Static and Dynamic Properties of the Unitary Gas

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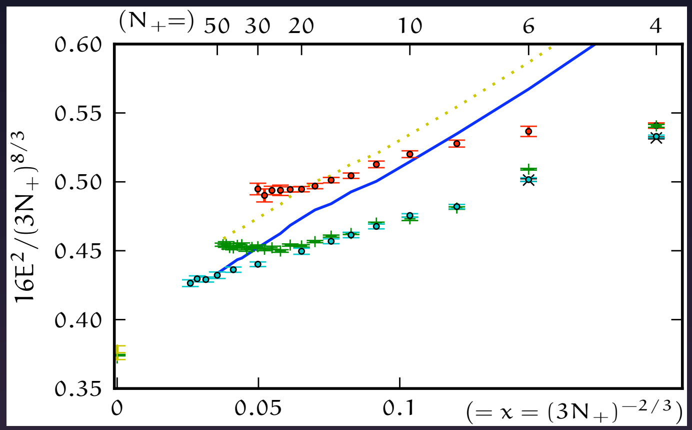
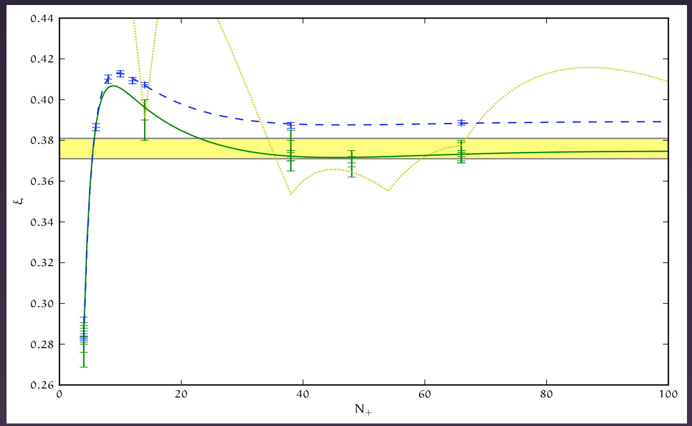
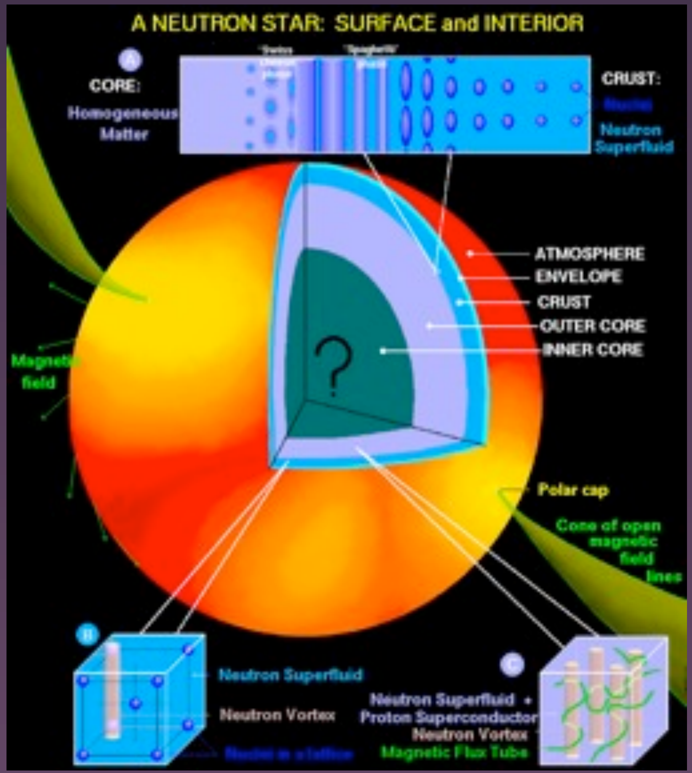
Outline

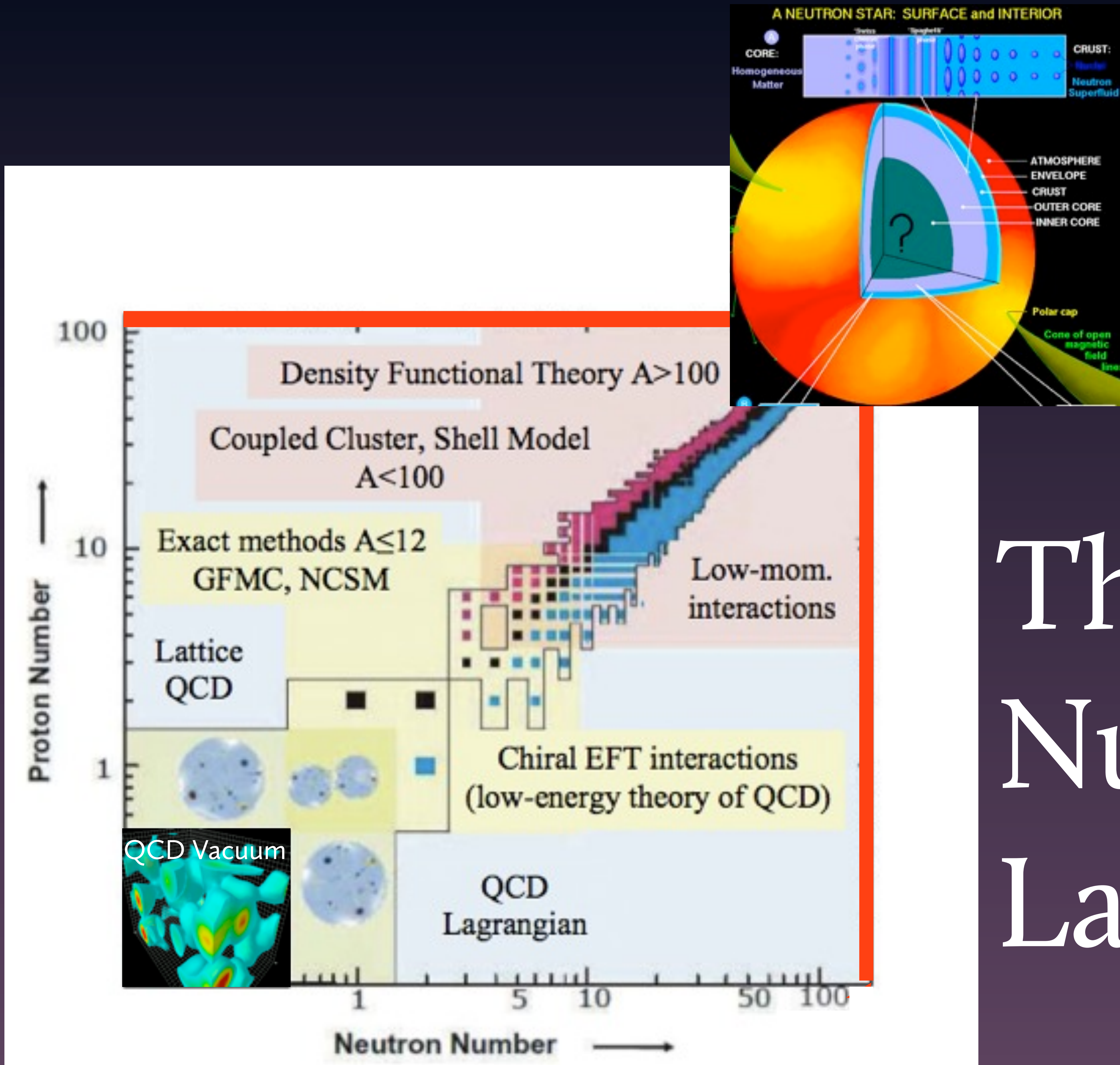
- DFT for Unitary Fermi Gas
  - Static: boxes and traps
  - Dynamics: via linear response and real time dynamics (TDDFT)
- Gross-Pitaevskii–Equation (GPE) to scale up to neutron stars (glitching)



