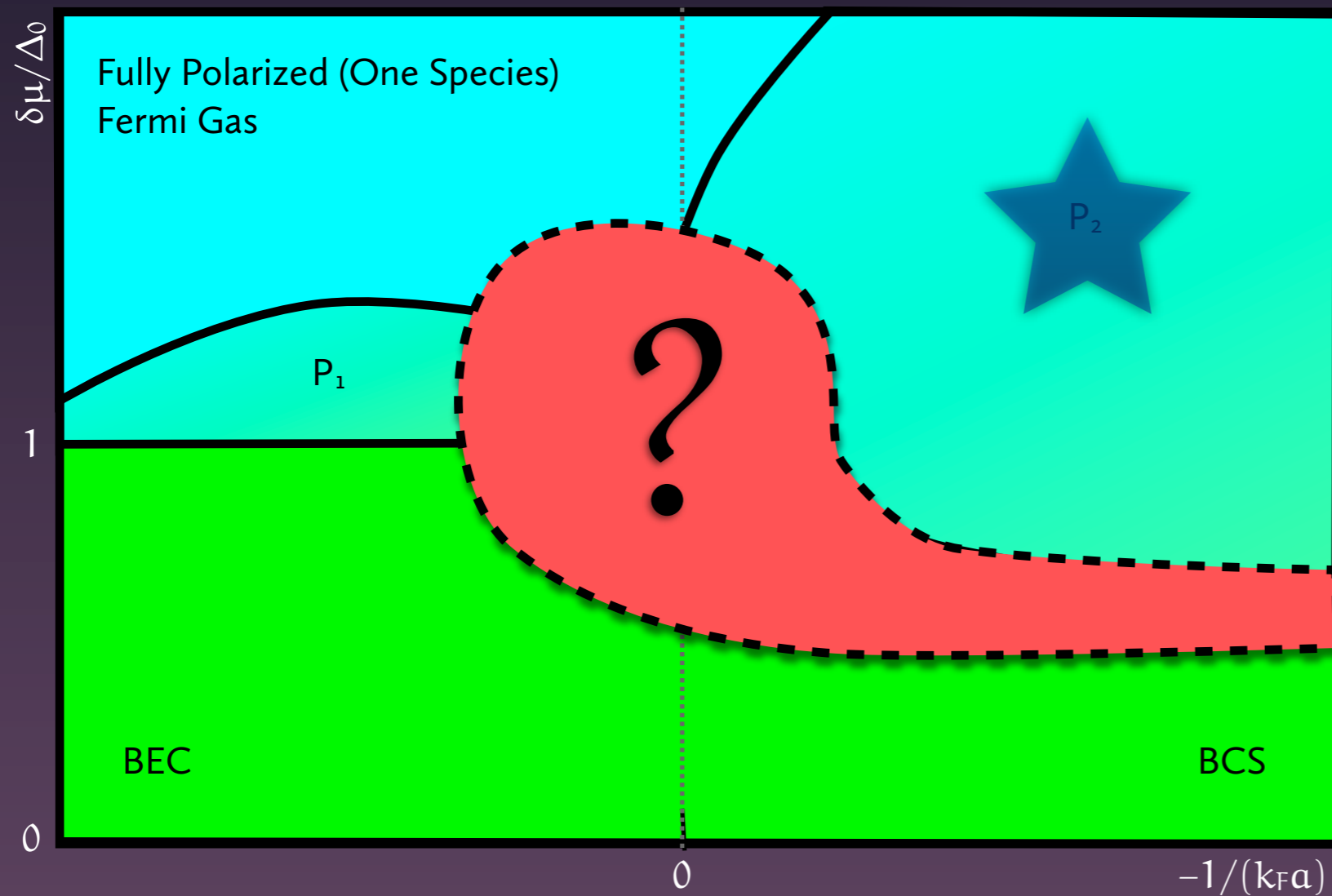


Unequal Fermi surfaces
 • Frustrates pairing

D.T. Son and M. Stephanov (2005)

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

Asymmetric P-wave pairs

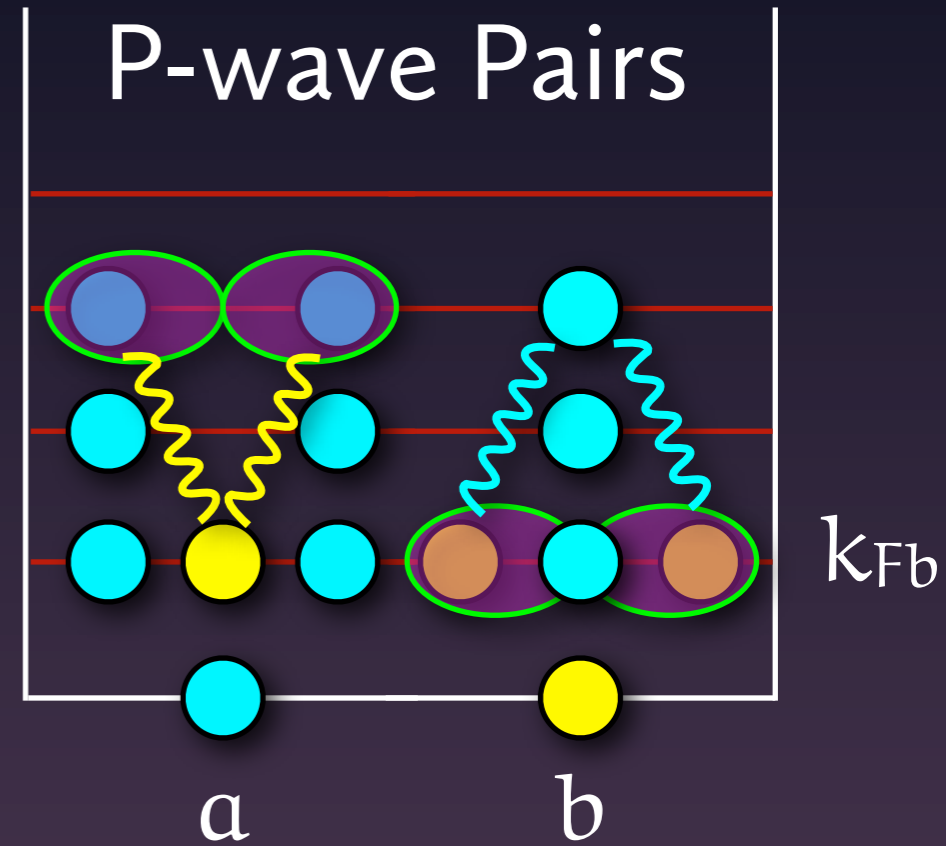


D.T. Son and M. Stephanov (2005)

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

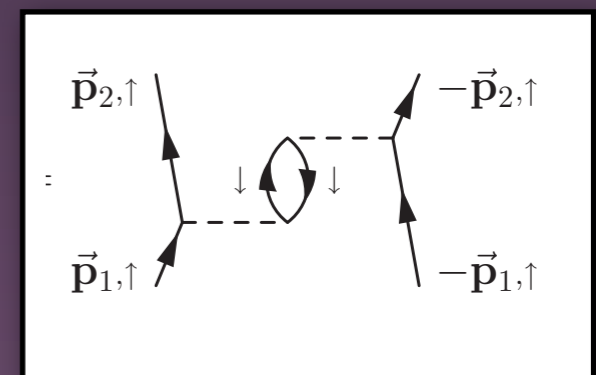
k_{Fa}

Intra-species P-wave Pairs

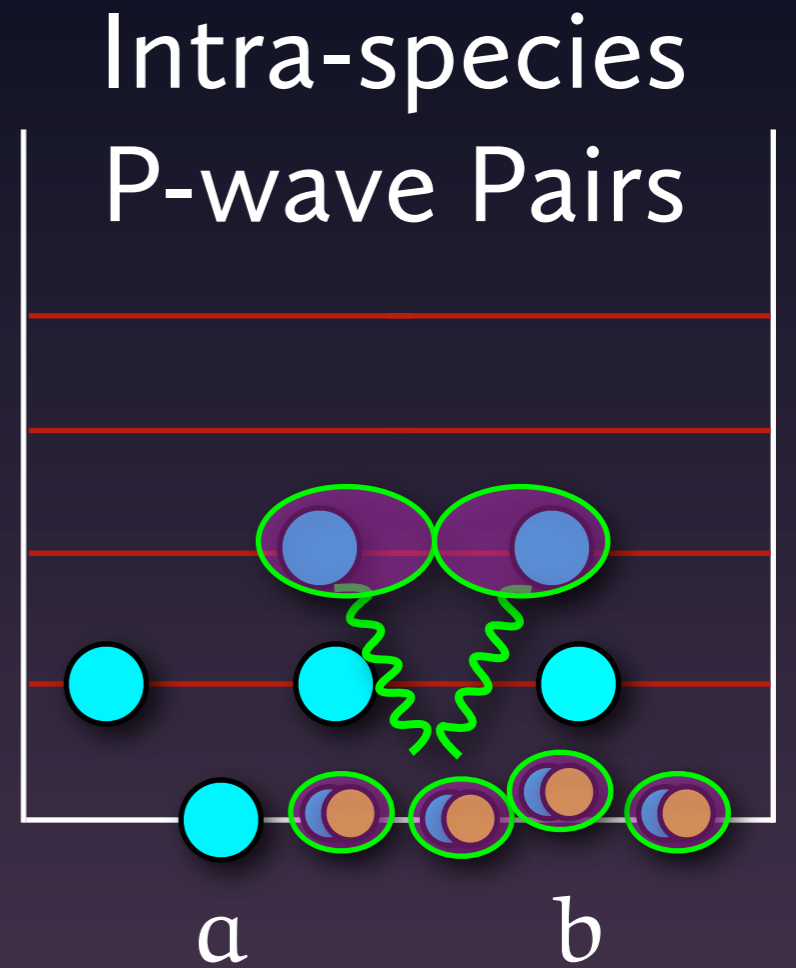
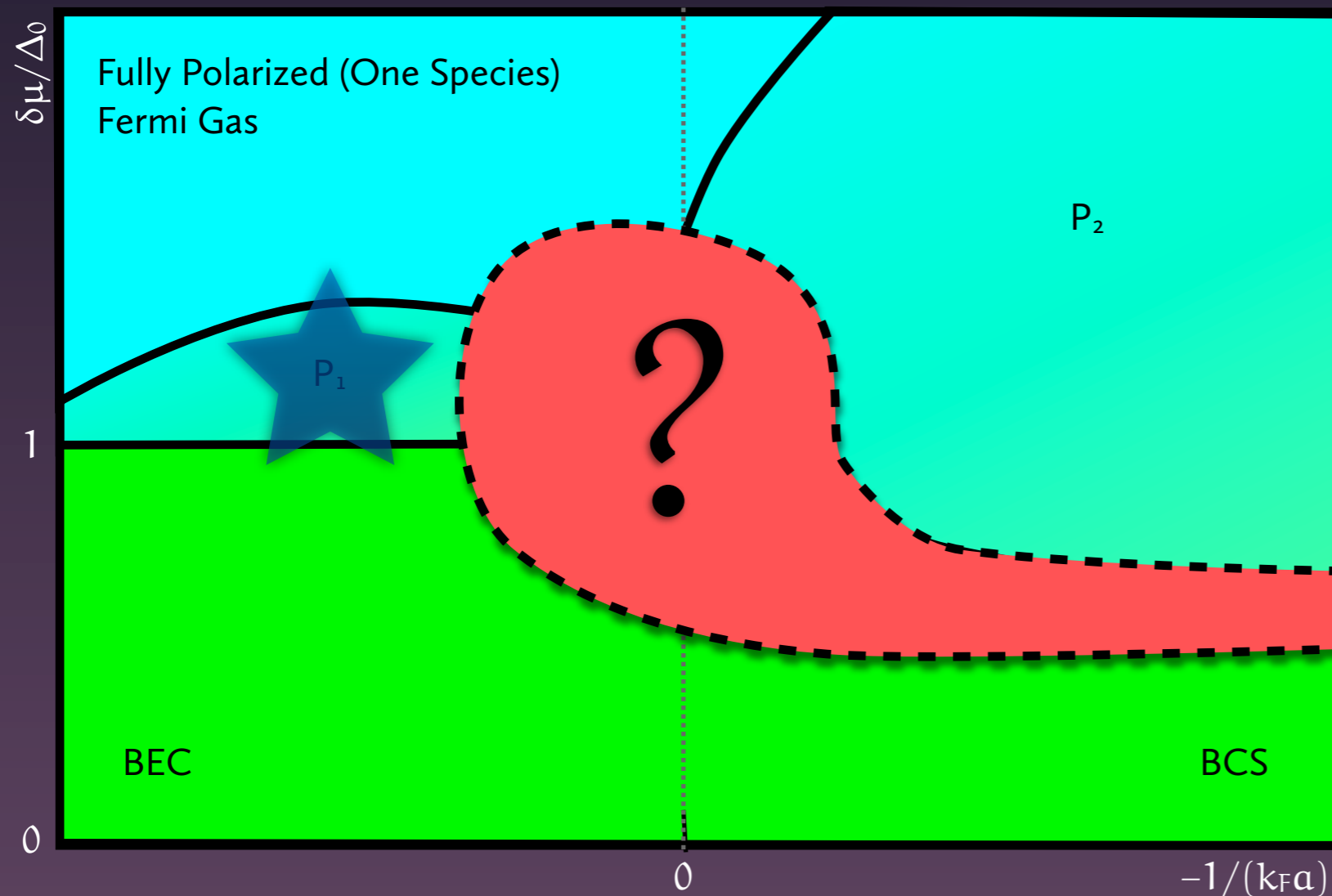


Kohn-Luttinger implies attractive at some l

Two coexisting superfluids



Asymmetric P-wave BEC

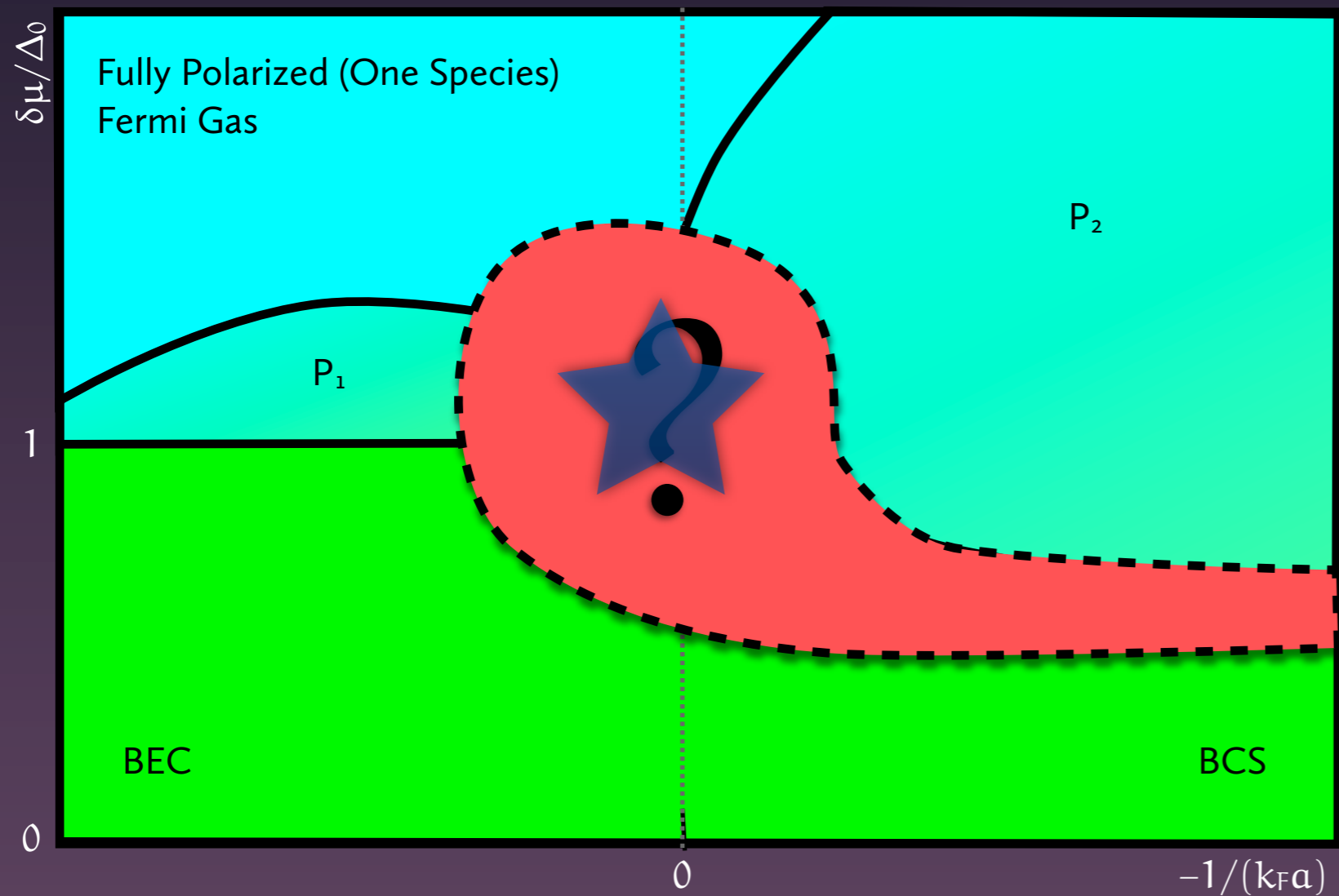


BEC and P-wave
superfluids coexist
homogeneously

D.T. Son and M. Stephanov (2005)

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

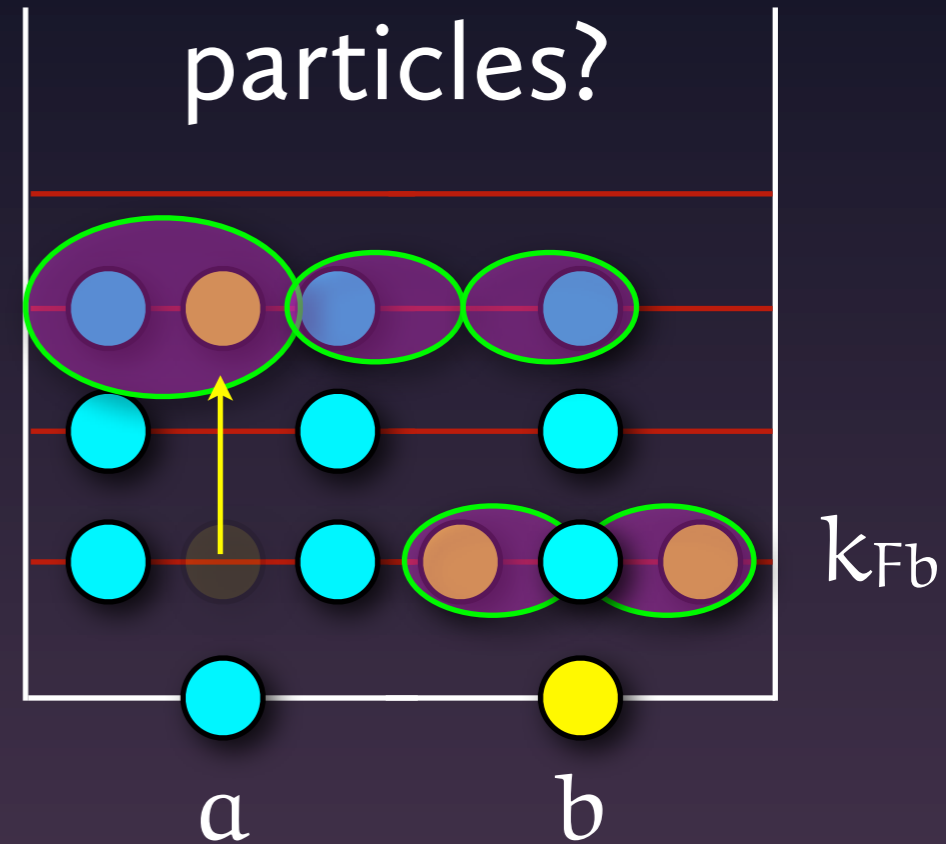
Asymmetric Gapless SF



D.T. Son and M. Stephanov (2005)

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

Pairing promotes
particles?

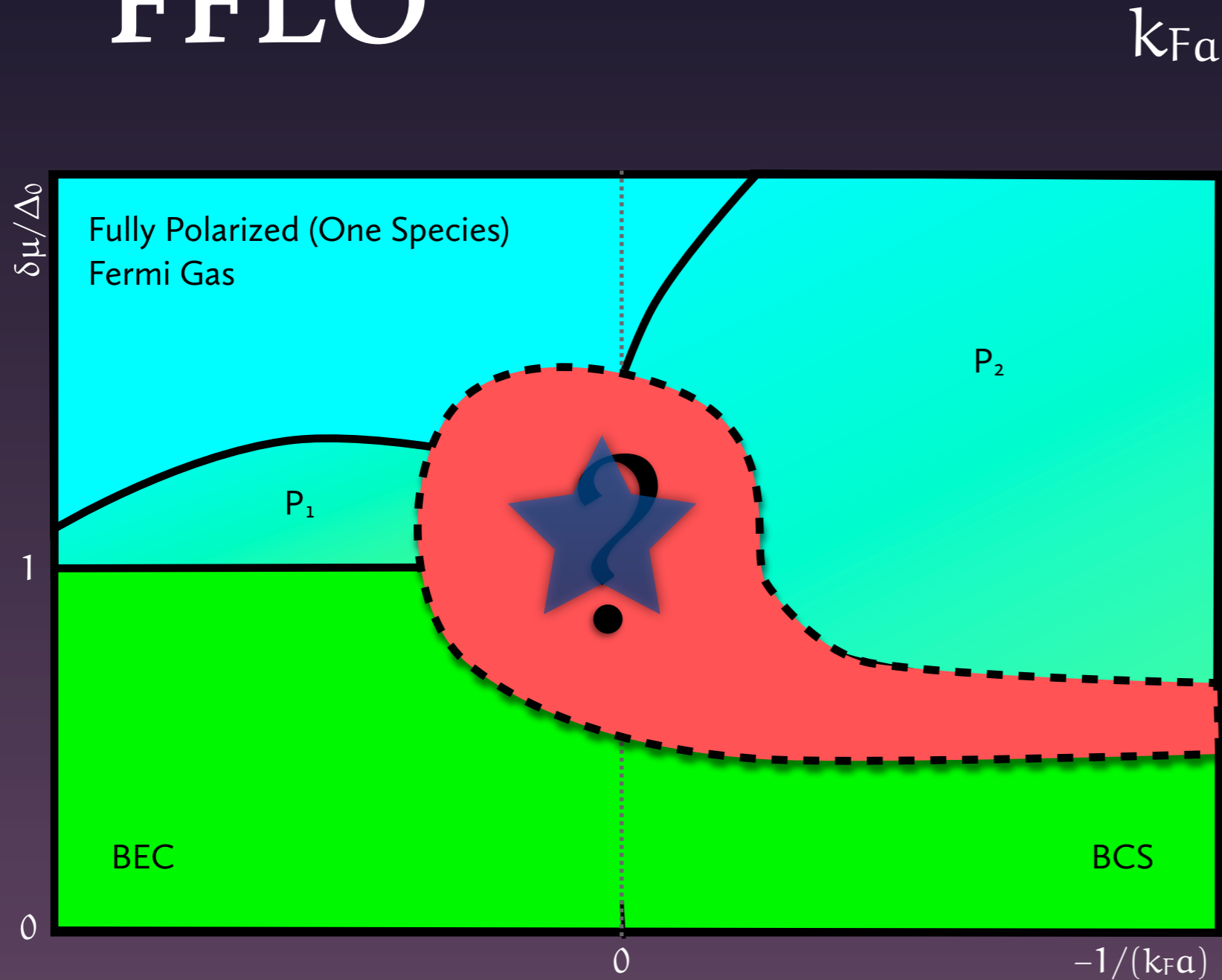


“Breach” in pairing

Still induced P-wave

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

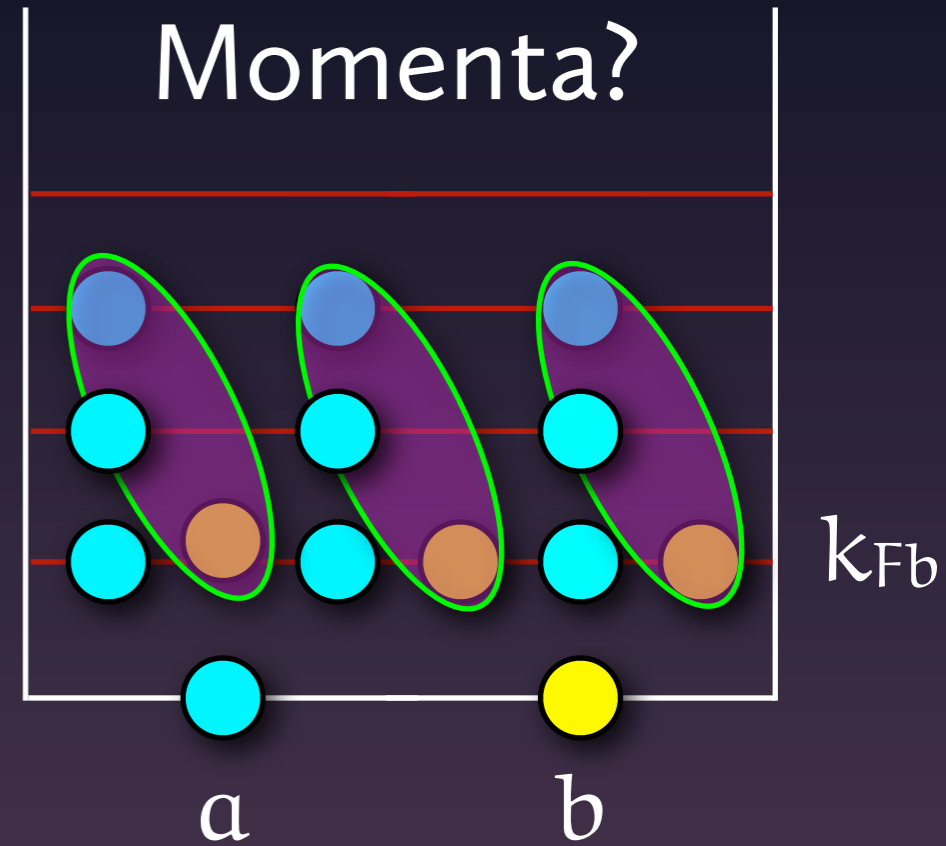
Asymmetric FFLO



D.T. Son and M. Stephanov (2005)

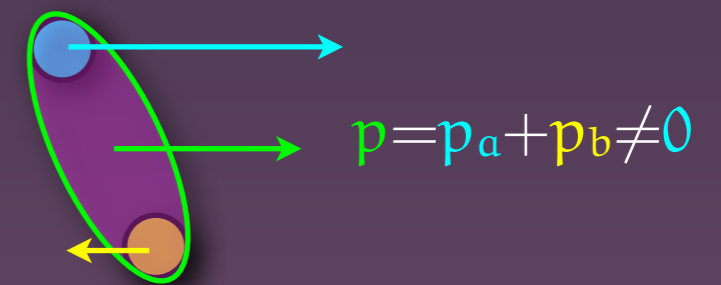
P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk (PRL 2006)

Pairs have
Momenta?

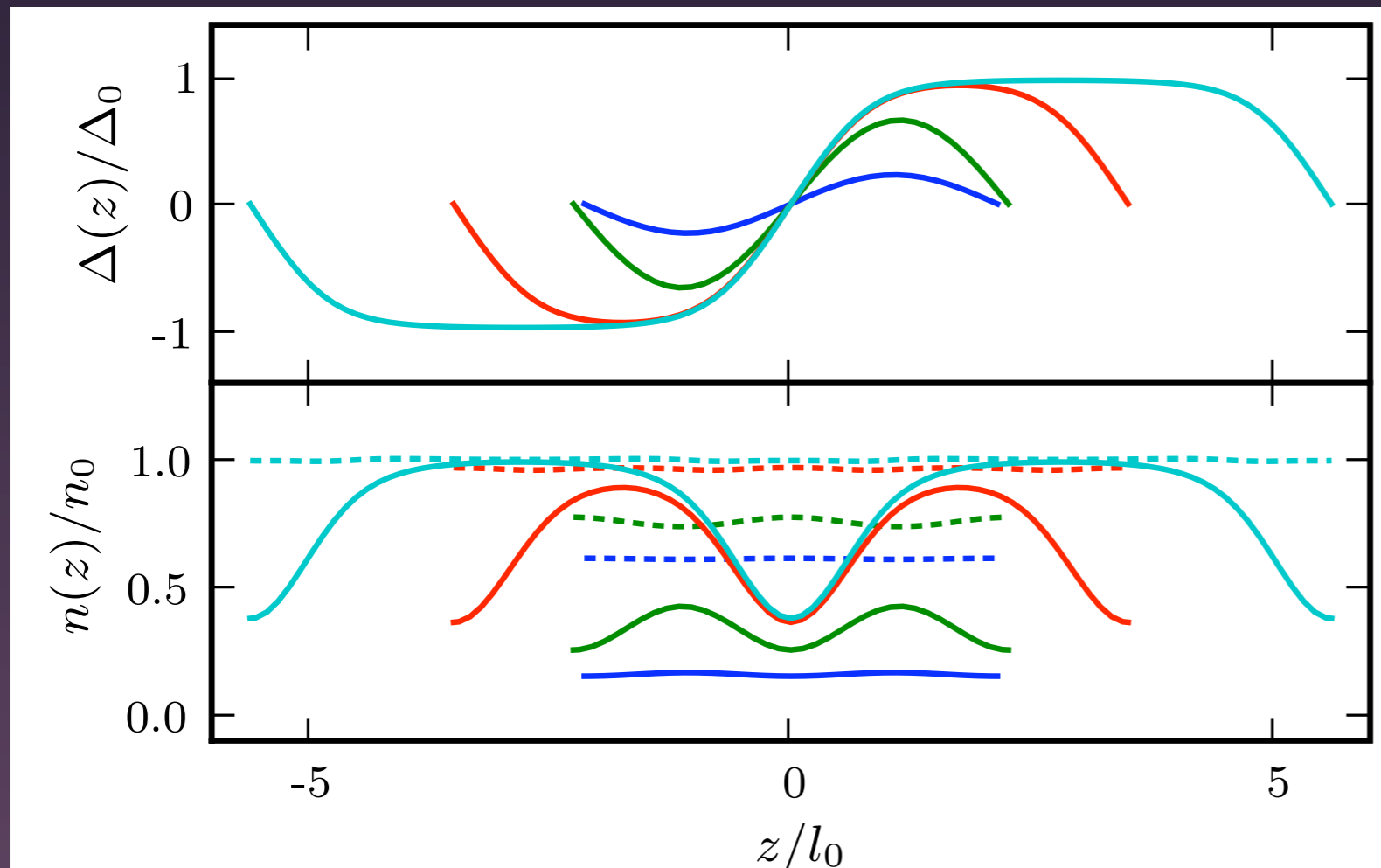


State (LO) is crystal
(supersolid)

Pairs have momentum

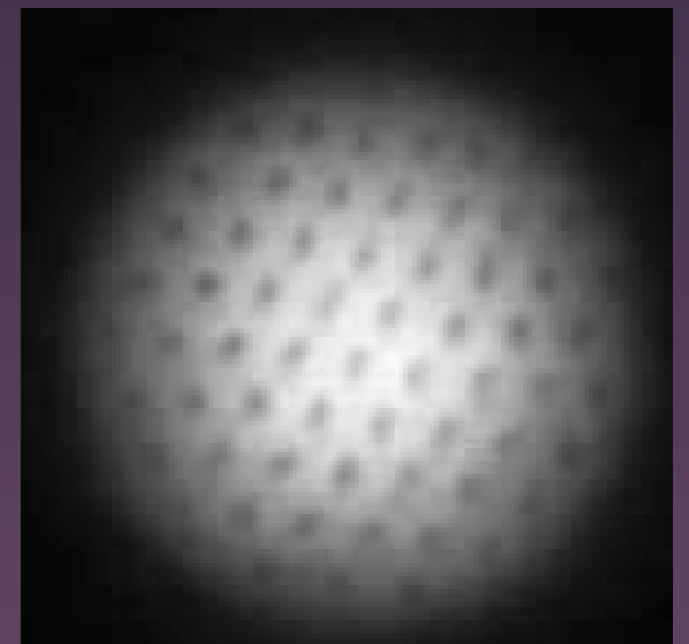


DFT predicts (FF)LO at Unitarity: Supersolid!



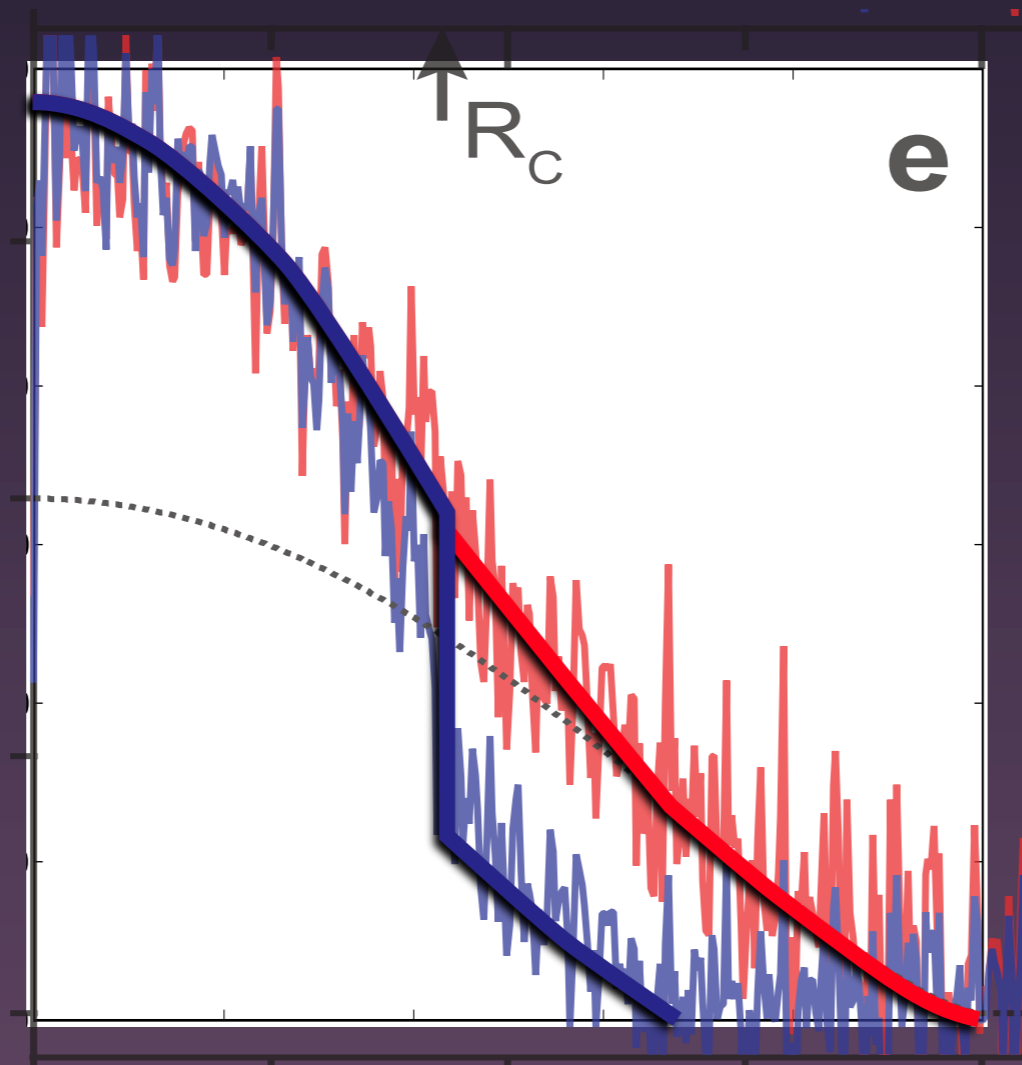
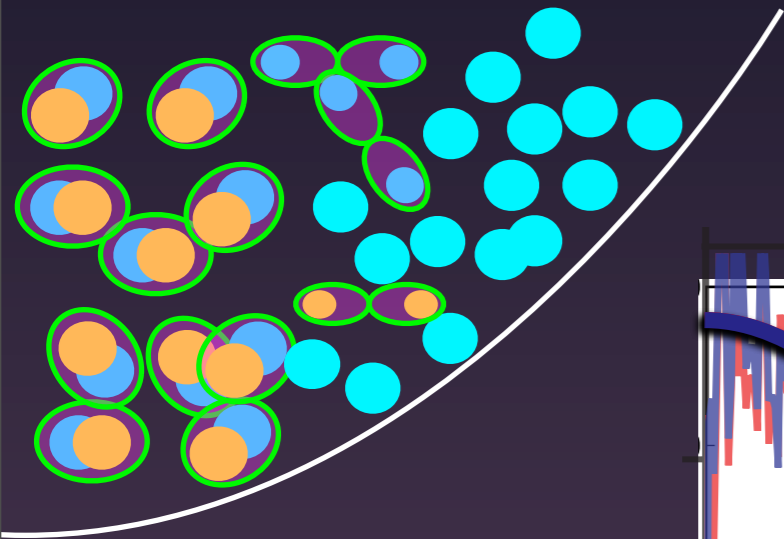
Large density contrast
(factor of 2)

Similar to contrast of
vortex core



Bulgac and Forbes PRL 101 (2008) 215301

Observations: Nothing?



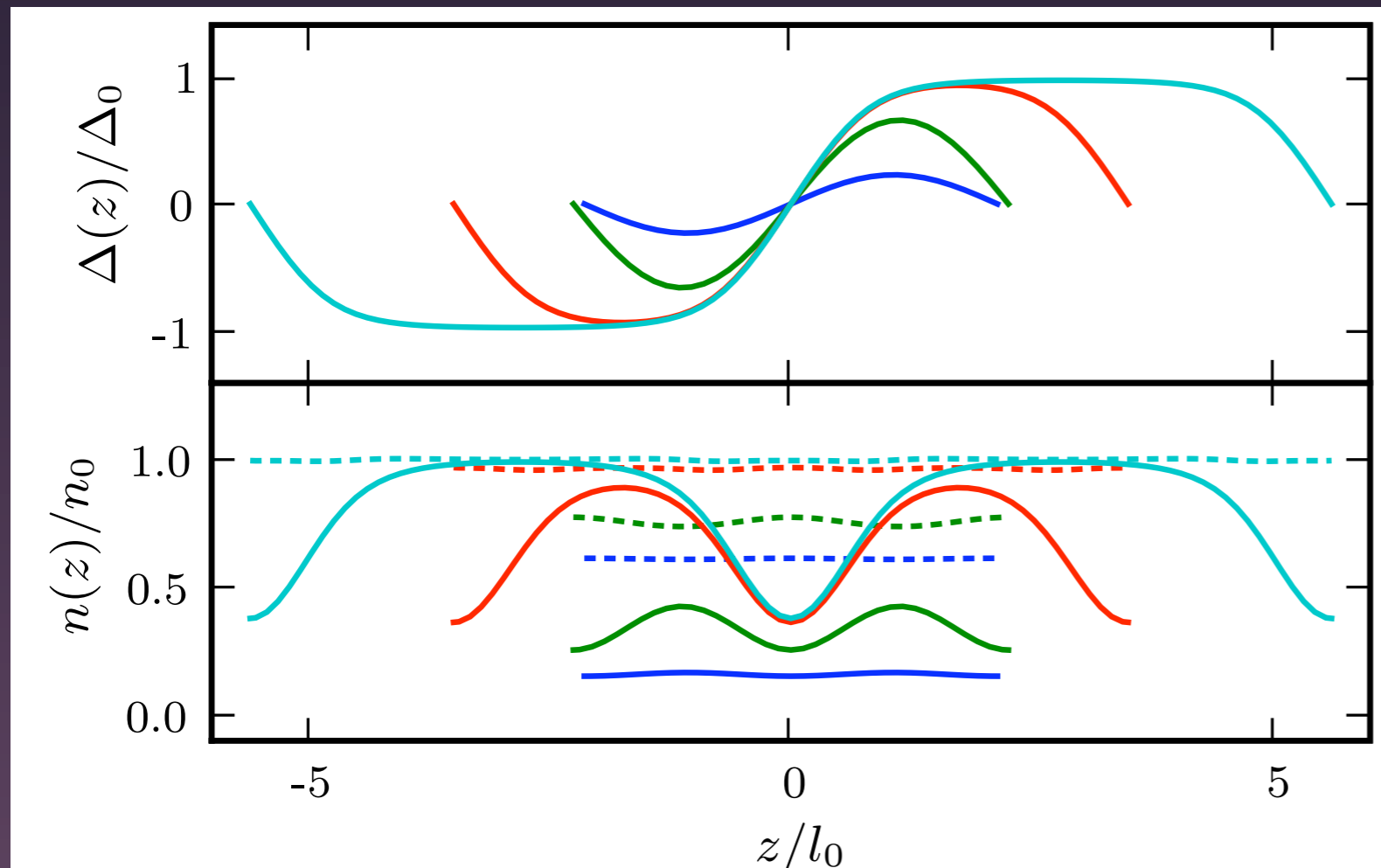
Paired core

Polarized wings

Maybe there are no interesting polarized superfluid phases?

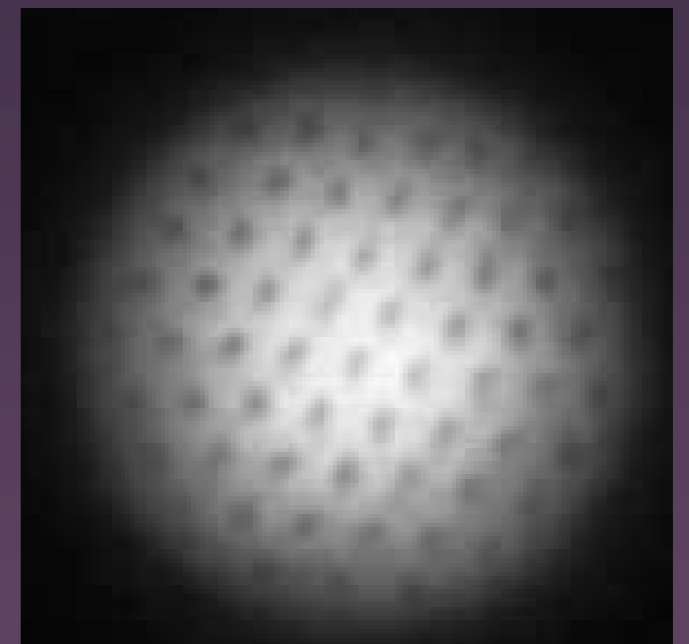
MIT Experimental data from Shin et. al (2008)

DFT predicts (FF)LO at Unitarity: Supersolid!