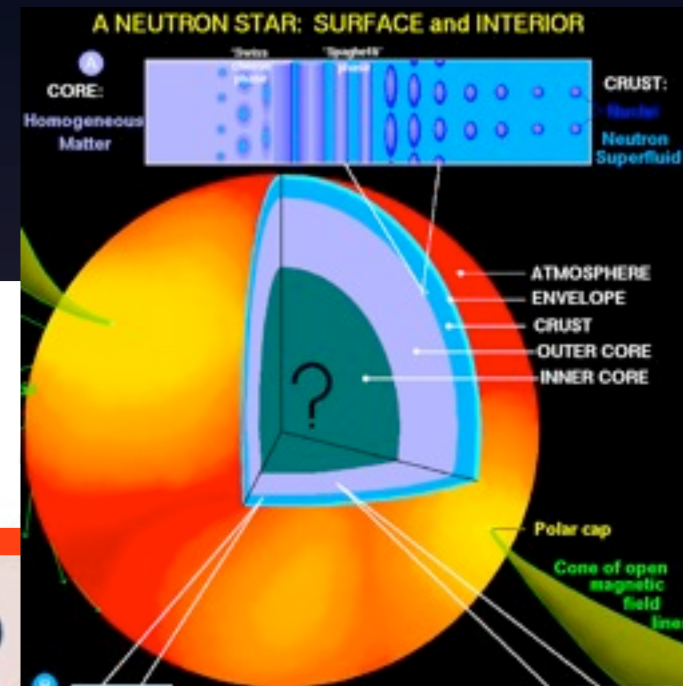


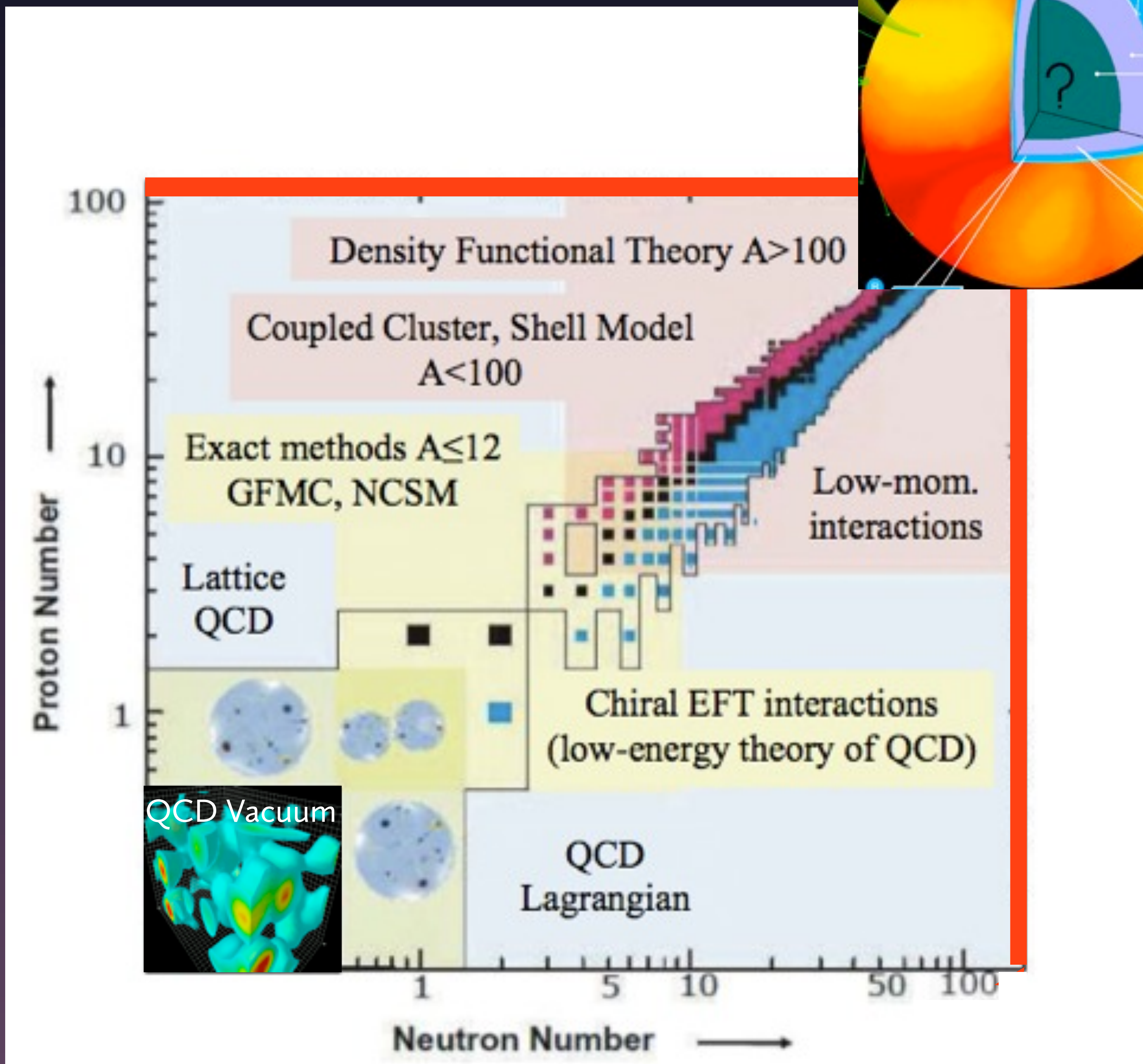


The Nuclear Landscape



QCD Vacuum Animation: Derek B. Leinweber (http://www.physics.adelaide.edu.au/~dleinweb/VisualQCD/Nobel/index.html)
Neutron Star Structure: (Dany Page) Landscape: (modified from a slide of A. Richter)





- Lattice QCD,
  nucleons, interactions
- QMC, etc.
  small to medium nuclei
- DFT,
  medium to large nuclei
- Neutron stars?
  Molecular Dynamics
  Hydrodynamics

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Application: Vortex Pinning

- Pulsar glitching (neutron stars)
  - Massive vortex unpinning events?
    Anderson and Itoh (1975)
- Large scale events (thousands of vortices)
  - Too big for DFT – use GPE
- Need Vortex-Defect interactions (force)
  - Use DFT to calculate and then fit GPE

Cold Atoms Benchmarking

- Theoretically clean and simple (universal)
- Well constrained
- Remarkably diverse phase structure
- Convergence of theory, simulation and experiment
- Benchmark for many-body techniques

Unitary Fermi Gas (UFG)

$$\hat{\mathcal{H}} = \int \left(\hat{\mathbf{a}}^\dagger \hat{\mathbf{a}} E_a + \hat{\mathbf{b}}^\dagger \hat{\mathbf{b}} E_b\right) - g \int_\Lambda \hat{\mathbf{a}}^\dagger \hat{\mathbf{b}}^\dagger \hat{\mathbf{b}} \hat{\mathbf{a}}$$

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

- 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)
- Universal physics:
  - $\mathcal{E}(\rho) = \xi \mathcal{E}_{FG}(\rho) \propto \rho^{5/3}$, $\xi = 0.376(5)$
- Good model of dilute neutron matter in neutron stars

Statics

Density Functional Theory (DFT)

- The (exact) ground state density in any external potential $V(x)$ minimizes a functional (Hohenberg Kohn):

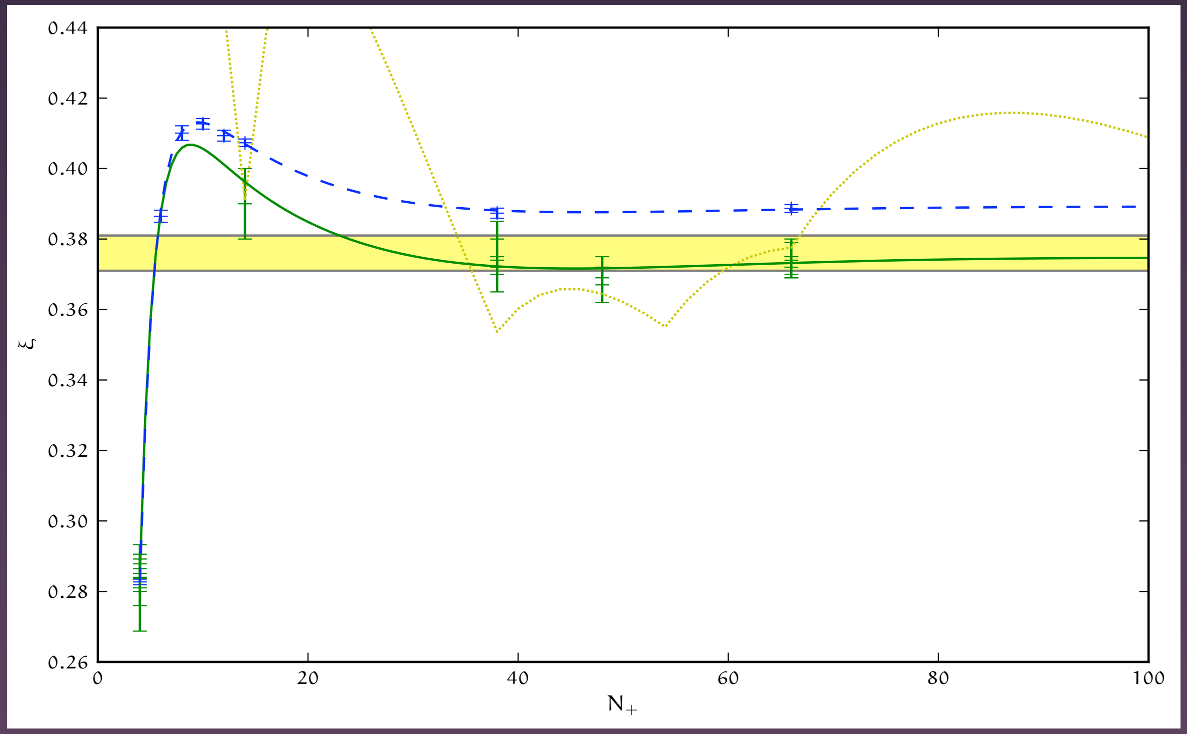
$$\int d^3x \{\mathcal{E}[n(x)] + V(x)n(x)\}$$

- Functional may be complicated (non-local)
  - Need to find physically motivated approximations

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

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

- 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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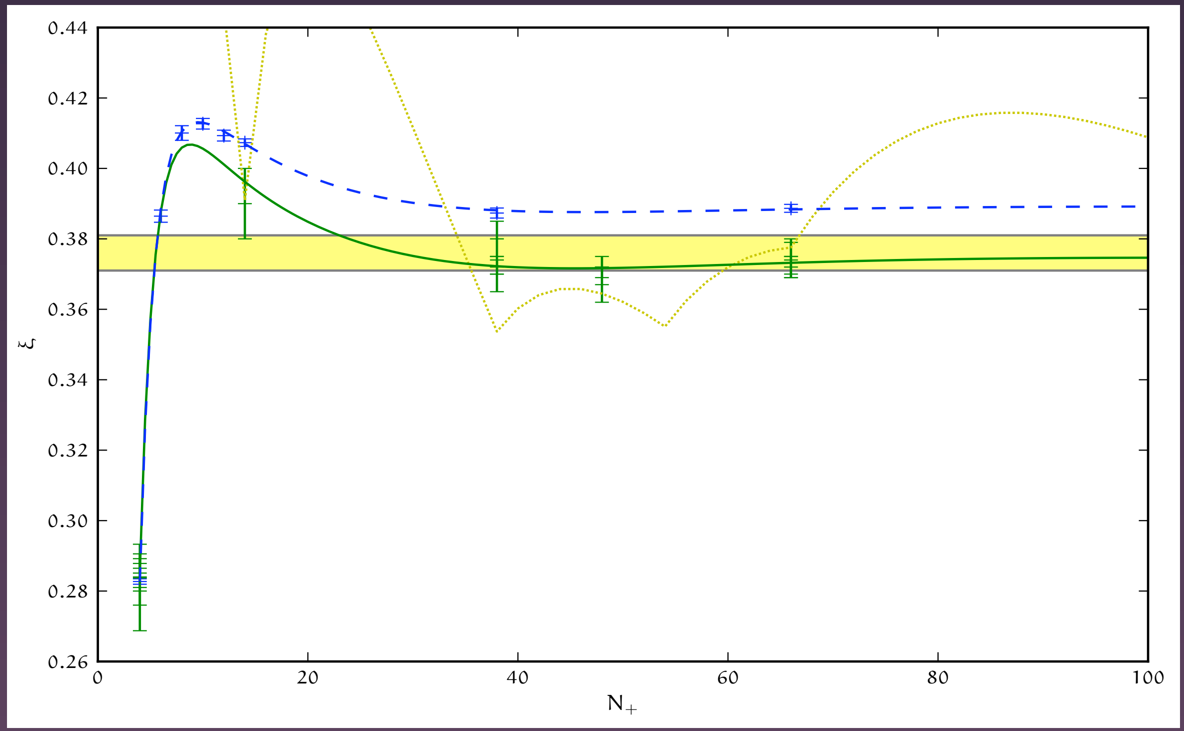
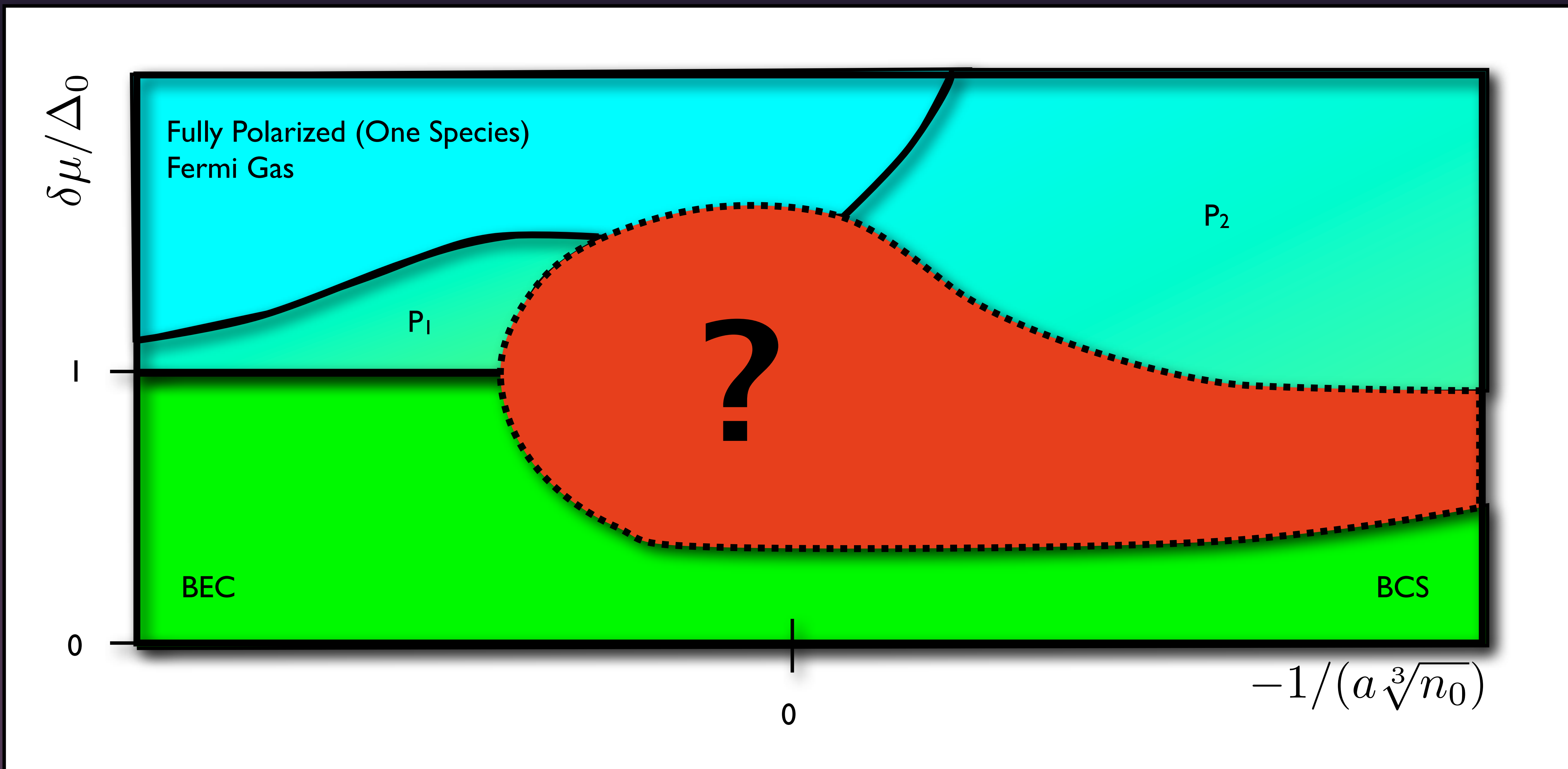
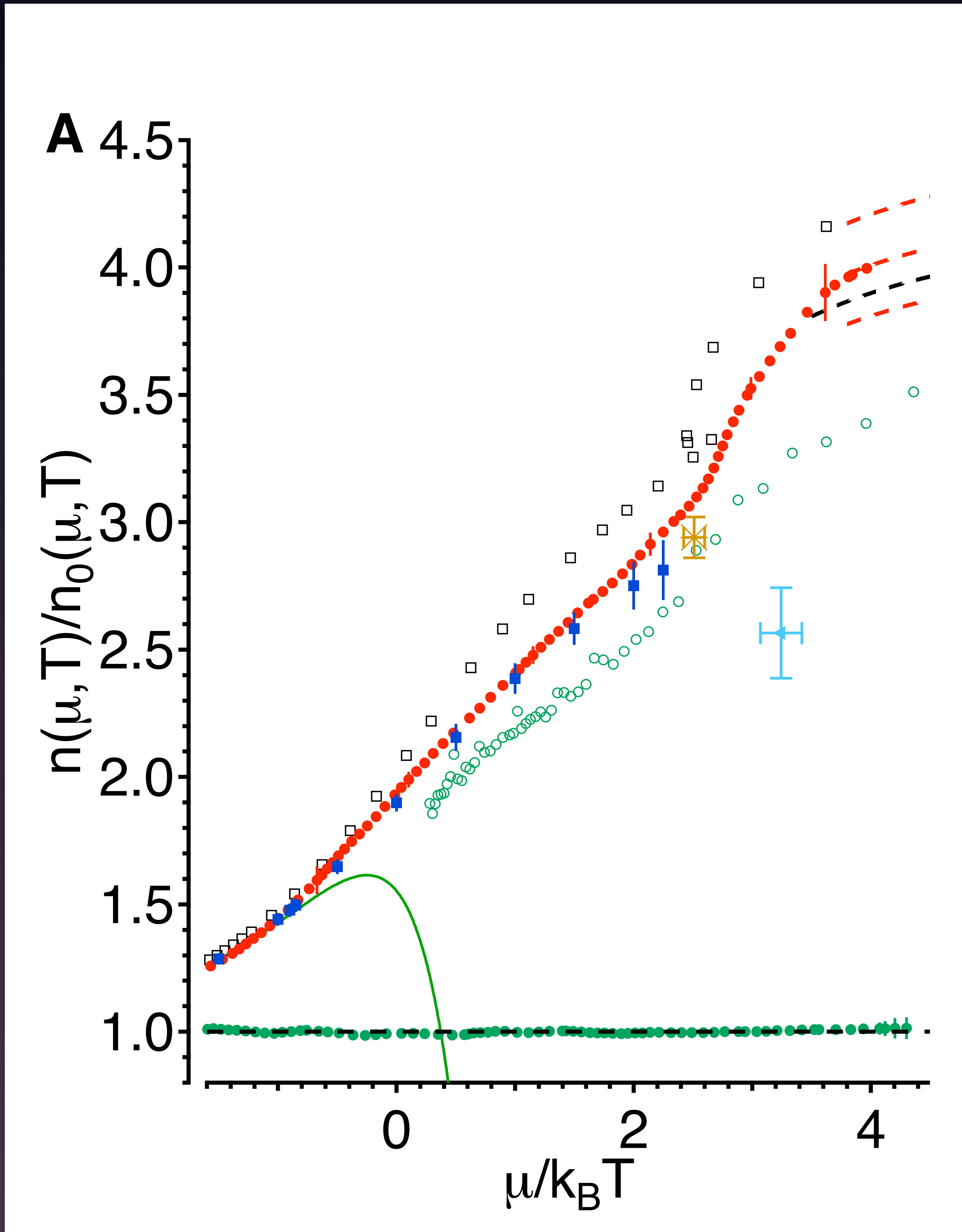


Forbes, Gandolfi, Gezerlis (2012)

Phase Structure



Based on D.T. Son and M. Stephanov (2005)
P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk PRL 97 020402 (2006)



Unitary Equation of State

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

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

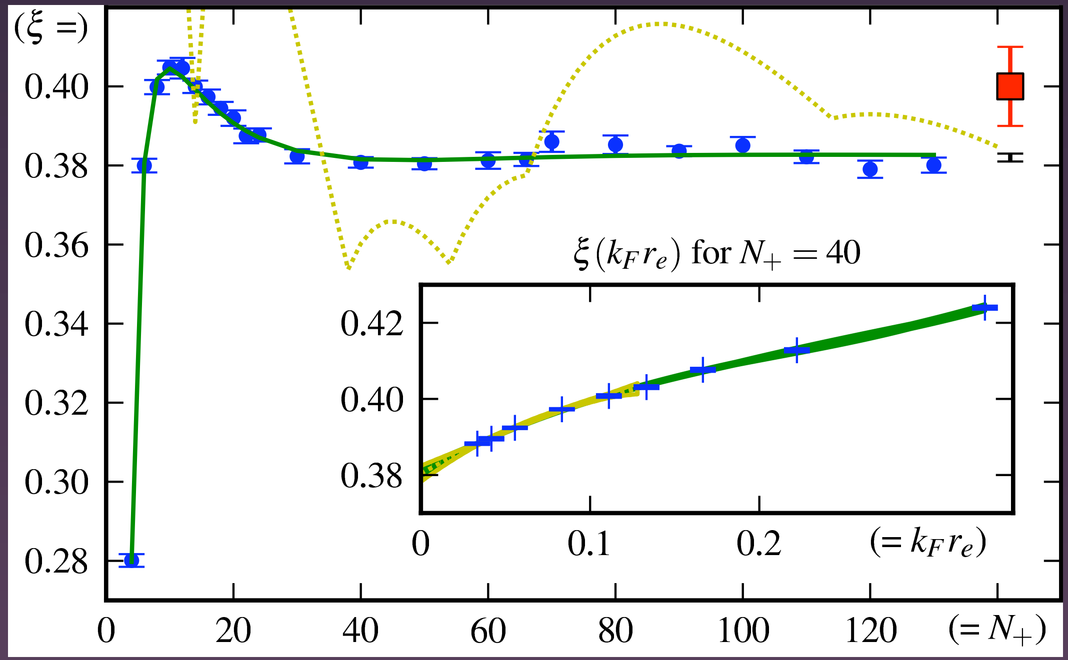
- Measured to percent level:
  - $\xi_{exp} = 0.376(5)$

Ku, Sommer, Cheuk, and Zwierlein 2012

SLDA: Fit to QMC using $r_{\text{eff}} = 0$ Extrapolation

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

- Three parameters, but
- Independent fits of each N
  - (lots of parameters)
- Can we model range?