Large density contrast
(factor of 2)

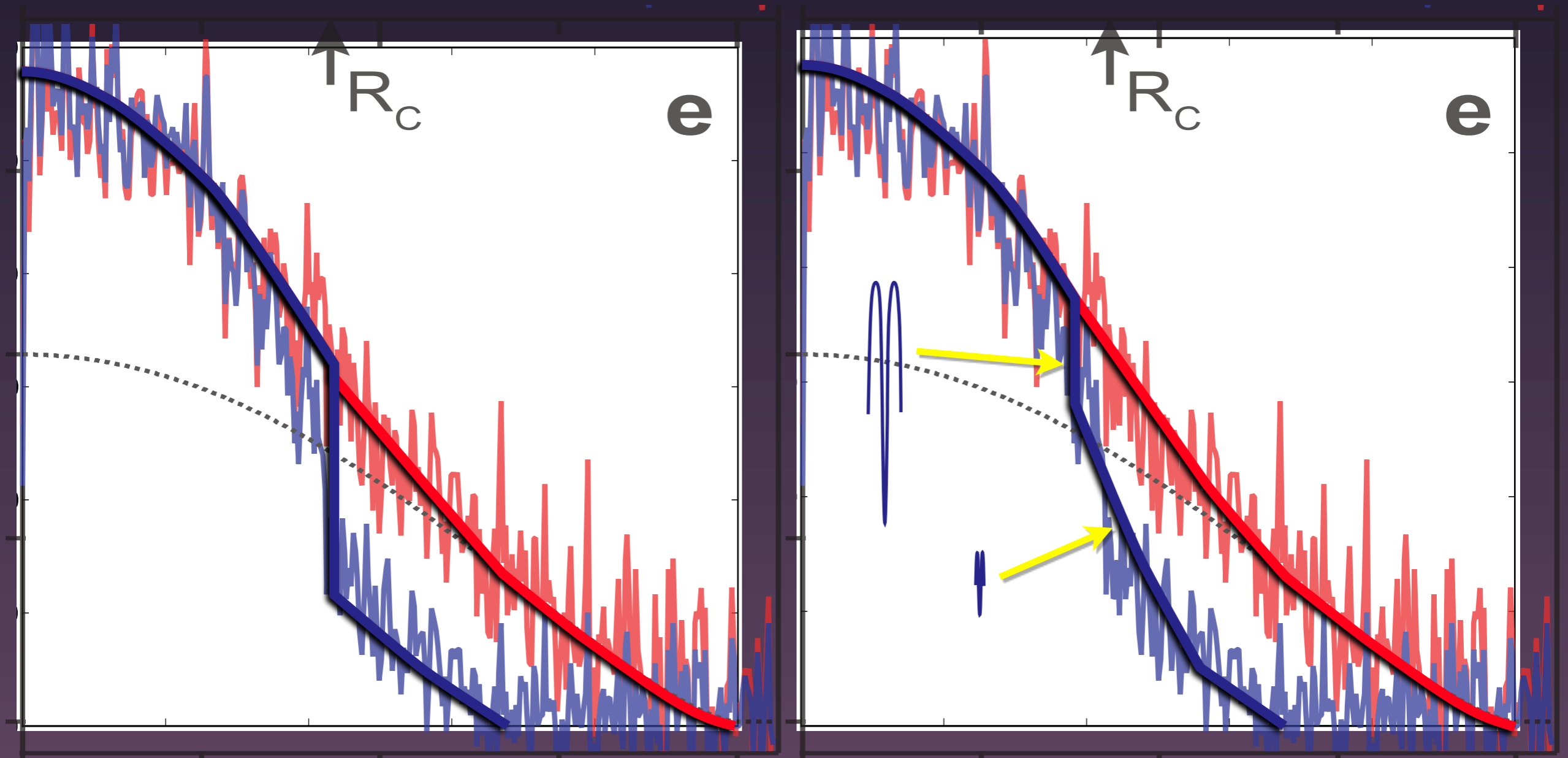
Similar to contrast of
vortex core



Bulgac and Forbes PRL 101 (2008) 215301

Observations: Inconclusive

- Need detailed structure or novel signature



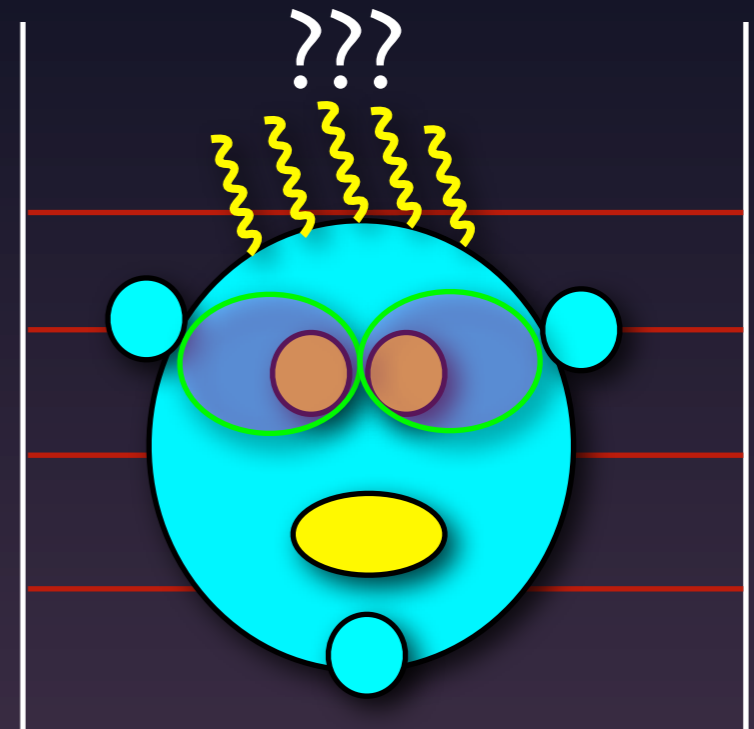
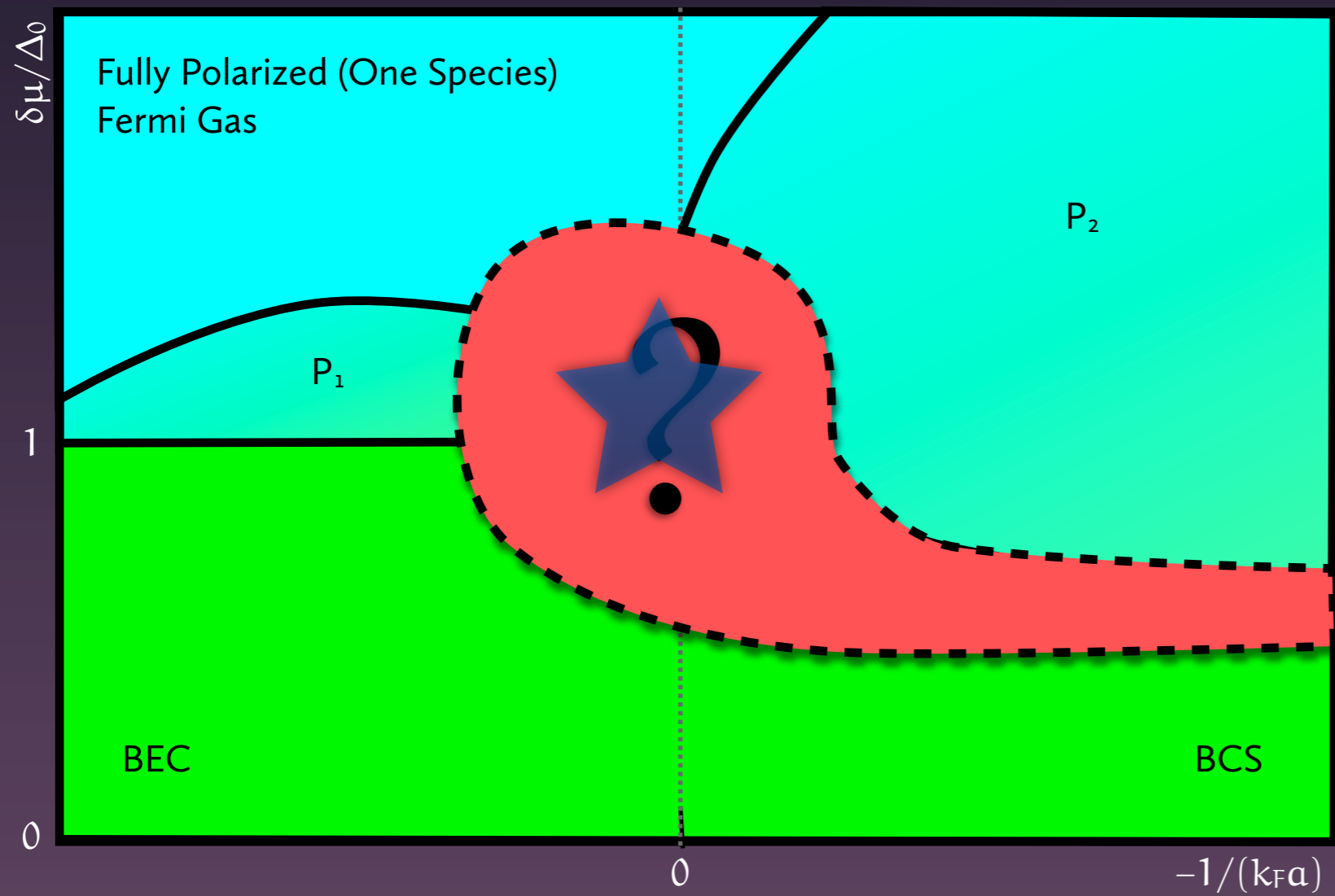
MIT Experimental data from Shin et. al (2008)

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, Delehayé, Chevy, and Stringari PRA 90 (2014) 043608

Asymmetric Exotica?



Need IR structure

Sign problem

Please benchmark!

Computational Costs

Classical: $6N N_t$

Quantum: $N_x^{3N} N_t$

Fermionic DFT: $N N_x^3 N_t$

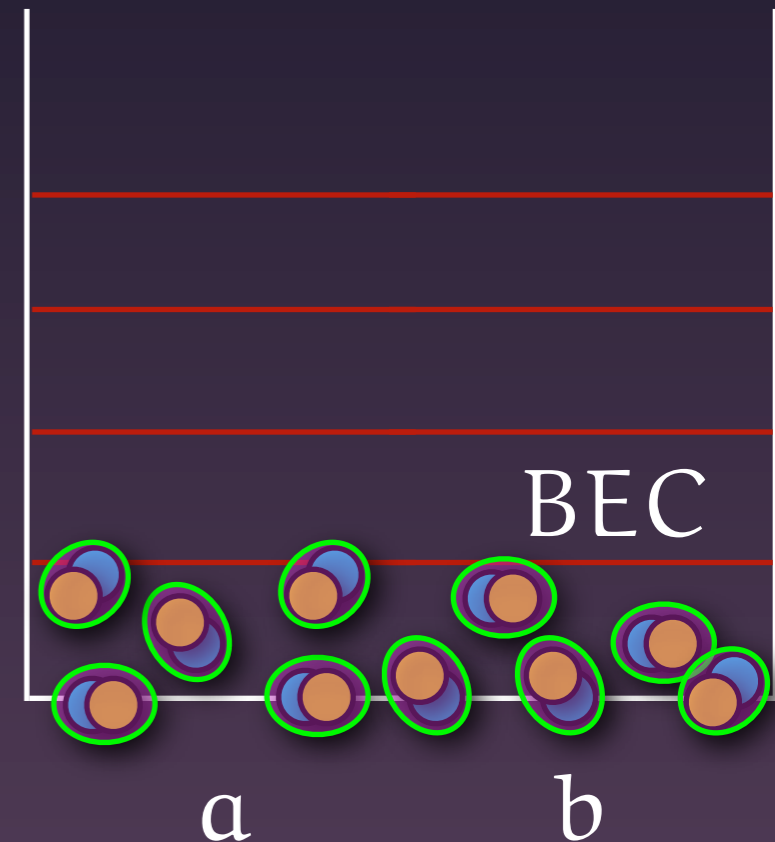
Bosonic DFT: $N_x^3 N_t$

Bosons are “easy”

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

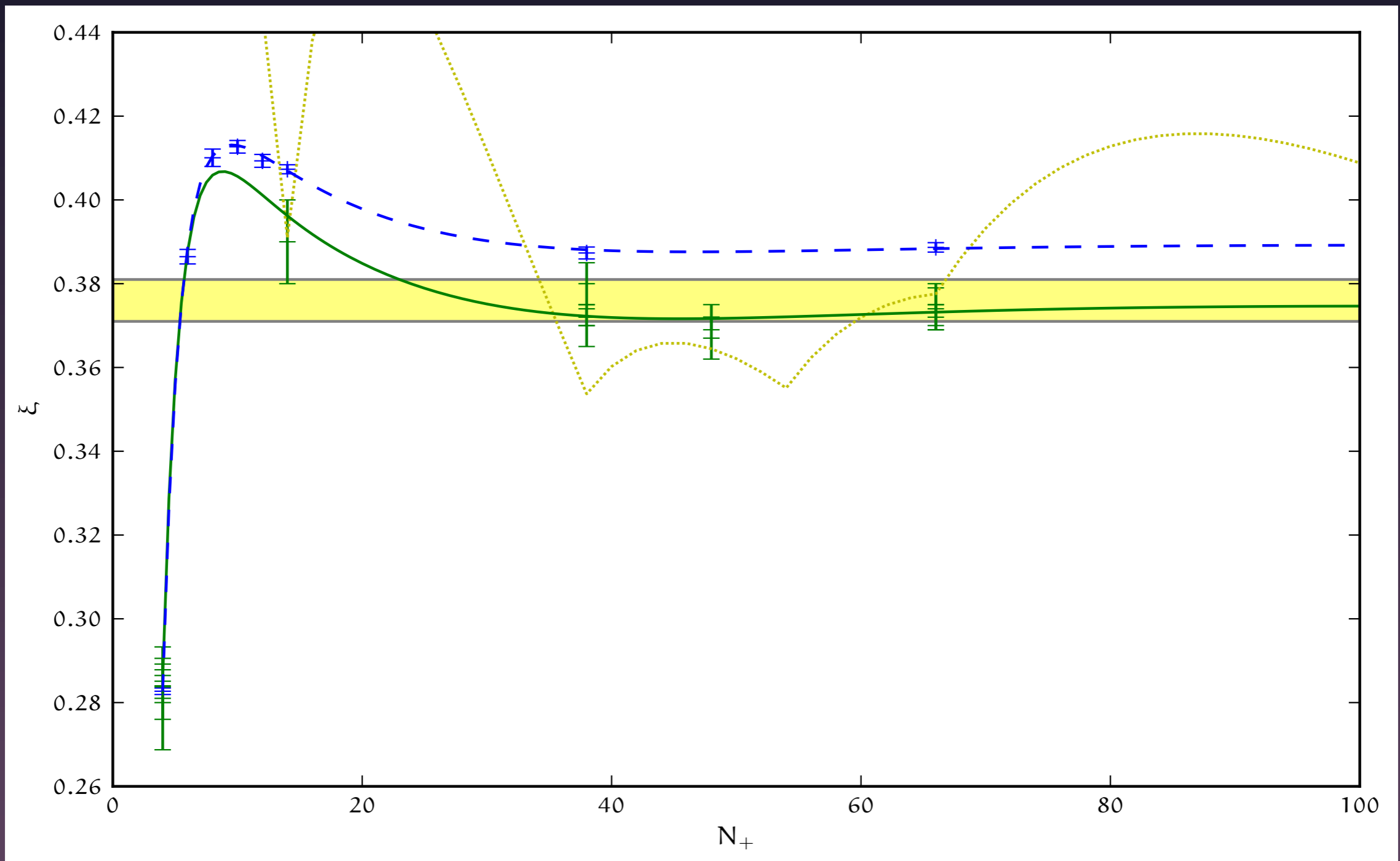
$$i\partial_t\Psi = \left(-\frac{\nabla^2}{2m_B} + [V + g|\Psi|^2] \right) \Psi$$

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



$$N_x^3 N_t$$

Misses “shell” effects



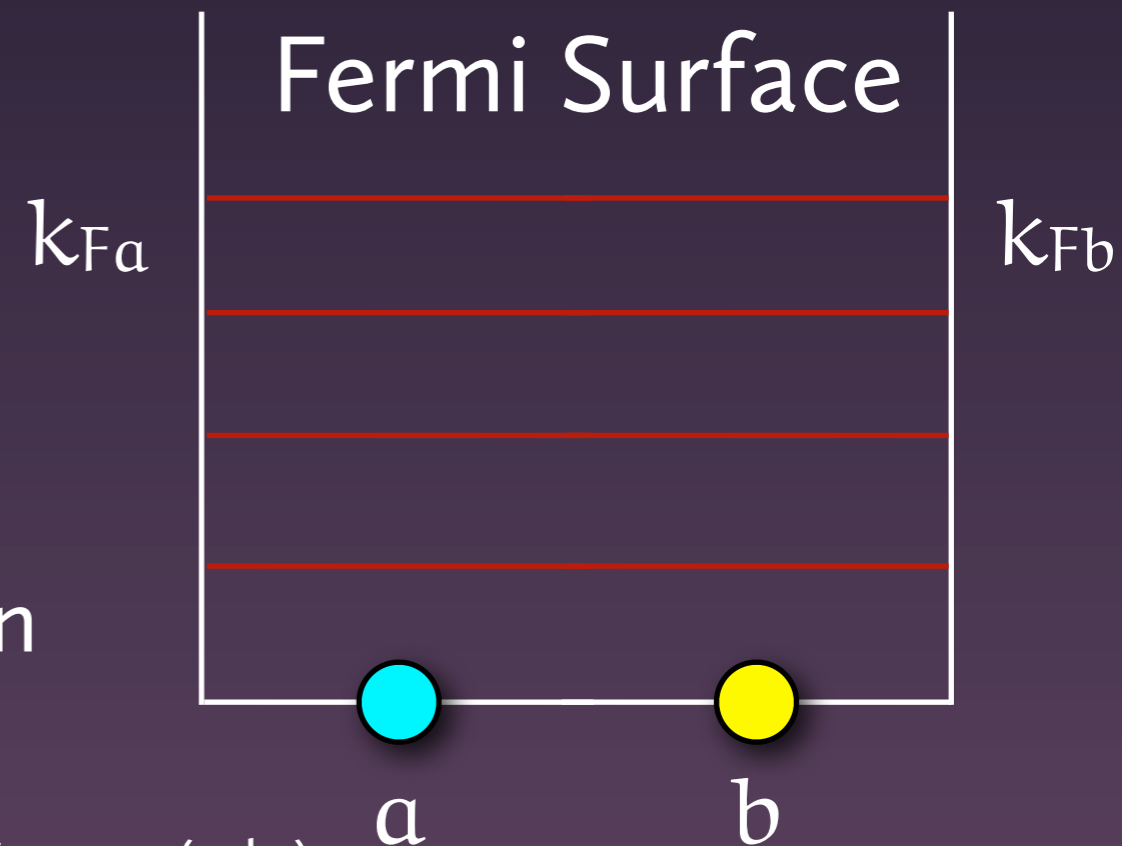
Forbes, Gandolfi, Gezerlis [PRA 86 (2012) 053603]

Fermions are harder

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

- 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



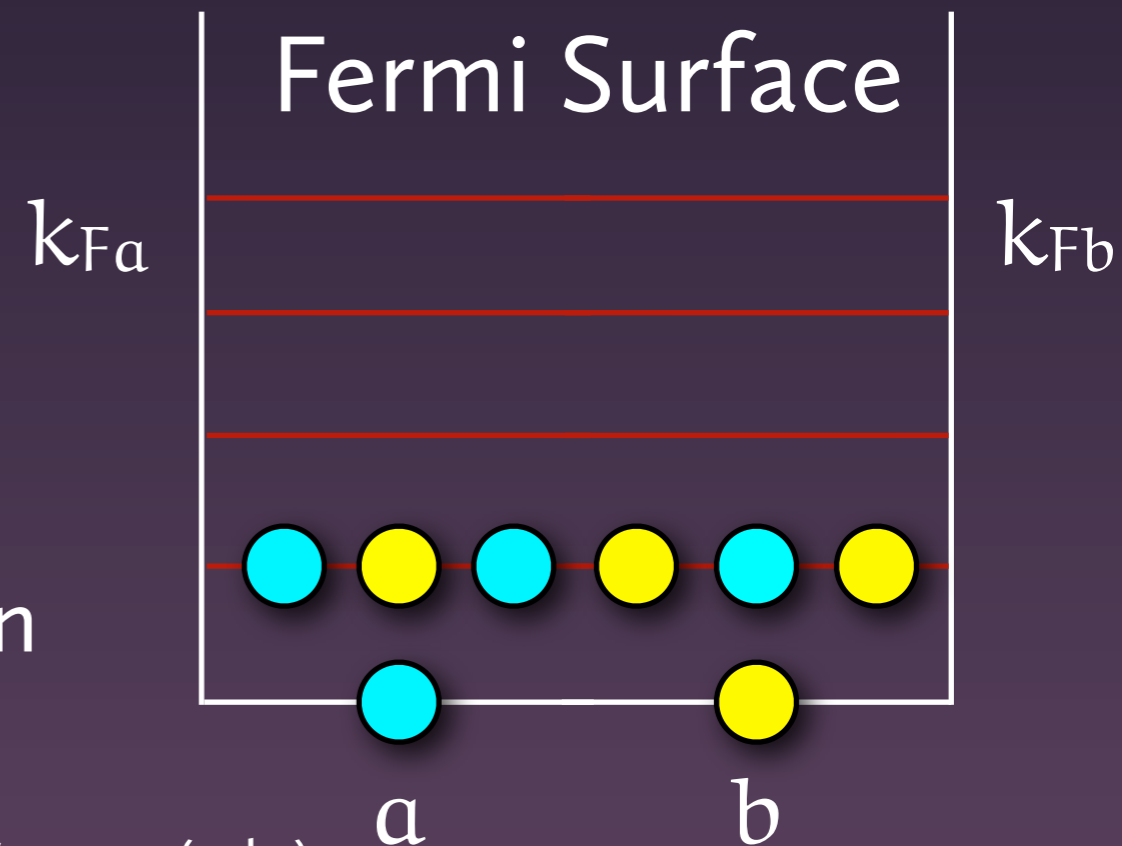
$$(N) N_x^3 N_t$$

Fermions are harder

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

- 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



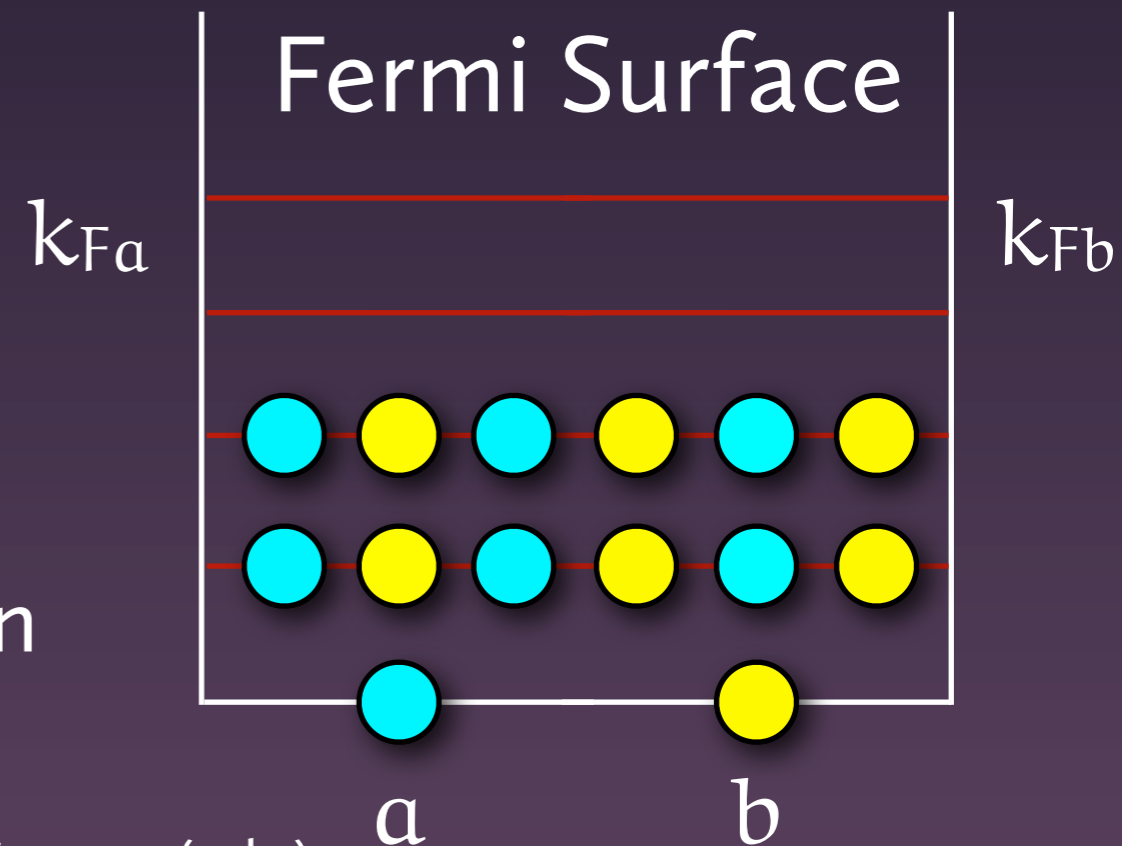
$$(N) N_x^3 N_t$$

Fermions are harder

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

- 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

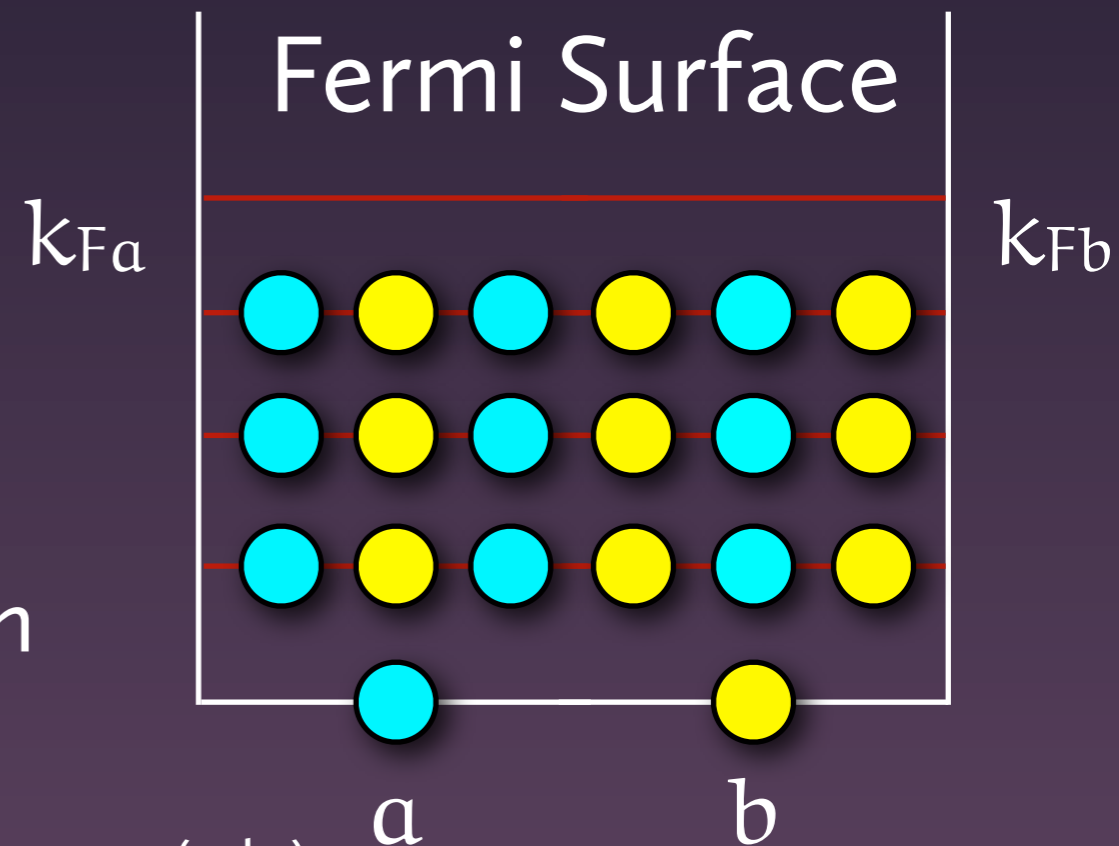
$$(N) N_x^3 N_t$$

Fermions are harder

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

- 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

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

- Evolution: $(N) N_x^3 N_t$

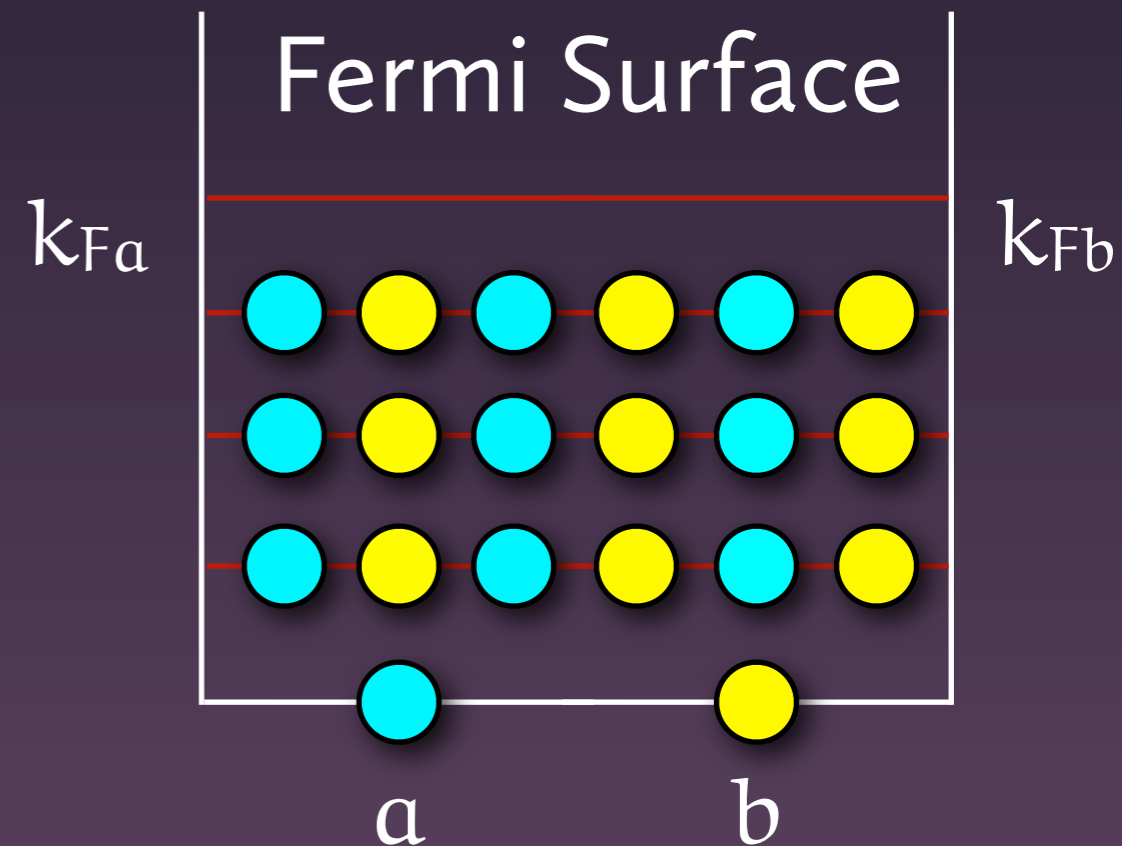
Scales reasonably well

- Ground state

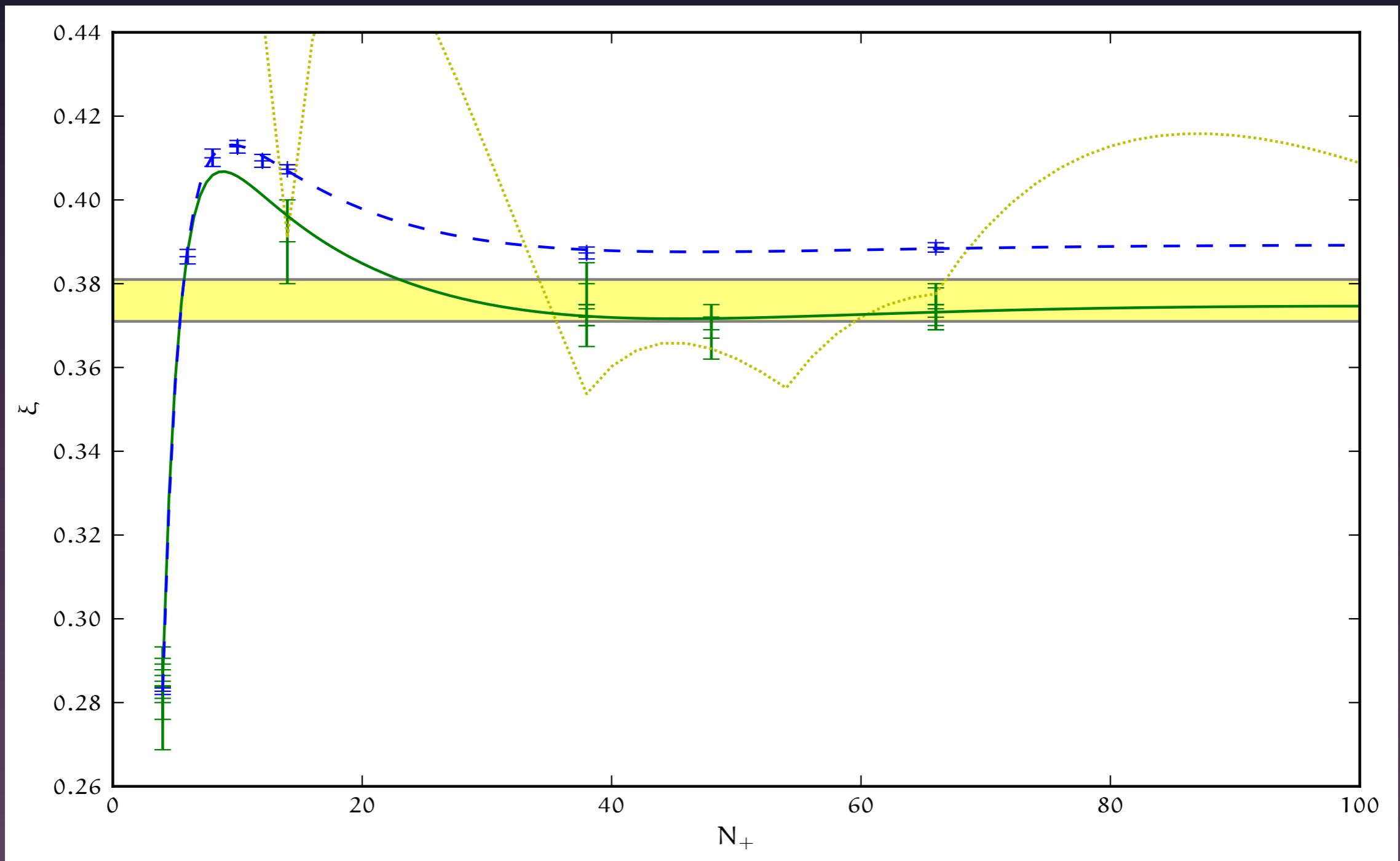
Need repeated diagonalization!

$$(N N_x^3)^3$$

(or does it...)



Correct “shell” effects

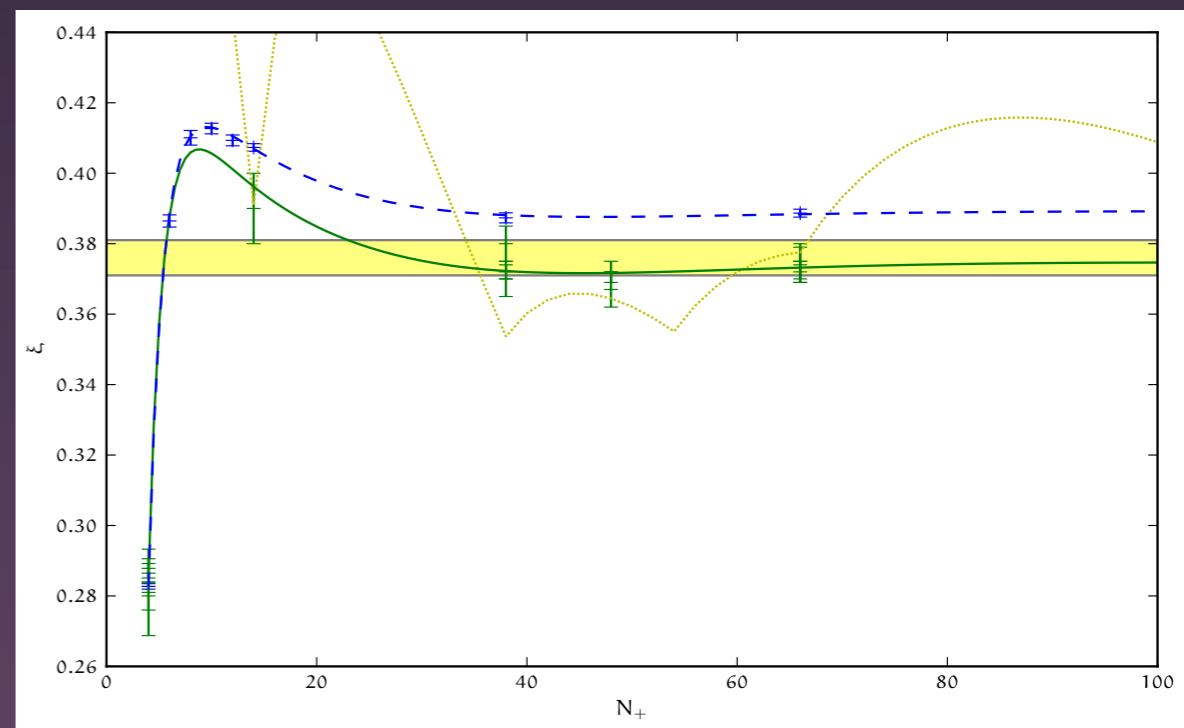


Forbes, Gandolfi, Gezerlis [PRA 86 (2012) 053603]

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/α)
 - Hartree (β), Pairing (g)



Forbes, Gandolfi, Gezerlis [PRA 2012]

BdG: contained in SLDA

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

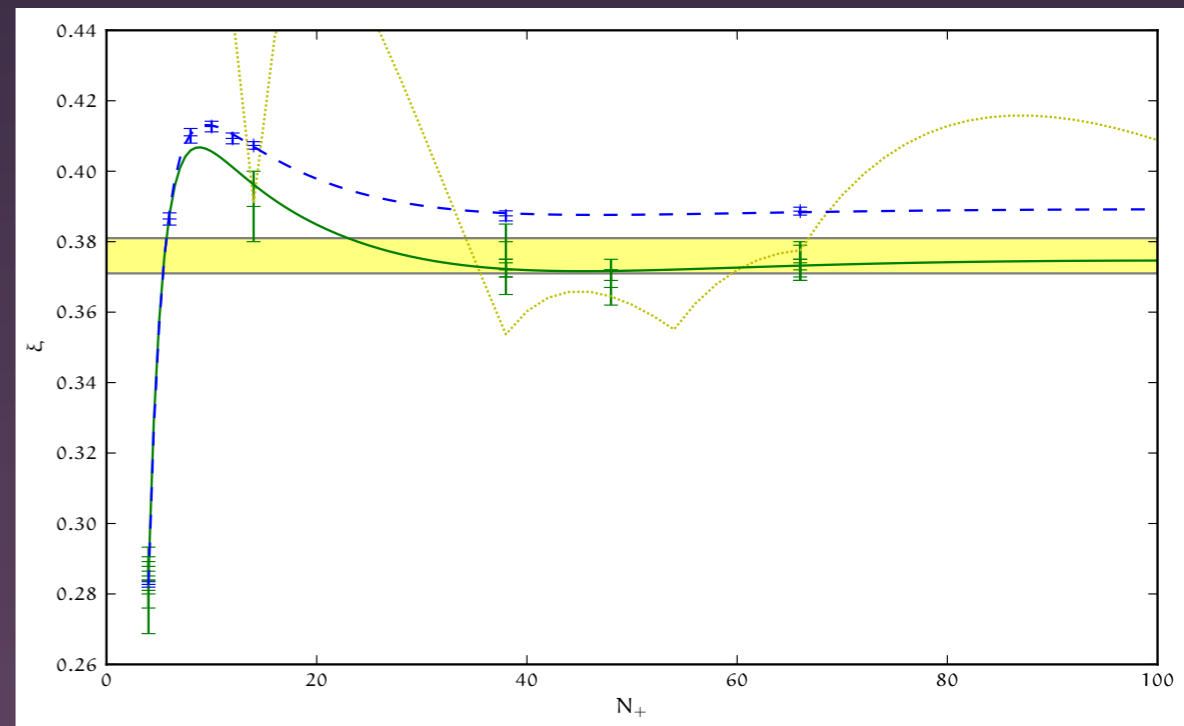
$\langle \nabla \hat{a}^\dagger \nabla \hat{a} \rangle + \langle \nabla \hat{b}^\dagger \nabla \hat{b} \rangle$ $\langle \hat{a}^\dagger \hat{b}^\dagger \rangle \langle \hat{b} \hat{a} \rangle$

- 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

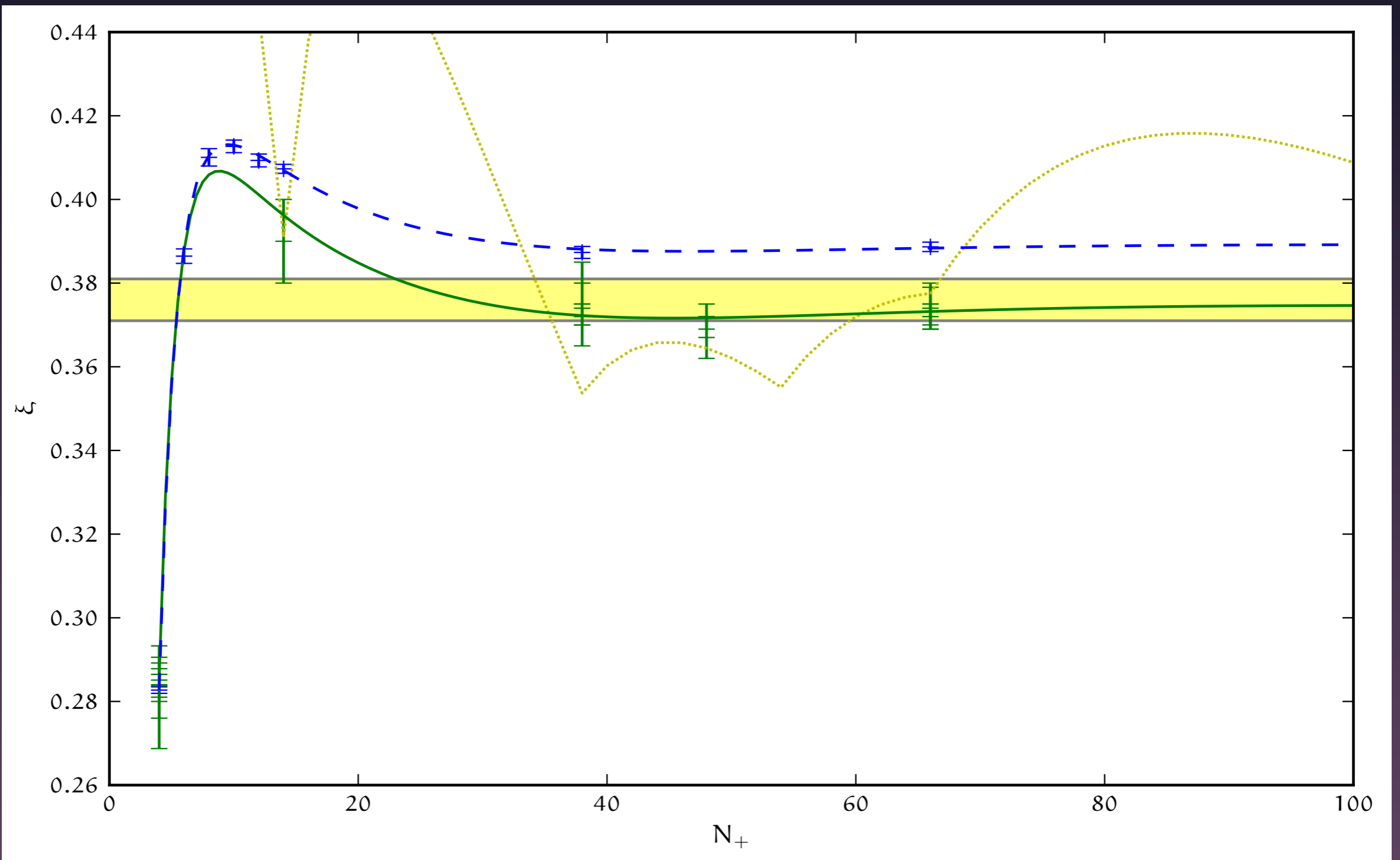
$$\mathcal{E}(n, \tau, \nu) = \alpha \frac{\tau}{m} + \beta \frac{(3\pi^2 n)^{5/3}}{10m\pi^2} + g_{\text{eff}} \nu^\dagger \nu$$

- 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)

SLDA: Superfluid Local

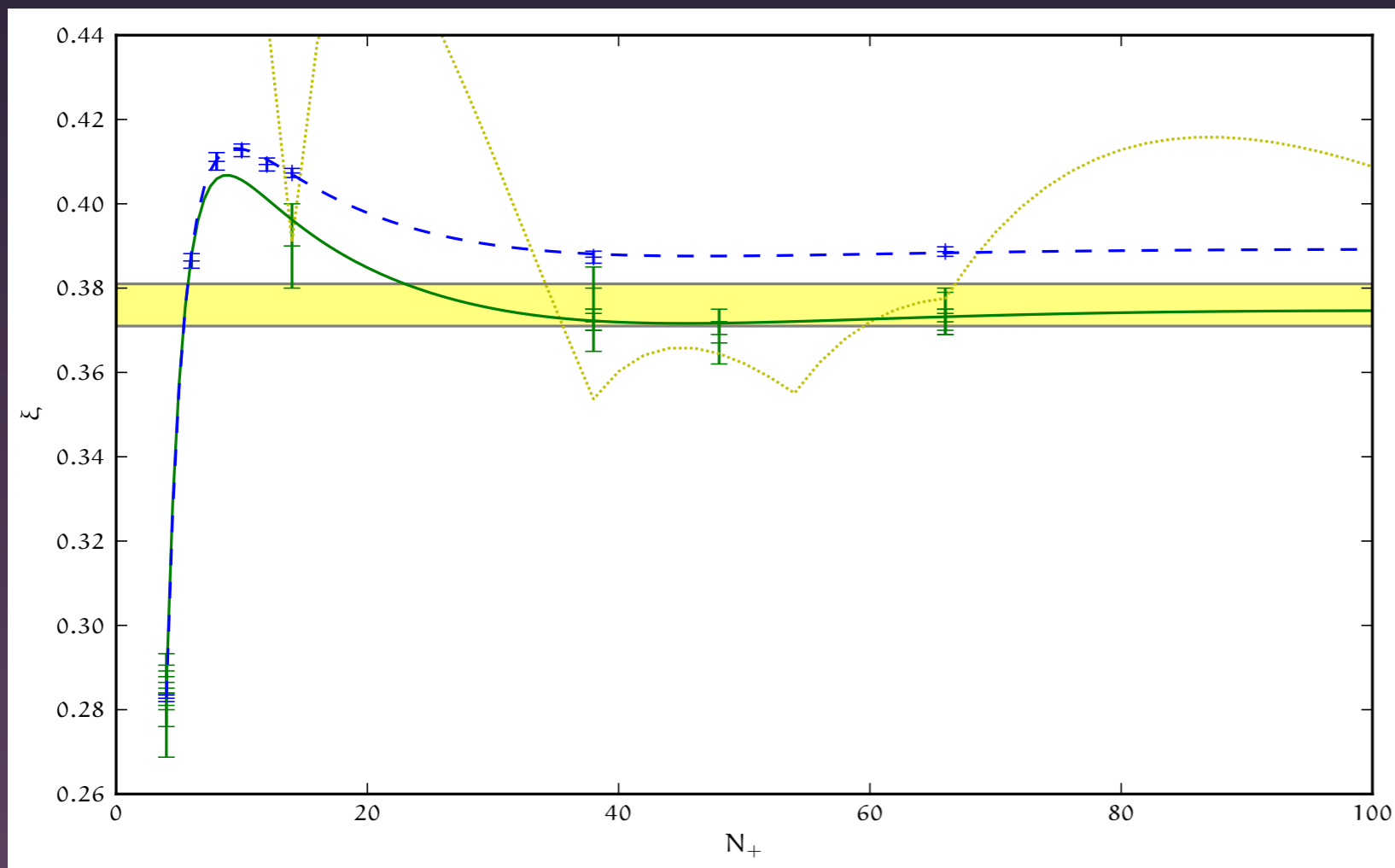


Forbes, Gandolfi, Gezerlis (2012)

Unbiased SLDA fit at

$$r_{\text{eff}} = 0$$

N_+	ξ_{N_+}	Method
2	-0.415332919...	exact (see section II C)
4	0.288(3), 0.286(3)	exact diagonalization [18]
"	0.28(1)	AFMC [18]
"	0.280(4)	AFMC [12]
14	0.39(1)	AFMC [12]
38	0.370(5), 0.372(2), 0.380(5)	AFMC [12]
48	0.372(3), 0.367(5)	AFMC [12]
66	0.374(5), 0.372(3), 0.375(5)	AFMC [12]
10^6	0.376(5)	experiment [5]



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)

Normal State				Superfluid State			
(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)	(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)
(3,1)	6.6 ± 0.01	6.687	1.3%	(1,1)	2.002 ± 0	2.302	15%
(4,1)	8.93 ± 0.01	8.962	0.36%	(2,2)	5.051 ± 0.009	5.405	7%
(5,1)	12.1 ± 0.1	12.22	0.97%	(3,3)	8.639 ± 0.03	8.939	3.5%
(5,2)	13.3 ± 0.1	13.54	1.8%	(4,4)	12.573 ± 0.03	12.63	0.48%
(6,1)	15.8 ± 0.1	15.65	0.93%	(5,5)	16.806 ± 0.04	16.19	3.7%
(7,2)	19.9 ± 0.1	20.11	1.1%	(6,6)	21.278 ± 0.05	21.13	0.69%
(7,3)	20.8 ± 0.1	21.23	2.1%	(7,7)	25.923 ± 0.05	25.31	2.4%
(7,4)	21.9 ± 0.1	22.42	2.4%	(8,8)	30.876 ± 0.06	30.49	1.2%
(8,1)	22.5 ± 0.1	22.53	0.14%	(9,9)	35.971 ± 0.07	34.87	3.1%
(9,1)	25.9 ± 0.1	25.97	0.27%	(10,10)	41.302 ± 0.08	40.54	1.8%
(9,2)	26.6 ± 0.1	26.73	0.5%	(11,11)	46.889 ± 0.09	45	4%
(9,3)	27.2 ± 0.1	27.55	1.3%	(12,12)	52.624 ± 0.2	51.23	2.7%
(9,5)	30 ± 0.1	30.77	2.6%	(13,13)	58.545 ± 0.18	56.25	3.9%
(10,1)	29.4 ± 0.1	29.41	0.034%	(14,14)	64.388 ± 0.31	62.52	2.9%
(10,2)	29.9 ± 0.1	30.05	0.52%	(15,15)	70.927 ± 0.3	68.72	3.1%
(10,6)	35 ± 0.1	35.93	2.7%	(1,0)	1.5 ± 0.0	1.5	0%
(20,1)	73.78 ± 0.01	73.83	0.061%	(2,1)	4.281 ± 0.004	4.417	3.2%
(20,4)	73.79 ± 0.01	74.01	0.3%	(3,2)	7.61 ± 0.01	7.602	0.1%
(20,10)	81.7 ± 0.1	82.57	1.1%	(4,3)	11.362 ± 0.02	11.31	0.49%
(20,20)	109.7 ± 0.1	113.8	3.7%	(7,6)	24.787 ± 0.09	24.04	3%
(35,4)	154 ± 0.1	154.1	0.078%	(11,10)	45.474 ± 0.15	43.98	3.3%
(35,10)	158.2 ± 0.1	158.6	0.27%	(15,14)	69.126 ± 0.31	62.55	9.5%
(35,20)	178.6 ± 0.1	180.4	1%				

Within few % except for smallest systems

Can add gradients

Forbes [arXiv:1211.3779]

From Bulgac, Forbes, and Magierski [arXiv:1008.3933] with FNDMC data from Blume, von Stecher, and Greene, PRL 99, 233201 (2007) and Blume, PRA 78, 013635 (2008)

What about Dynamics?