Forbes, Gandolfi, Gezerlis (2012)

Fit directly to QMC

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

- Each parameter becomes a quadratic polynomial:
  - $\alpha(k_F r_e)$, $\beta(k_F r_e)$, $\gamma(k_F r_e)$
- we actually use physical parameters $\xi(k_F r_e)$, $\Delta(k_F r_e)$, $\alpha(k_F r_e)$
- 9 total parameters for all N

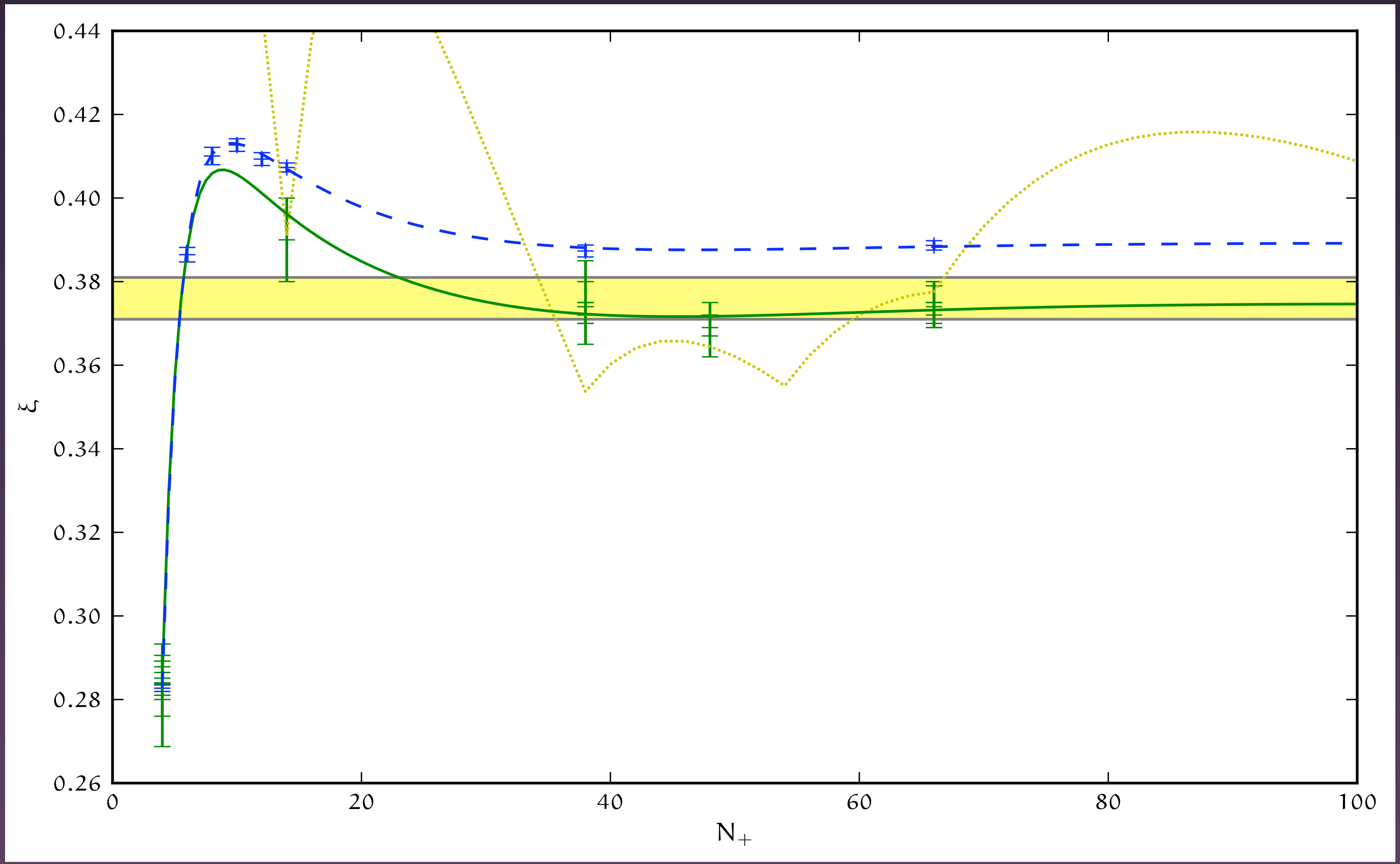
Fit directly to QMC

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

- Not complete story for modeling range:
  - Does not regulate theory
  - No structure for gap (Δ_p)

    probably requires non-local functional

Fit SLDA to box QMC



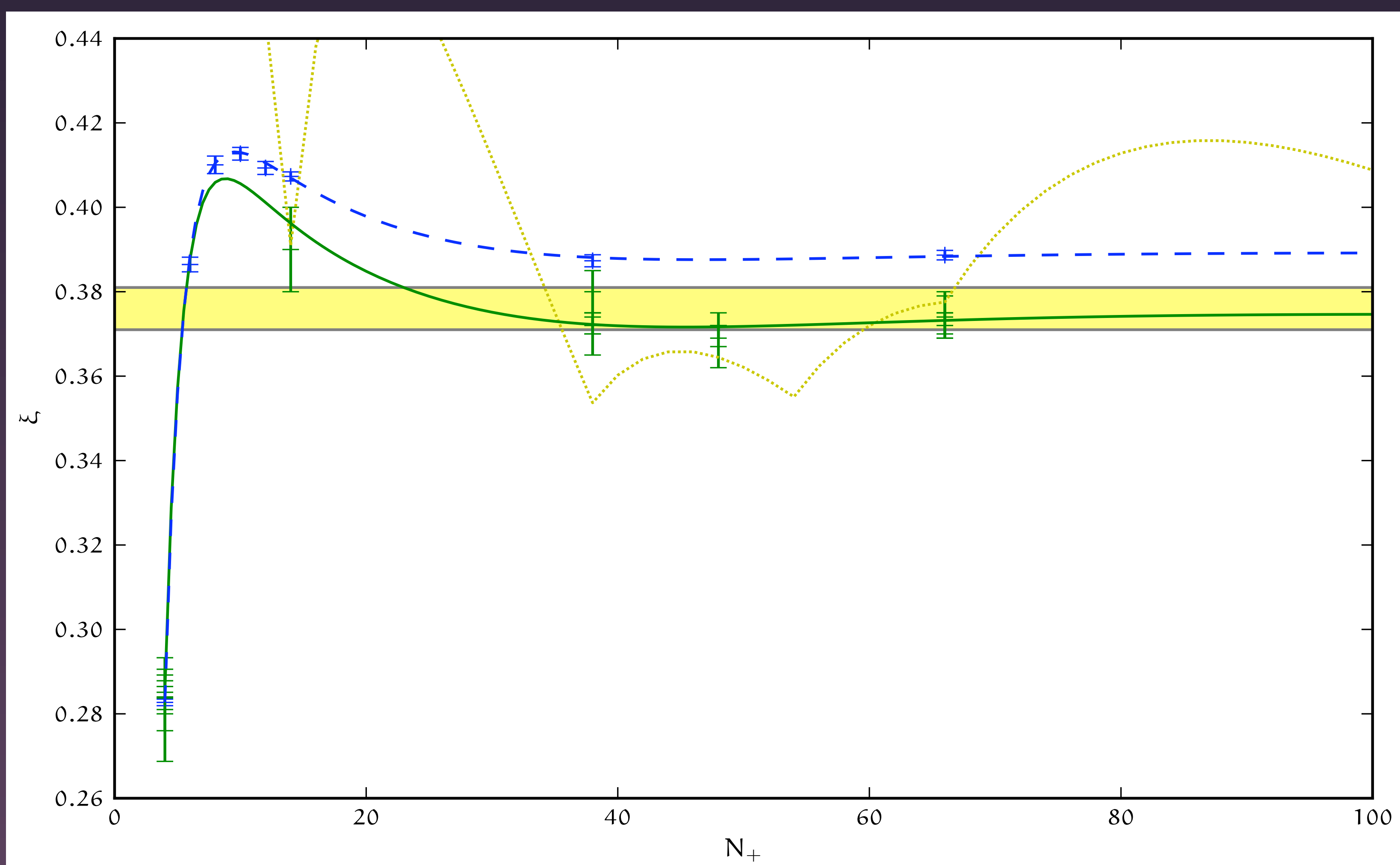
- Fit 60 QMC with 9 parameter model
- Directly use QMC with sub-percent errors
  - $\chi^2 = 6$

Forbes, Gandolfi, Gezerlis PRL (2011)

SLDA parameters

$$\alpha, \xi, \eta = a_0 + a_1 k_F r_e + a_2 (k_F r_e)^2$$

	a_0	a_1	a_2
ξ_{PT}	0.3903(7)	0.121(10)	0.00(3)
	0.3911(4)	0.111(3)	
ξ_{2G}	0.3890(4)	0.128(4)	−0.06(1)
	0.3900(3)	0.111(2)	
η_{PT}	0.99(3)	−2.1(4)	3(1)
	0.90(1)	−0.85(7)	
η_{2G}	0.879(7)	−0.84(3)	0.00(3)
	0.875(8)	−0.82(4)	
α_{PT}	1.34(2)	−1.6(4)	5(2)
	1.303(10)	−0.71(8)	
α_{2G}	1.292(7)	−0.73(6)	0.1(2)
	1.289(7)	−0.69(3)	