Realtime Evolution

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

- No diagonalization needed for evolution

Just apply Hamiltonian

Use FFT for kinetic term

- Efficient realtime evolution the scales well

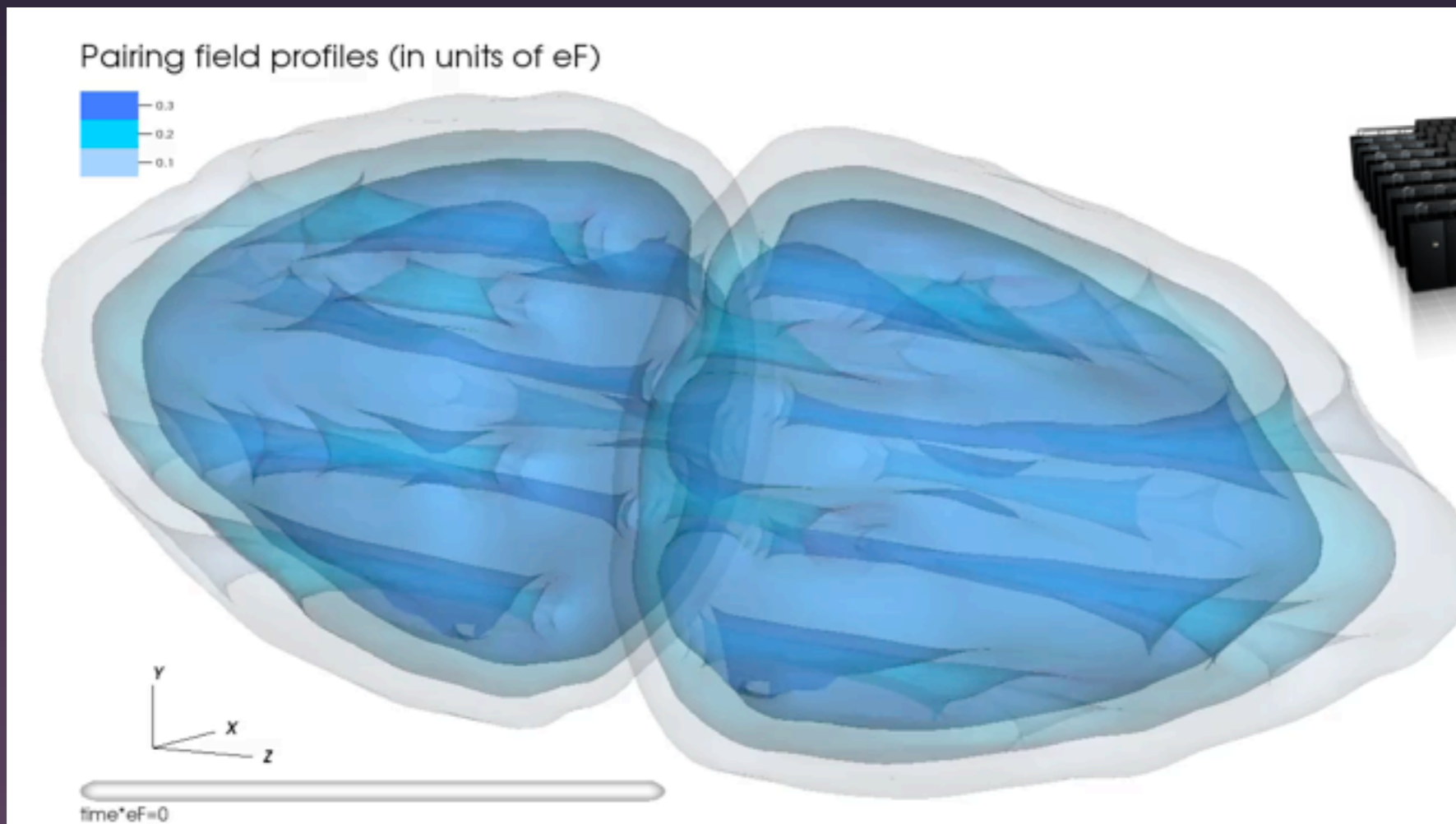
Distribute wavefunctions over nodes

Utilize GPUS

- Split Operator or ABM evolution

DFT: Fermion still hard

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

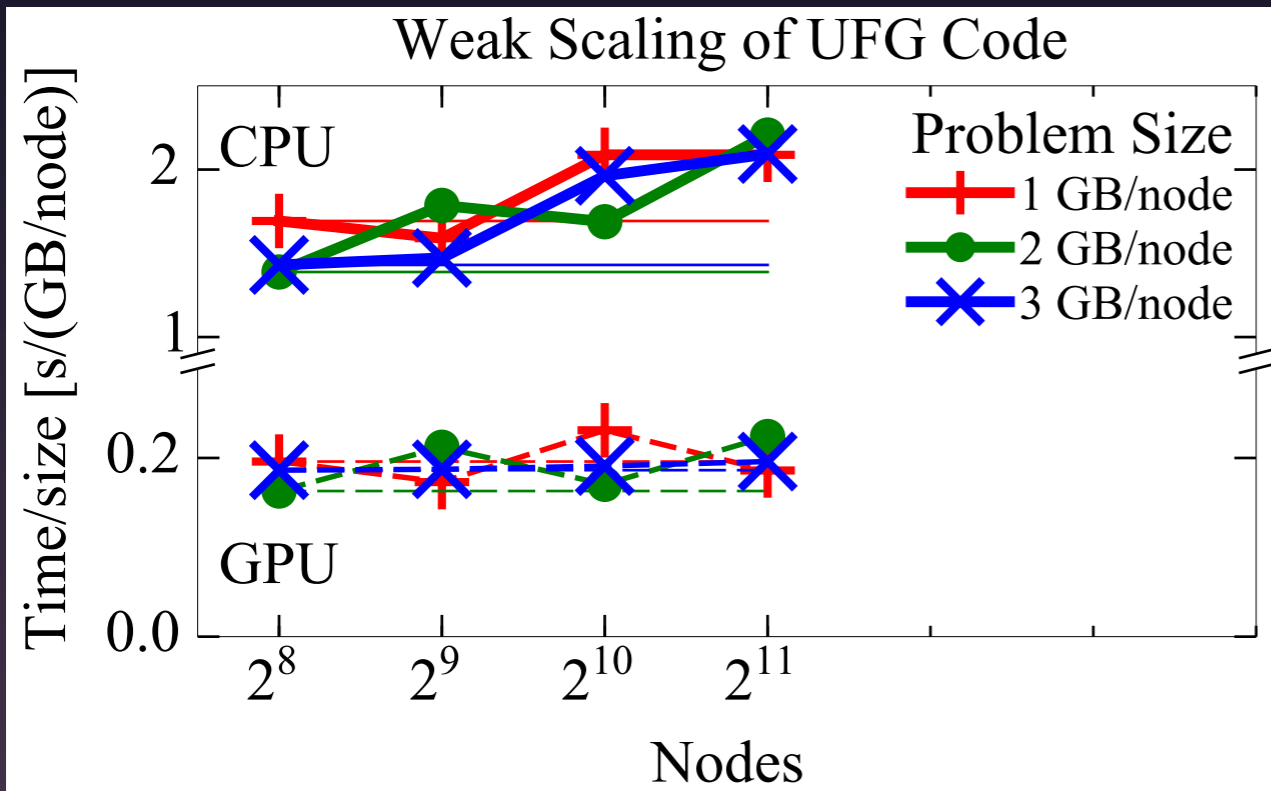


- 48×48×128 lattice
- 131 629 two-component wavefunctions
- 1TB per state

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

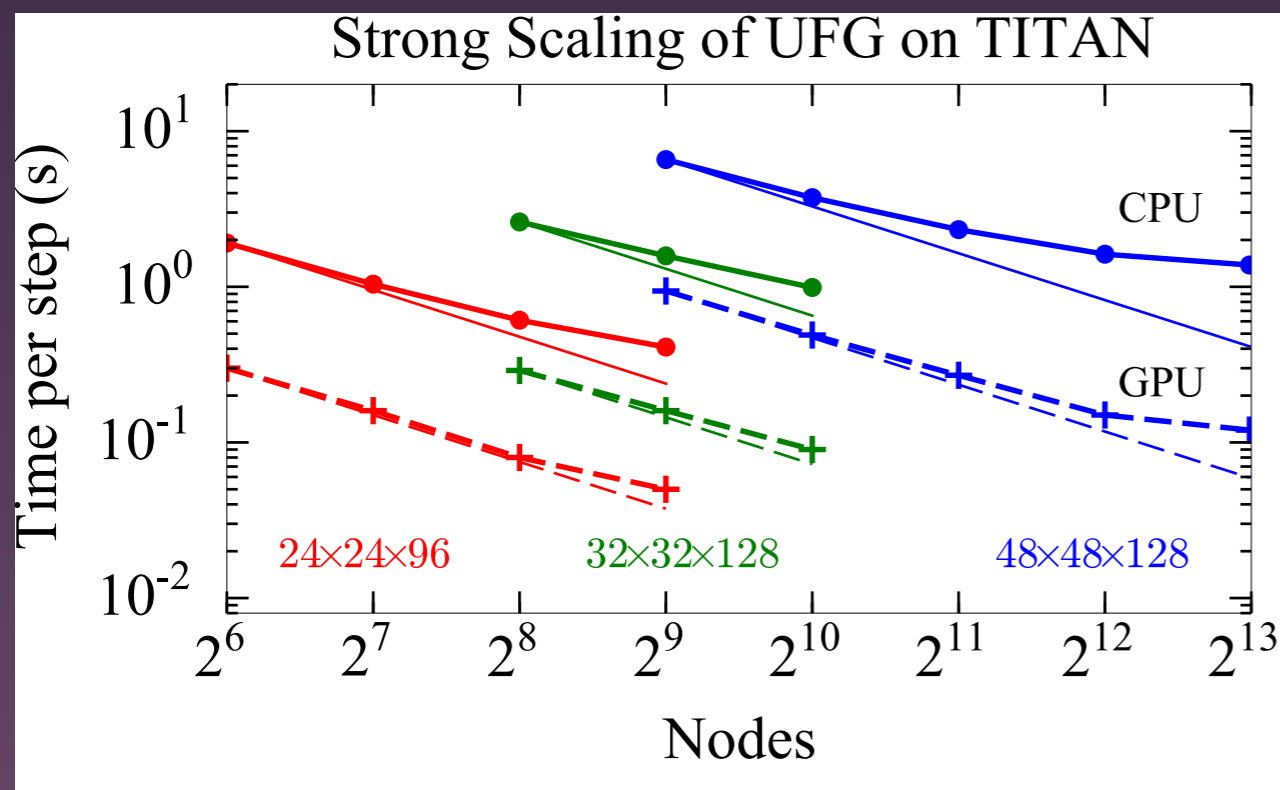
$N N_x^3 N_t$

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

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

- 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

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

- 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: $V_t = \text{diag}(i[H, \rho]^\dagger)$

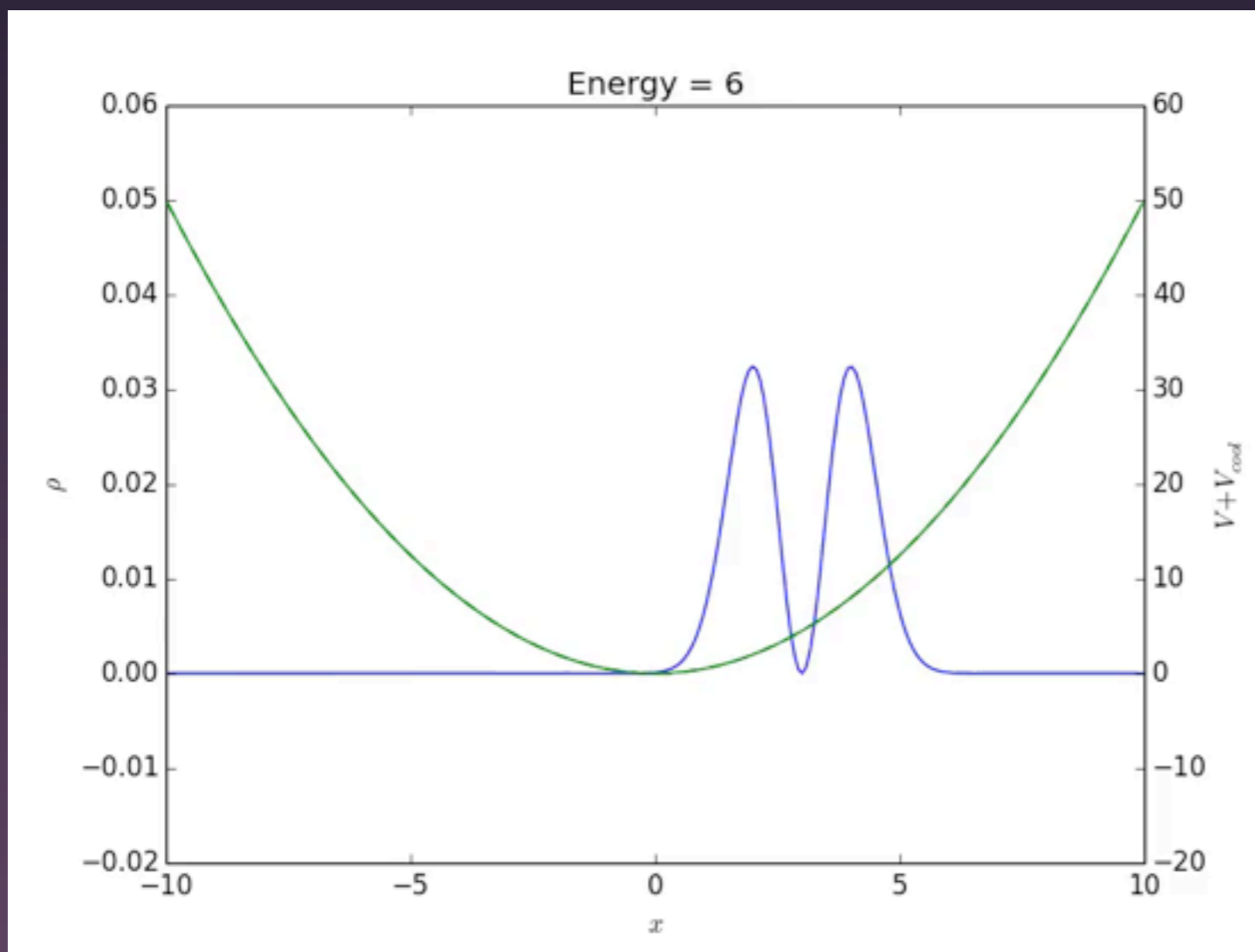
Quantum Friction

Potential counteracts
currents

Use with dynamics to
minimize energy

Harmonic oscillator with an excited state

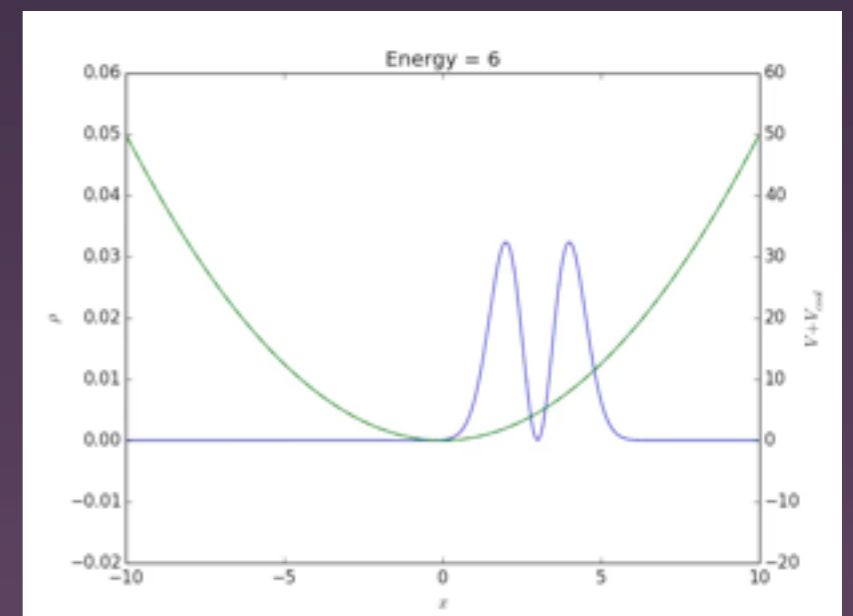
Quantum Friction



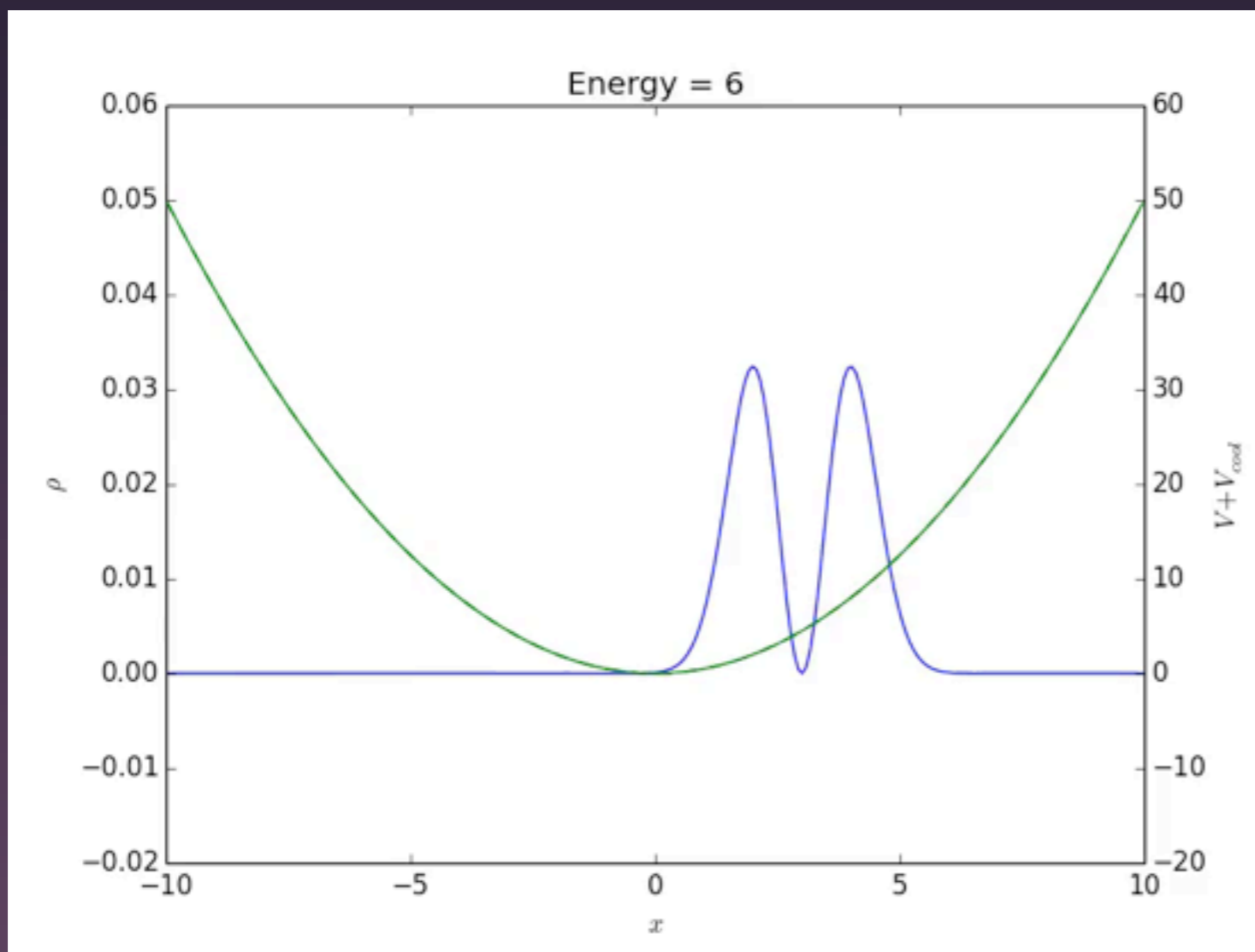
Harmonic oscillator with an excited state

Potential counteracts currents

Use with dynamics to minimize energy



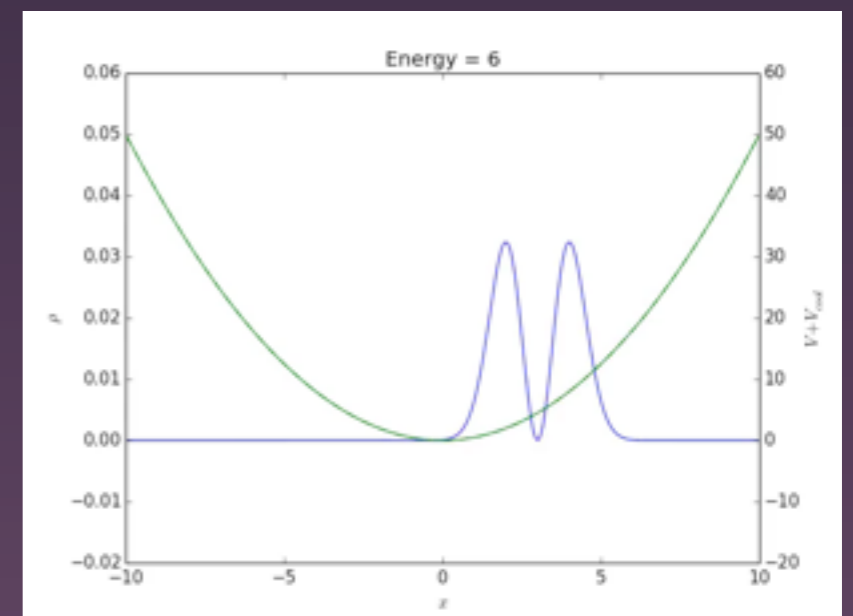
Quantum Friction



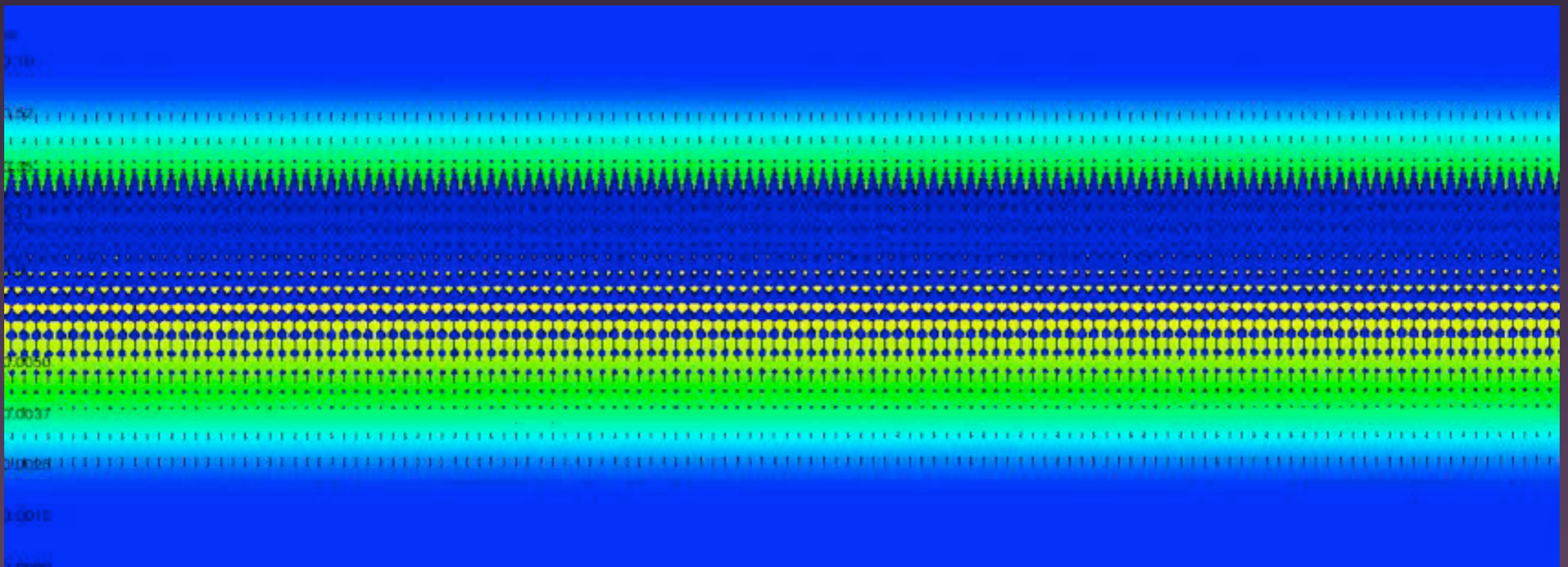
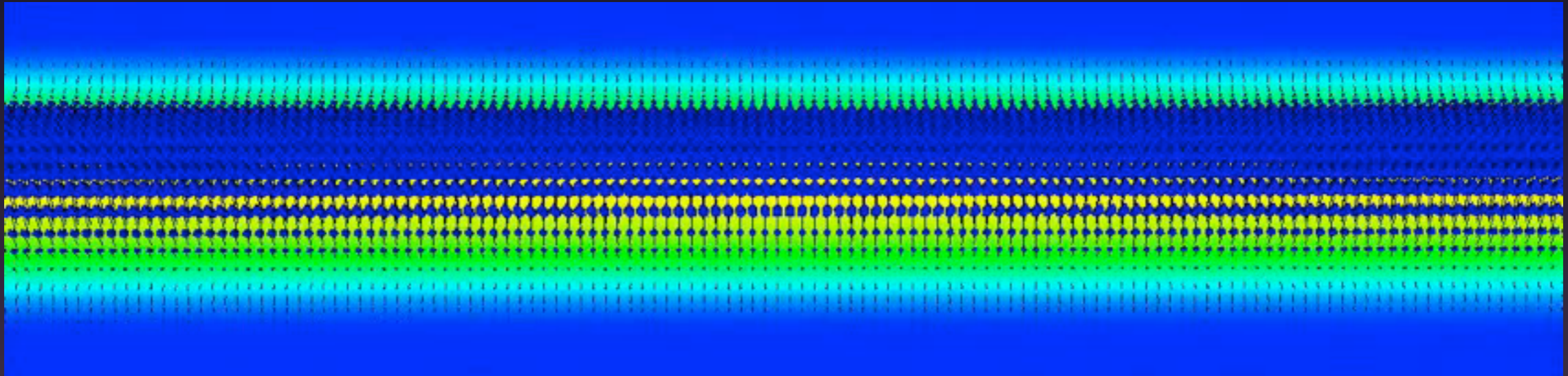
Harmonic oscillator with an excited state

Potential counteracts currents

Use with dynamics to minimize energy



State Preparation



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

Quantum Friction

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

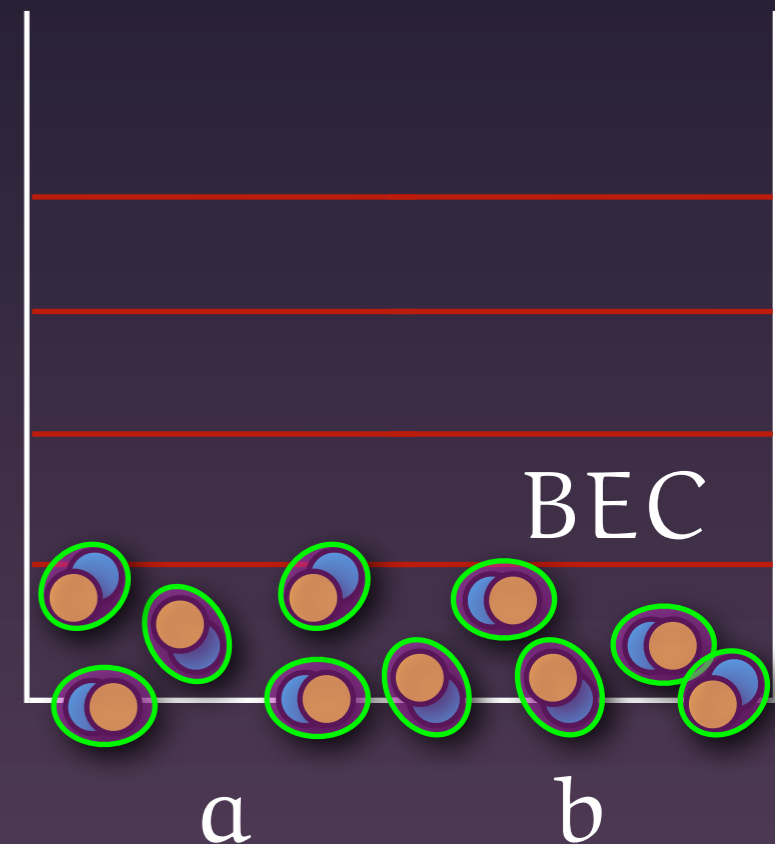
- General method: (works for many problems)
Needs a good initial state to ensure reasonable occupation numbers
- Easy to compute: local time-dependent potential
Acts to remove local currents
- Couple with quasi-adiabatic state preparation
Bulgac, Forbes, Roche, and Wlazłowski (2013) [arXiv:1305.6891]

Bosons are “easy”

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

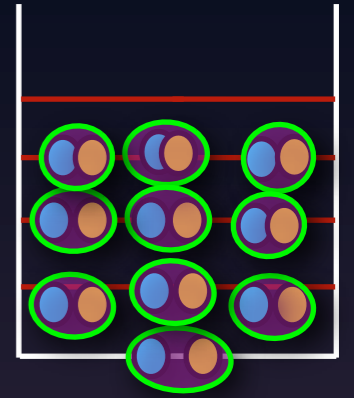
$$i\partial_t\Psi = \left(-\frac{\nabla^2}{2m_B} + [V + g|\Psi|^2] \right) \Psi$$

- 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



$$N_x^3 N_t$$

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

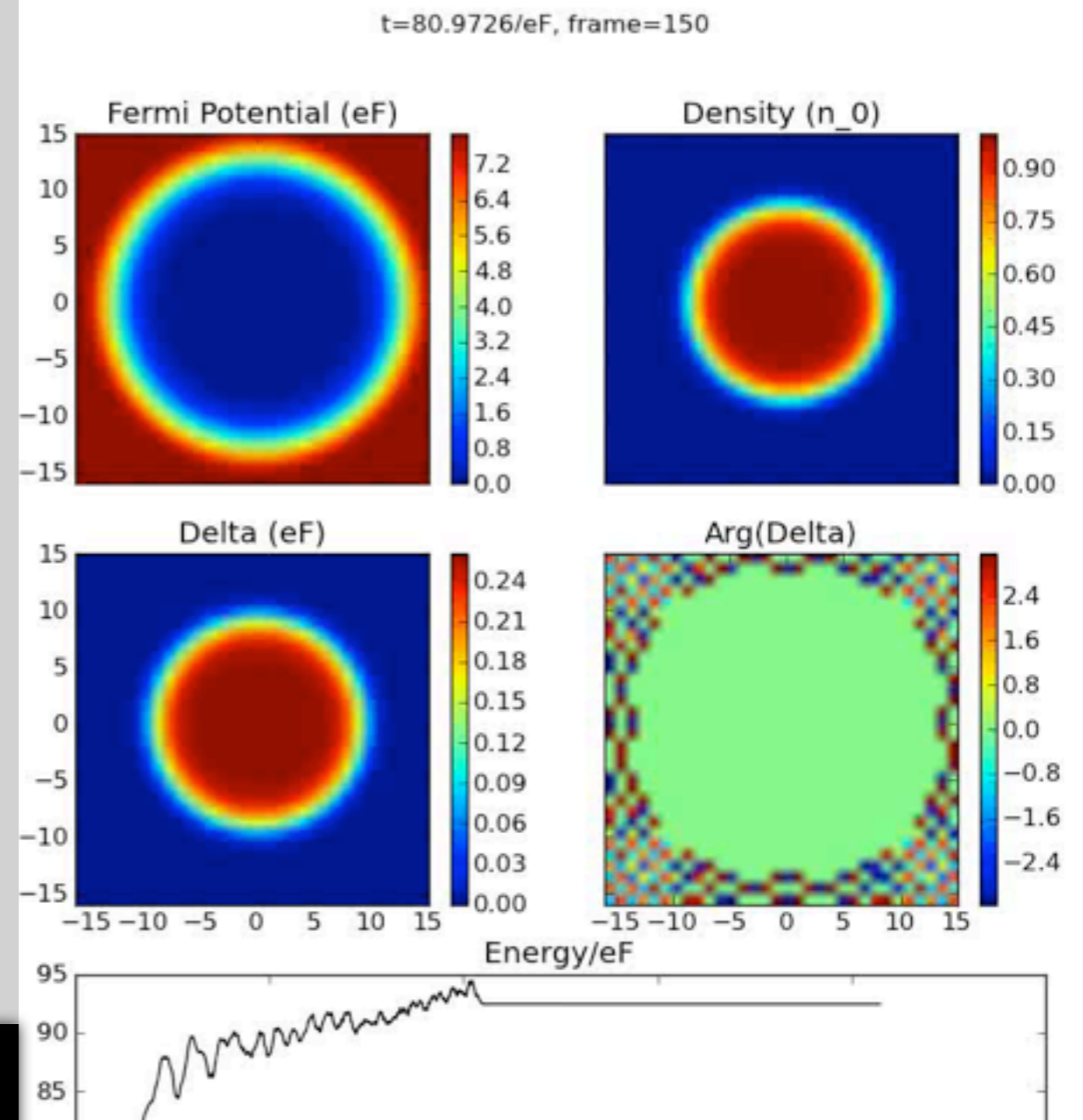
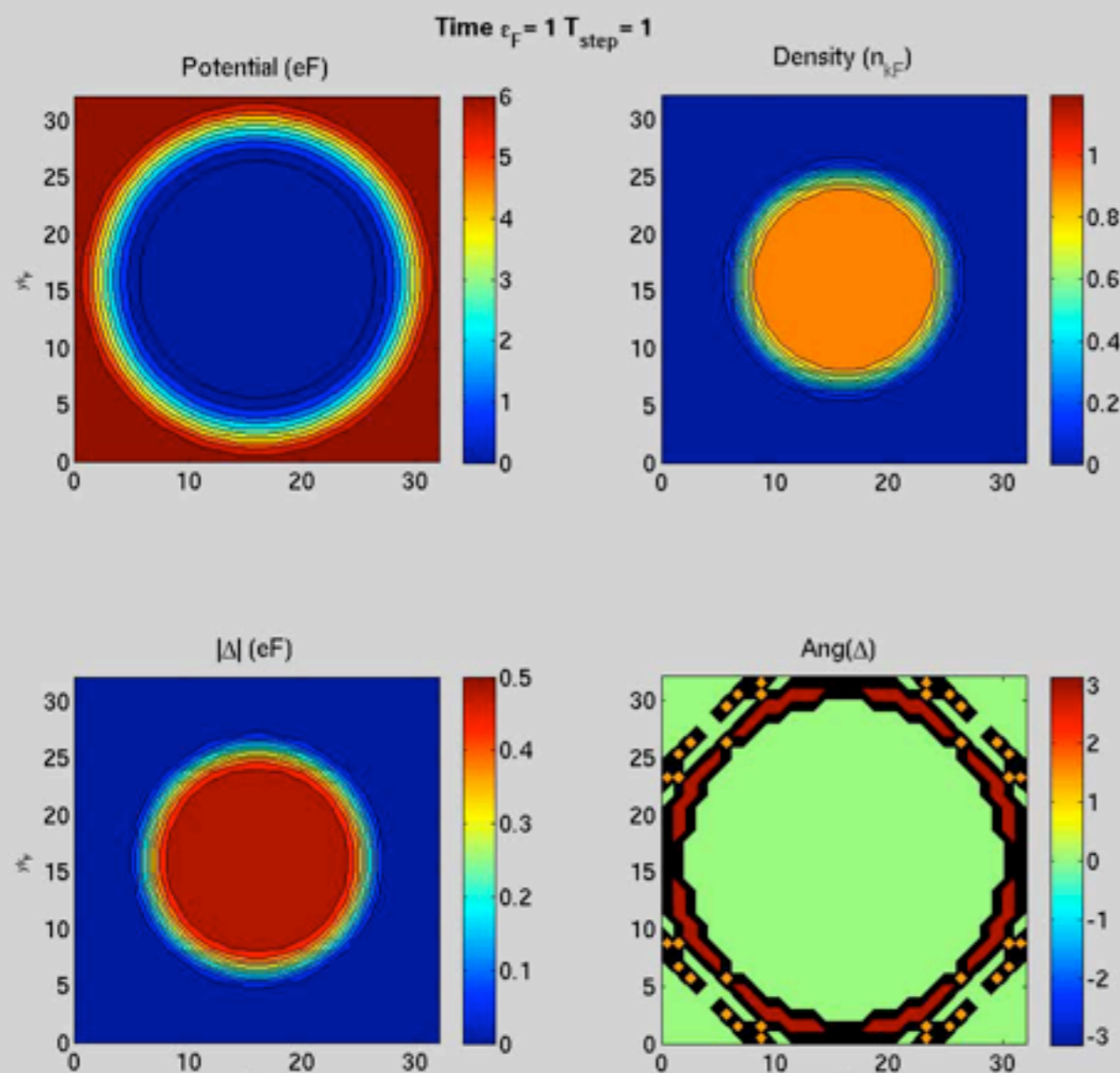
$$\epsilon_F = \mathcal{E}'_{FG}(\rho_F) \propto \rho_F^{3/2}$$

- “Extended Thomas-Fermi” (ETF) model

Comparison

Fermions
SLDA TDDFT

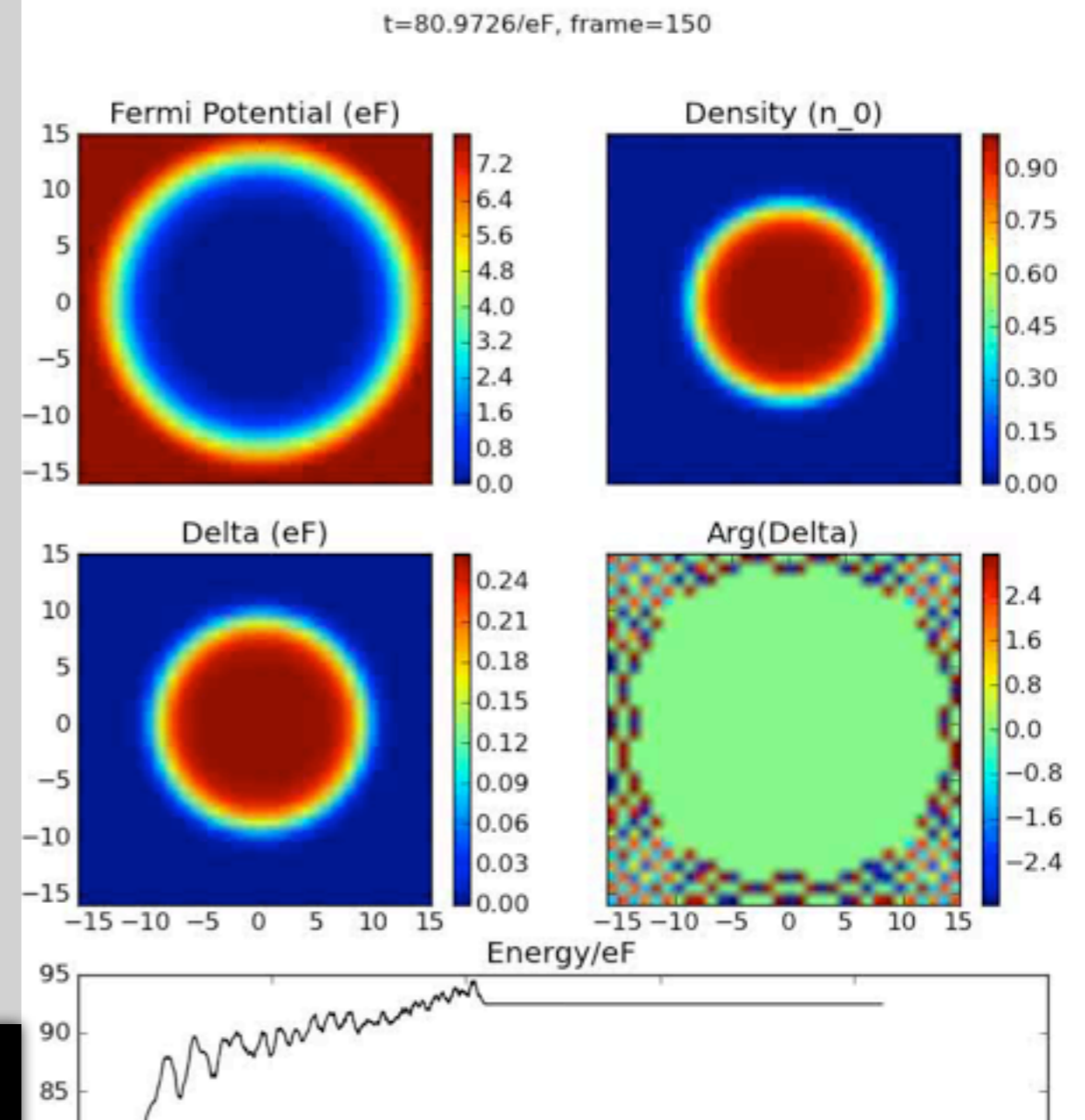
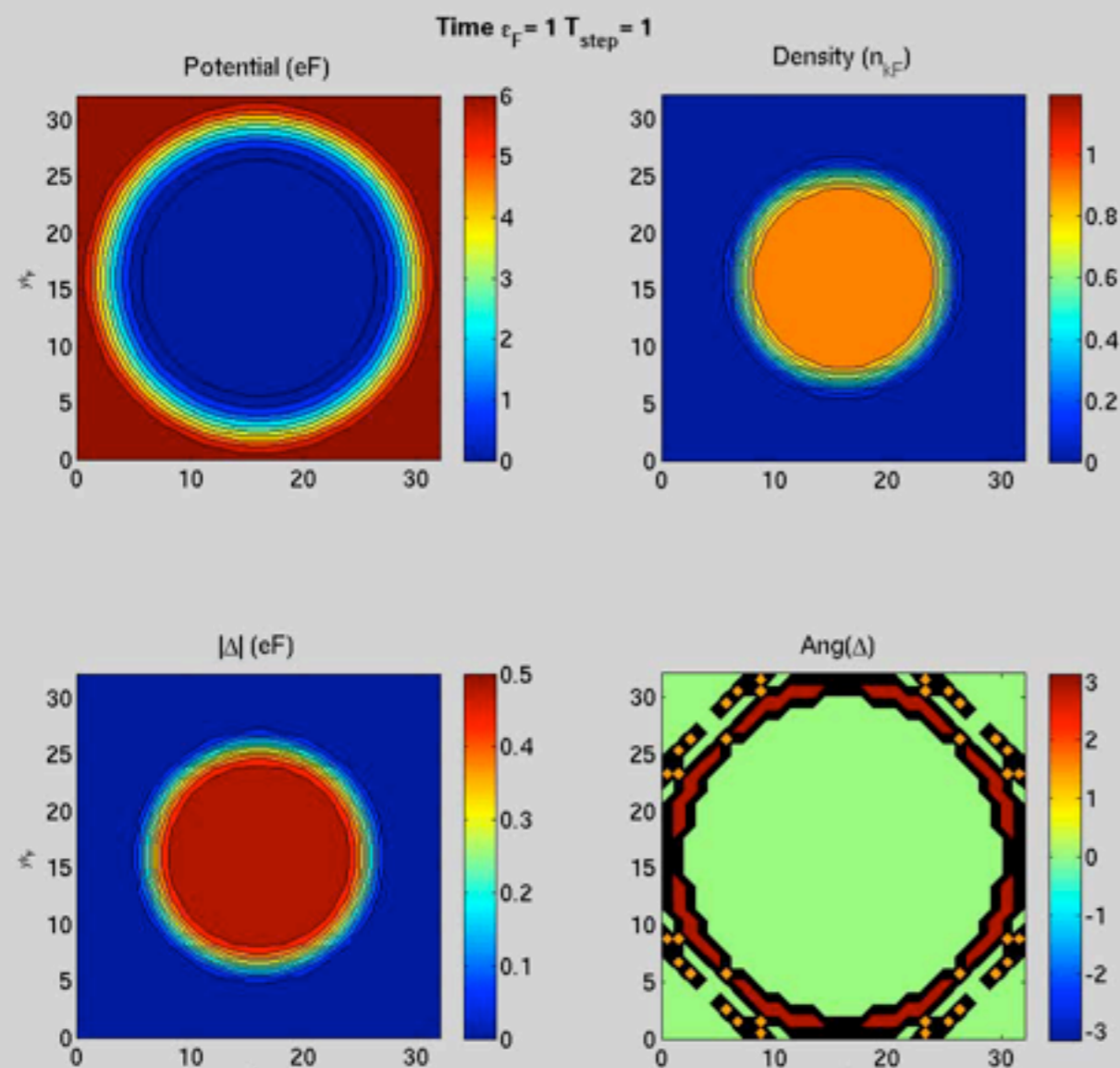
Gross Pitaevskii
model



Bulgac et al. (Science 2011)

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

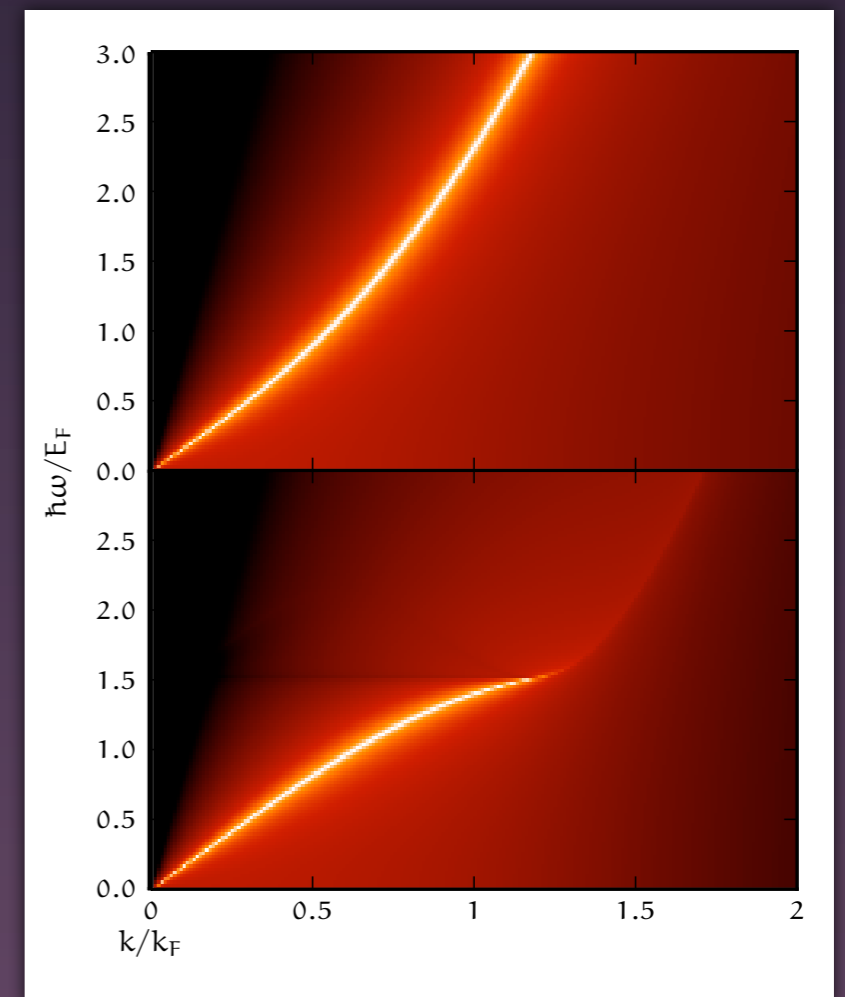
- GPE:
- Simulation much easier!
- Evolve 1 wavefunction
- Use supercomputers to study large volumes



Bulgac et al. (Science 2011)

Matching Theories: The Good

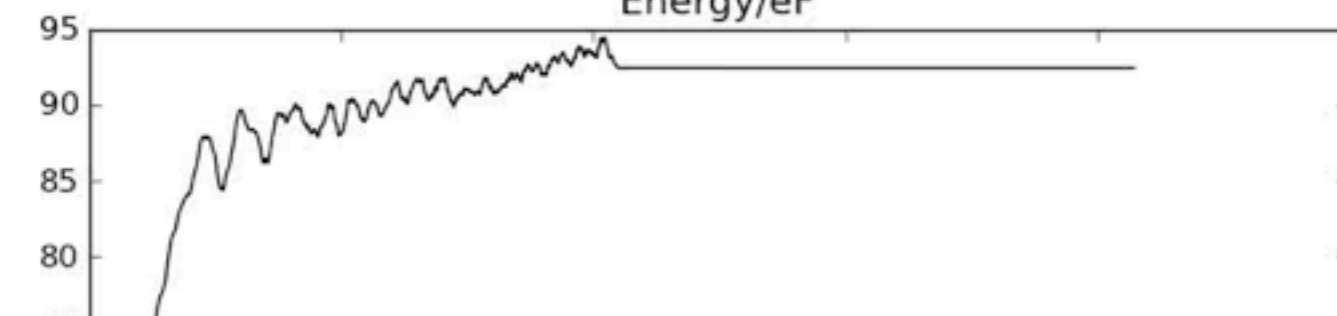
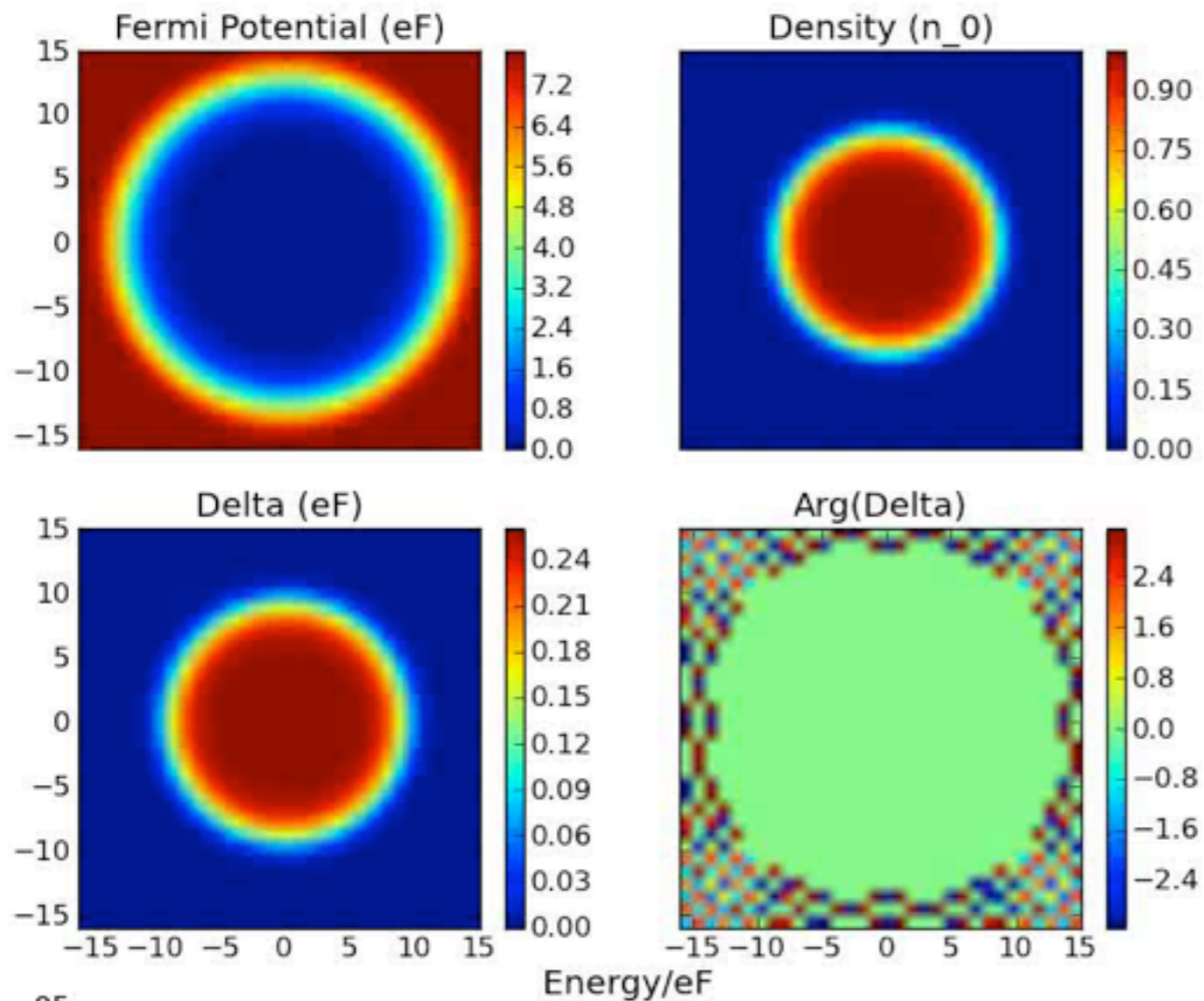
- Galilean Covariance (fixes mass/density relationship)
- Equation of State
- Hydrodynamics
 - speed of sound (exact)
 - phonon dispersion (to order q^3)
 - static response (to order q^2)



Forbes and Sharma (PRA 2014)

What is missing?