Universal slope

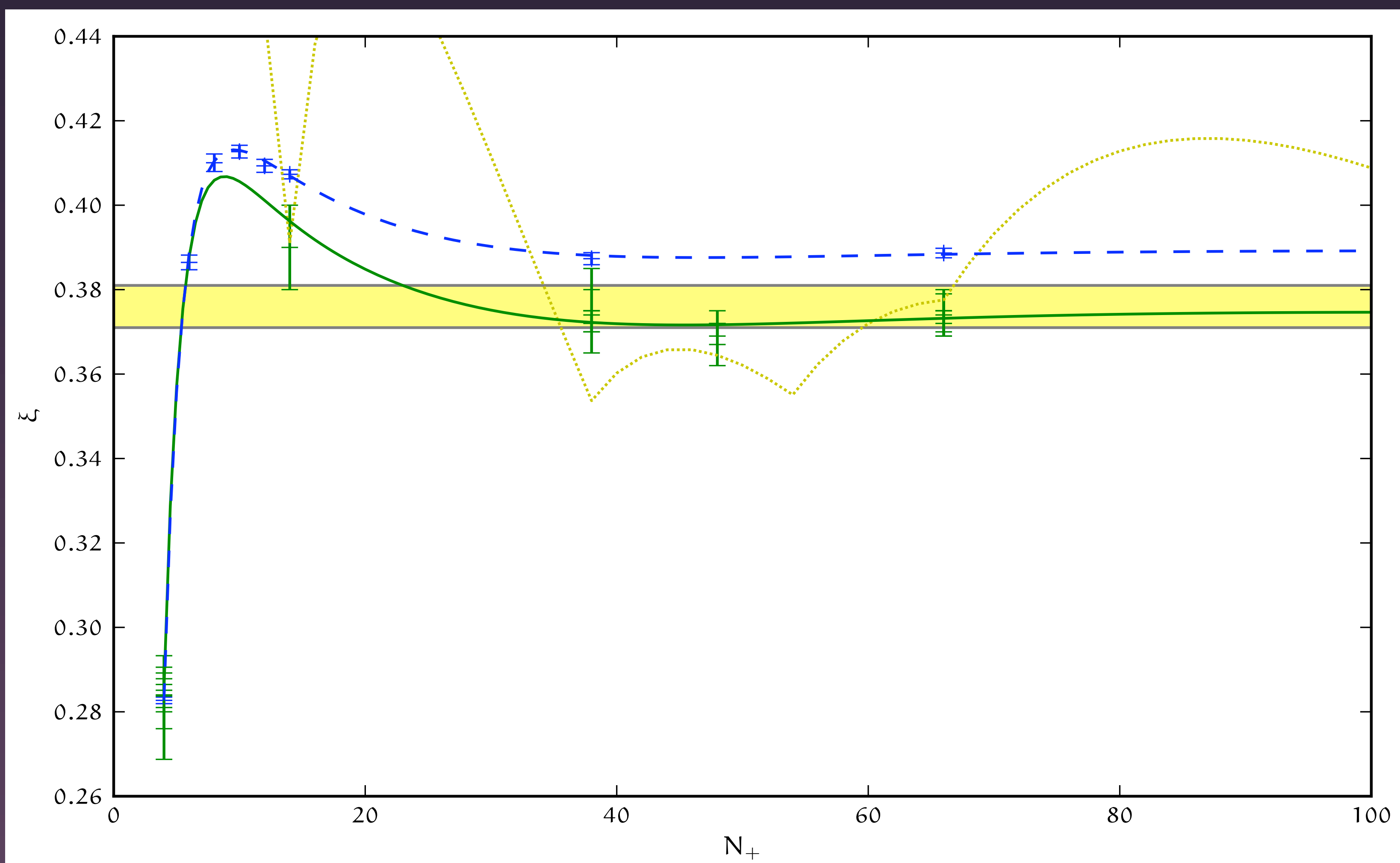
$$\xi = \xi + (k_F r_e) S$$

S=0.12(1)

Forbes, Gandolfi, Gezerlis (2012)

SLDA parameters

$$\alpha, \xi, \eta = a_0 + a_1 k_F r_e + a_2 (k_F r_e)^2$$



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Gap and inverse mass seem too large

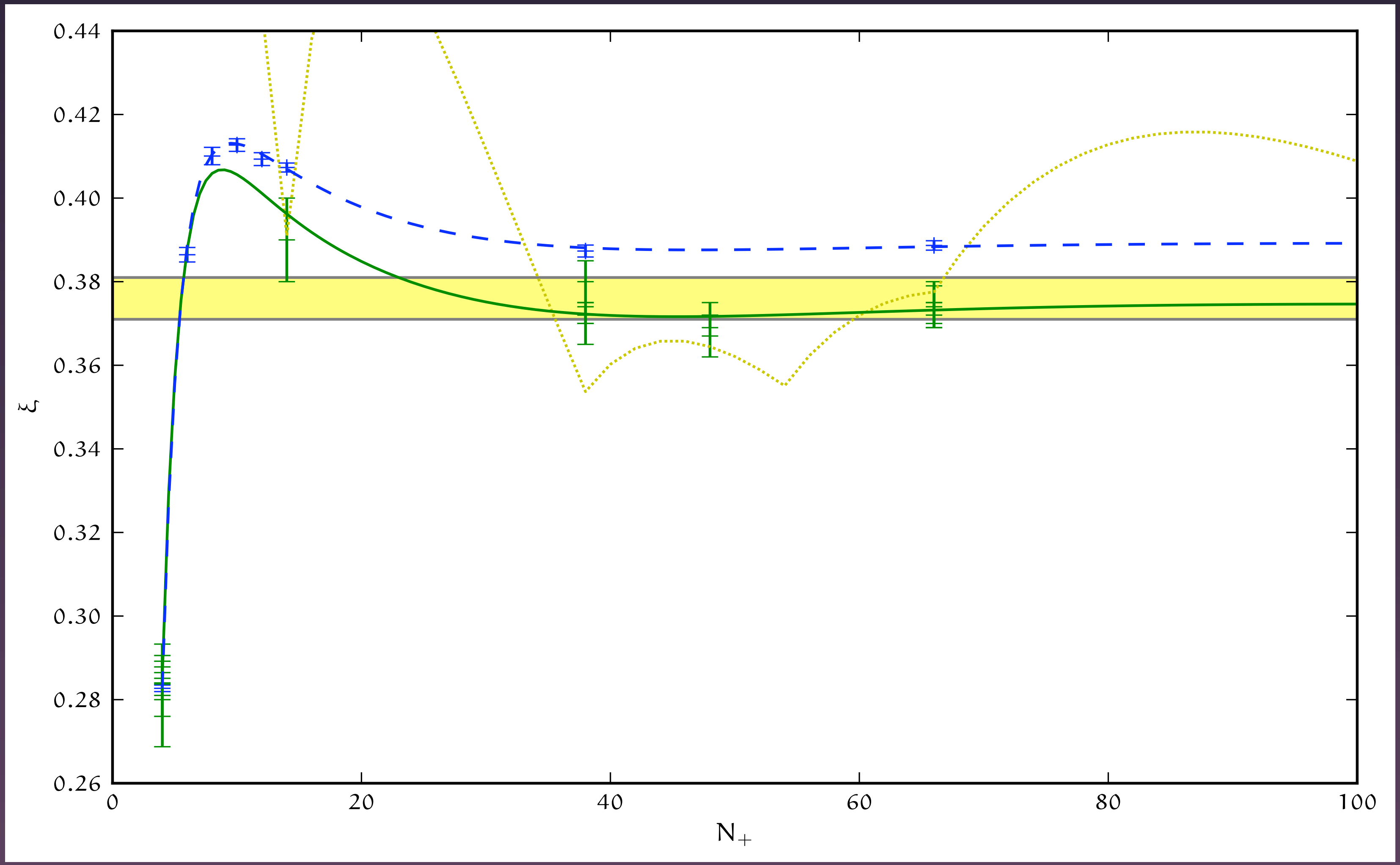
Limitation of fixed node approximation?

Forbes, Gandolfi, Gezerlis (2012)

Unbiased SLDA fit

$$\alpha, \xi, \eta = a_0 + a_1 k_F r_e + a_2 (k_F r_e)^2$$

N_+	ξ_{N_+}	Method
2	$-0.415332919\cdots$	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]

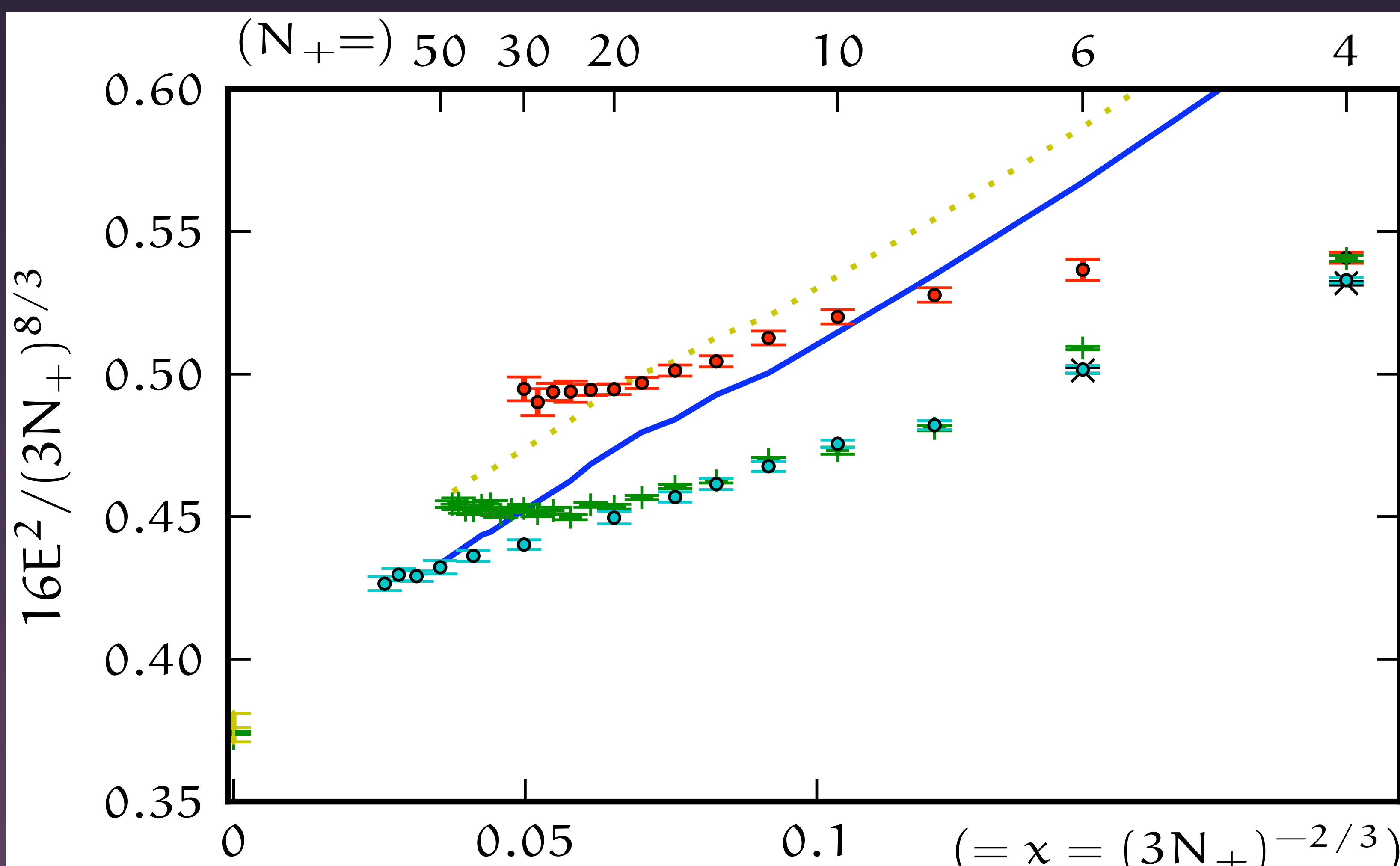


Fit to unbaised results

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

Forbes, Gandolfi, Gezerlis (2012)

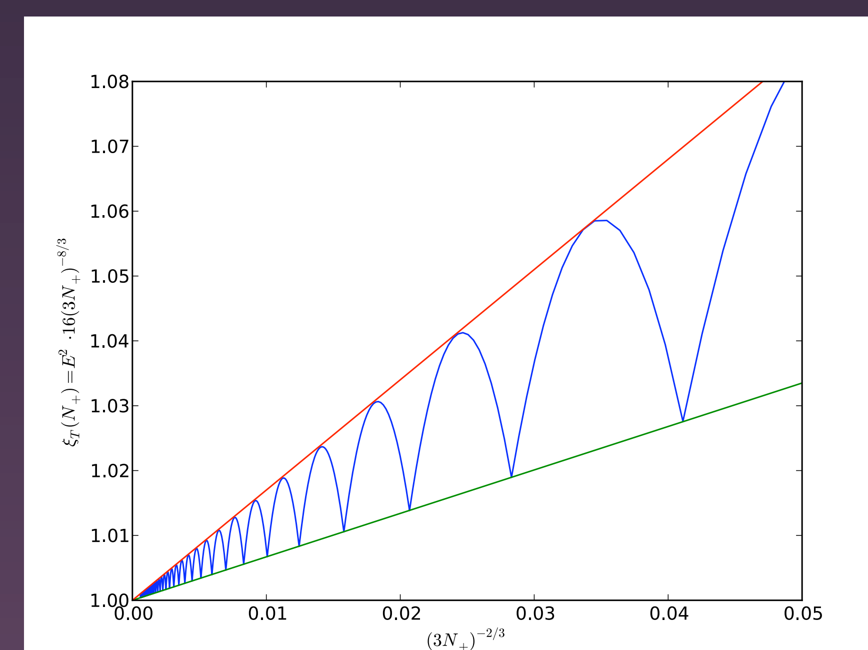
Harmonic Traps



First correct asymptotic behaviour

Almost no shell effects

Check Gradient terms

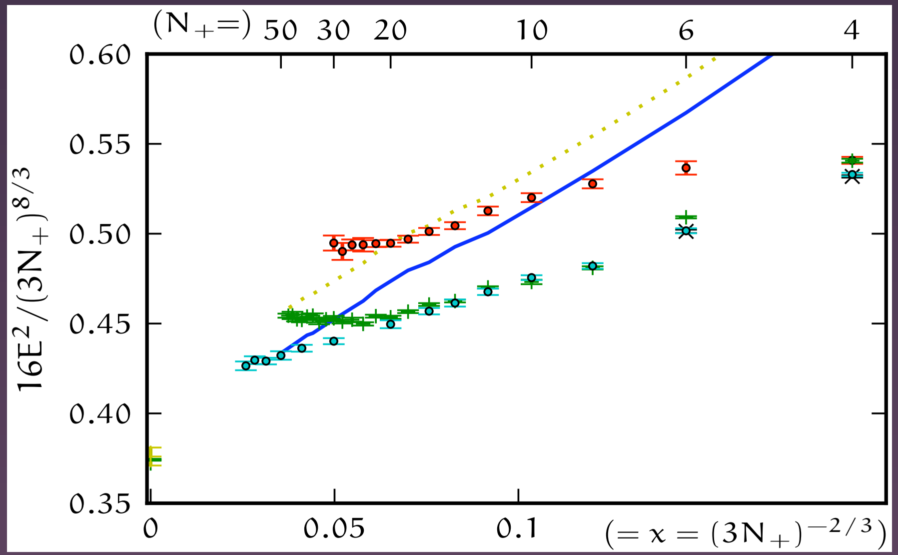


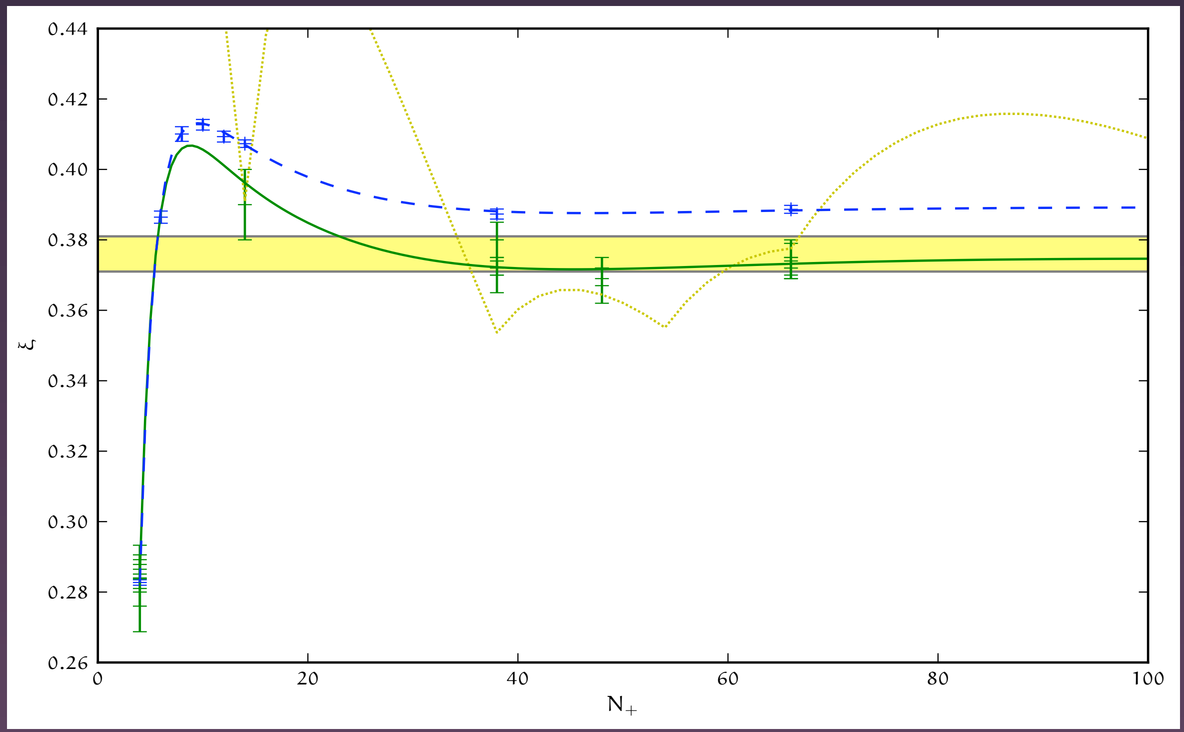
Forbes, Gandolfi, Gezerlis (2012)

SLDA Summary

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

- Works remarkably well





Forbes, Gandolfi, Gezerlis (2012)

Dynamics

TDDFT (TDSLDA)

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

- Need to evolve each hundreds of thousands of wavefunctions
- Possible for moderate systems (nuclei) using supercomputers
  - resonances (GDR Stetcu et al. 2012), induced fission
- Probably not for glitching dynamics

GPE model for UFG

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

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

- Think:
  - Boson = Fermion pair (dimer)
- 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)

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

$$\mathcal{E}(\rho_F, \{\nabla\rho_F\}) = \xi\mathcal{E}_{FG}(\rho_F) + \frac{4\lambda - 1}{8m}(\nabla\sqrt{\rho_F})^2$$

- In the absence of currents (i.e. no vortices), kinetic and Weizsäcker terms behave the same
- See Salasnich for a discussion

GPE model for UFG

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

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

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

Low Energy Theory

$$\mathcal{L}_{\text{LO+NLO}} = \xi^{-3/2} P_{FG}(X) + c_1 m^{1/2} \frac{(\nabla X)^2}{\sqrt{X}} + c_2 \frac{(\nabla^2\phi)^2 - 9m\nabla^2 A_0}{\sqrt{m}} \sqrt{X}$$

$$X = \mu - V(t,\vec{x}) - \partial_t \phi - \frac{(\nabla\phi)^2}{2m} \qquad \langle ab \rangle = |\Delta| e^{2i\phi}$$

- Low energy theory of phonons (Son and Wingate 2006)
- Strongly constrained by General Coordinate Covariance
  - generalizes Galilean covariance
  - reduces NLO to 2 new coefficients c_1, c_2
- Three universal coefficients:
  - ξ, c_1, c_2