$t=80.9726/eF$, frame=150

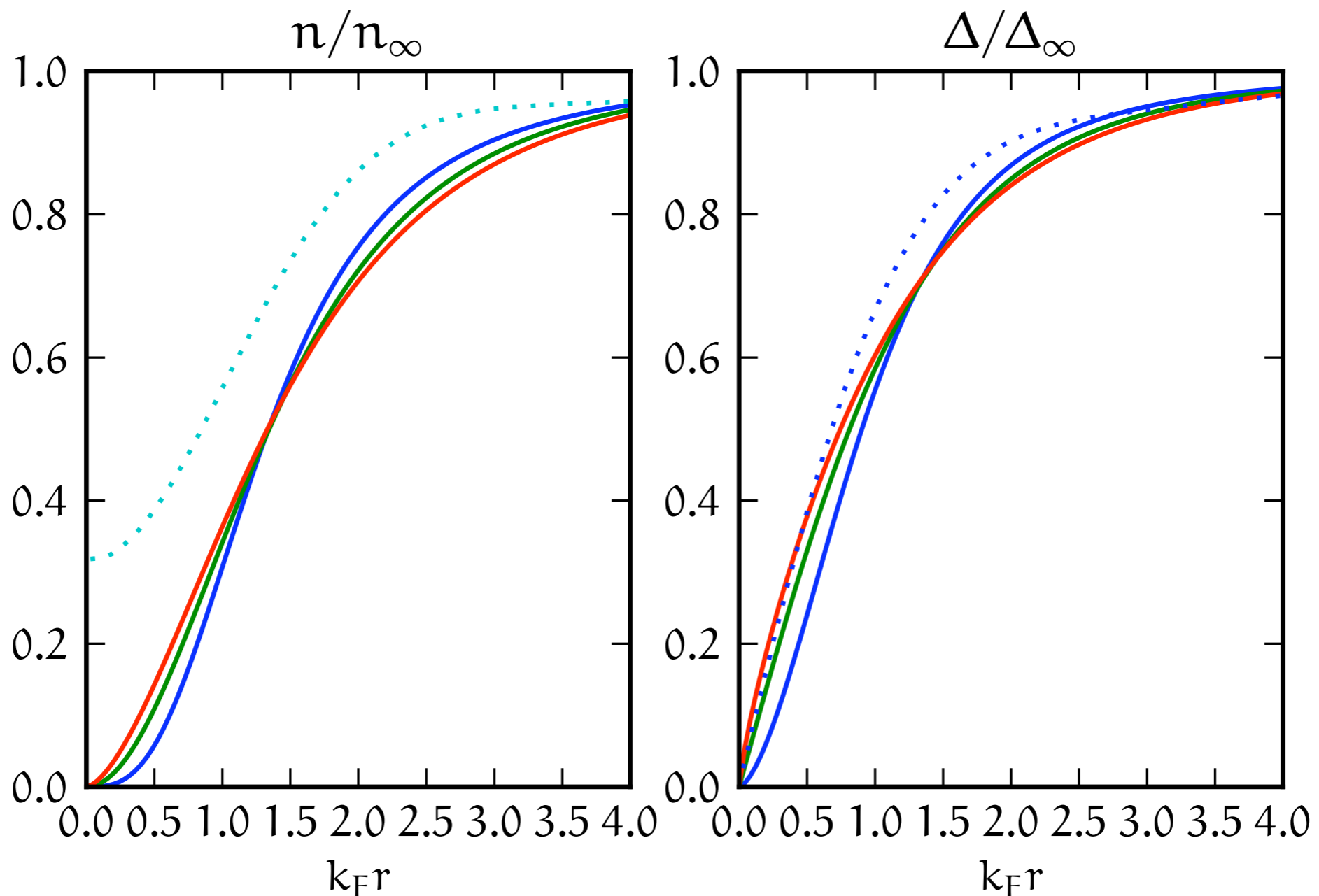


- Excessive phonon noise
- Short-wavelength
- Dissipation
- Vortex lattice doesn't crystallize
- Incorrect vortex mass
- Vortices move too slowly

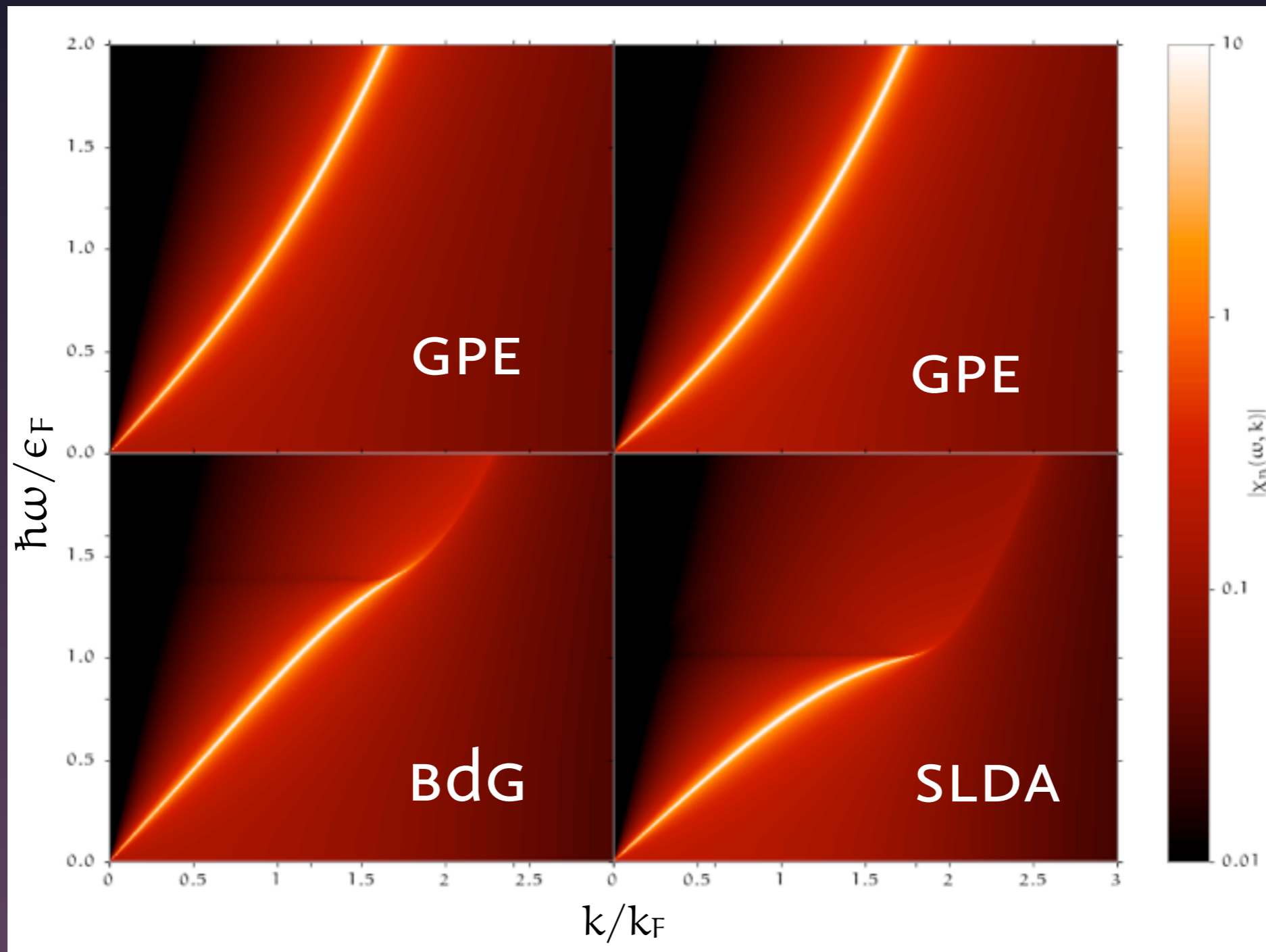
Matching Theories: The Bad

- GPE has $\rho=2|\Psi|^2$
 - 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)

Vortex Structure (empty core)

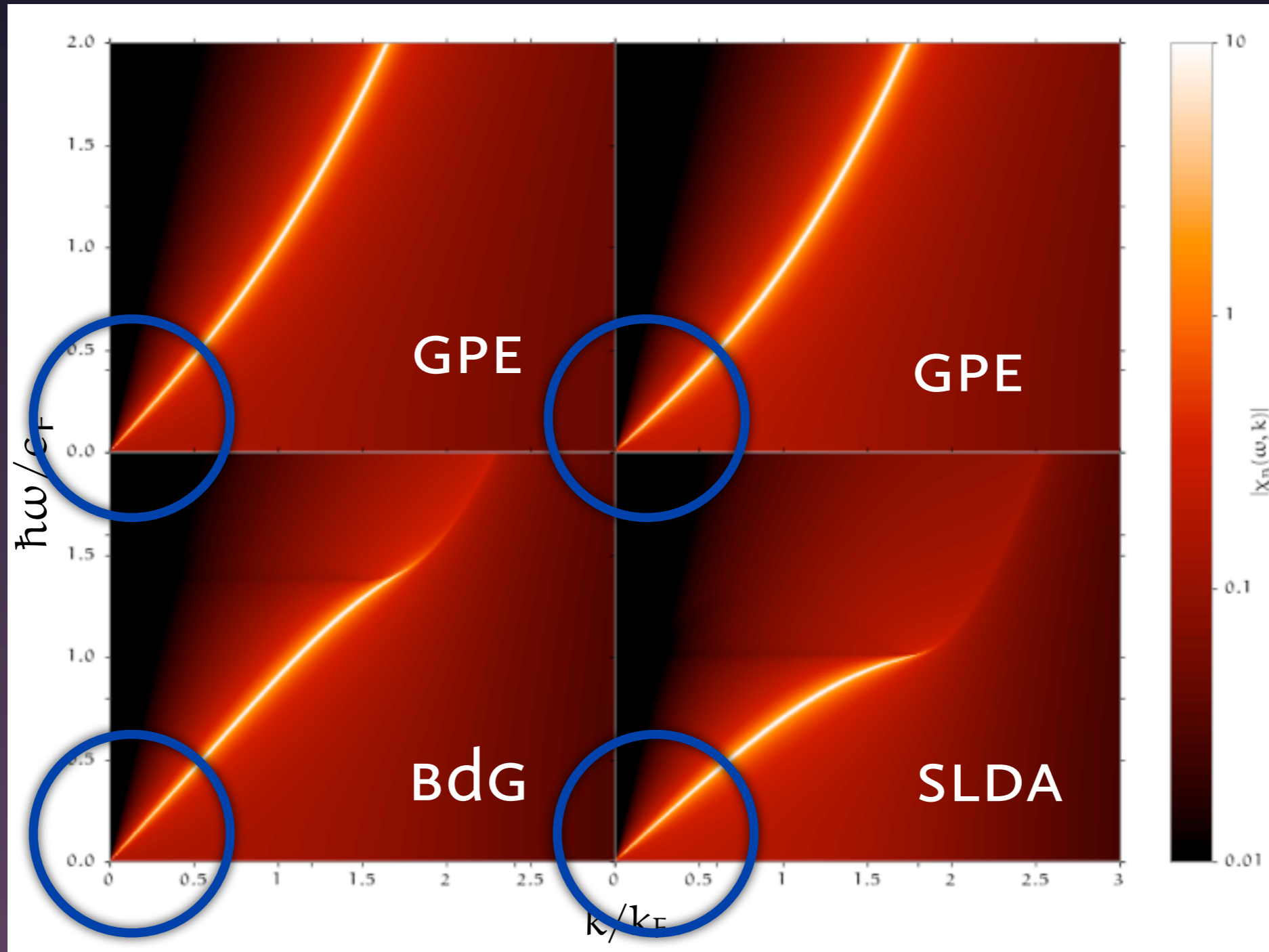


Linear Response



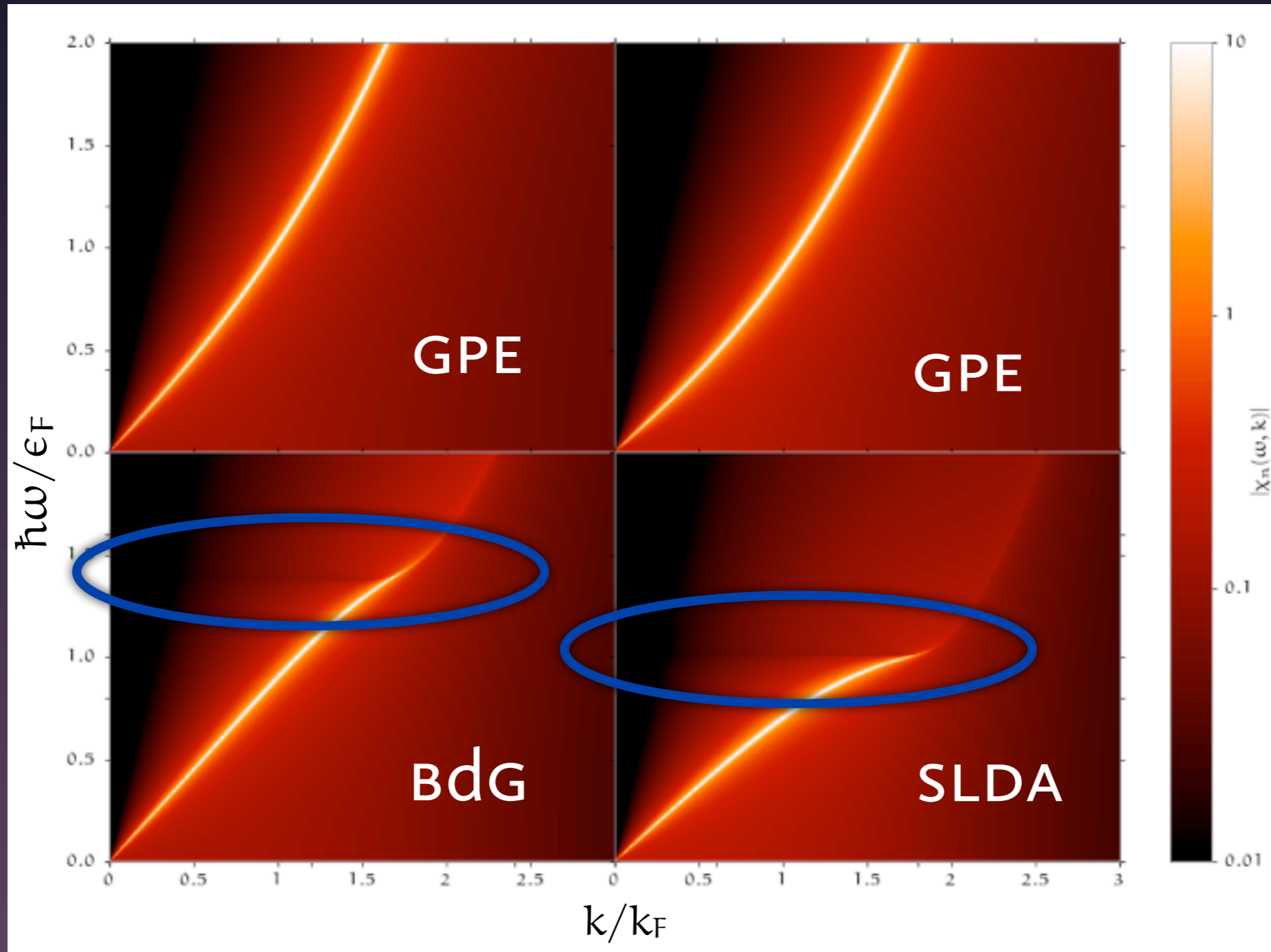
Michael Forbes and Rishi Sharma PRA 90 (2014) 043638

Low energy Phonons



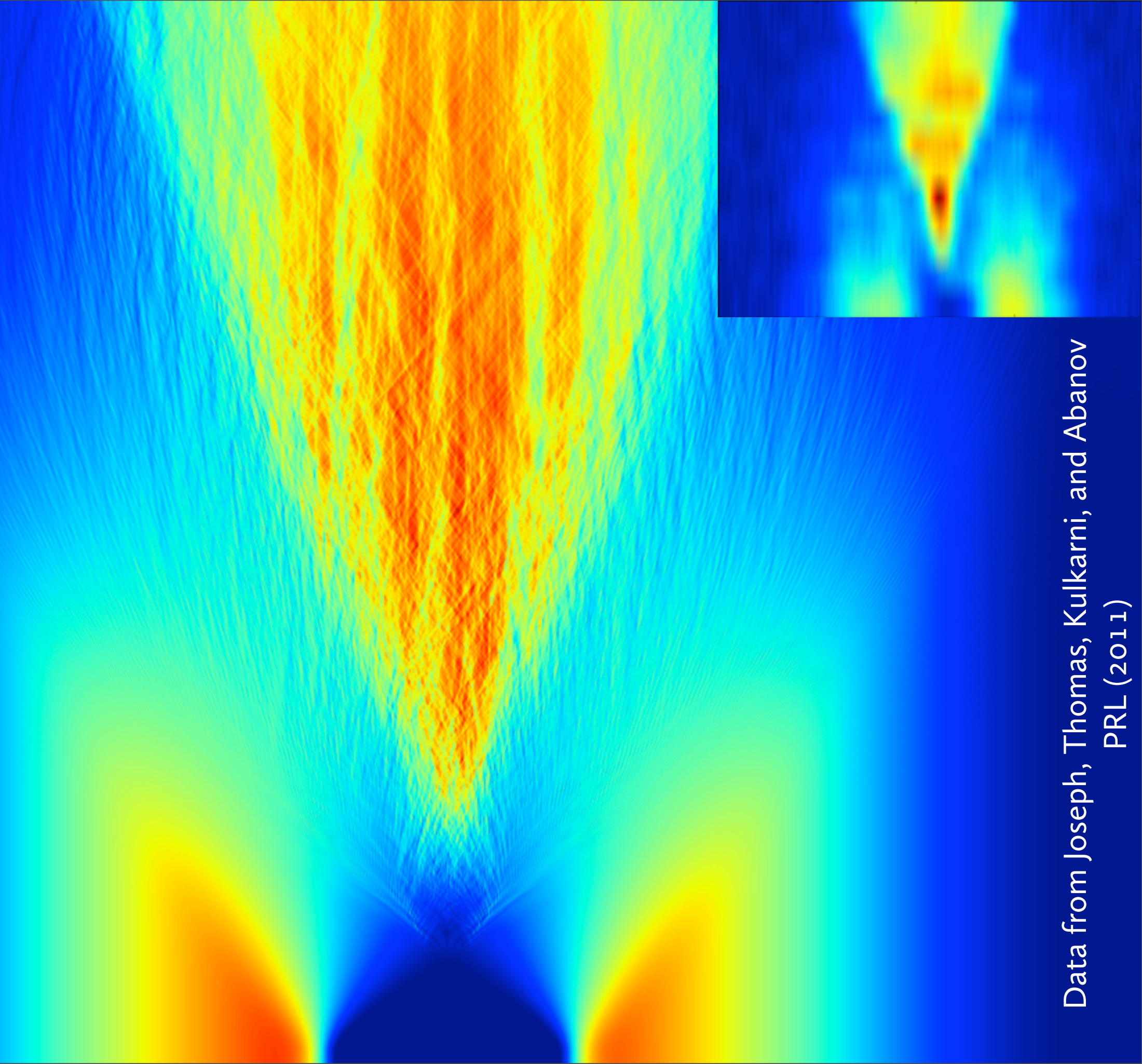
Michael Forbes and Rishi Sharma PRA 90 (2014) 043638

Missing Pair-breaking



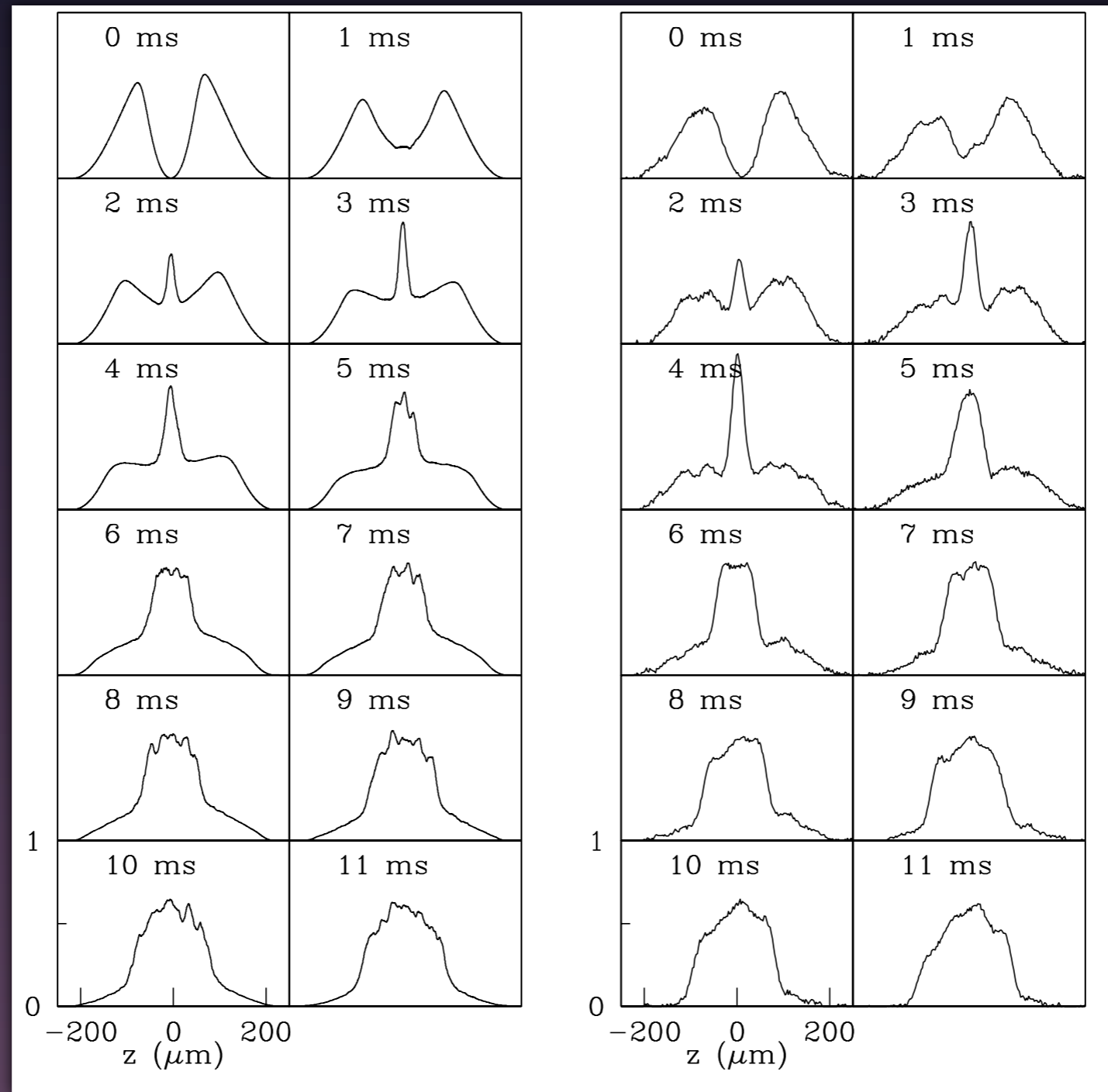
Michael Forbes and Rishi Sharma PRA 90 (2014) 043638

2D GPE simulation



Data from Joseph, Thomas, Kulkarni, and Abanov
PRL (2011)

GPE vs. Experiment



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

Conjecture

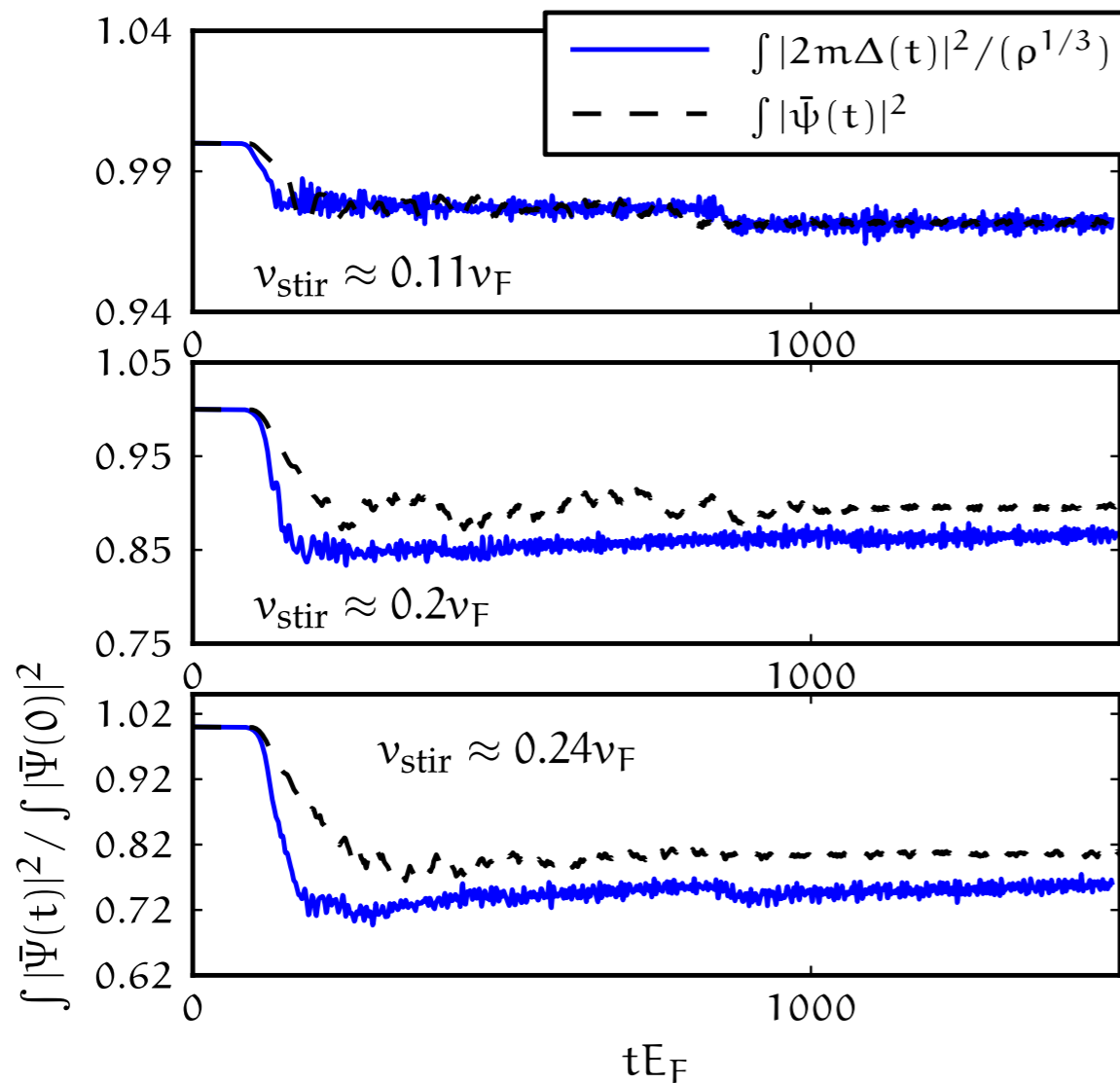


FIG. 8. (Color online) Conservation of the integrated squared pairing gap (squared smoothed ψ) for the simulations for $v_{\text{stir}} = 0.1v_F$ ($v_{\text{stir}} = 0.11v_F$), $v_{\text{stir}} = 0.2v_F$ ($v_{\text{stir}} = 0.197v_F$), and $v_{\text{stir}} = 0.25v_F$ ($v_{\text{stir}} = 0.242v_F$) for 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%.

Resolve with:

Two-fluid hydrodynamics
Normal + Superfluid

Conversion via coarse-graining/
condensation

Provide dissipation - mocks pair-
breaking

Normal fluid will fill vortices

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

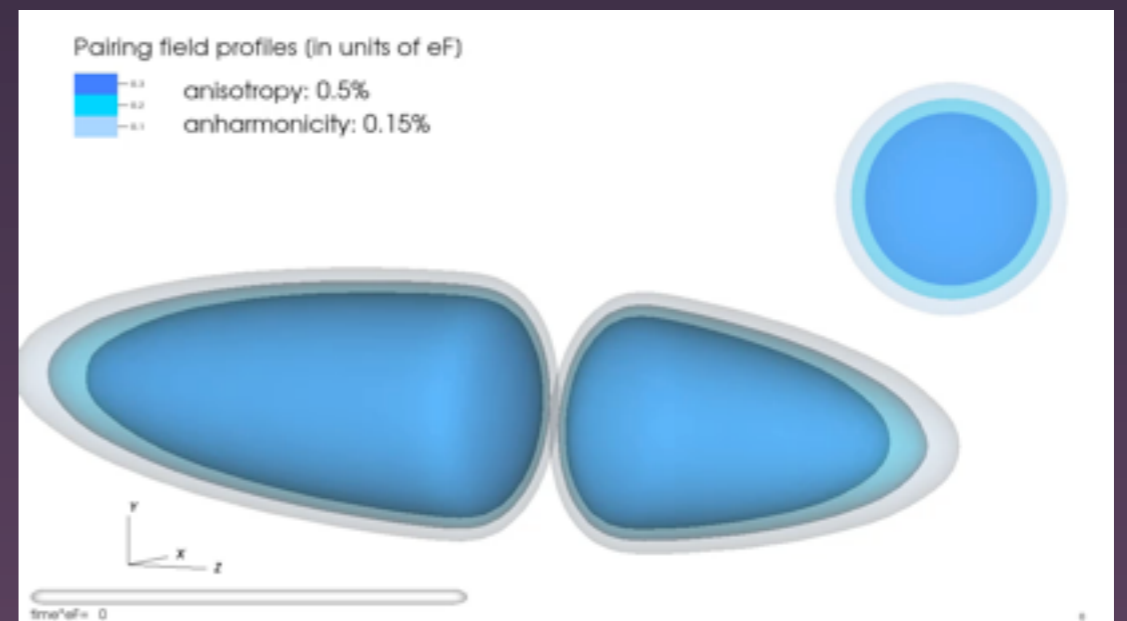
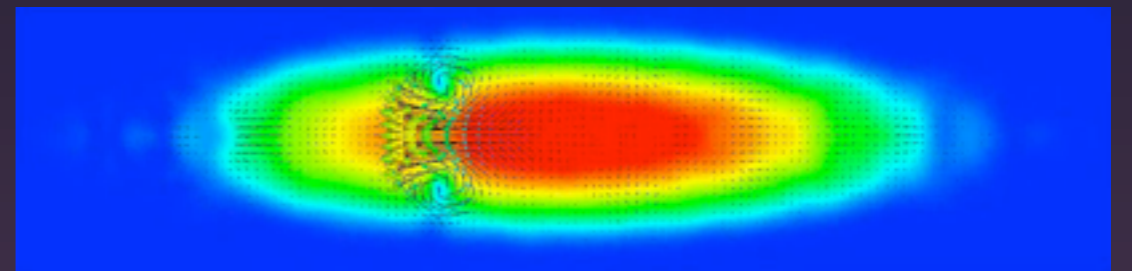
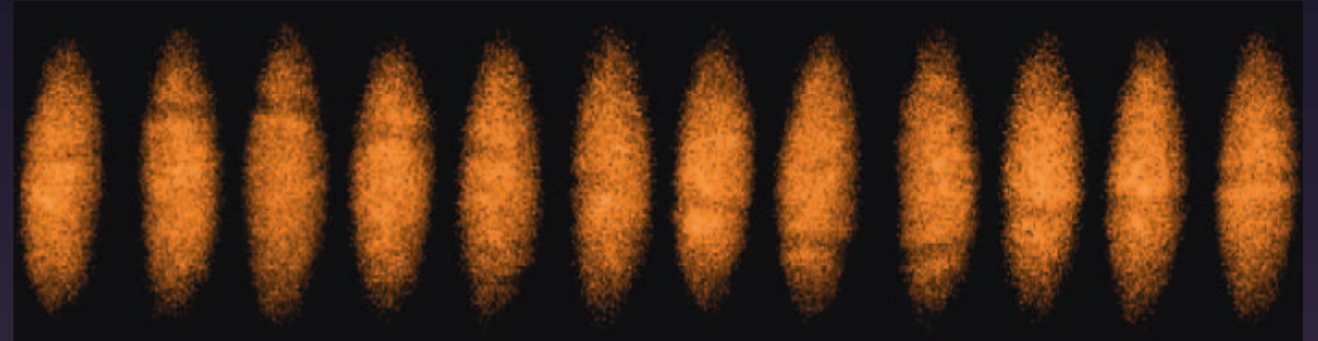
- Vortex Reconnection
- Quantum Turbulence

New arena:

Strong interactions (unlike BECs)

Experiments

Reliable theory (unlike He)



MIT Experiment

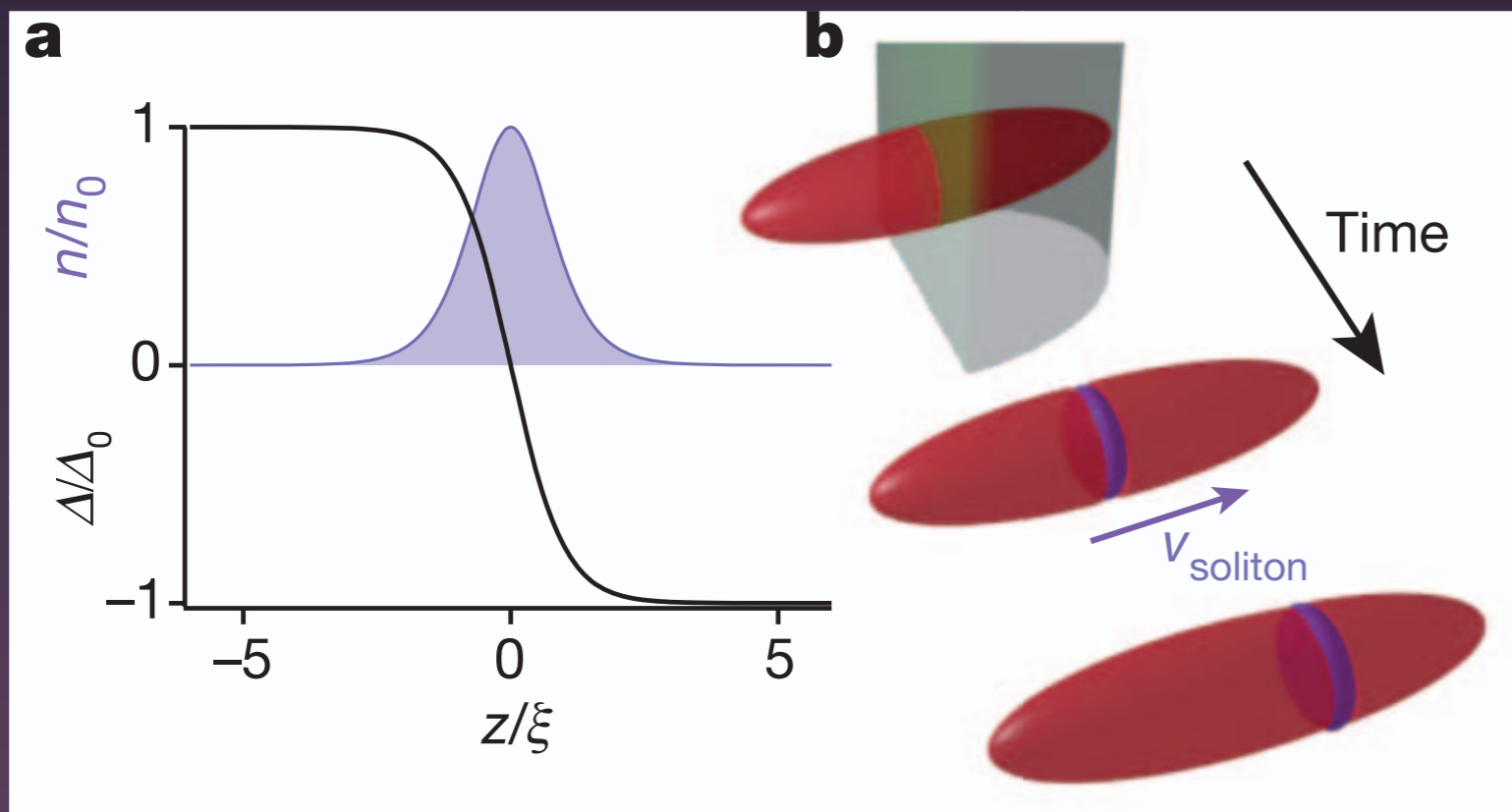
- ${}^6\text{Li}$ atoms ($N \approx 10^6$) cooled in harmonic trap
- Step potential used to imprint a soliton
- Let system evolve
- Image after ramping magnetic field B and expanding
- Observe an oscillating soliton with long period $T \approx 12T_z$
 - Bosonic solitons (BECs) oscillate with $T \approx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

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

Ku et al. PRL 113 (2014) 065301

MIT Experiment

$$\hbar\partial_t(\delta\varphi) = \delta V \quad (\text{phase difference on either side of trap})$$



Imprint soliton

Step potential
phases evolve to
 π phase shift

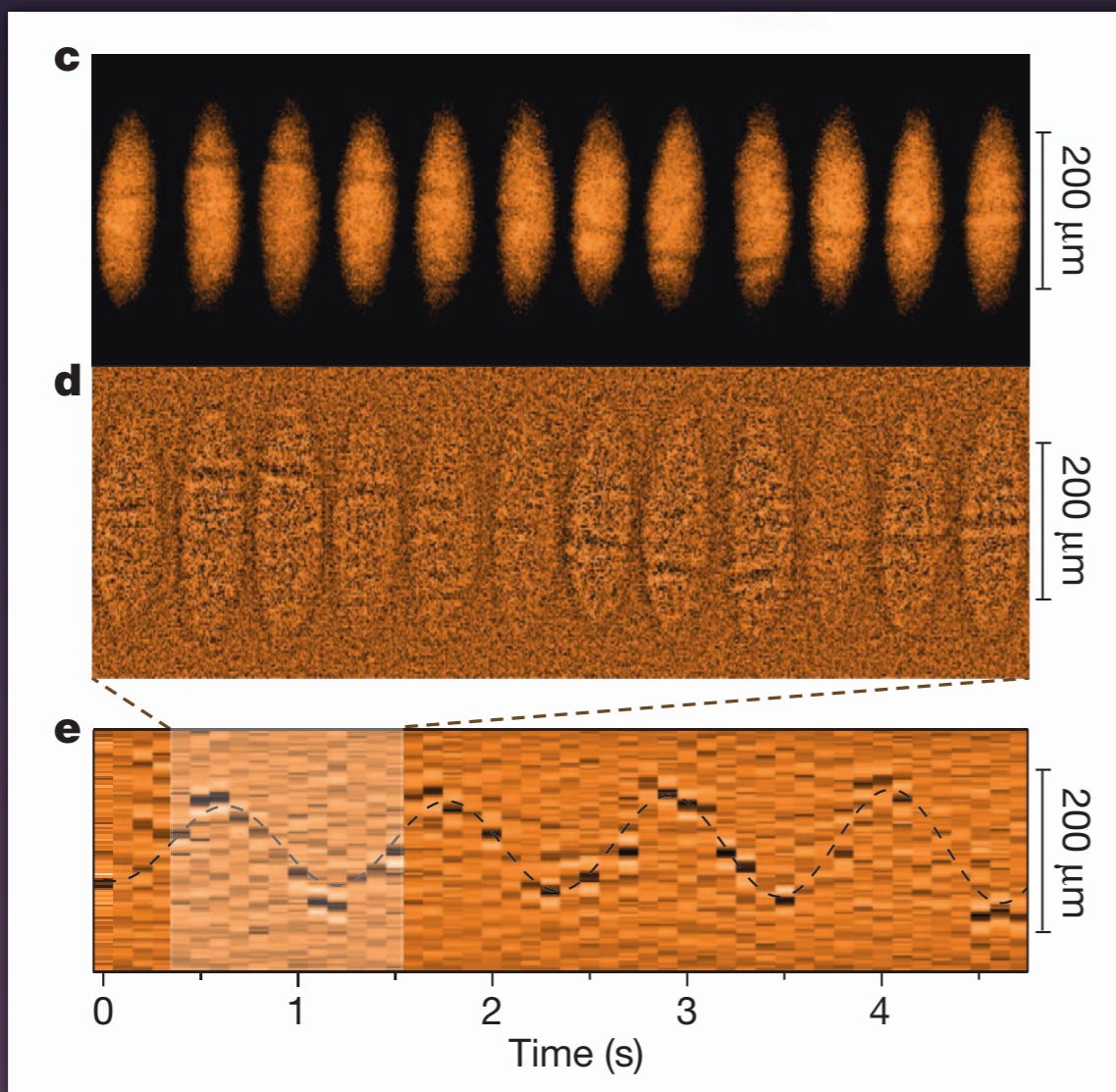
Flat domain wall
(dark/grey soliton)

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

Ku et al. PRL 113 (2014) 065301

MIT Experiment

(each image is a different run)



Thick solitons

- $10 \times$ coherence length

Slowly moving

$$T \approx 12T_z$$

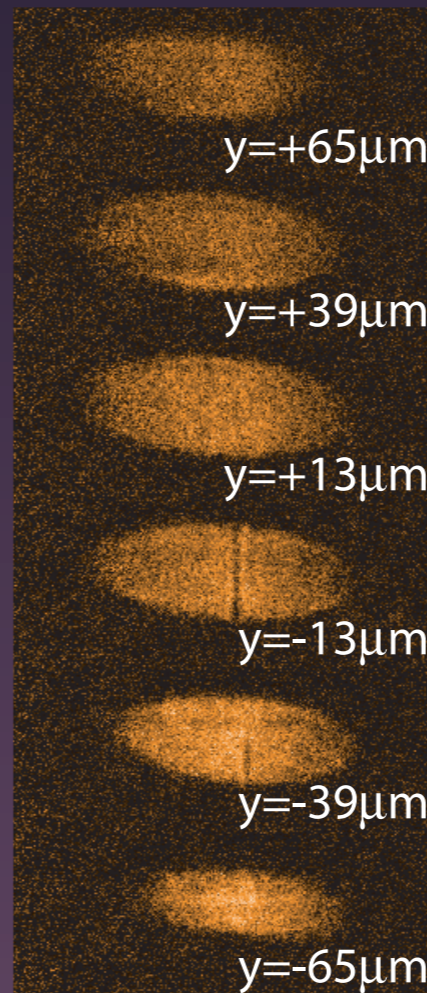
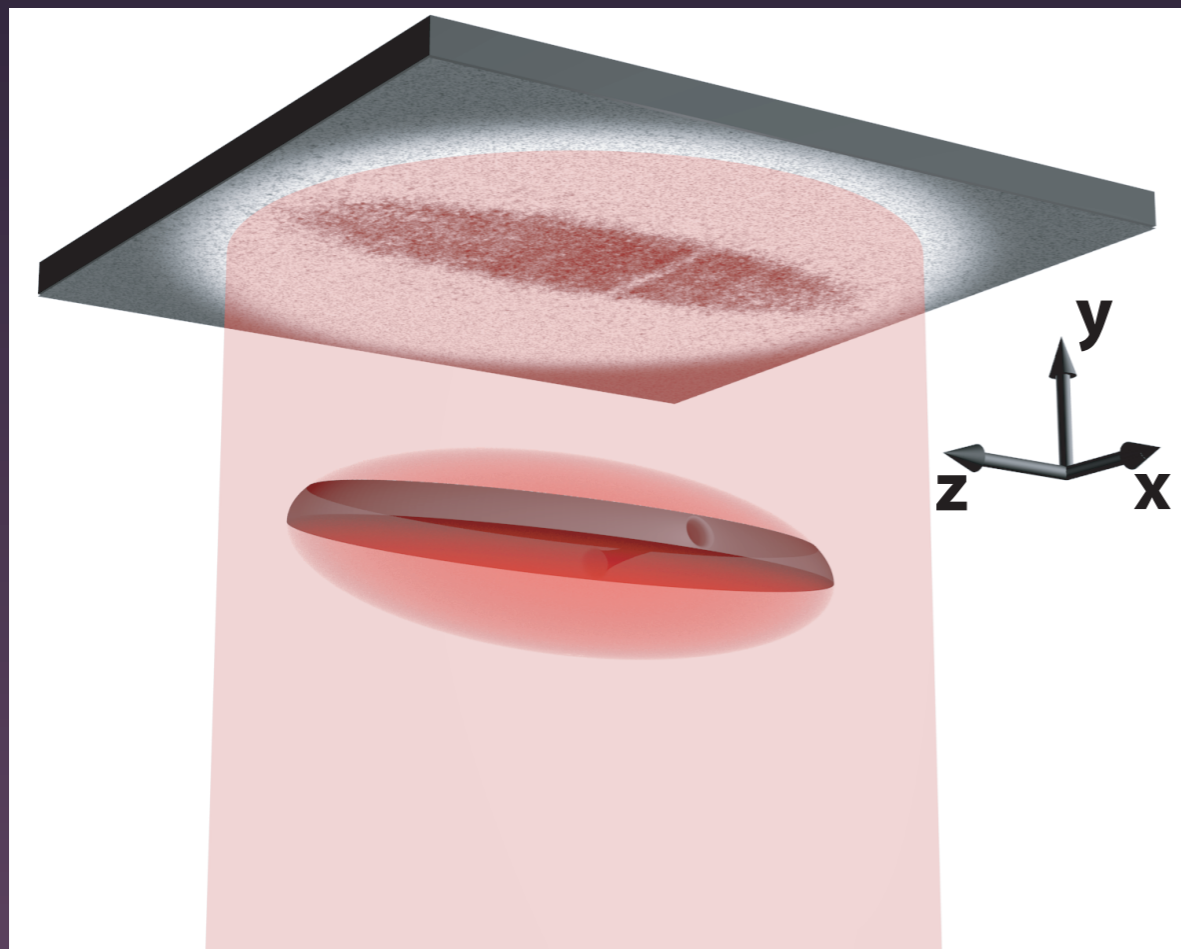
Theory (Walls):

$$T \sim 1.2 - 1.4T_z$$

Is theory wrong?