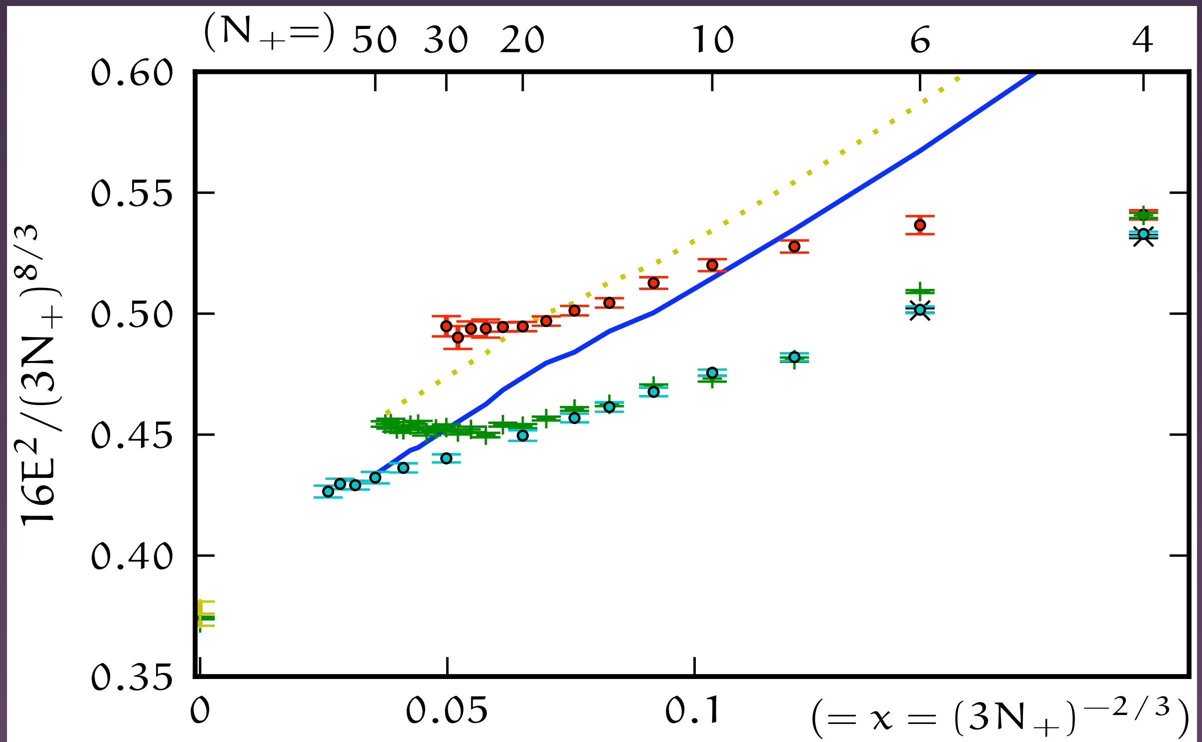
Static Response

$$\chi(q) = \frac{-mk_F}{\pi^2\xi}\left[1 + 2\pi^2\sqrt{2\xi}\left(c_1 - \tfrac{9}{2}c_2\right)\frac{q^2}{k_F^2}\right] + O(q^4 \ln q),$$

$$\chi^T(q) = -9c_2\sqrt{\frac{\xi}{2}}v_F q^2 + O(q^4 \ln q)$$

- Epsilon expansion at NLO (Rupak and Schäfer 2007):
  - $c_1 = -0.004776\ \xi^{-3/2} + O(\epsilon^2)$
  - $c_2 = 0 + O(\epsilon^2)$
- Asymptotic slope of HO trap:

$$E(N_+) = \frac{\sqrt{\xi}}{4}\omega(3N_+)^{4/3} + \\ -\sqrt{2}\pi^2\xi\left(c_1 - \tfrac{9}{2}c_2\right)\omega(3N_+)^{2/3} \\ + O(N_+^{5/9})$$



Phonon Dispersion

$$\omega_q = c_s q \left[1 - \pi^2 \sqrt{2\xi_S}\left(c_1 + \tfrac{3}{2}c_2\right)\frac{q^2}{k_F^2}\right] + O(q^5 \ln q), \qquad c_s = \sqrt{\frac{\xi_S}{3}} v_F$$

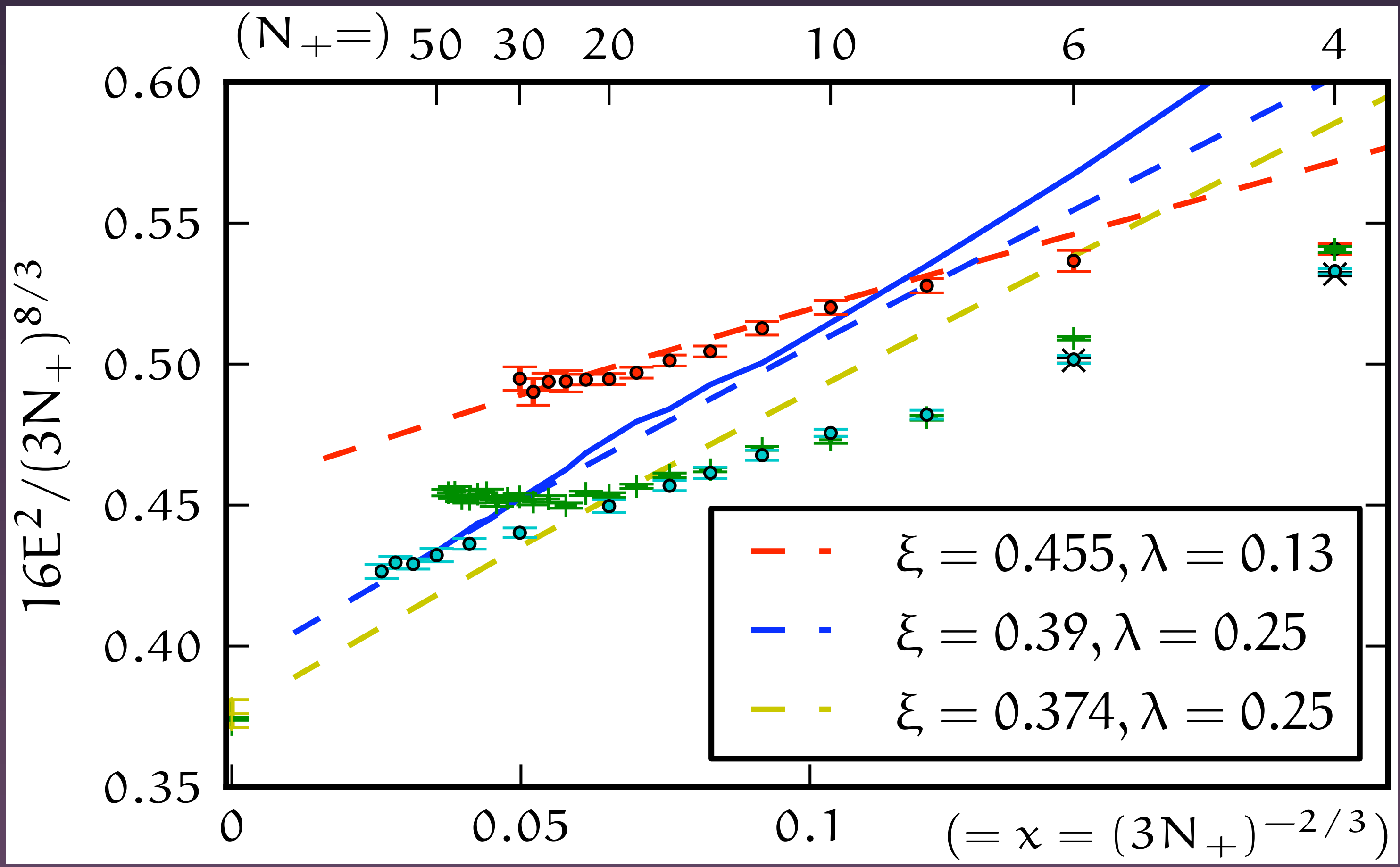
- Different combination than static response if $c_2 \neq 0$

GPE/ETF Model

$$\omega_q = \sqrt{\frac{\xi}{3}} v_F q \left(1 + \frac{3\lambda\hbar^2}{8\xi}\frac{q^2}{k_F^2} + \cdots\right), \quad \chi(\vec{q}) = -\frac{mk_F}{\pi^2\xi}\left[1 - \frac{3\lambda}{4\xi}\frac{q^2}{k_F^2} + \cdots\right]$$