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

Objects are Vortices



Better tomographic imaging reveals vortex

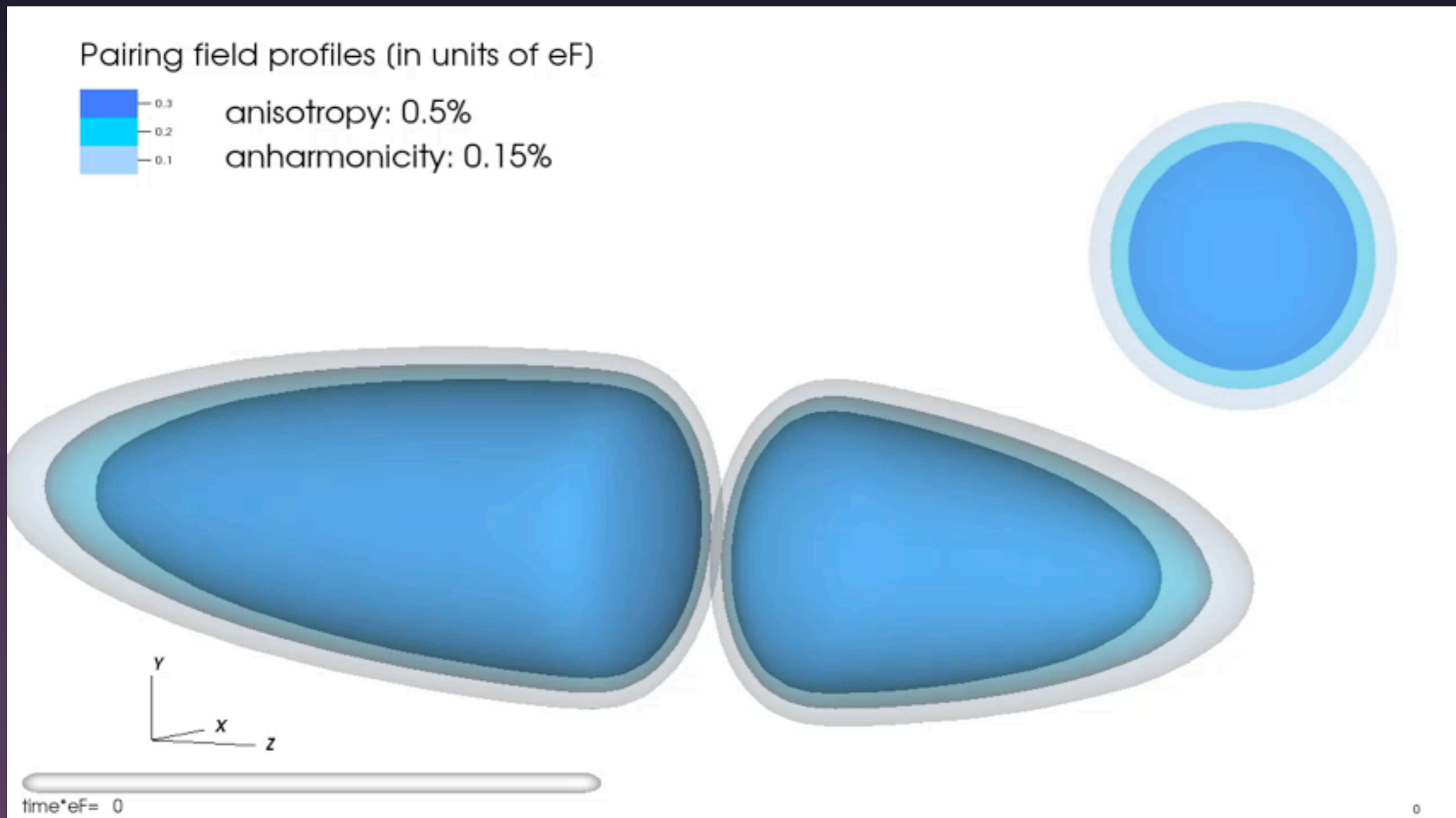
Gravity breaks trap asymmetry

Only imaged in one direction

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

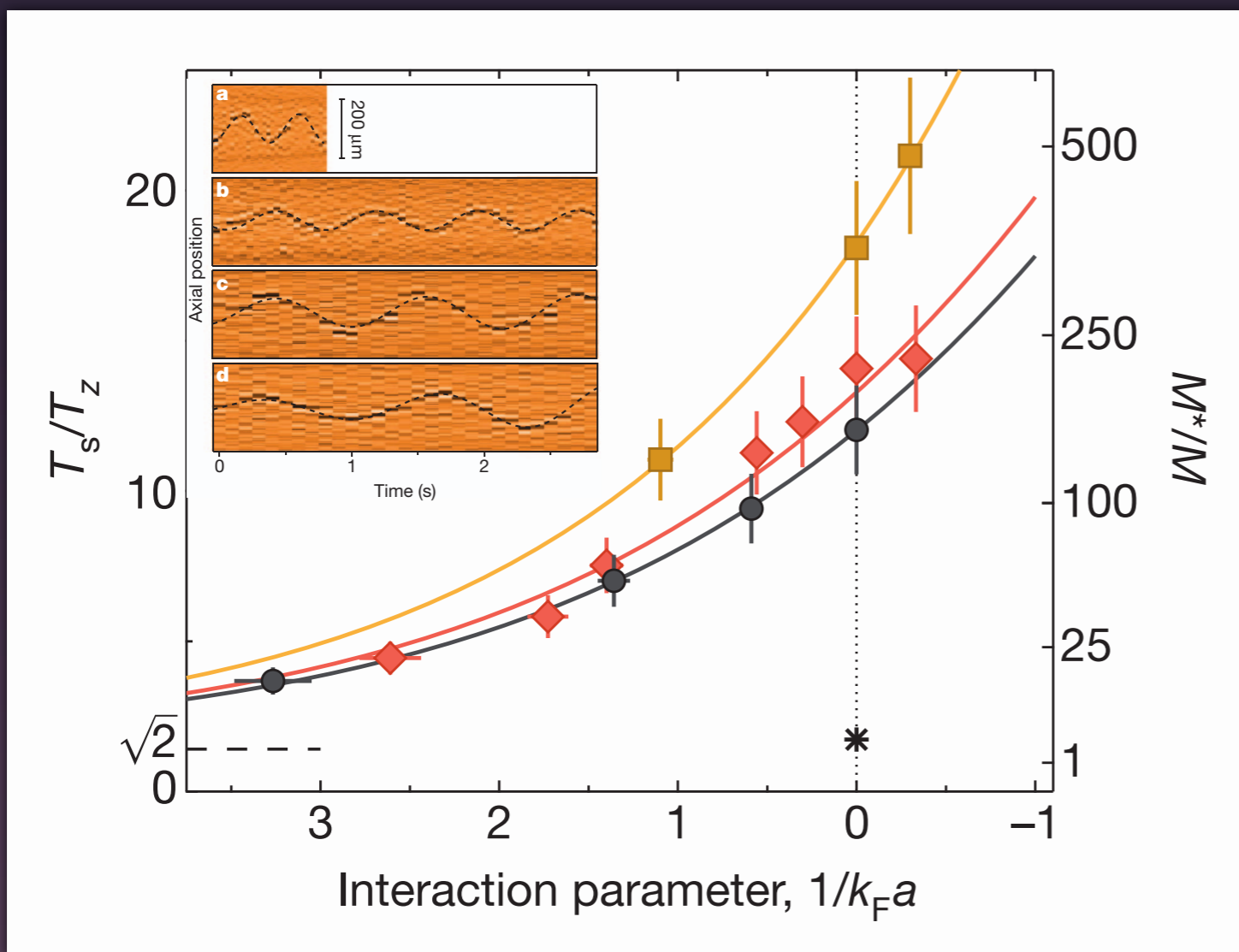
Ku et al. PRL 113 (2014) 065301

Wall, Ring, Vortex



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

MIT Experiment



Period depends on:

- Aspect ratio

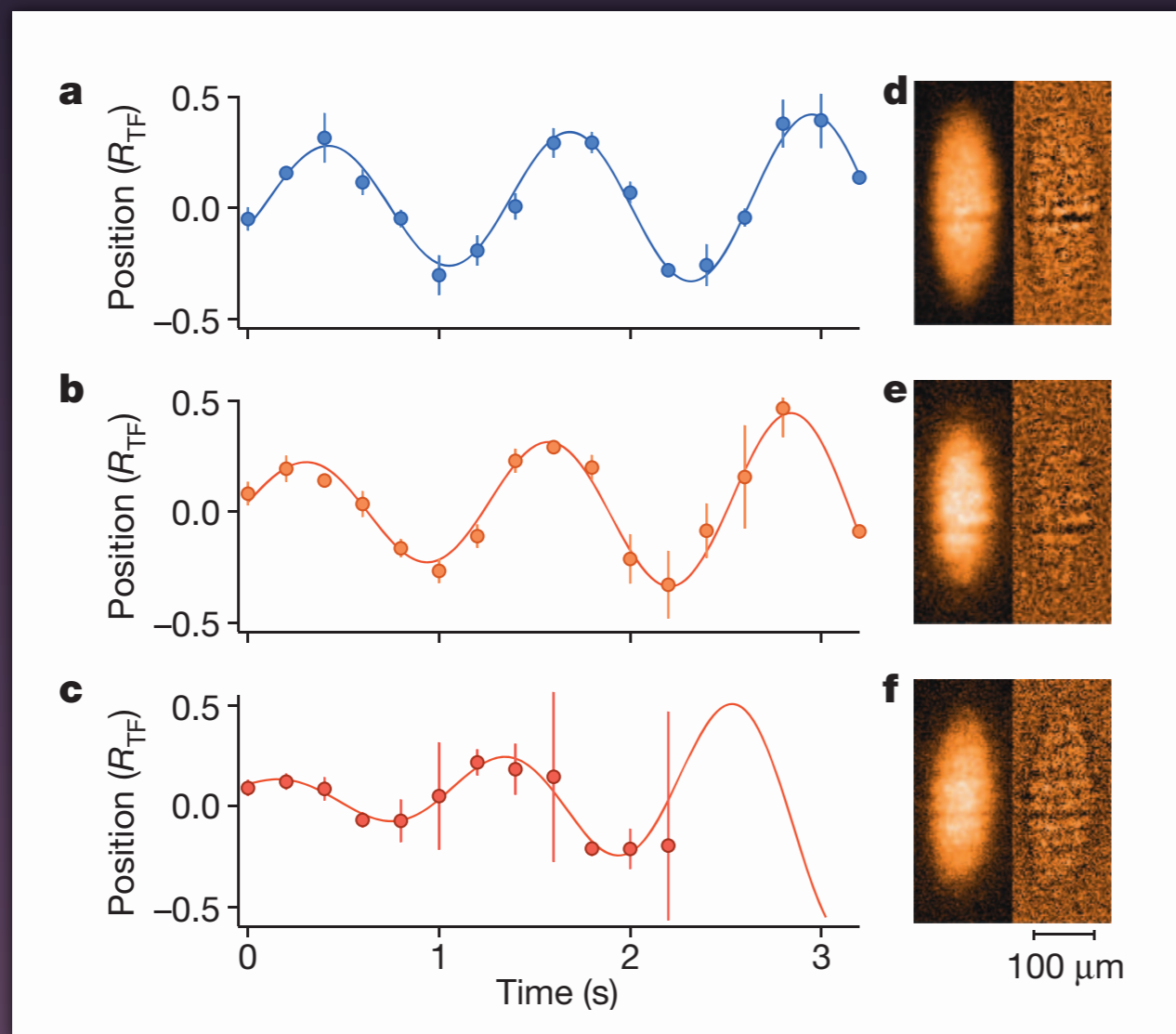
$$\lambda \in \{3.3, 6.2, 12\}$$

- Interaction

Much longer than predicted for domain walls

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

MIT Experiment



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

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

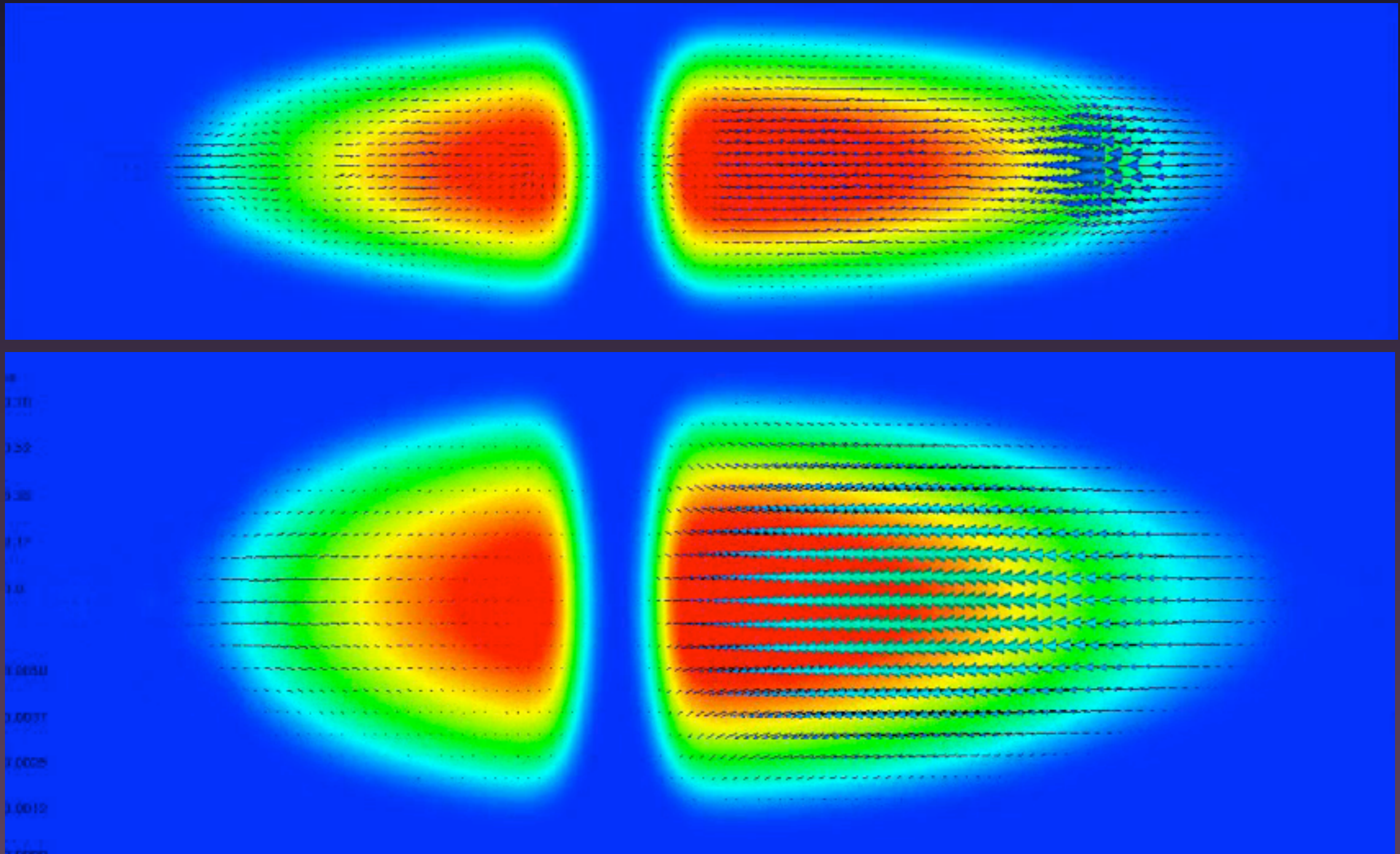
Density Functional Theory (DFT)

- 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

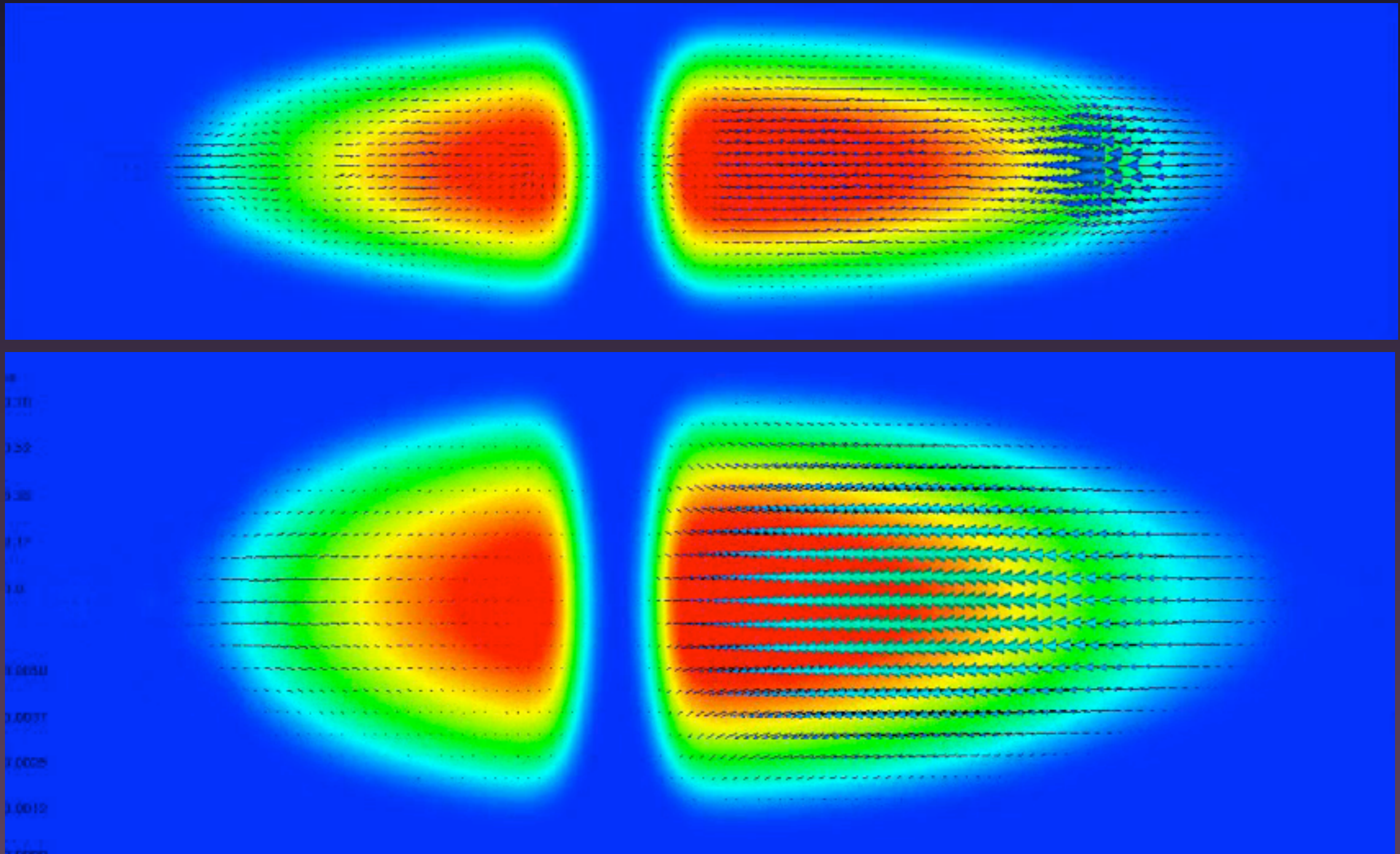
Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]:
32x32x128

State Preparation



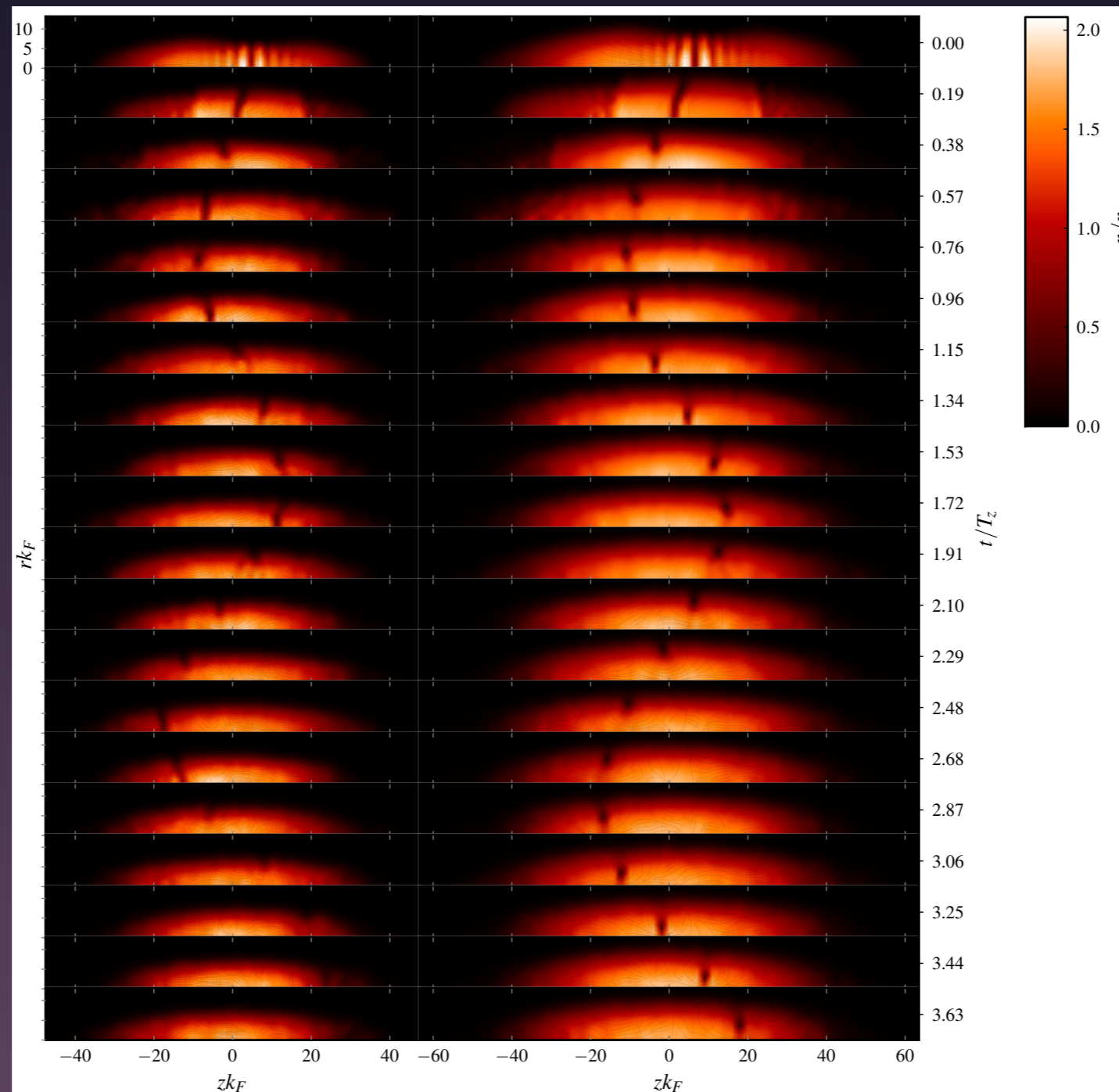
Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]:
32x32x128

State Preparation



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

Vortex Ring Oscillation



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

Vortex Rings

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

- 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

$$M_I = \frac{F}{\dot{v}} \sim 8\pi^2 m n R^3 \left(\ln \frac{R}{l_{\text{coh}}} \right)^{-1}$$

$$M_{\text{VR}} = m N_{\text{VR}} \sim m n 2\pi R \pi l_{\text{coh}}^2$$

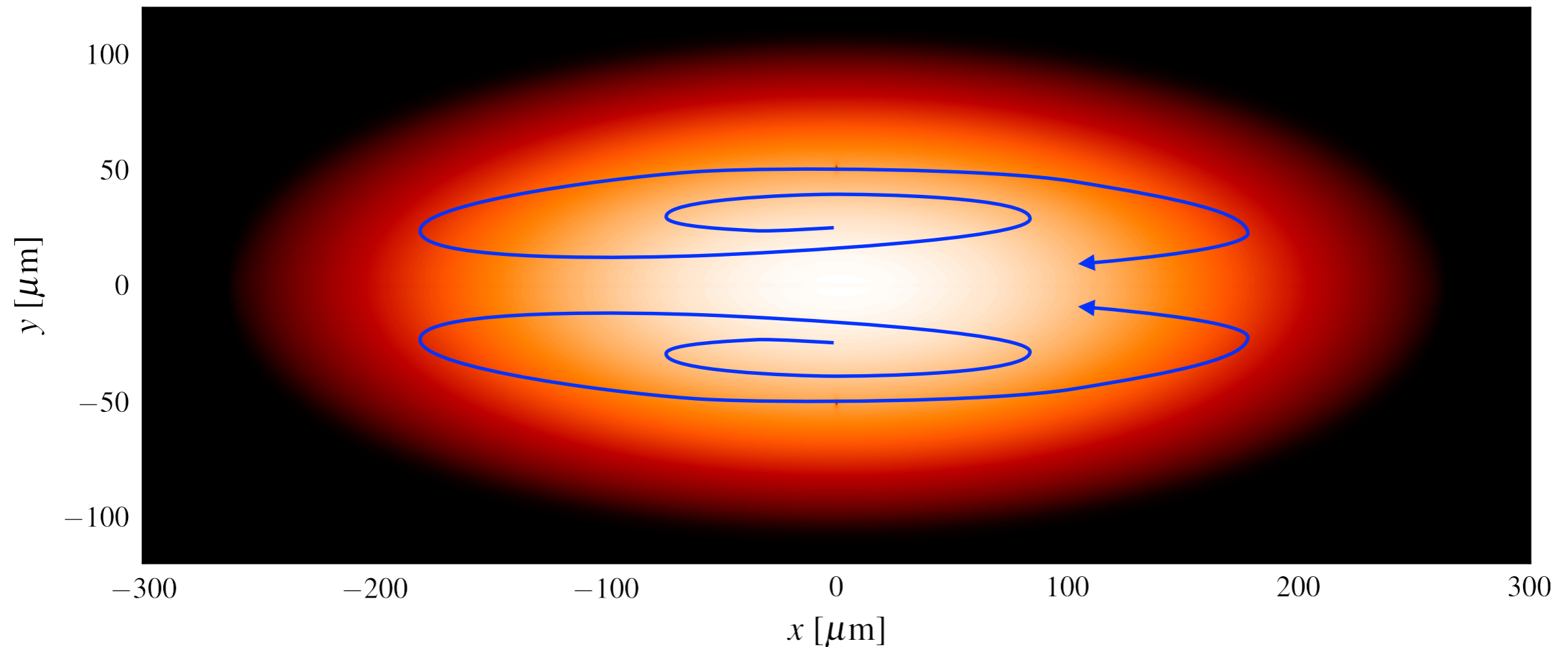
- M_I : Inertial (kinetic mass) differs significantly from
- M_{VR} : Mass depletion
- Long periods

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

Vortex Rings in a Trap

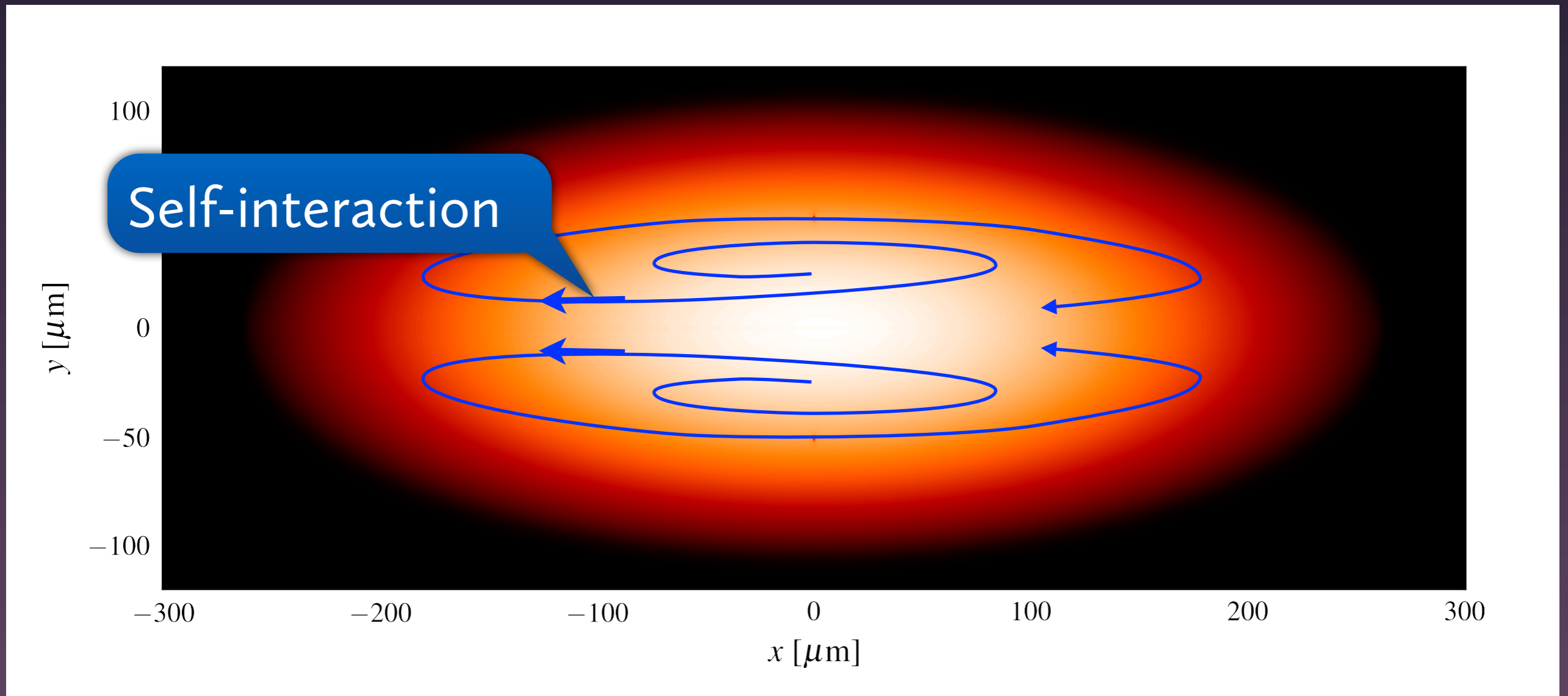
- Behaviour depends on $T \sim R/l_{\text{coh}} \sim k_{\text{F}}R$
- Large traps have long periods ($k_{\text{F}}R \sim 20$ for experiment)
- Small (narrow) approach domain wall $T \approx \sqrt{2}T_z$
Formula does not apply
- Depends on l_{coh}
Characterizes dependence on scattering length

Vortex Ring Motion



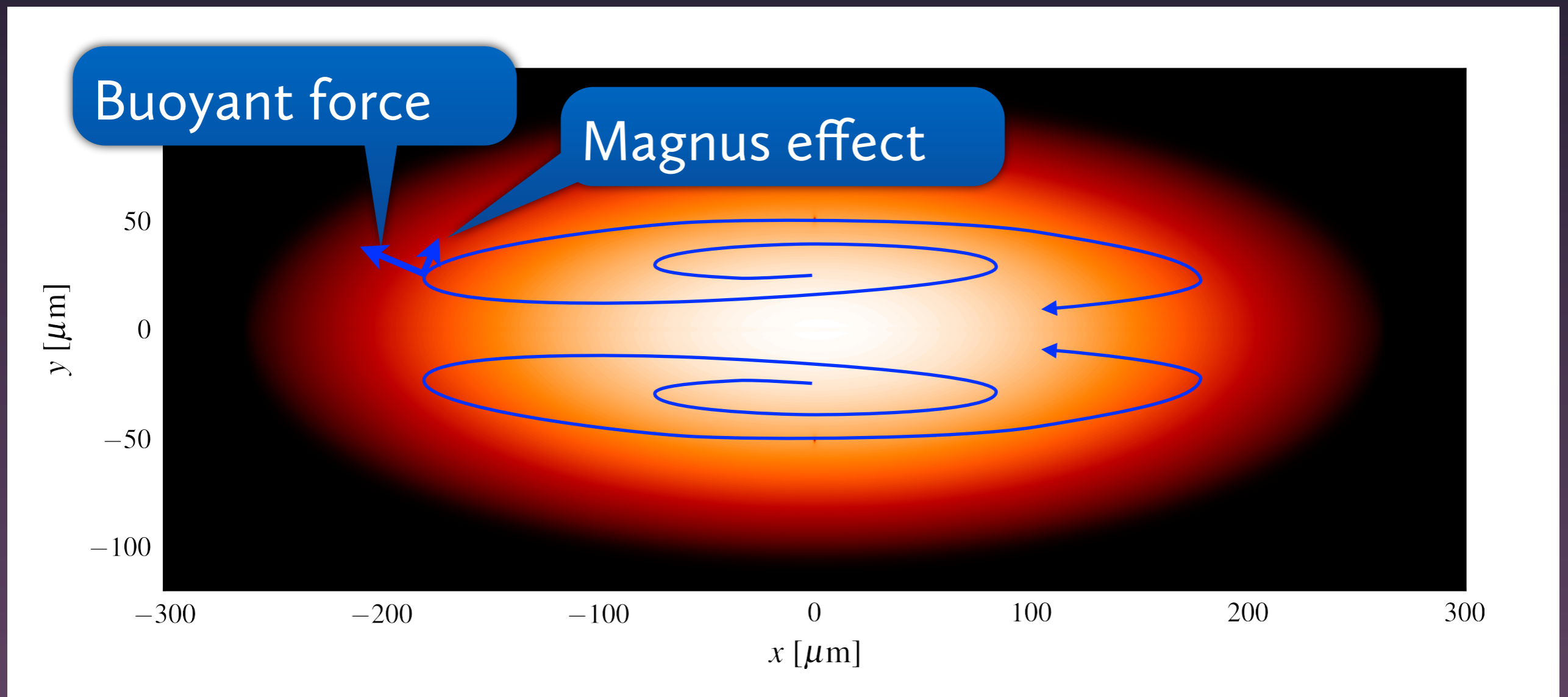
Vortex ring motion (here in the presence of “thermal” noise, hence the inverse decay)

Vortex Ring Motion



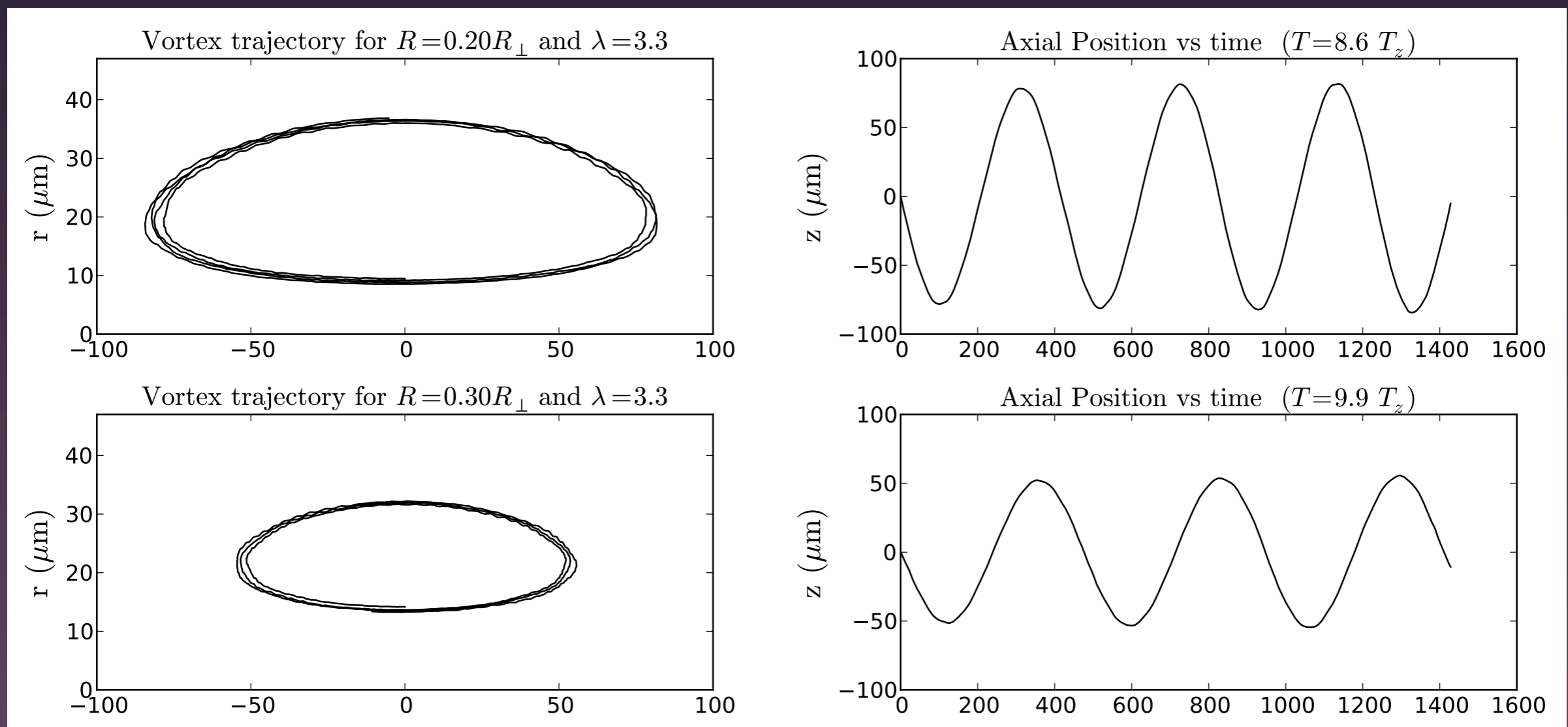
Vortex ring motion (here in the presence of “thermal” noise, hence the inverse decay)

Vortex Ring Motion



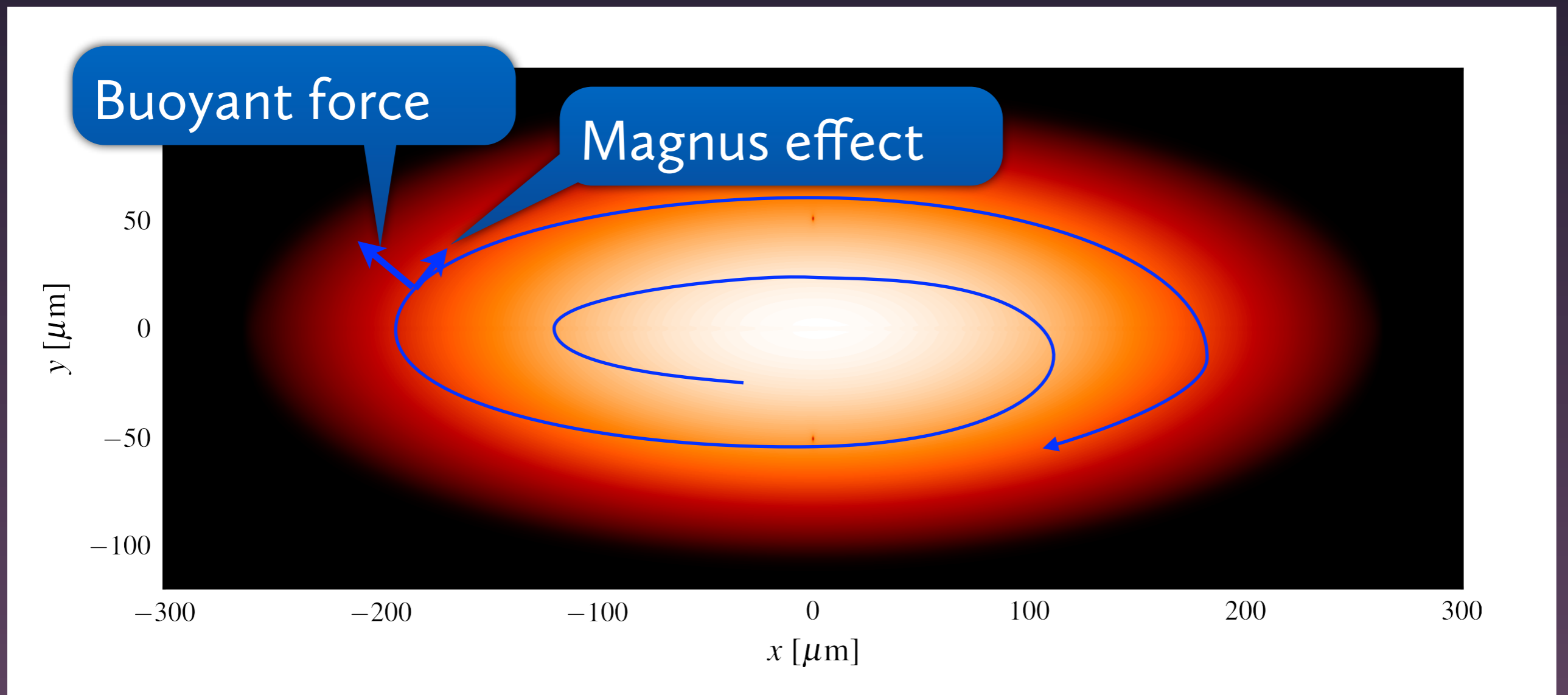
Vortex ring motion (here in the presence of “thermal” noise, hence the inverse decay)

Near-Harmonic Motion

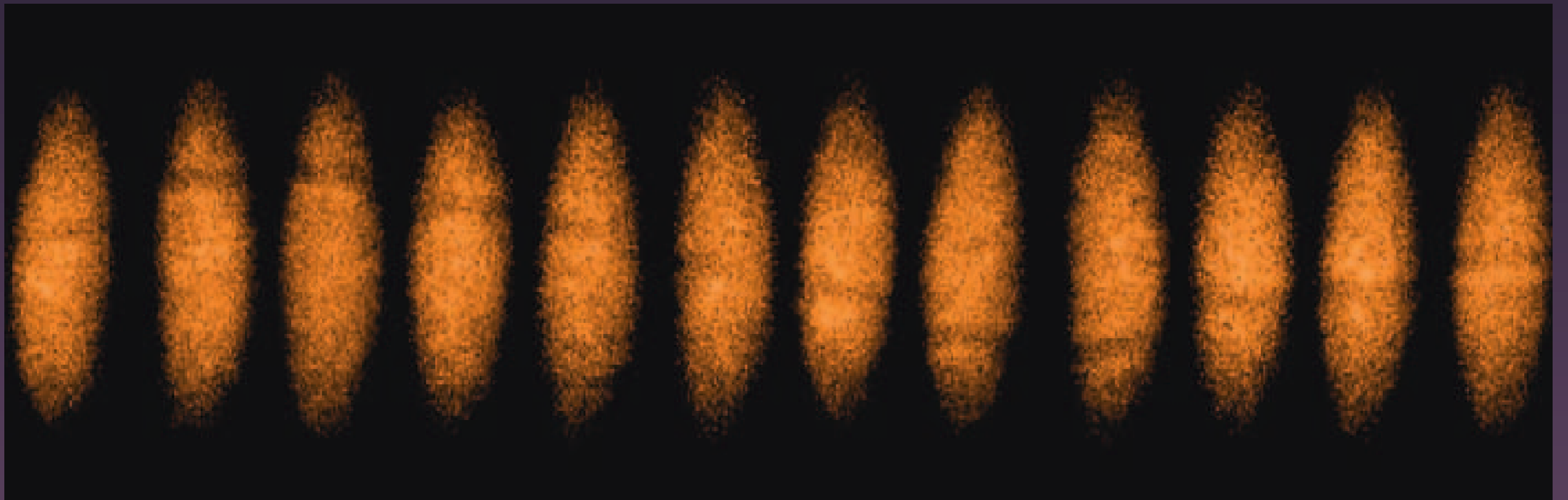


Bulgac, Forbes, Kelley, Roche, Wlazłowski (2013) [arXiv:1306.4266]

Vortex Motion

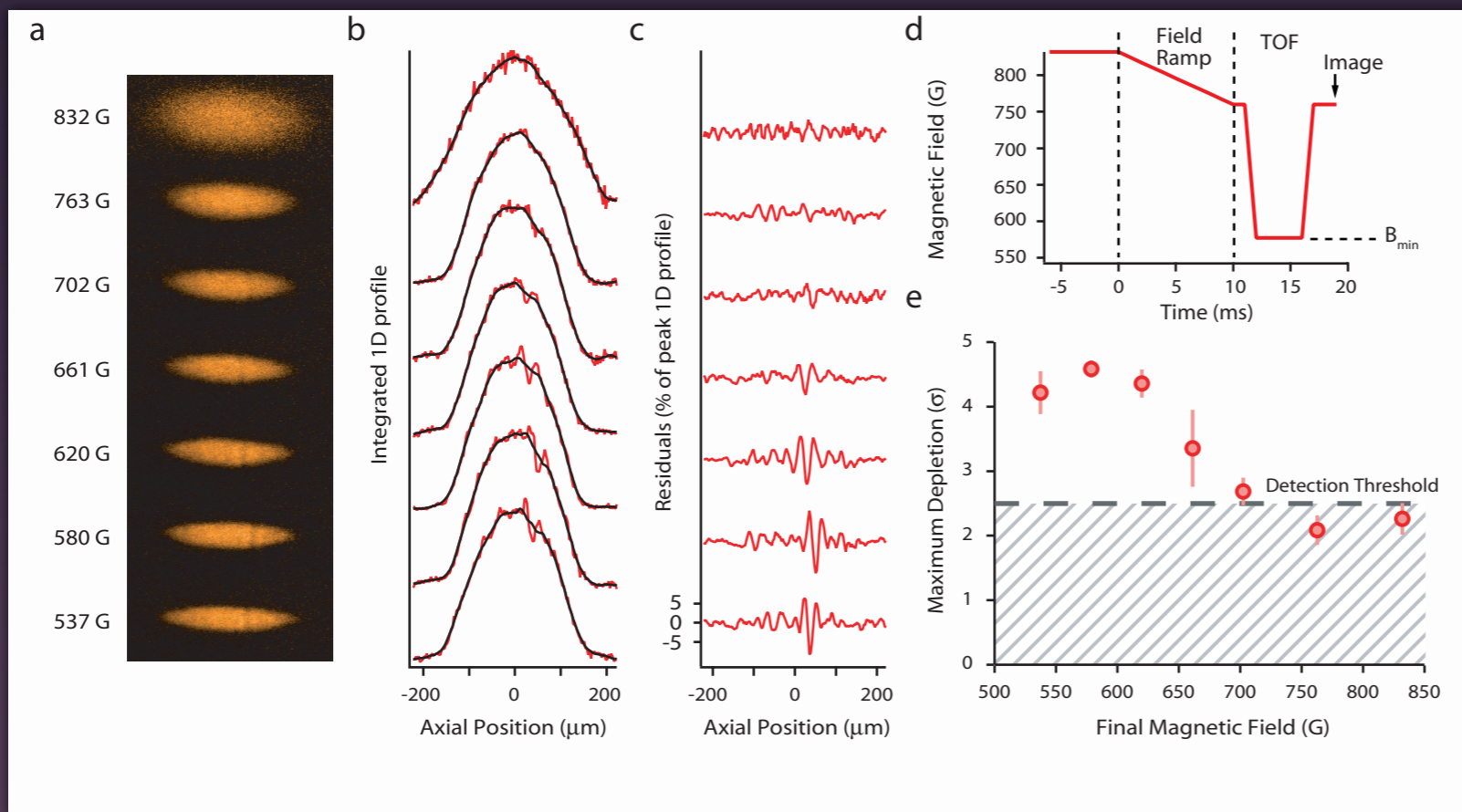


“Too Thick” for Vortex Rings?



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

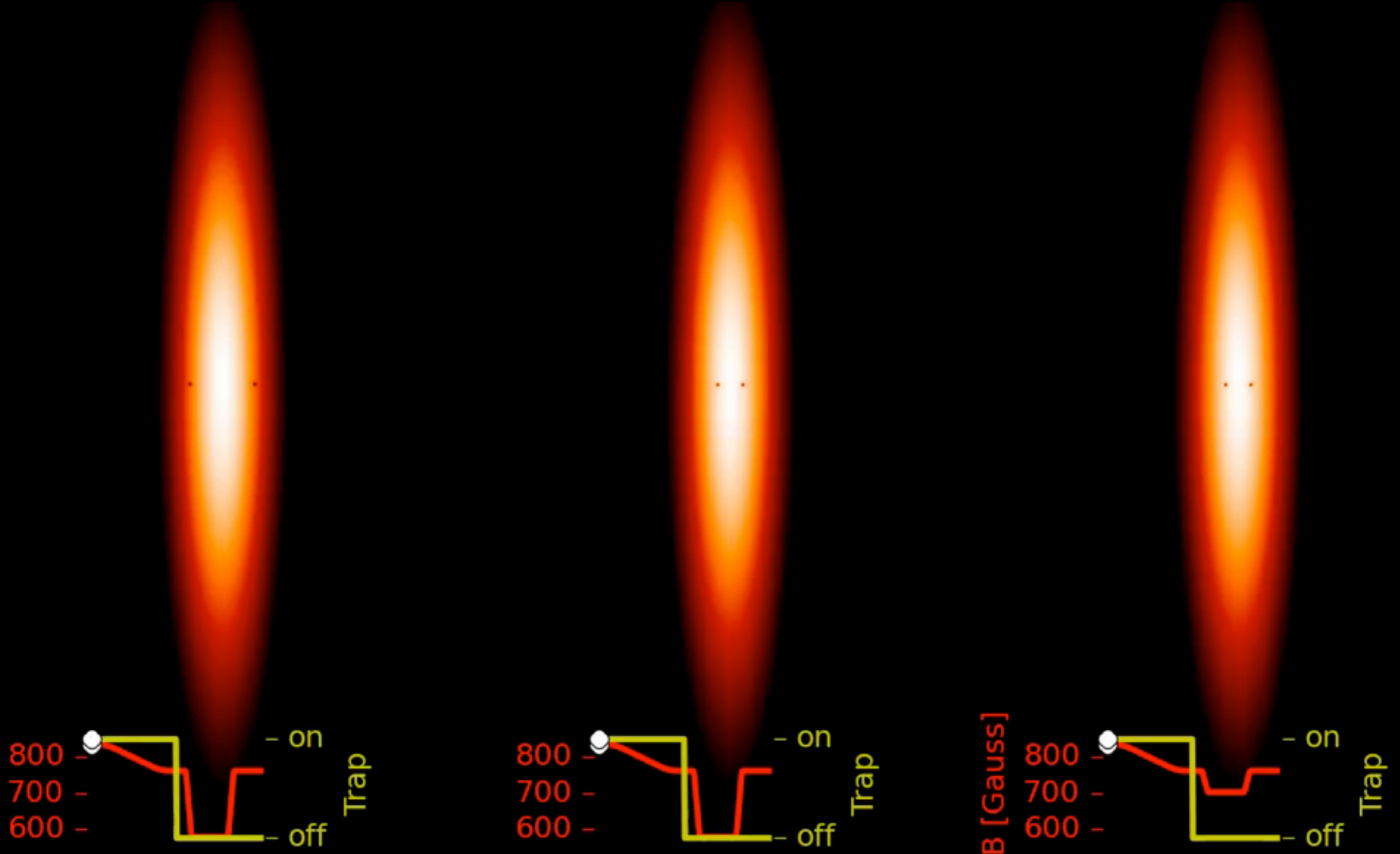
MIT Experiment



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

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

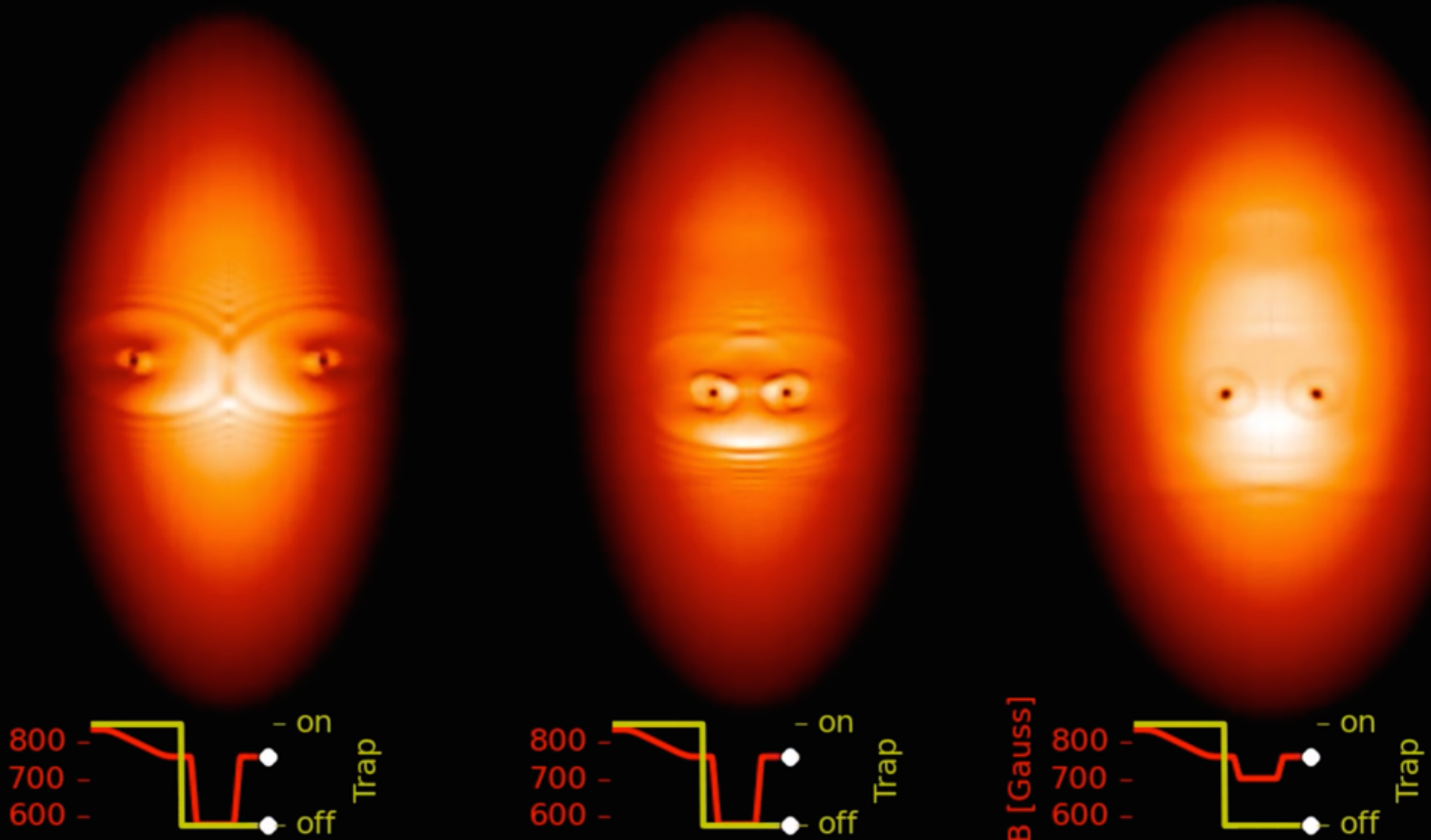
Imaging Vortex Rings



A.Bulgac, M.M.Forbes, M.M.Kelley, K.J.Roche, and G.Wazłowski
Phys. Rev. Lett. 112, 025301 (2014)

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

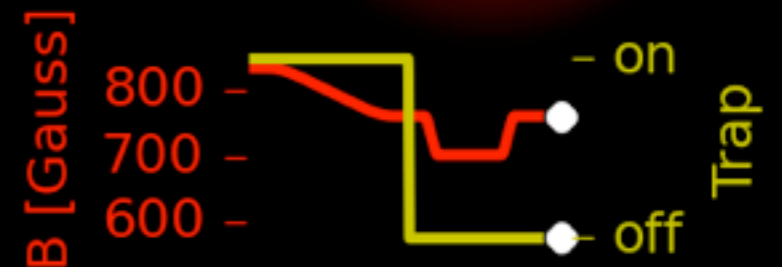
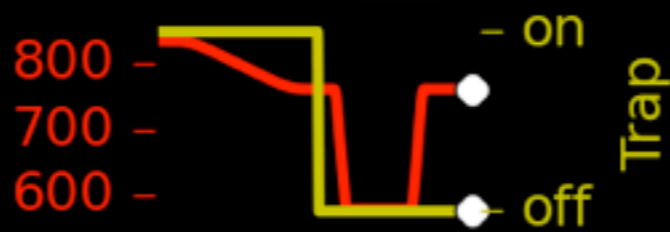
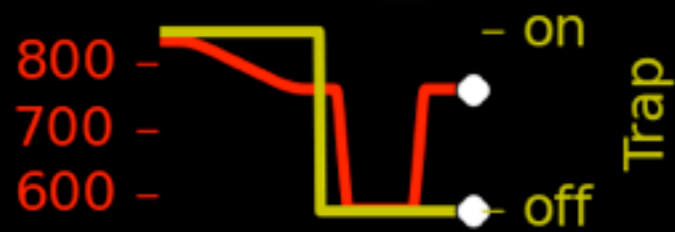
Imaging Vortex Rings



A. Bulgac, M.M. Forbes, M.M. Kelley, K.J. Roche, and G. Wazłowski
Phys. Rev. Lett. 112, 025301 (2014)

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

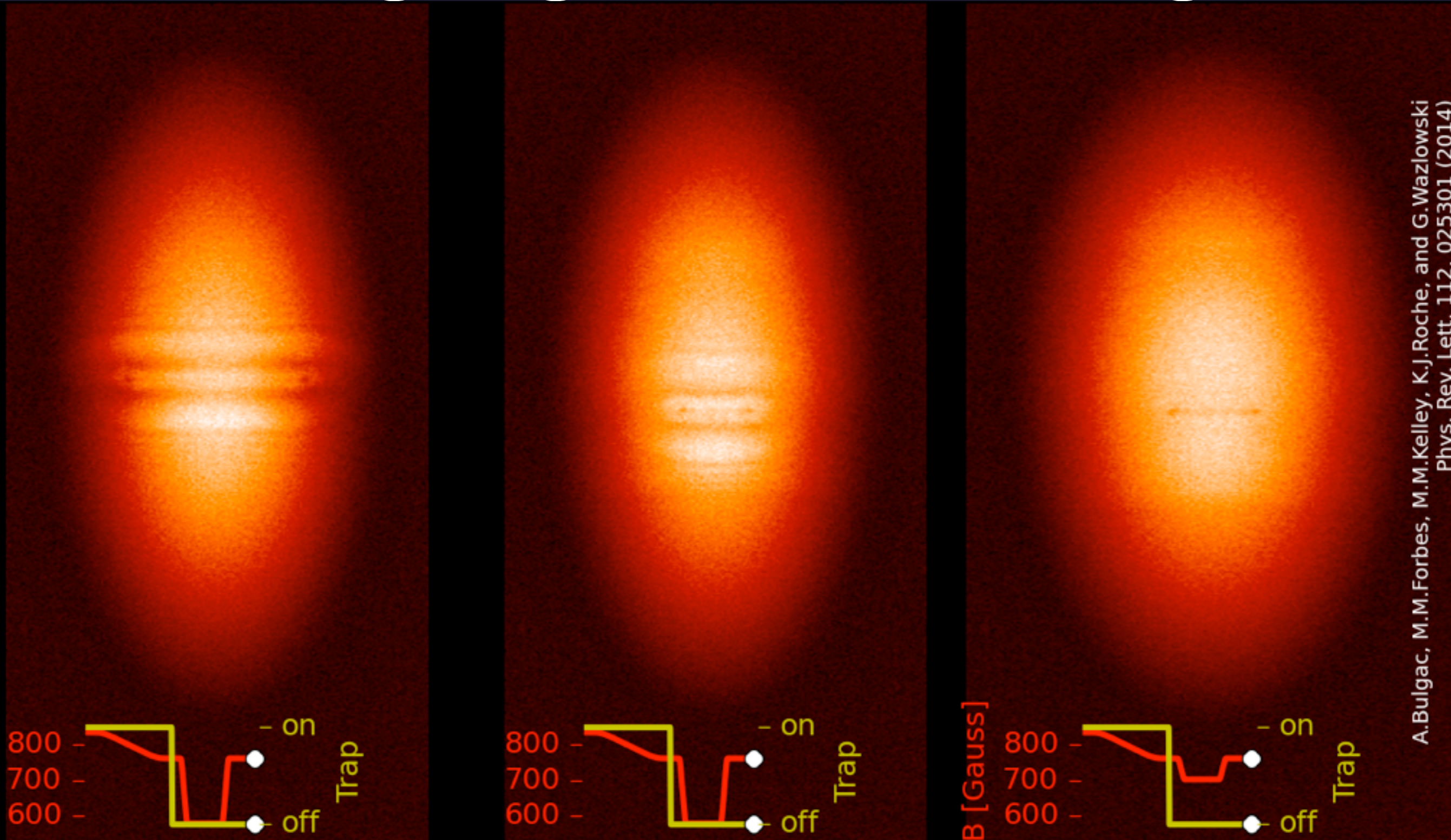
Imaging Vortex Rings



A. Bulgac, M.M. Forbes, M.M. Kelley, K.J. Roche, and G. Wazłowski
Phys. Rev. Lett. 112, 025301 (2014)

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

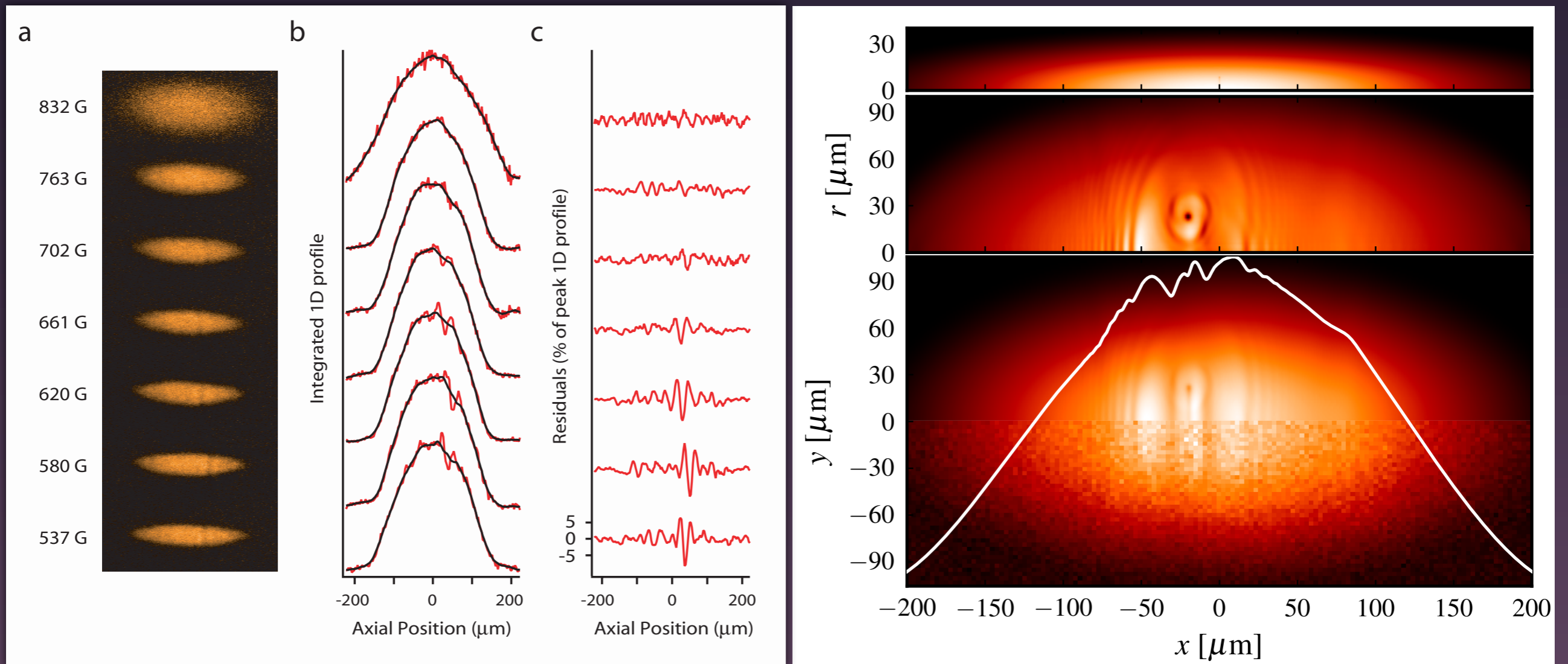
Imaging Vortex Rings



A.Bulgac, M.M.Forbes, M.M.Kelley, K.J.Roche, and G.Wazlowski
Phys. Rev. Lett. 112, 025301 (2014)

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

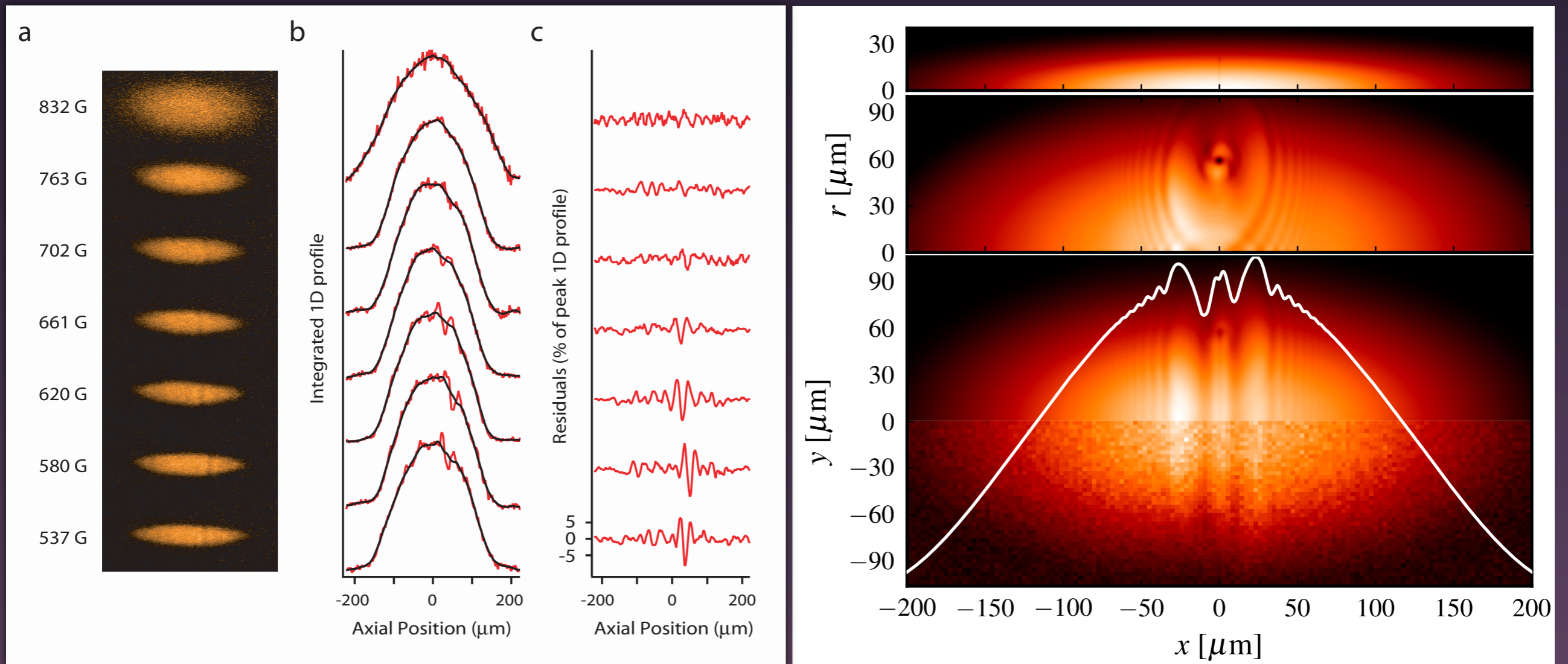
Explains Dependence on B_{\min}



Yefsah et al. Nature 499 (426) 2013

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

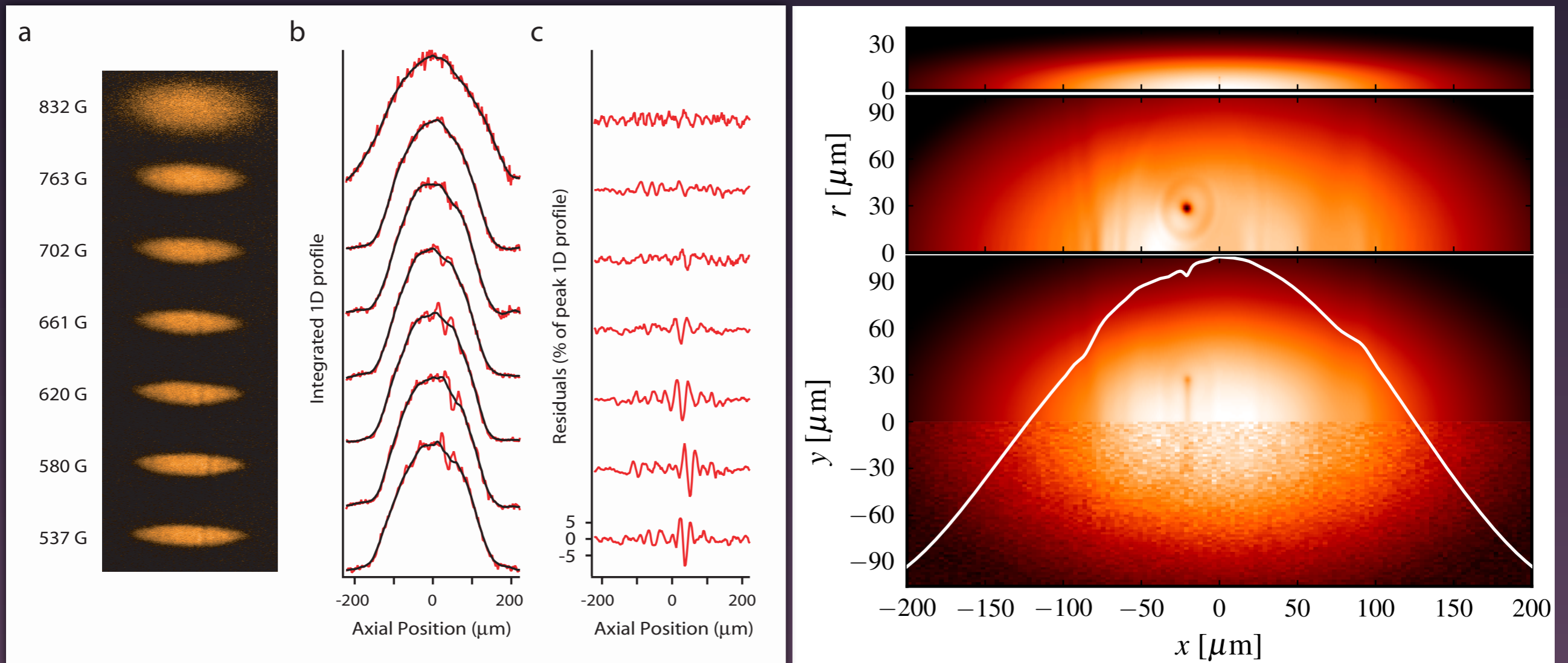
Explains Dependence on B_{\min}



Yefsah et al. Nature 499 (426) 2013

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

Explains Dependence on B_{\min}



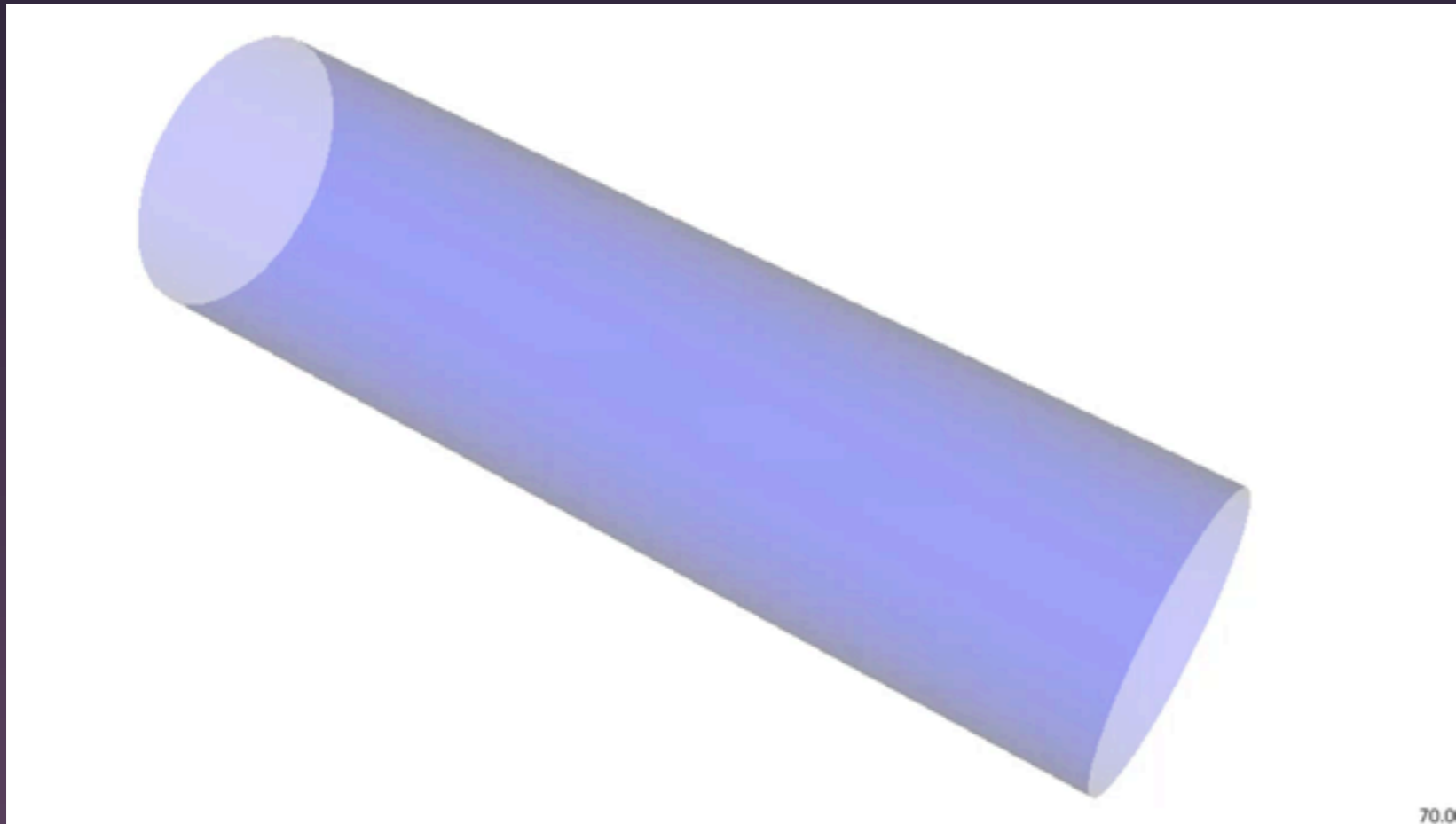
Yefsah et al. Nature 499 (426) 2013

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

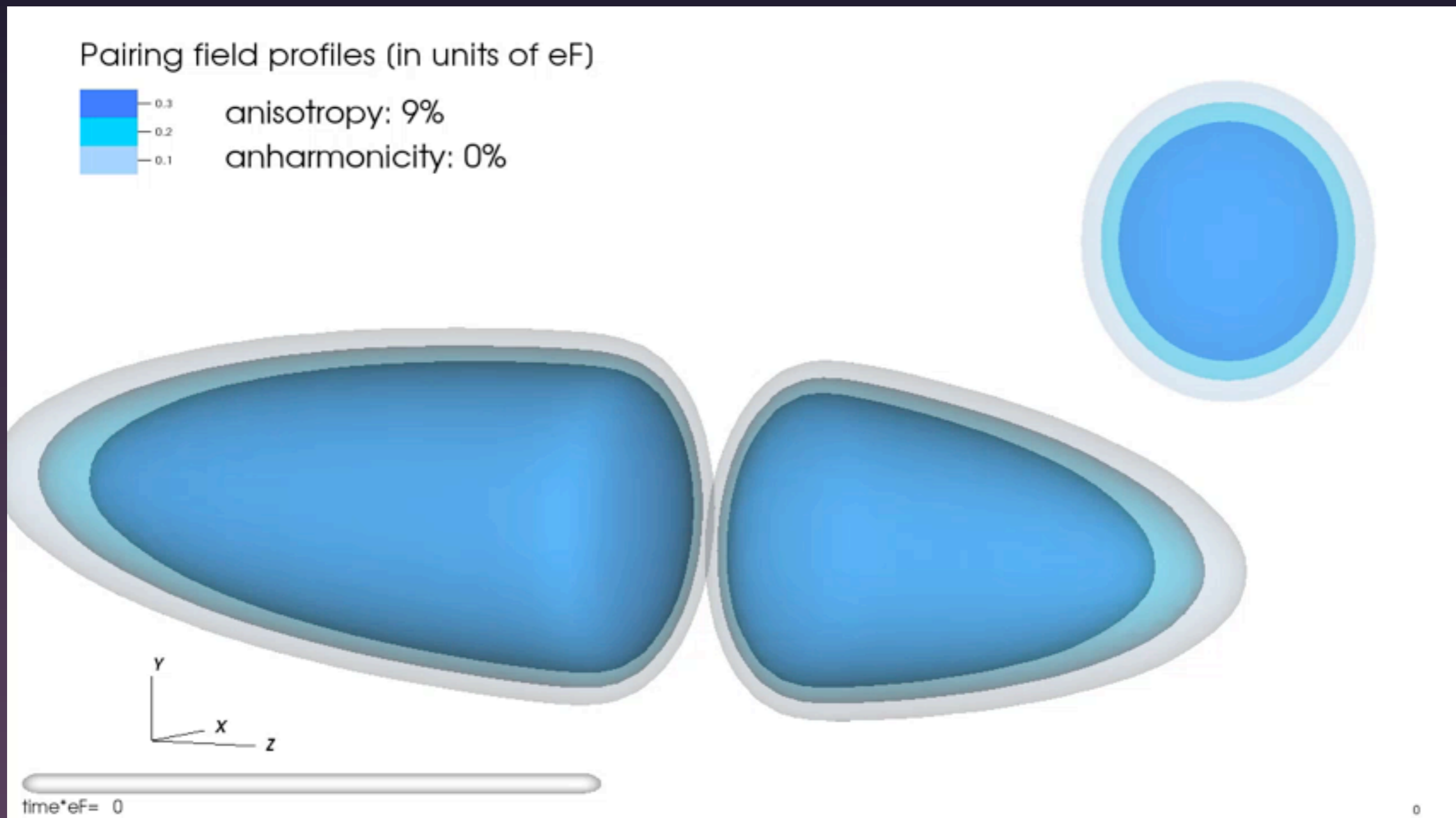
See online supplemental material to Bulgac, Luo, Magierski, Roche, and Yu,
Science, 332, 1288 (2011)

Asymmetric Rings Decay to Vortices

Reconnection
• Quantum turbulence

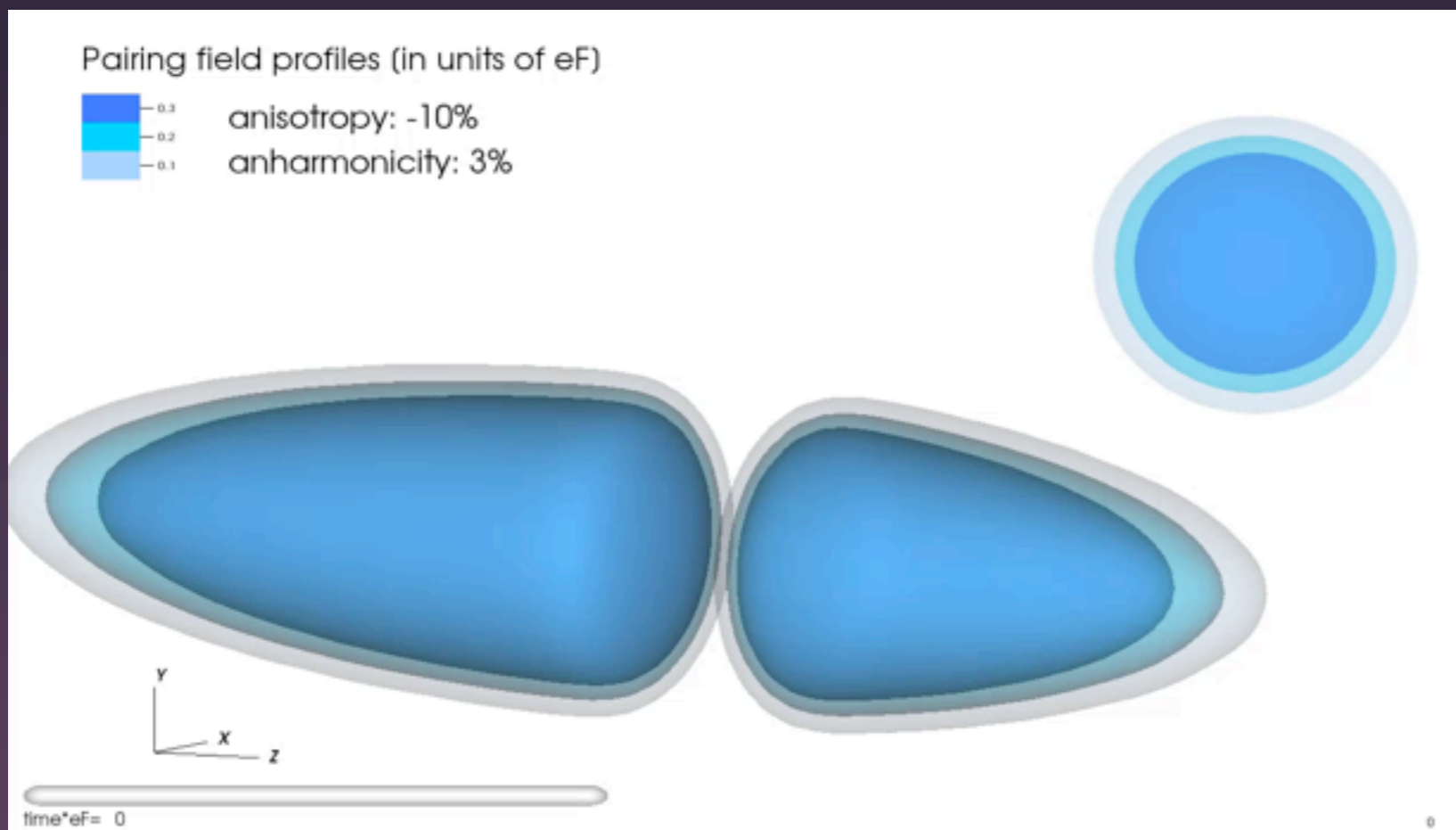
See online supplemental material to Bulgac, Luo, Magierski, Roche, and Yu,
Science, 332, 1288 (2011)

Evolution of a Vortex



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

Consistent Alignment?



Short vortex = lower E

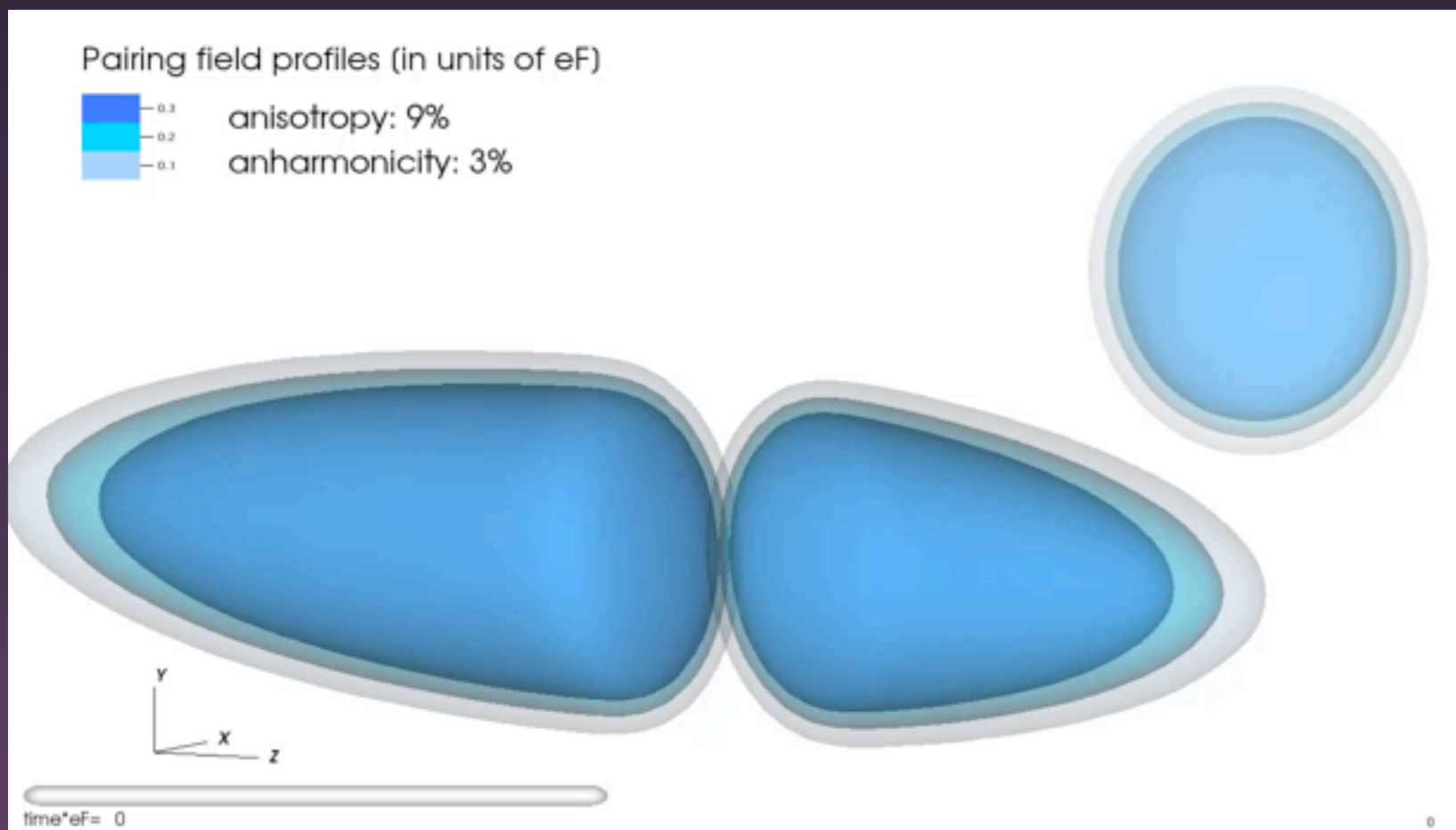
No vortex = lowest E!

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

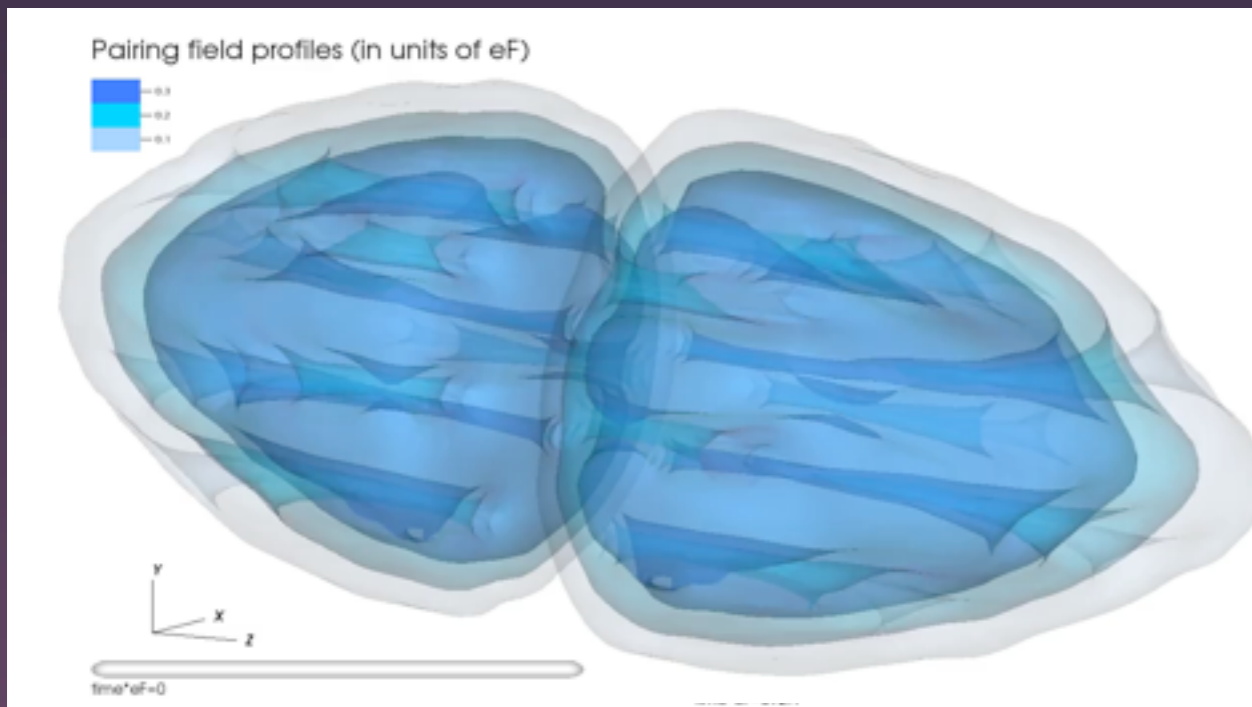
Oblique vortex rotates

Alignment needs
dissipation

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

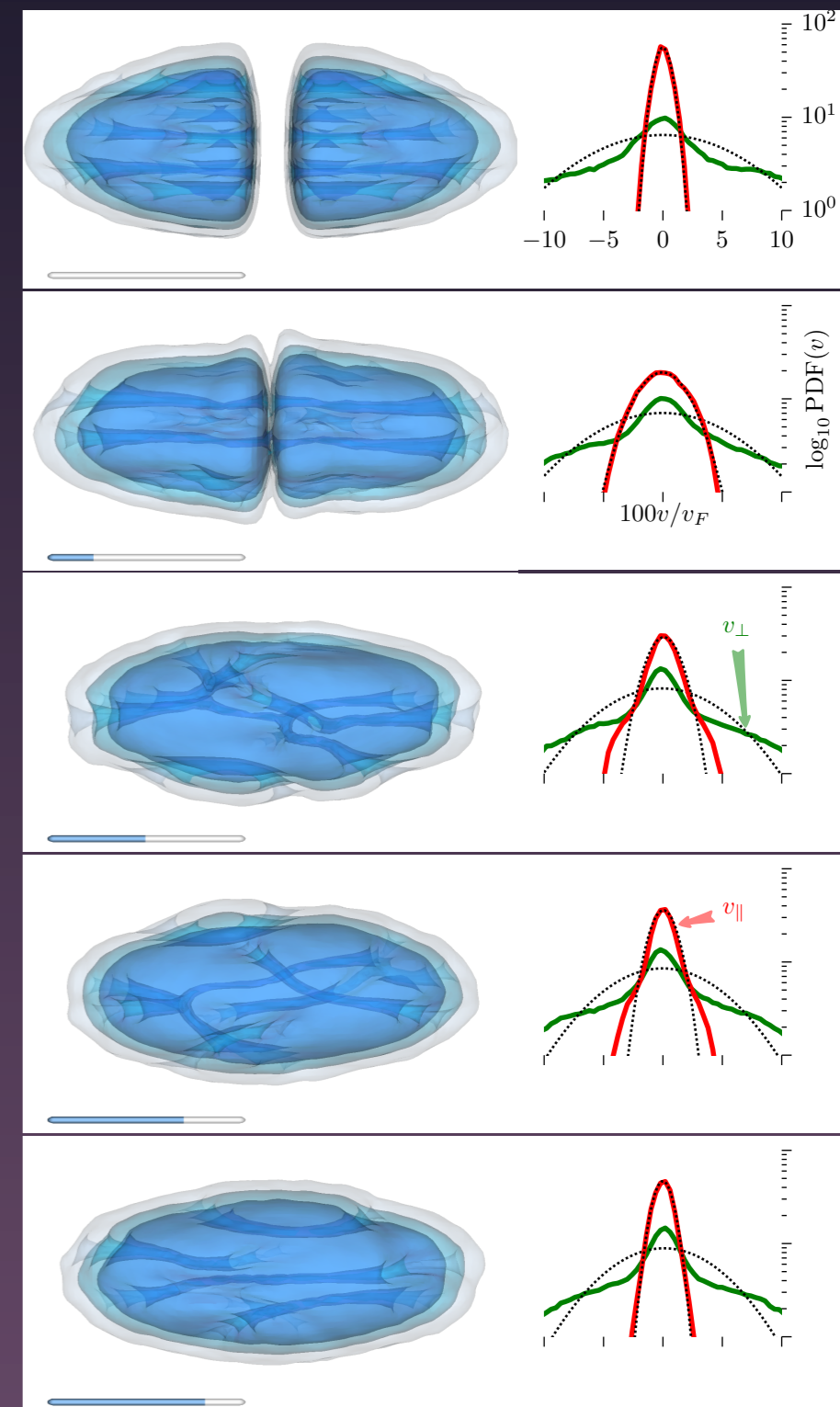
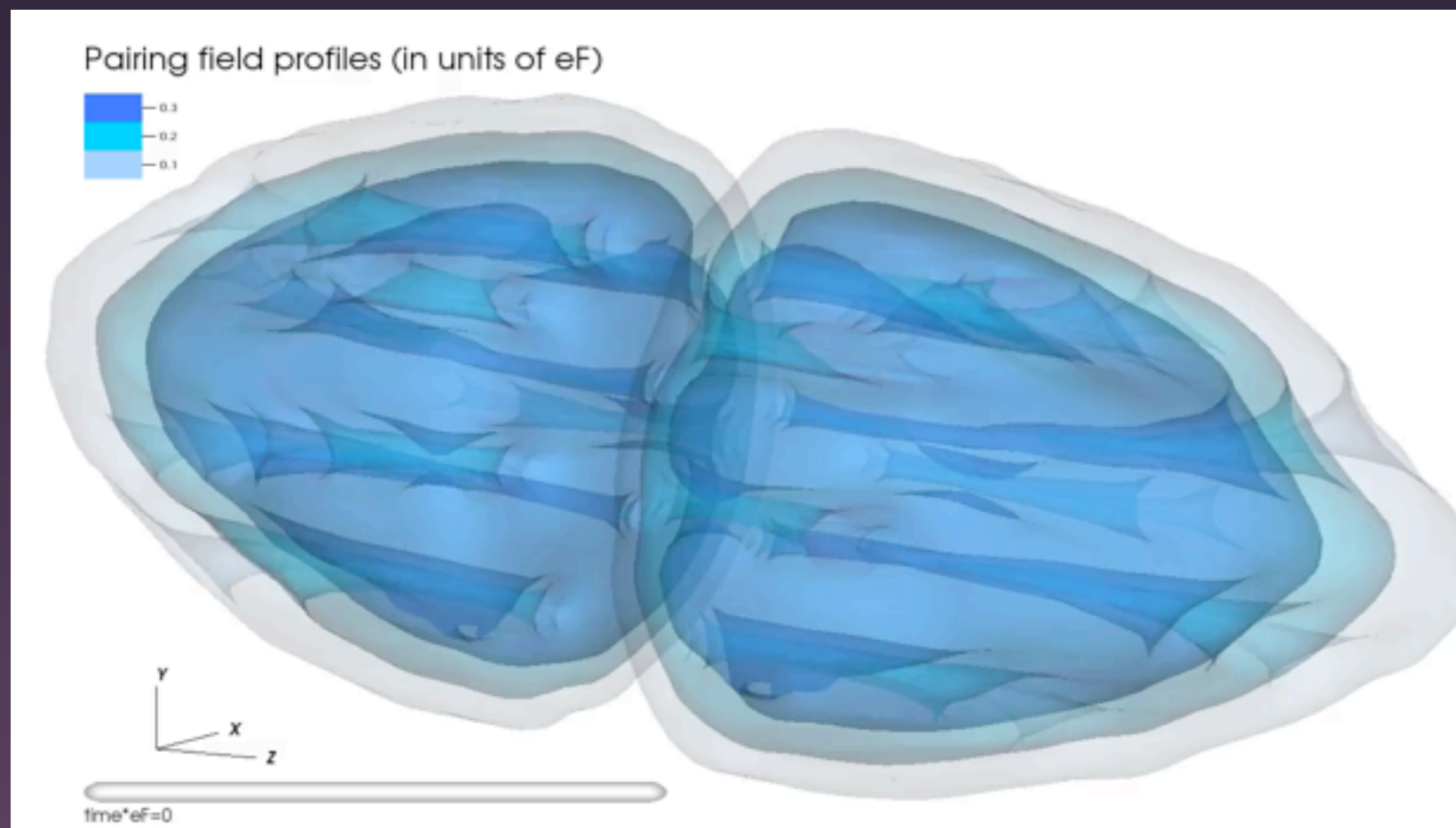
Vortex Reconnection Quantum Turbulence

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



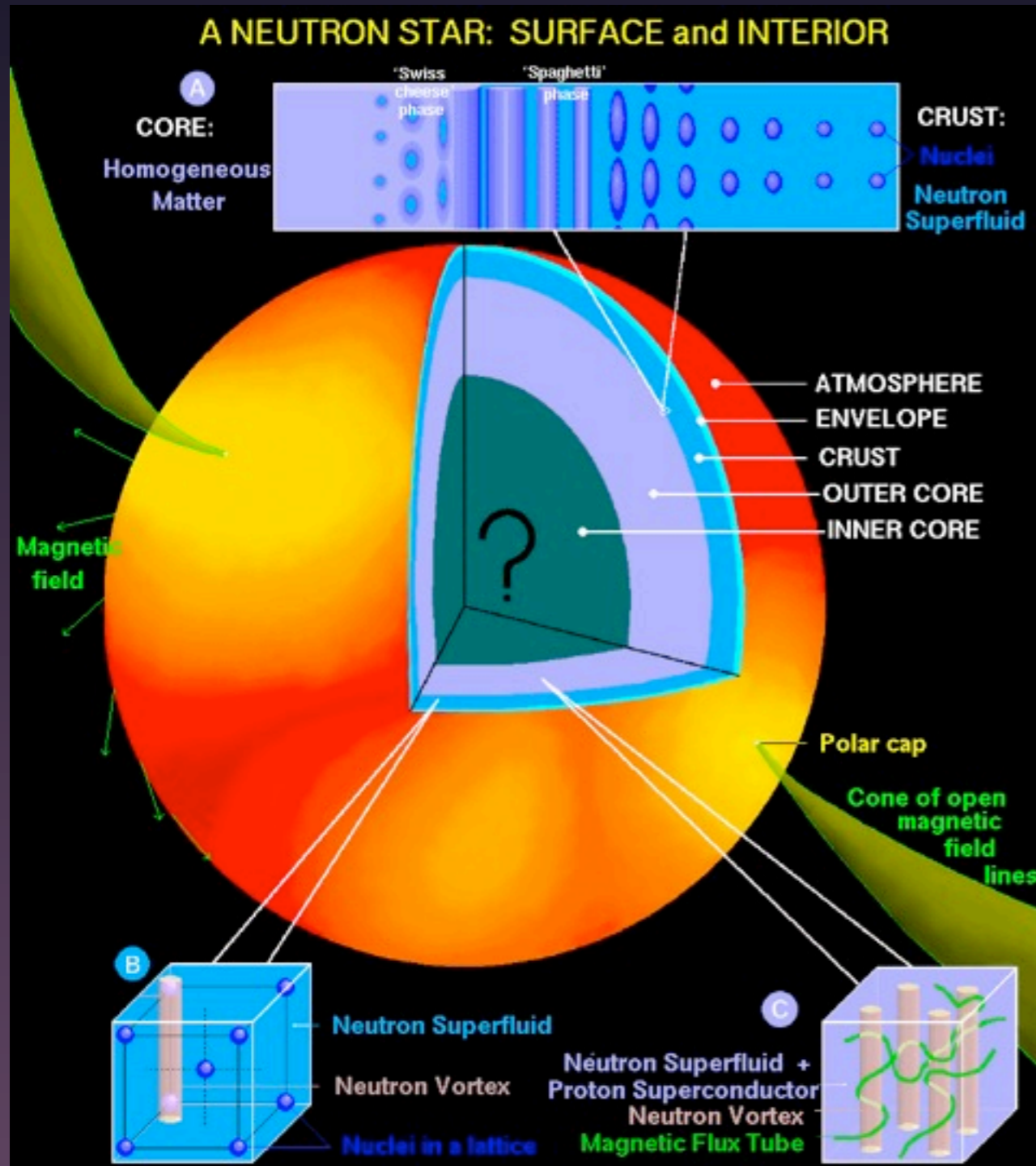
Paoletti, Fisher, Sreenivasan, and Lathrop,
PRL 101, 154501 (2008)

Quantum Turbulence with Fermions

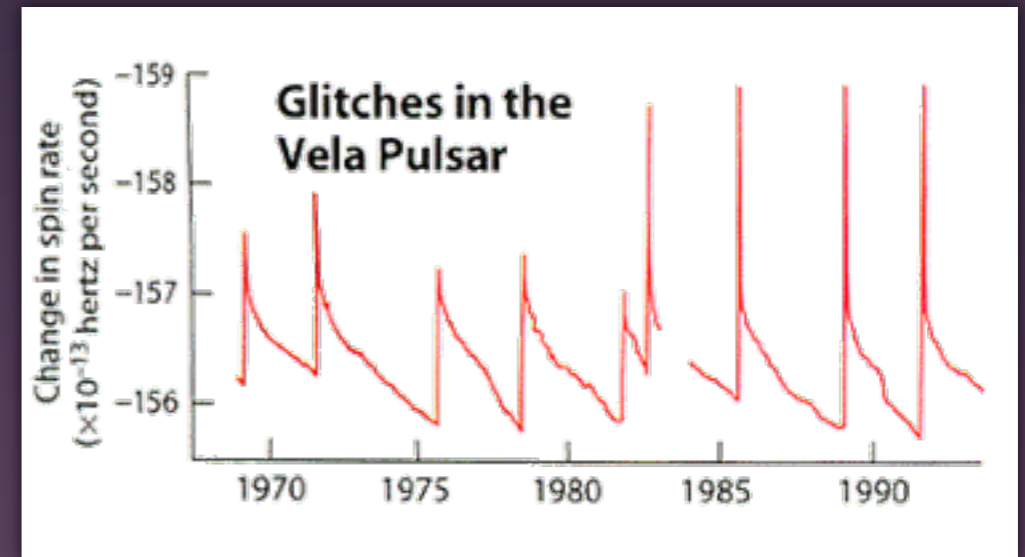


Wlazłowski, Bulgac, Forbes, and Roche [arXiv:1404.1038]

Neutron Star Glitches



- Rapid increase in pulsation rate
- Anderson and Itoh (1975) suggested pinned superfluid vortices



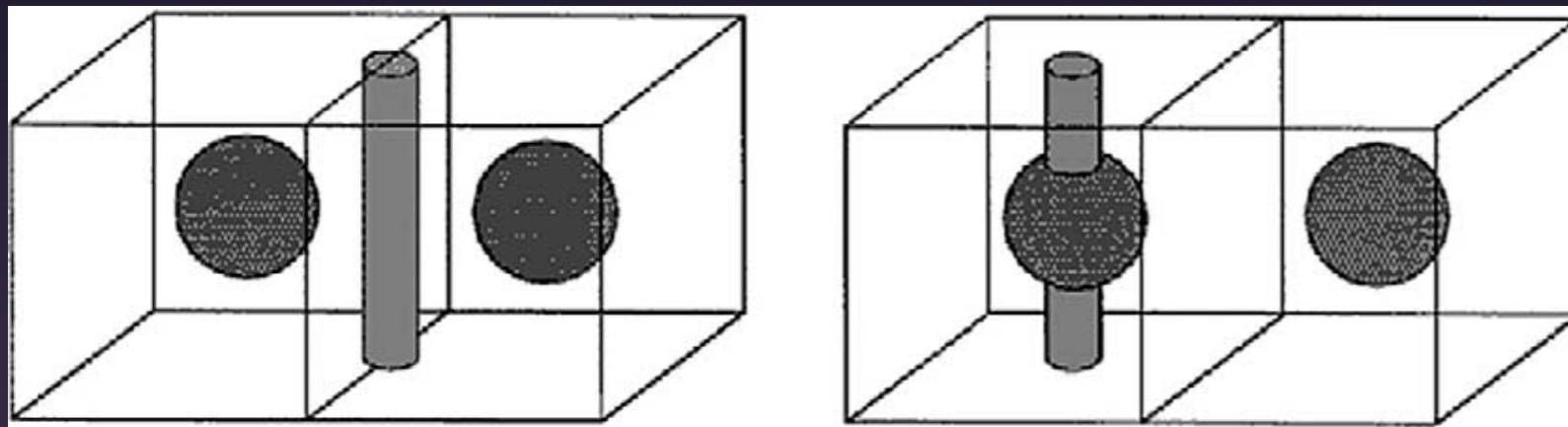
Pulsar Astronomy by Andrew G. Lyne and Francis Graham-Smith

Dany Page: <http://www.astroscu.unam.mx/neutrones/NS-Picture/NS-Picture.html>

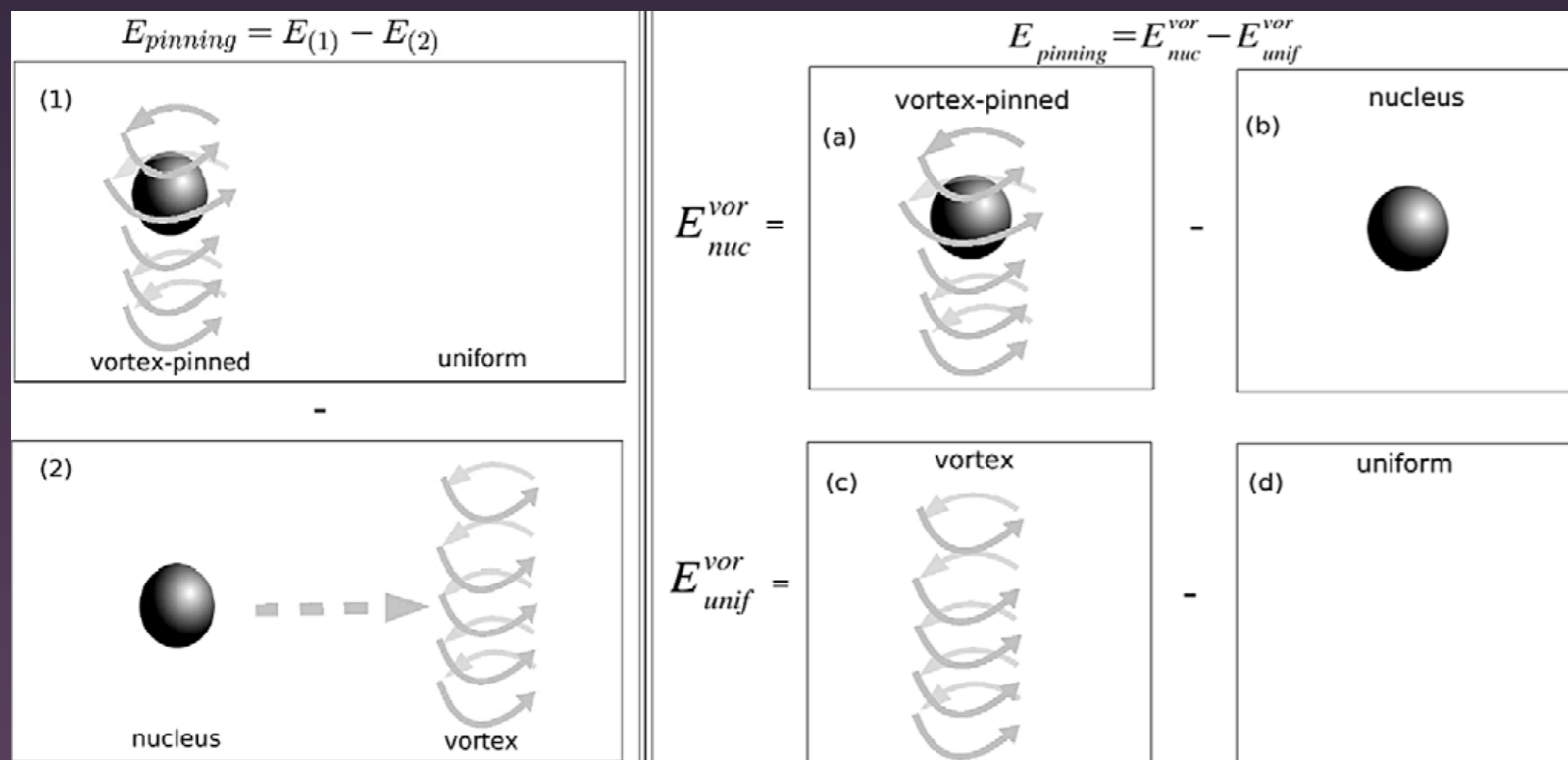
Understanding Pinning

- 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 \rightarrow hydrodynamics \rightarrow filament models

Pinning from Statics



Energy calculations



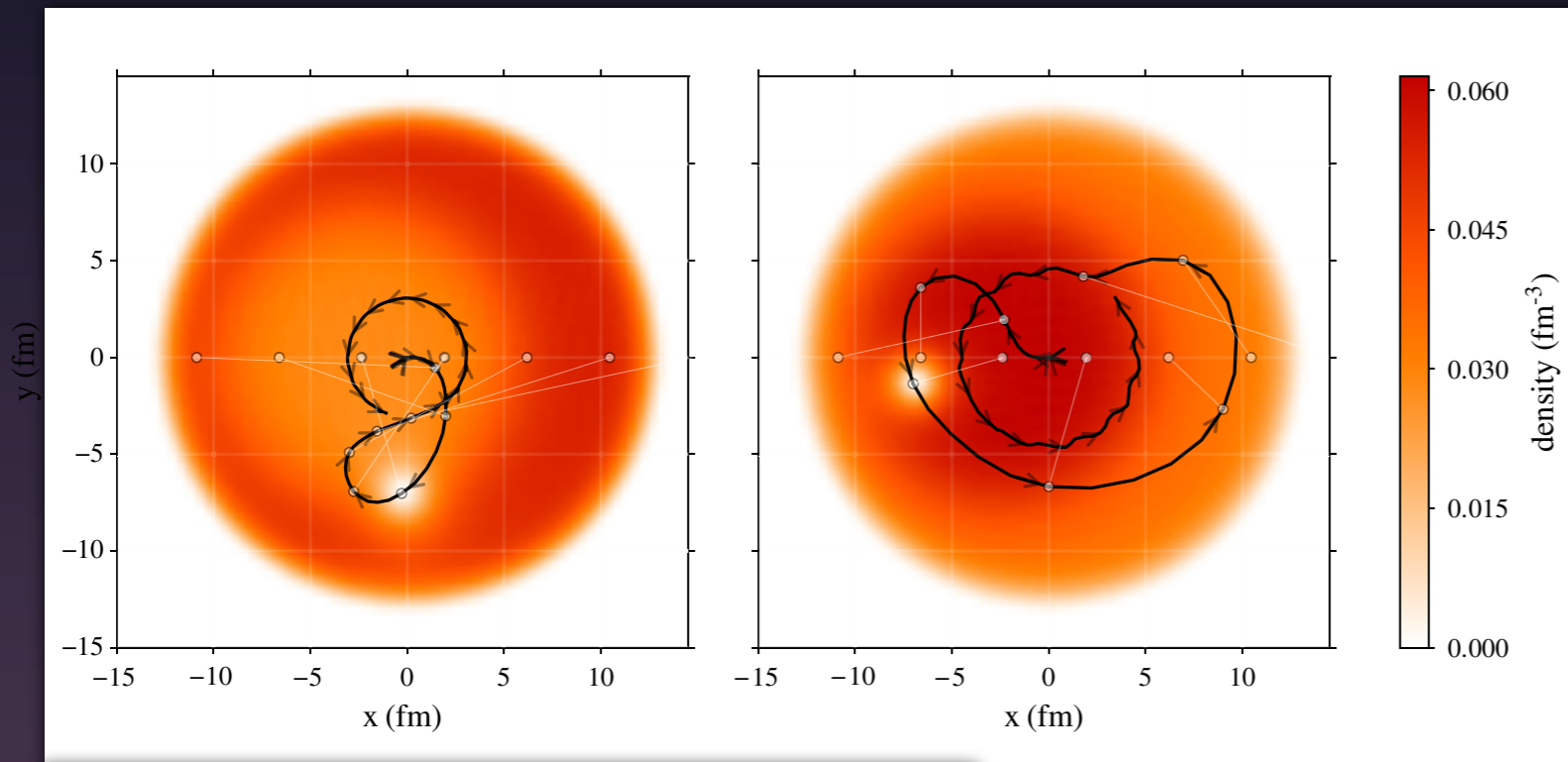
Must diagonalize to high precision
(subtraction involved)

How to extract $F(r)$?

P. Donati, P.M. Pizzochero Nucl. Phys. A742 (2004) 363

Avogadro, F. Barranco, R. A. Broglia, and E. Viguzzi, Nucl. Phys. A811 (2008) 378

Pinning: Dynamics

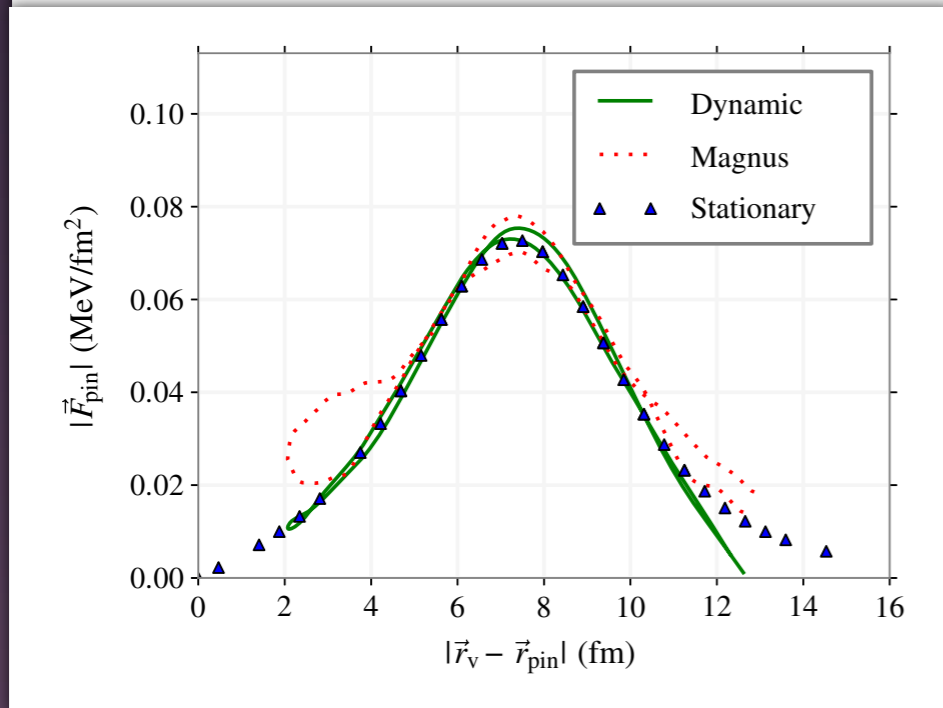


Extract force with dynamical methods

Scales well numerically:
No diagonalization

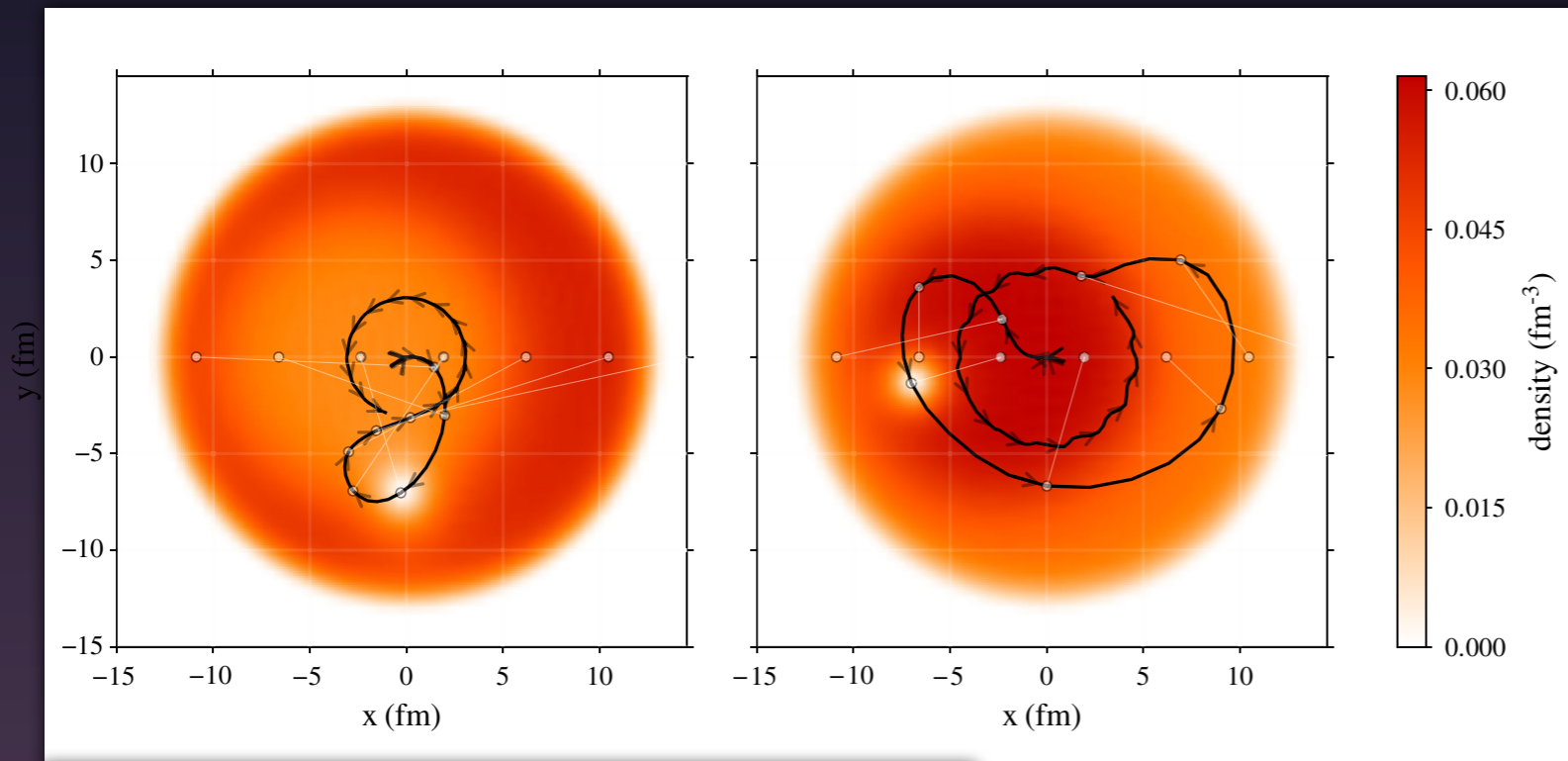
Extract force at any separation

Still needs fermion DFT



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

Pinning: Dynamics



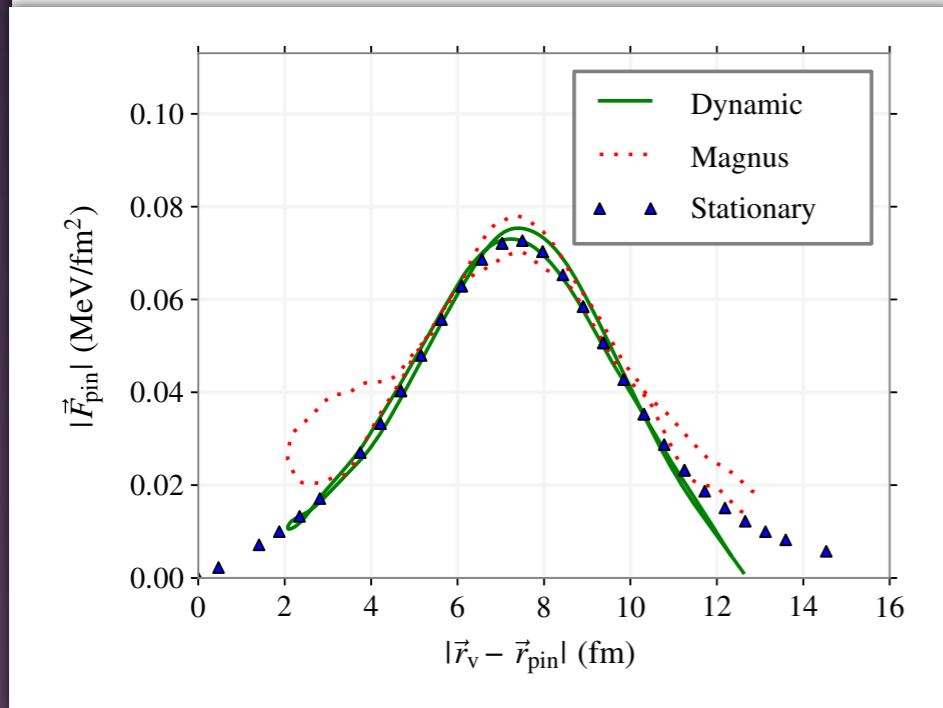
Extract force with dynamical methods

Scales well numerical:
No diagonalization

Extract force at any separation

Multiscale analysis:

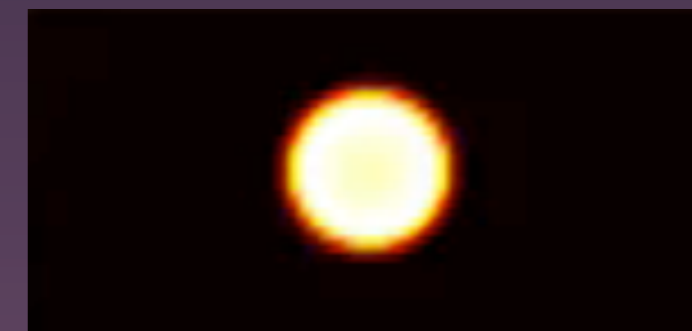
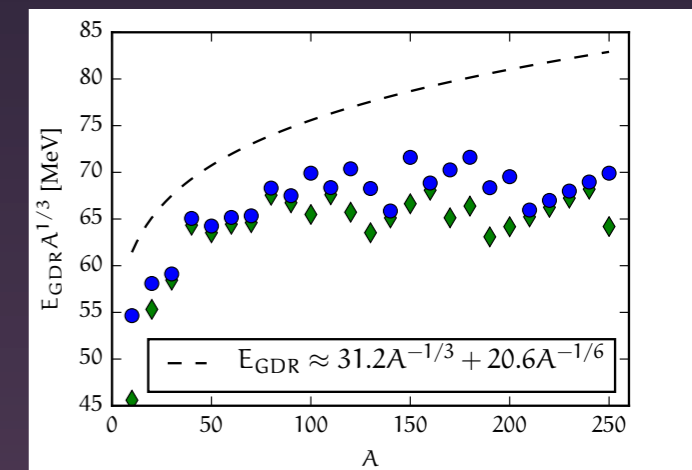
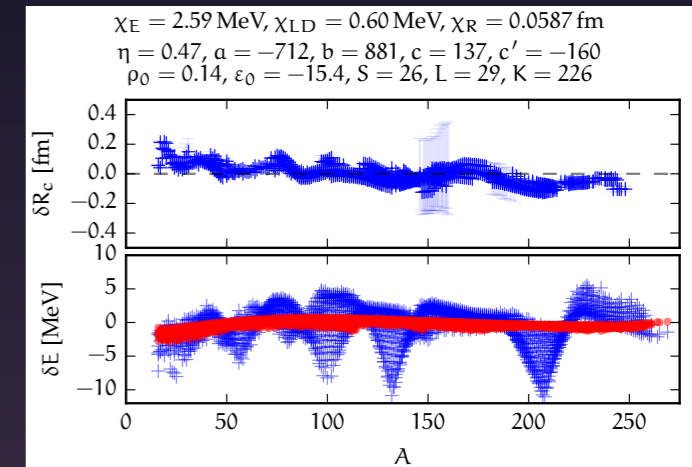
- Microscopic DFT
- Mesoscopic GPE
- Macroscopic hydro



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

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

- Extended Thomas-Fermi (ETF) form

- $\mathcal{E}(\rho_n, \rho_p)$

- Equation of state. Saturation and symmetry properties: 4 parameters

- $\mathcal{E}_\nabla(\nabla\rho_n, \nabla\rho_p, \dots)$

- 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

$$\begin{aligned} \mathcal{E}(\rho_{n,p}) = & \frac{3 \hbar^2 (3\pi^2 \rho_n)^{2/3}}{5} + \frac{3 \hbar^2 (3\pi^2 \rho_p)^{2/3}}{5} + \\ & + \left(a_0 \rho_+^{2/3} + a_1 \rho_+ + a_2 \rho_+^{4/3} + \dots \right) \rho_+ + \\ & + \left(b_0 \rho_+^{2/3} + b_1 \rho_+ + b_2 \rho_+^{4/3} + \dots \right) \rho_+ \left(\frac{\rho_n - \rho_p}{\rho_+} \right)^2 \end{aligned}$$

- Thomas-Fermi (TF) non-interacting

Equation of State

$$\begin{aligned} \mathcal{E}(\rho_{n,p}) = & \frac{3 \hbar^2 (3\pi^2 \rho_n)^{2/3}}{5} + \frac{3 \hbar^2 (3\pi^2 \rho_p)^{2/3}}{5} + \\ & + \left(a_0 \rho_+^{2/3} + a_1 \rho_+ + a_2 \rho_+^{4/3} + \dots \right) \rho_+ + \\ & + \left(b_0 \rho_+^{2/3} + b_1 \rho_+ + b_2 \rho_+^{4/3} + \dots \right) \rho_+ \left(\frac{\rho_n - \rho_p}{\rho_+} \right)^2 \end{aligned}$$

- Symmetric nuclear matter
- Exchange for saturation properties:

Equation of State

$$\begin{aligned}\mathcal{E}(\rho_{n,p}) = & \frac{3 \hbar^2 (3\pi^2 \rho_n)^{2/3}}{5} + \frac{3 \hbar^2 (3\pi^2 \rho_p)^{2/3}}{5} + \\ & + \left(a_0 \rho_+^{2/3} + a_1 \rho_+ + a_2 \rho_+^{4/3} + \dots \right) \rho_+ + \\ & + \left(b_0 \rho_+^{2/3} + b_1 \rho_+ + b_2 \rho_+^{4/3} + \dots \right) \rho_+ \left(\frac{\rho_n - \rho_p}{\rho_+} \right)^2\end{aligned}$$

- Symmetry Energy

Equation of State

$$\begin{aligned} \mathcal{E}(\rho_{n,p}) = & \frac{3 \hbar^2 (3\pi^2 \rho_n)^{2/3}}{5} + \frac{3 \hbar^2 (3\pi^2 \rho_p)^{2/3}}{5} + \\ & + \left(a_0 \rho_+^{2/3} + a_1 \rho_+ + a_2 \rho_+^{4/3} + \dots \right) \rho_+ + \\ & + \left(b_0 \rho_+^{2/3} + b_1 \rho_+ + b_2 \rho_+^{4/3} + \dots \right) \rho_+ \left(\frac{\rho_n - \rho_p}{\rho_+} \right)^2 \end{aligned}$$

- 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

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

$$\delta = \frac{\rho_0 - \rho}{3\rho_0}$$

- 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

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

$$Q = G_E^p * \rho_p + G_E^n * \rho_n$$

- 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

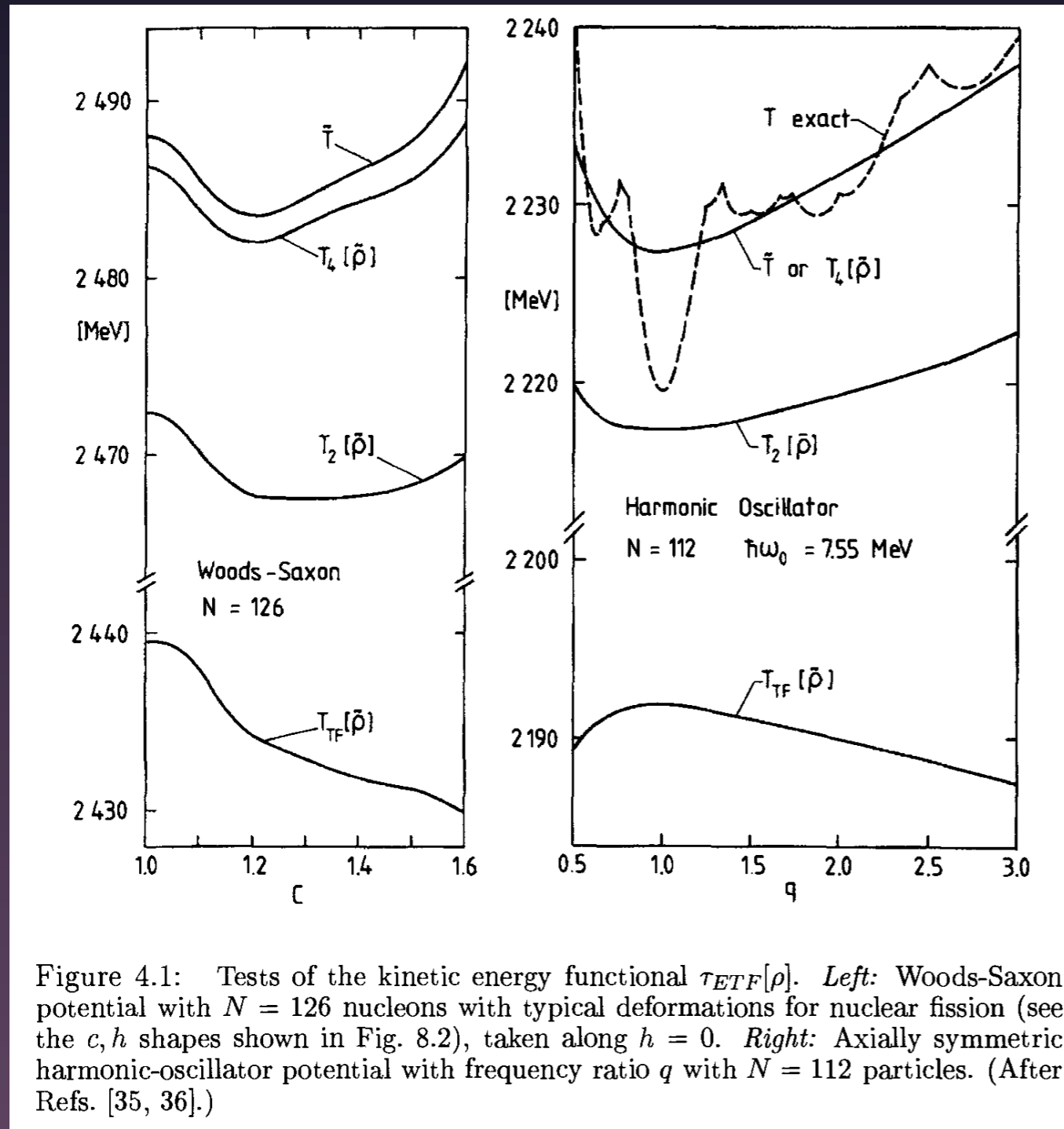
Semiclassical Expansion of Kinetic Energy

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

- $c_2 = 1/9$ (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)

Semiclassical Expansion



Brack and Bhaduri "Semiclassical physics" (1997)

Functional

$$\begin{aligned} \mathcal{E} = & \mathcal{E}_{\text{TF}}(\rho_n, \rho_p) + a_1 \rho^2 + a_2 \rho^{7/3} + \left(b_0 \rho^{5/3} + b_1 \rho^2 \right) \left(\frac{\rho_n - \rho_p}{\rho} \right)^2 \\ & + \eta \frac{\hbar^2}{2} \left(\frac{(\nabla \sqrt{\rho_n})^2}{m_n} + \frac{(\nabla \sqrt{\rho_p})^2}{m_p} \right) + c_4 \text{ terms} + \text{Coulomb} \end{aligned}$$

- 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

$\eta=1/4$ looks like dimers

- Fit: $\eta=1/2$

Liquid Drop Formula

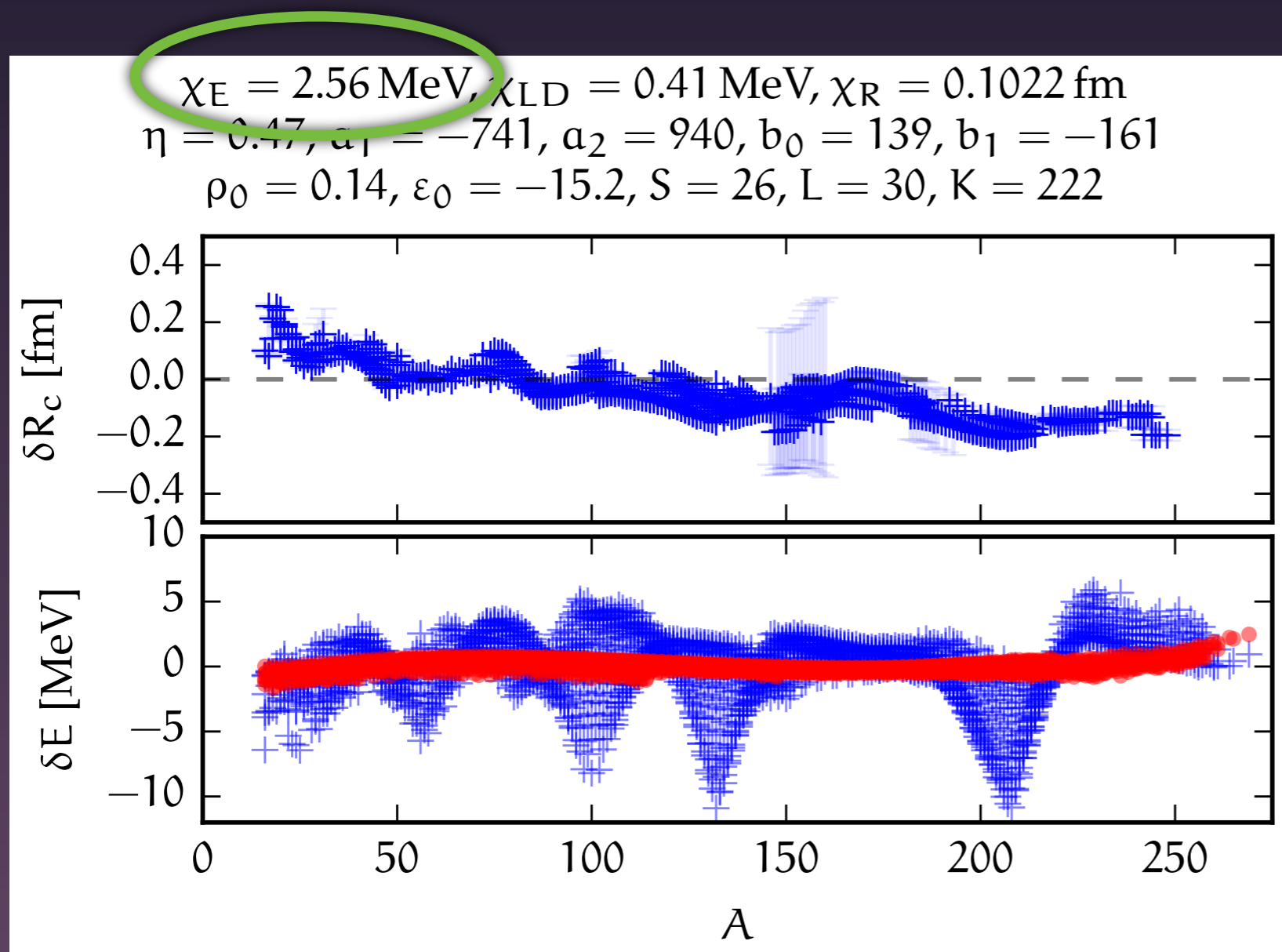
$$\begin{aligned} a_{\text{vol}}A + a_{\text{surf}}A^{2/3} + a_{\text{Coul}}\frac{Z^2}{A^{1/3}} + a_{\text{sym}}\frac{(Z - N)^2}{A} + a_{\text{pair}}\frac{(Z \bmod 2) + (N \bmod 2)}{A^{1/2}} \\ + a_{\text{CoulS}}\frac{Z^2}{A^{2/3}} + a_{\text{symS}}\frac{(Z - N)^2}{A^{4/3}} \end{aligned}$$

- 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

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



Just fit masses

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

Missing shell effects

Masses:

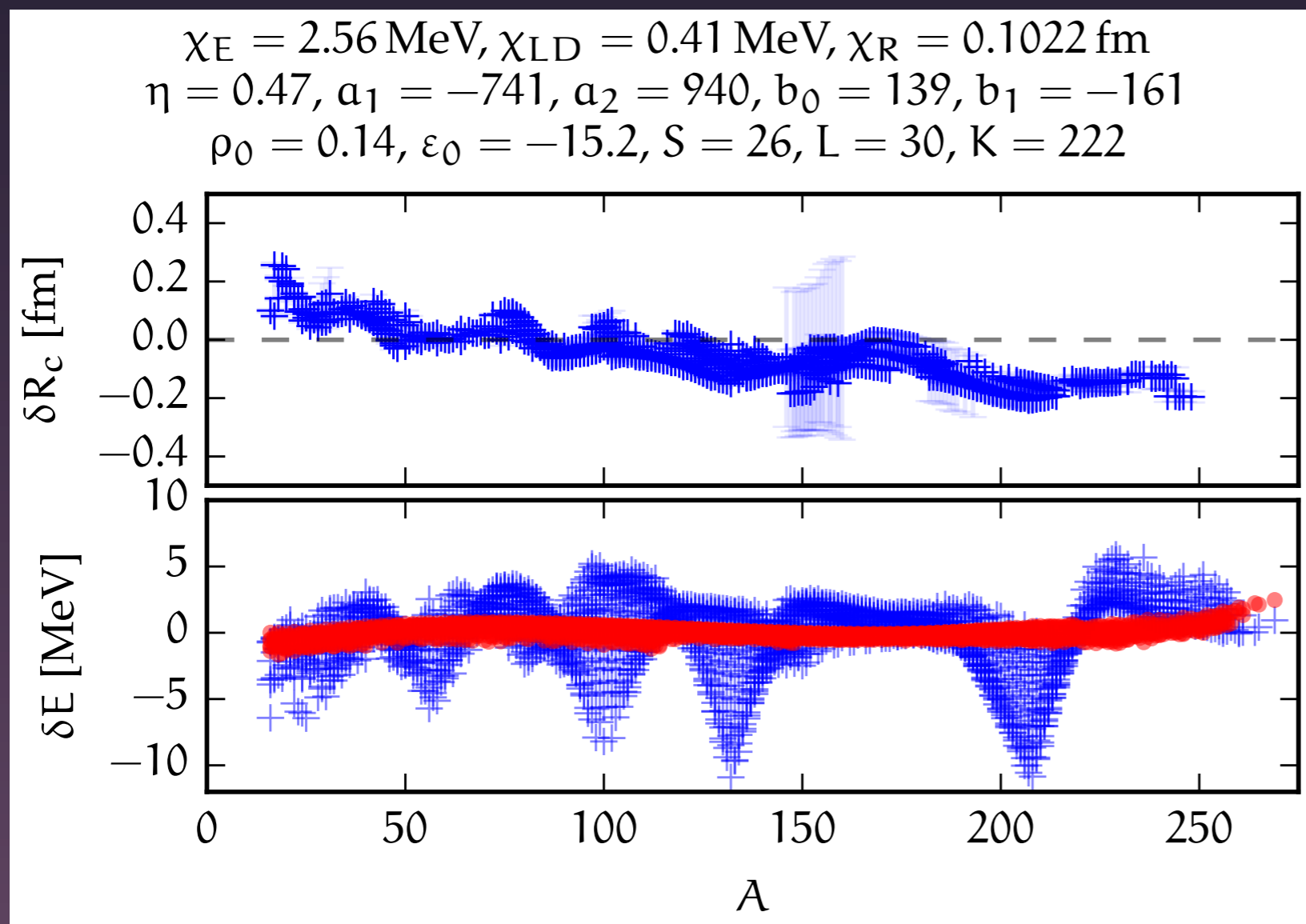
Audi (2012) - 2236 nuclei

Charge radii:

Angeli (2013) - 879 radii

No charge form-factors

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



Just fit masses

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

Missing shell effects

Masses:

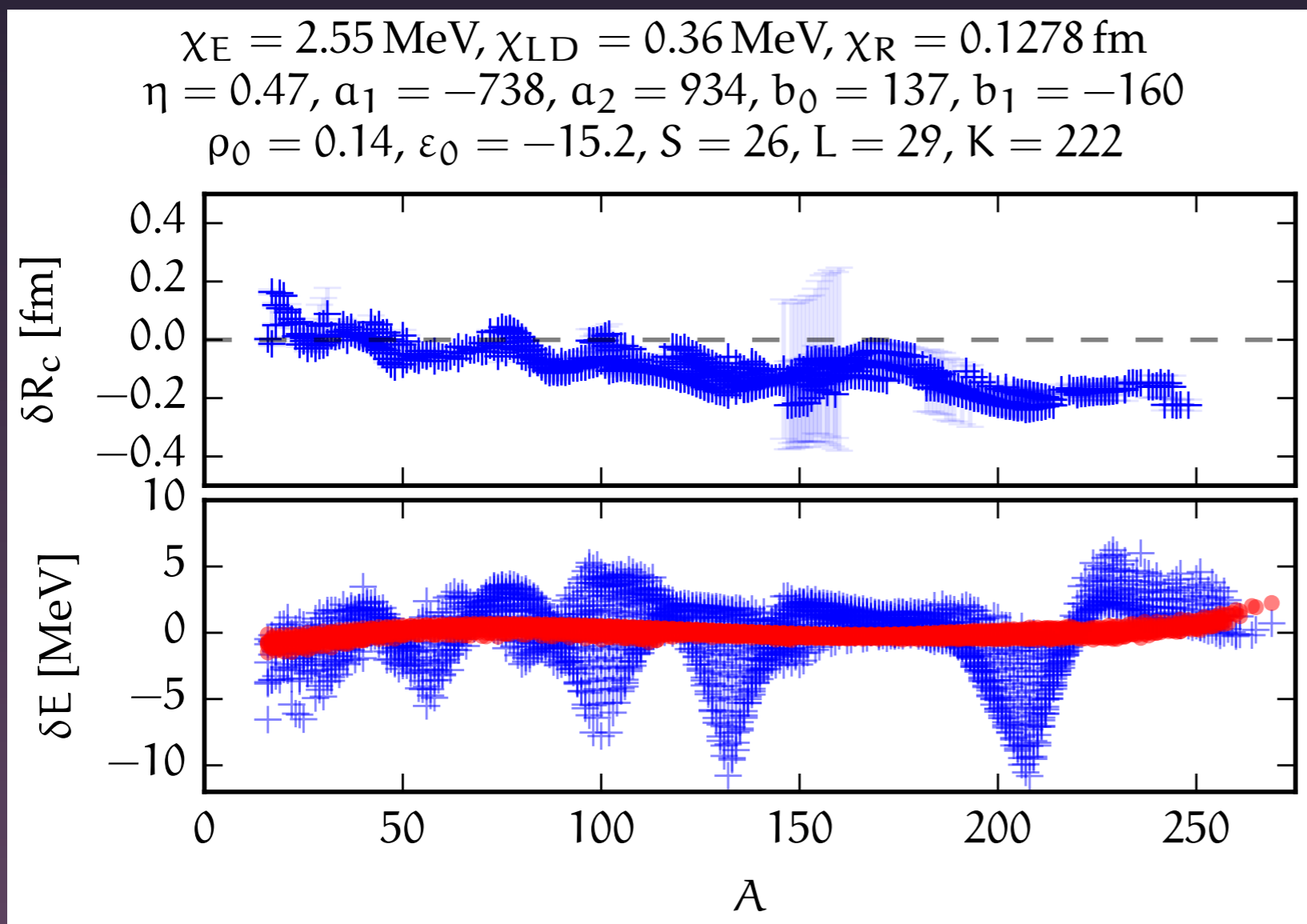
Audi (2012) - 2236 nuclei

Charge radii:

Angeli (2013) - 879 radii

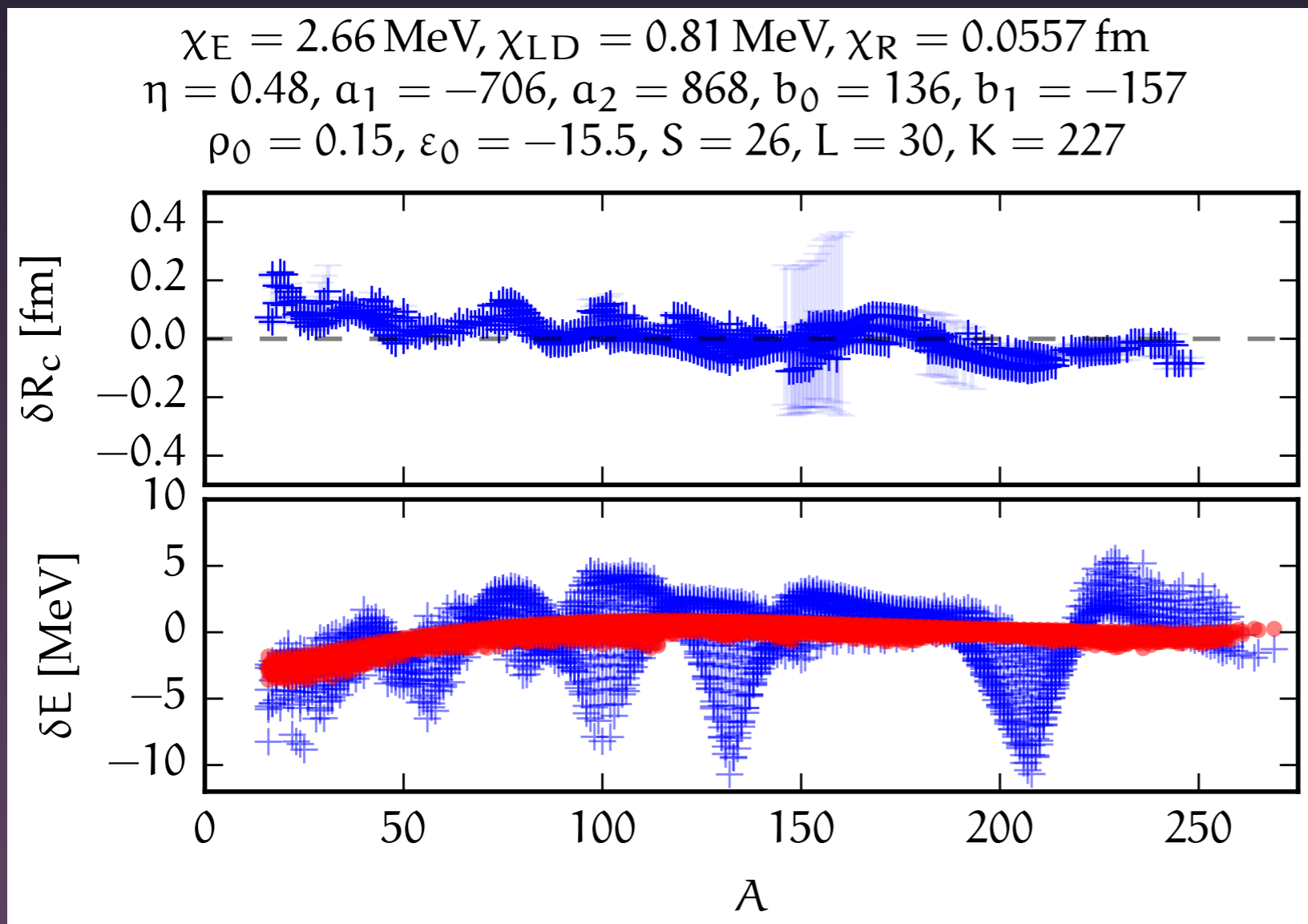
Add Charge form factors

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



Fit Charge Radii too

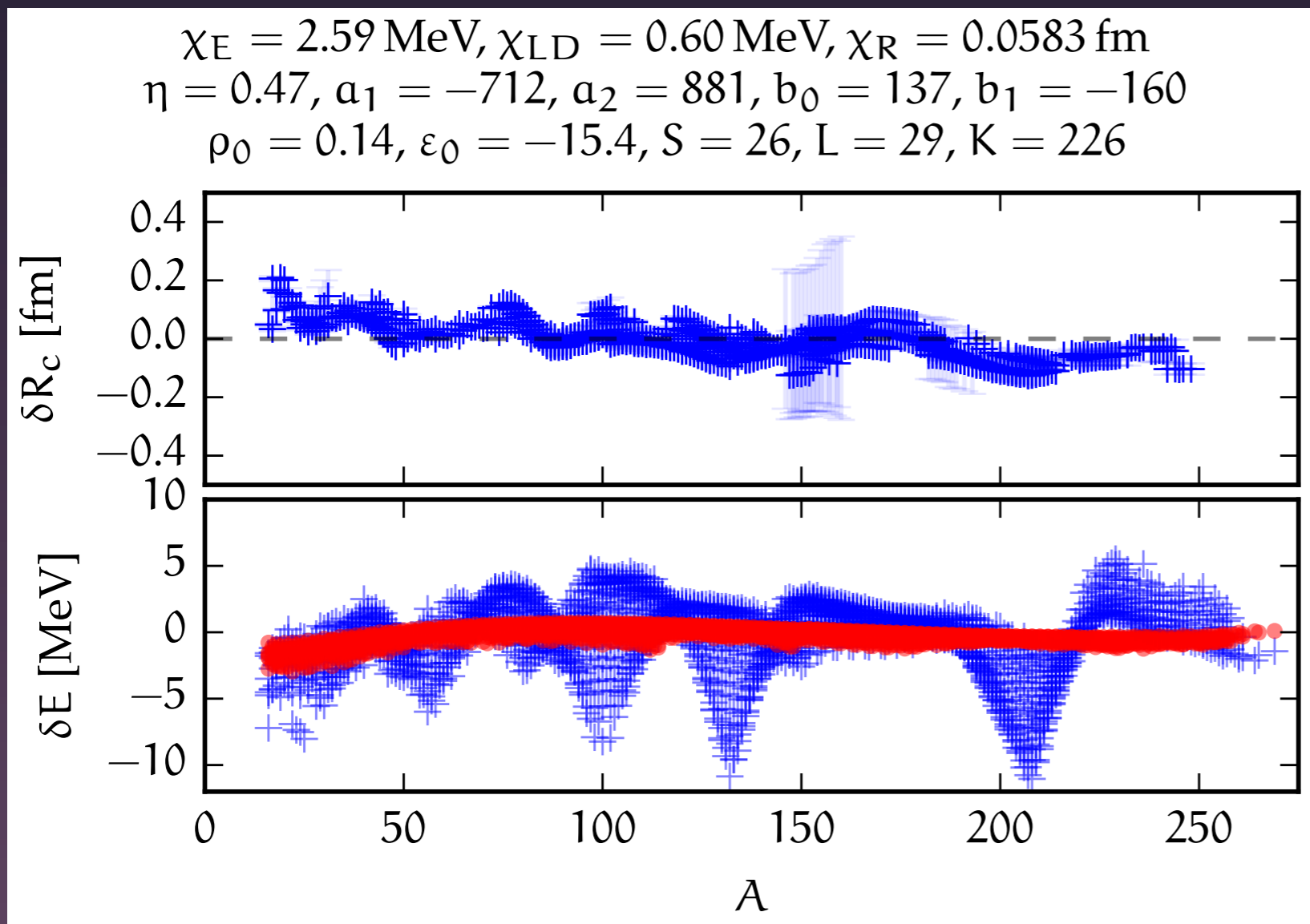
$$\varepsilon_{\text{TF}} + a_1 \rho^2 + a_2 \rho^{7/3} + \left(b_0 \rho^{5/3} + b_1 \rho^2 \right) \left(\frac{\rho_n - \rho_p}{\rho} \right)^2 + \eta \frac{\hbar^2}{2m} (\nabla \sqrt{\rho})^2 + \dots$$



Charge radii from
Angeli (2013)

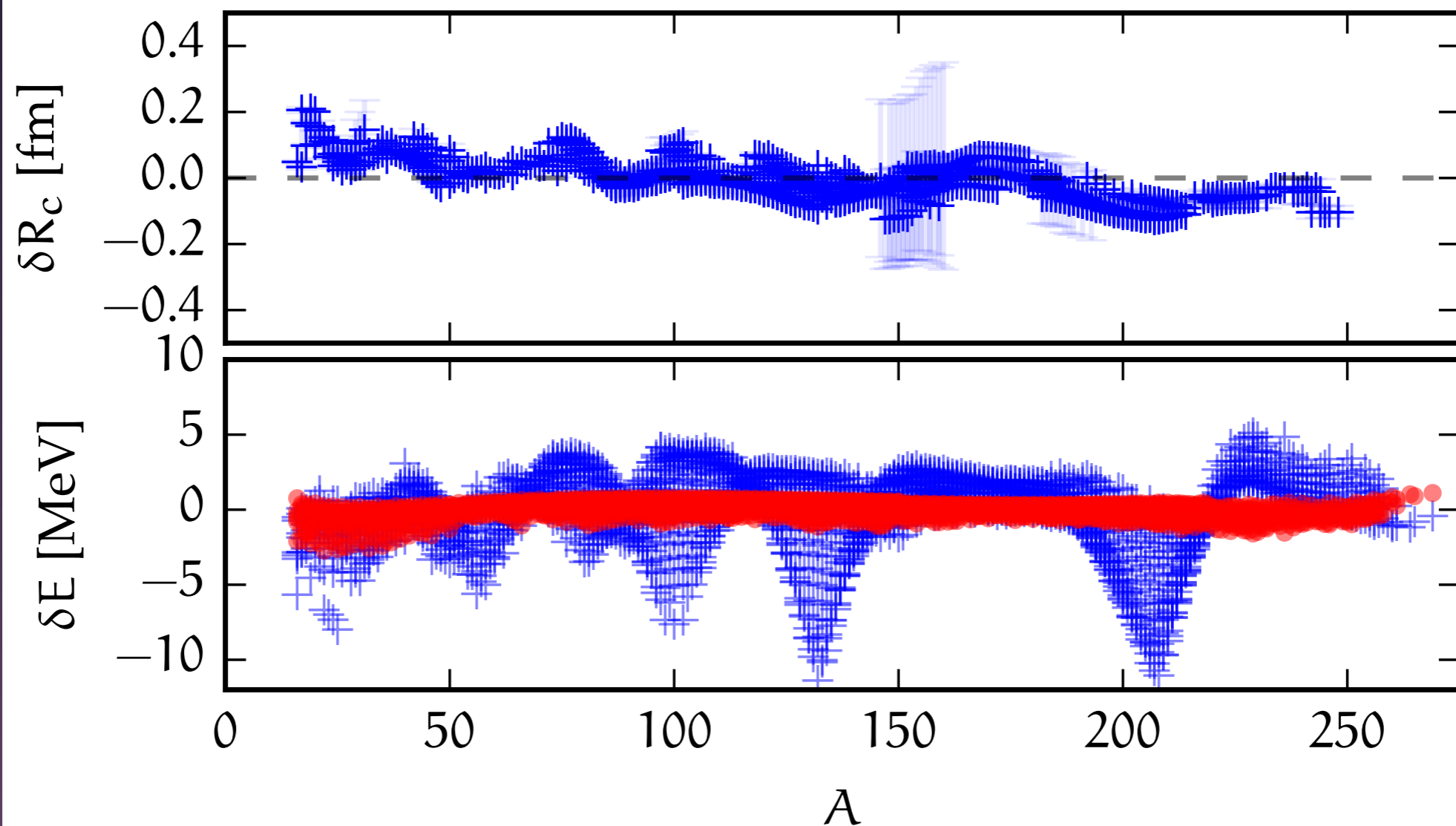
Fit individual c_4 terms

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



Missing Shell Effects

$$\begin{aligned} \chi_E &= 2.55 \text{ MeV}, \chi_{LD} = 0.51 \text{ MeV}, \chi_R = 0.0583 \text{ fm} \\ \eta &= 0.47, a_1 = -712, a_2 = 881, b_0 = 137, b_1 = -160 \\ \rho_0 &= 0.14, \varepsilon_0 = -15.4, S = 26, L = 29, K = 226 \end{aligned}$$



(Hydro)Dynamics

$$\partial_t \rho + \vec{\nabla} \cdot (\rho \vec{v}) = 0$$

$$m \left(\partial_t + \vec{v} \cdot \vec{\nabla} \right) \vec{v} + \vec{\nabla} \left(\frac{\delta \mathcal{E}(\rho, \nabla \rho, \dots)}{\delta \rho} \right) = 0$$

- 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

$$m \partial_t \vec{v} + \vec{\nabla} \left[\frac{m v^2}{2} + \frac{\delta \mathcal{E}(\rho, \nabla \rho, \dots)}{\delta \rho} \right] = 0$$



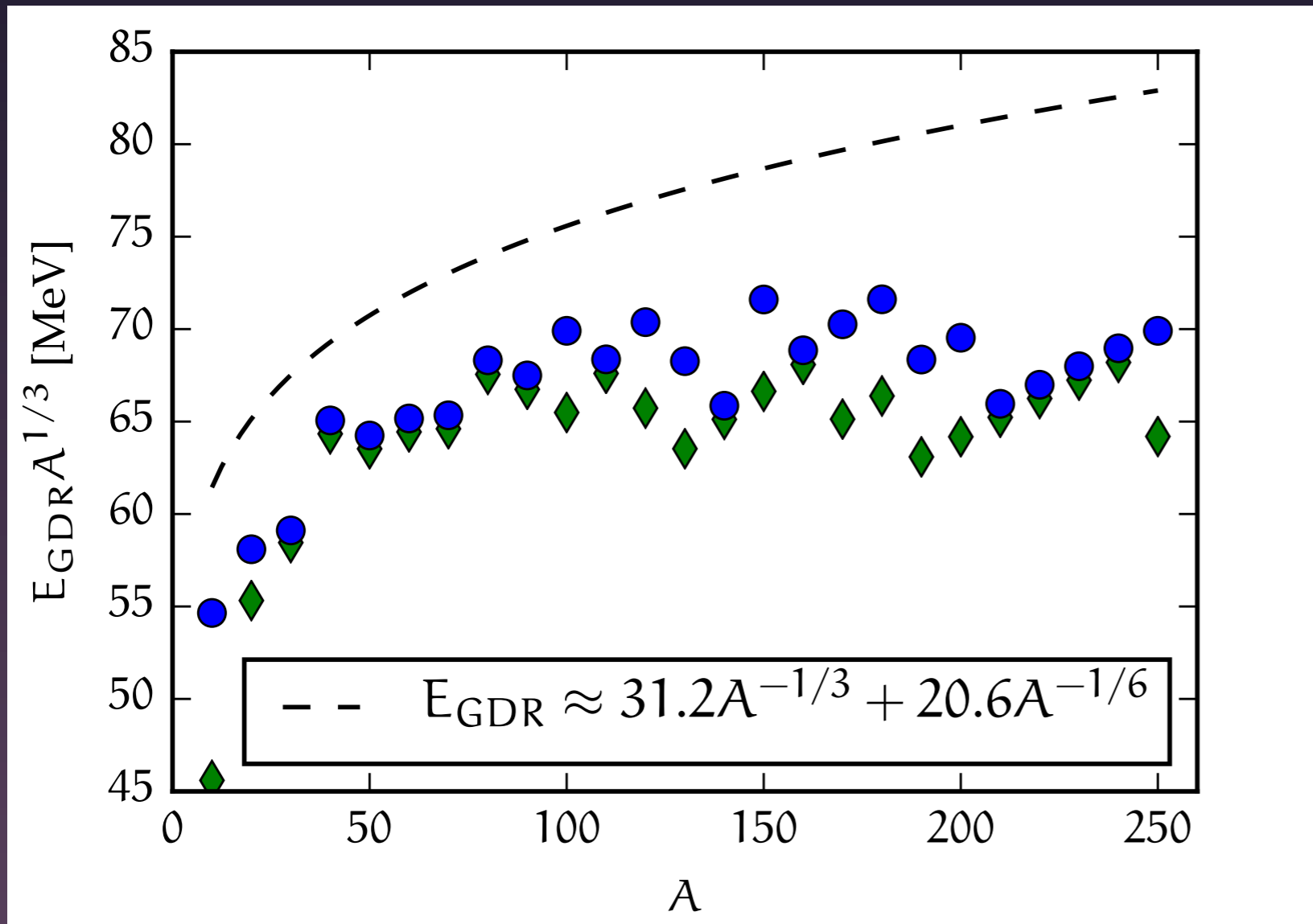
Implement as NLSEQ

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

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

- Numerically stable and efficient (same code as before)
(Some tricks with Coulomb)
- Artificial “quantization”
but $\eta=1/4$ looks like dimers...

Giant Dipole Resonance

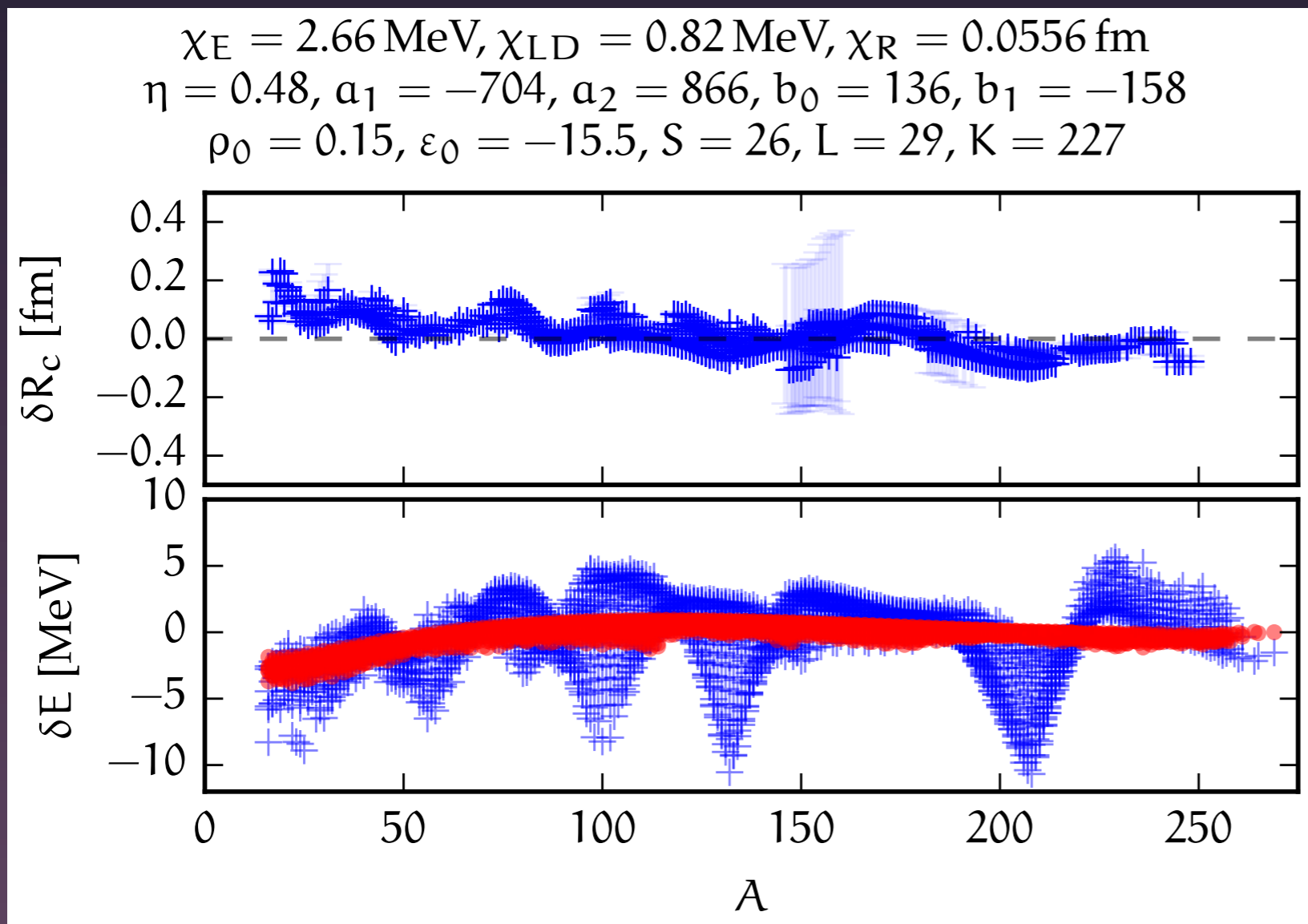


Preliminary results
~30% too low

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

Entrainment

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

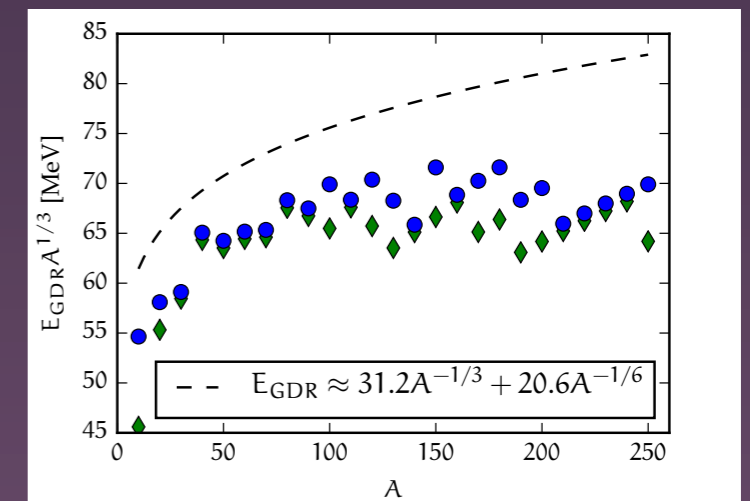


Galilean invariant

Best fit: $\alpha = -0.3$

30% to effective mass

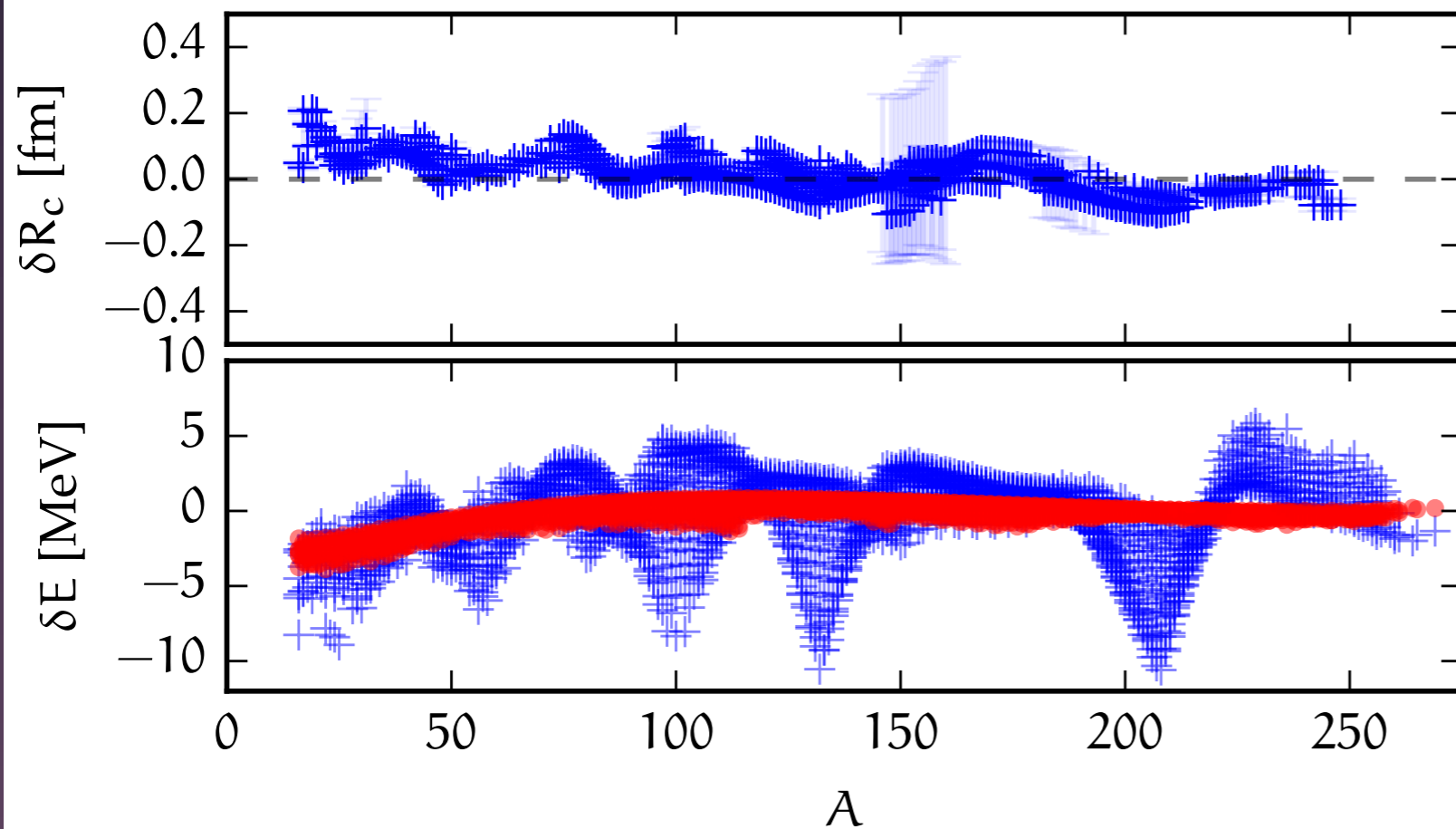
Time-dependent
Skyrme functionals do
not have this term...



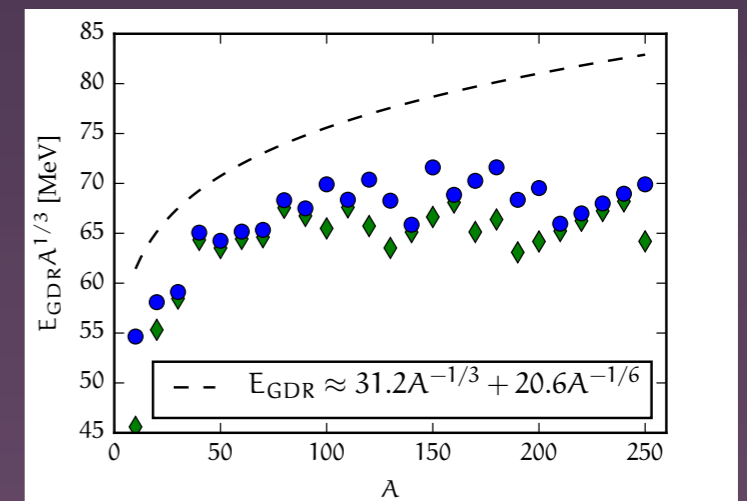
(no entrainment)

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

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



Entrainment does not spoil mass fits



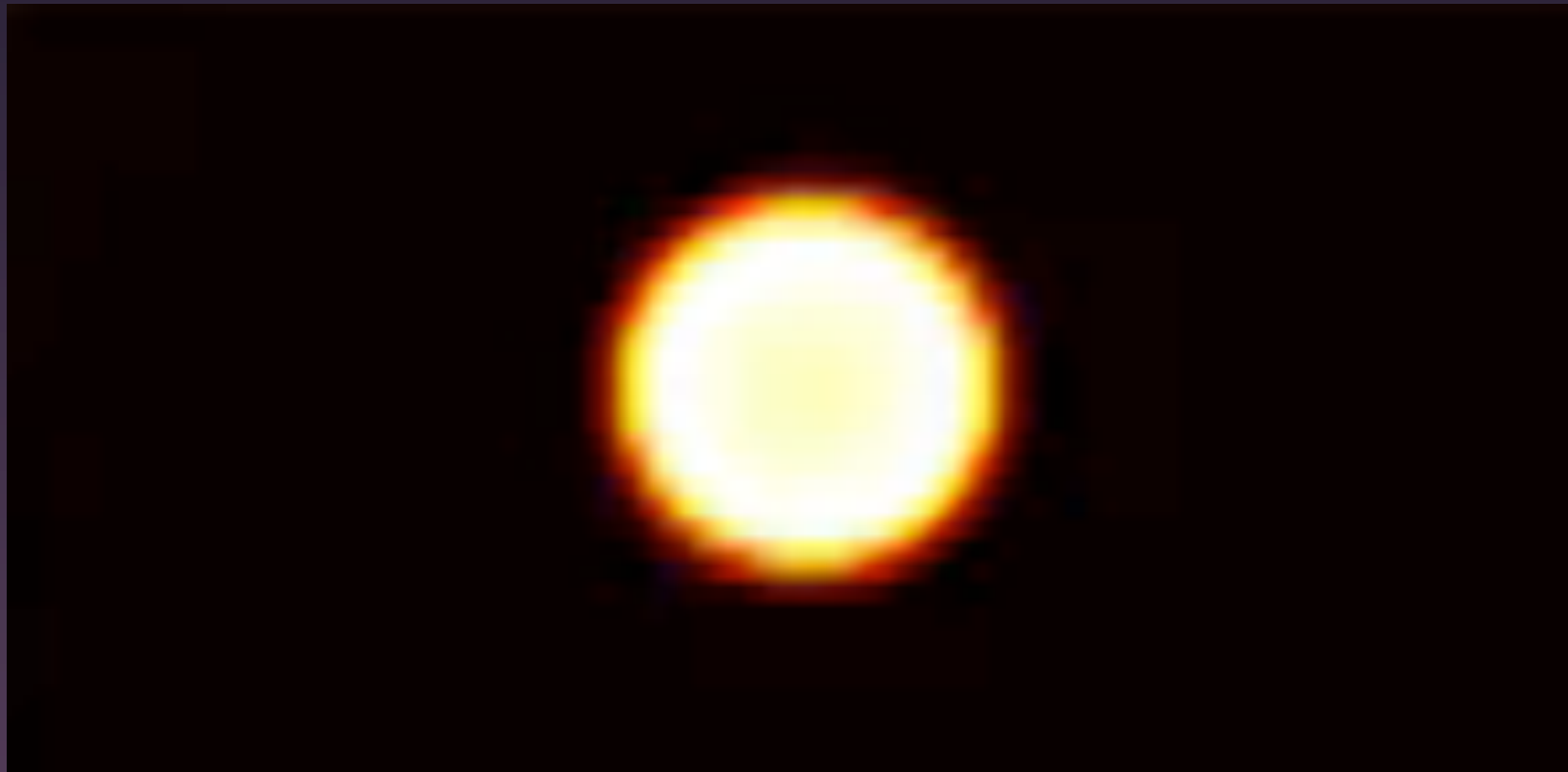
^{238}U Fission

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

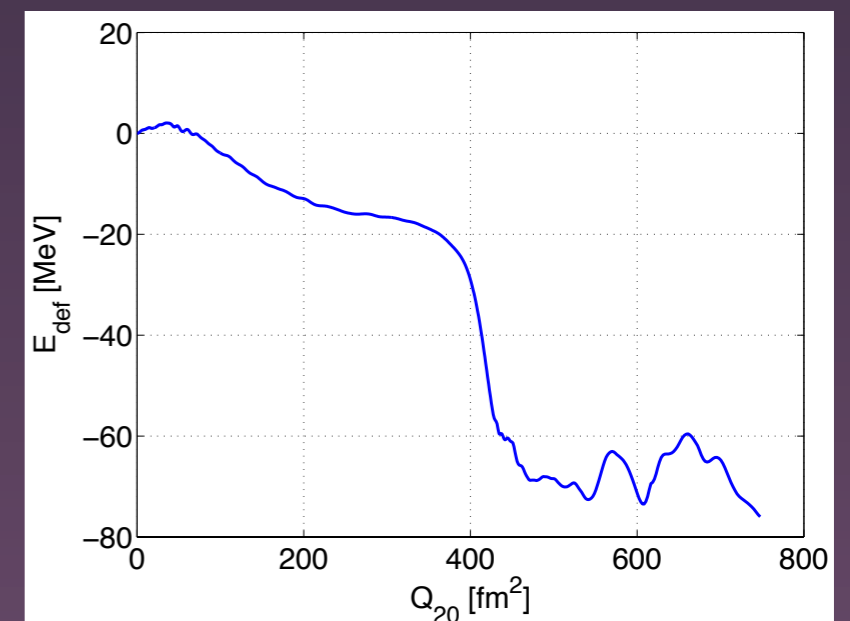
Quadrupole ν added

Fully 3D simulation
20 min on laptop

$32 \times 32 \times 64$
($dx=1\text{ fm}$)



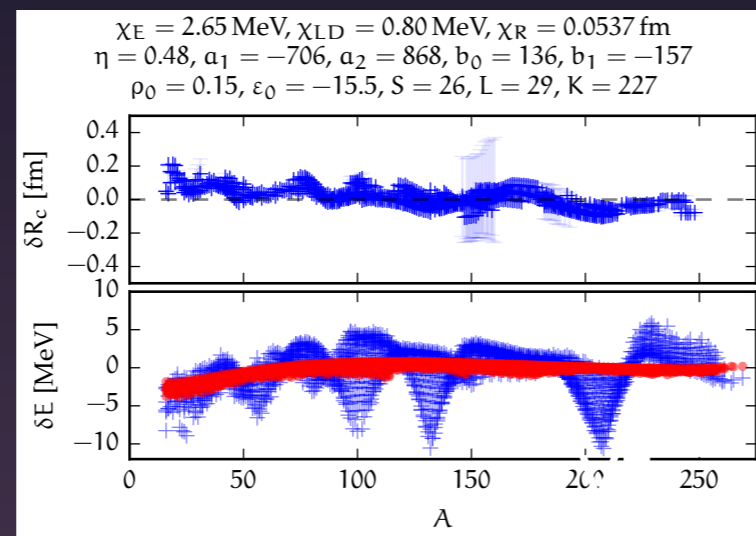
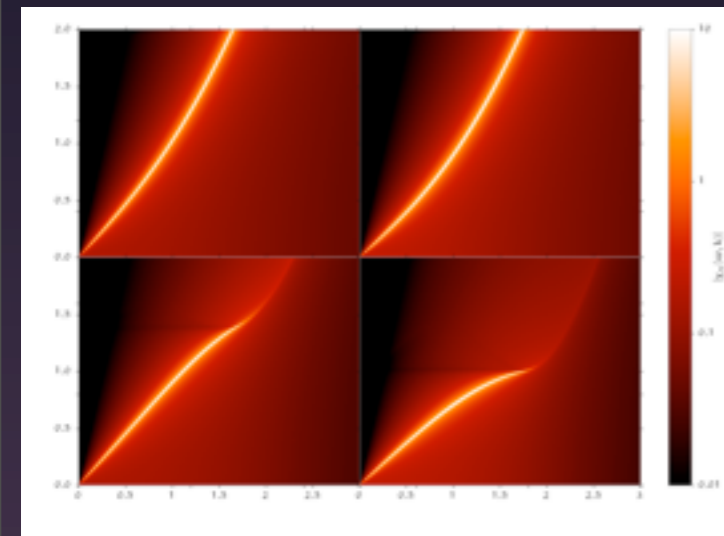
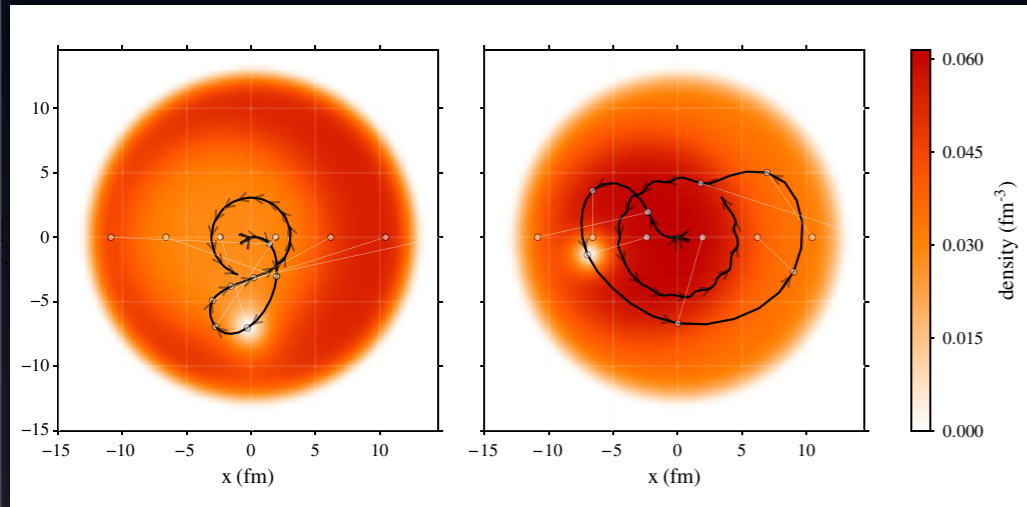
(Preliminary results)



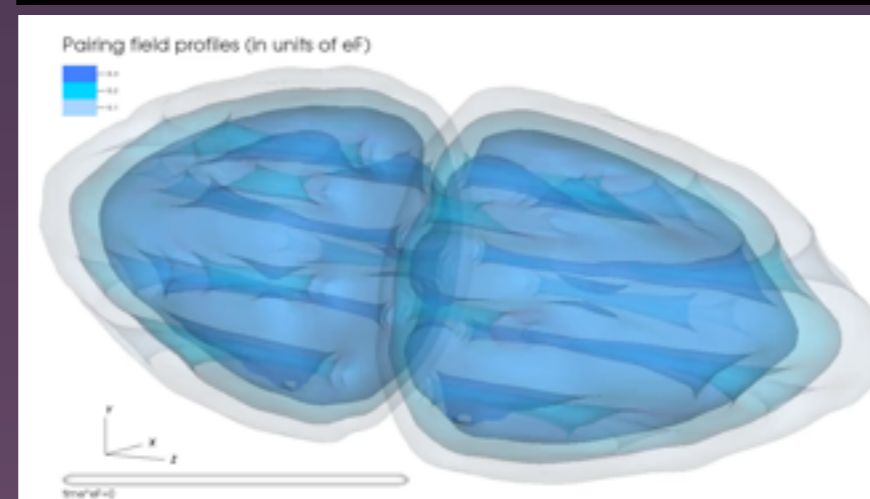
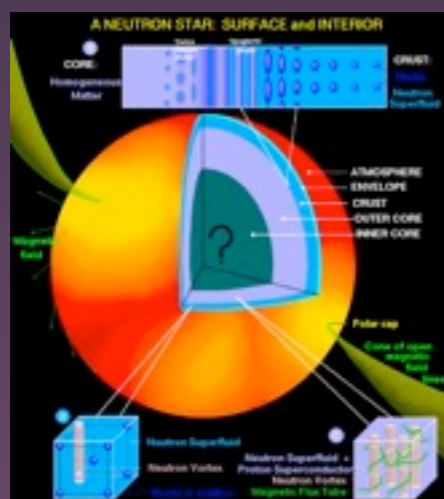
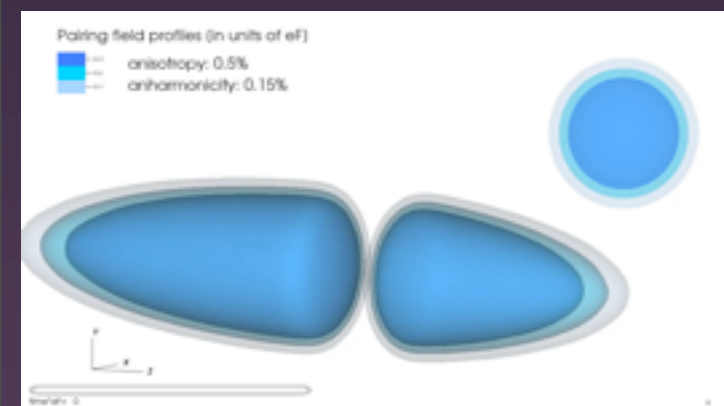
Can you simulate nuclei?

Boselets, Fermilets, ...

Realtime Methods



- Efficient
- DFT + Hydro.
 - Validated with cold atoms, nuclei
- New arena to study Quantum Turbulence and neutron star phenomenology



Realtime Methods

- Efficient
- DFT + Hydro.
 - Validated with cold atoms, nuclei
- New arena to study Quantum Turbulence and neutron star phenomenology