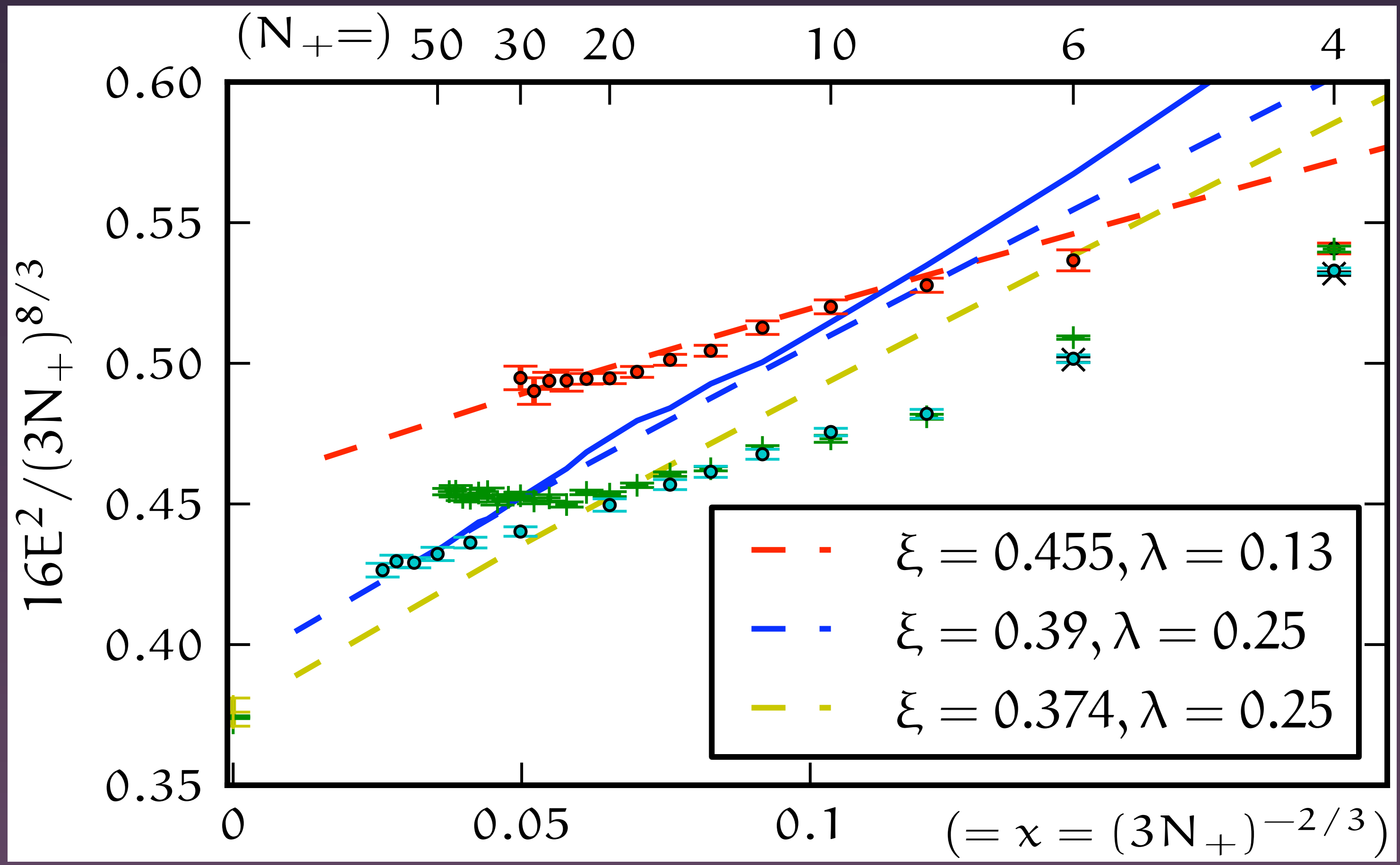
$$\lambda = \frac{-8\pi^2\sqrt{2\xi}\xi}{3}c_1$$

- Has $c_2 = 0$:
- Two Parameters (ξ, λ)
- "natural" λ=0.25
- Salasnich, Toigo (2008) fit to Blume
  (ξ=0.45, λ=0.13)



Gradient Corrections

- In principle, Weizsäcker term is leading gradient correction for SLDA. Will affect slope.
- "natural" λ=0.25 corresponds to no Weizsäcker term
- SLDA has almost the correct slope "built in"
- No need for leading gradient correction?



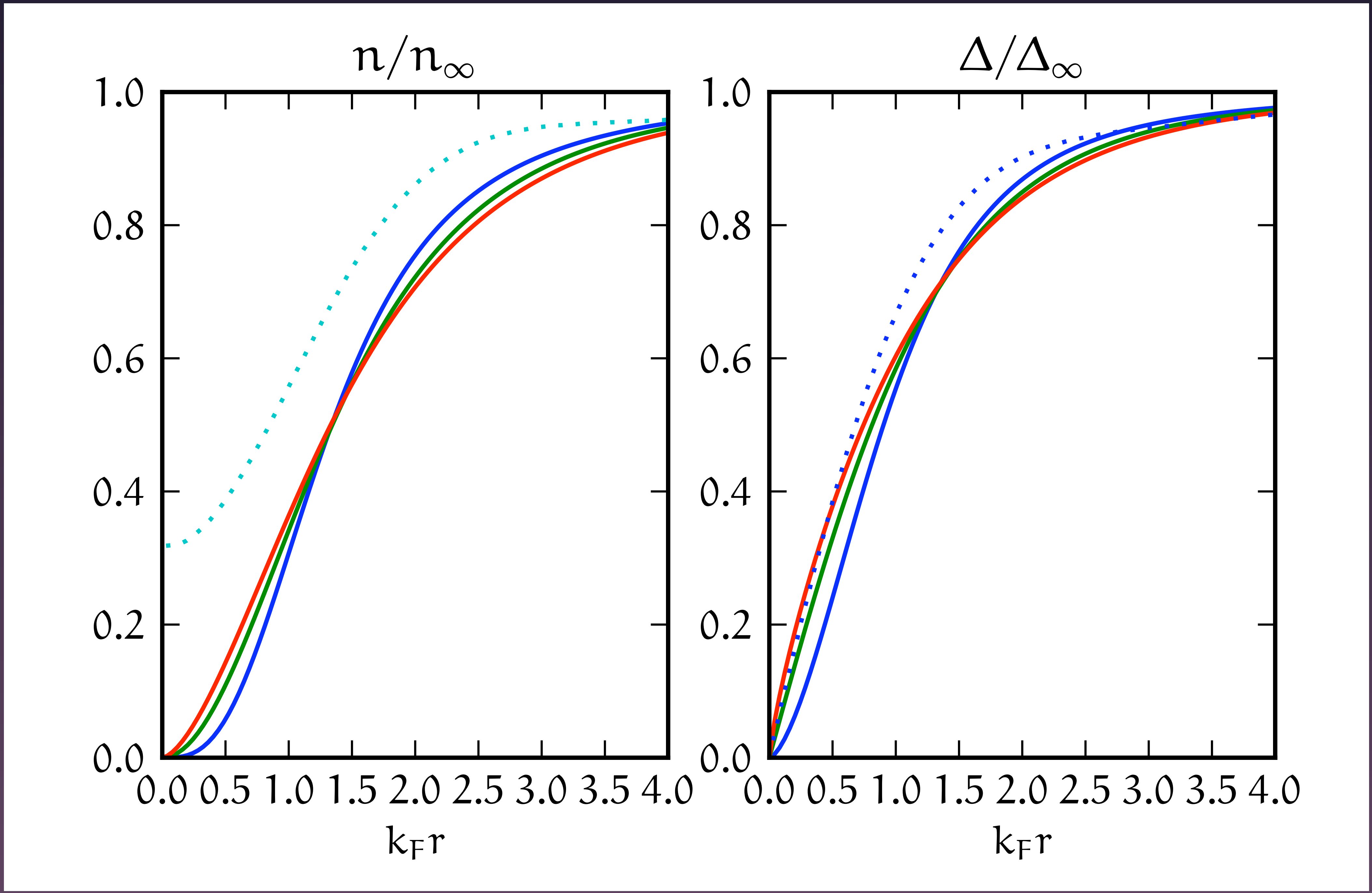
Matching Theories: The Good

- 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)

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)

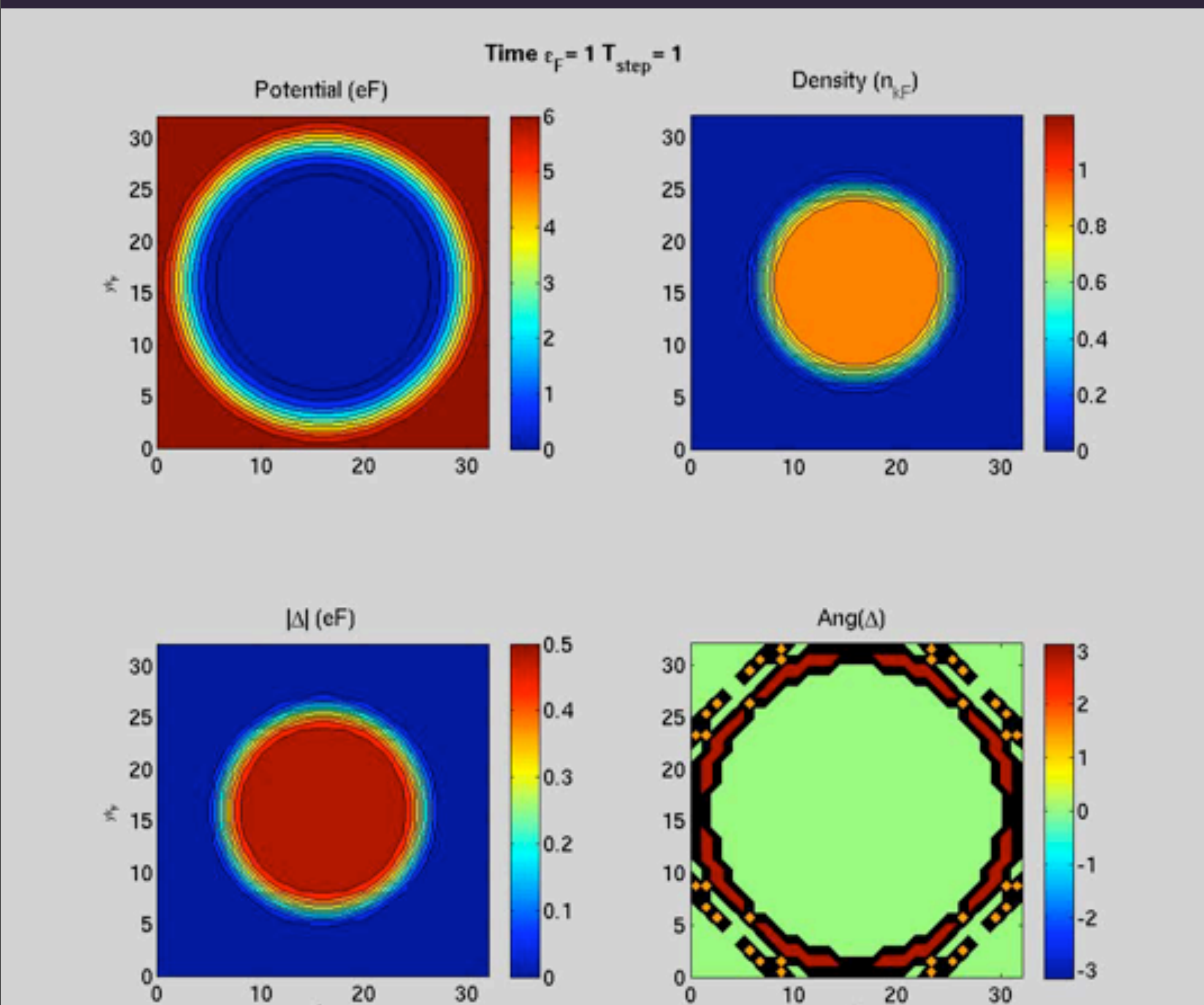
Vortex Structure



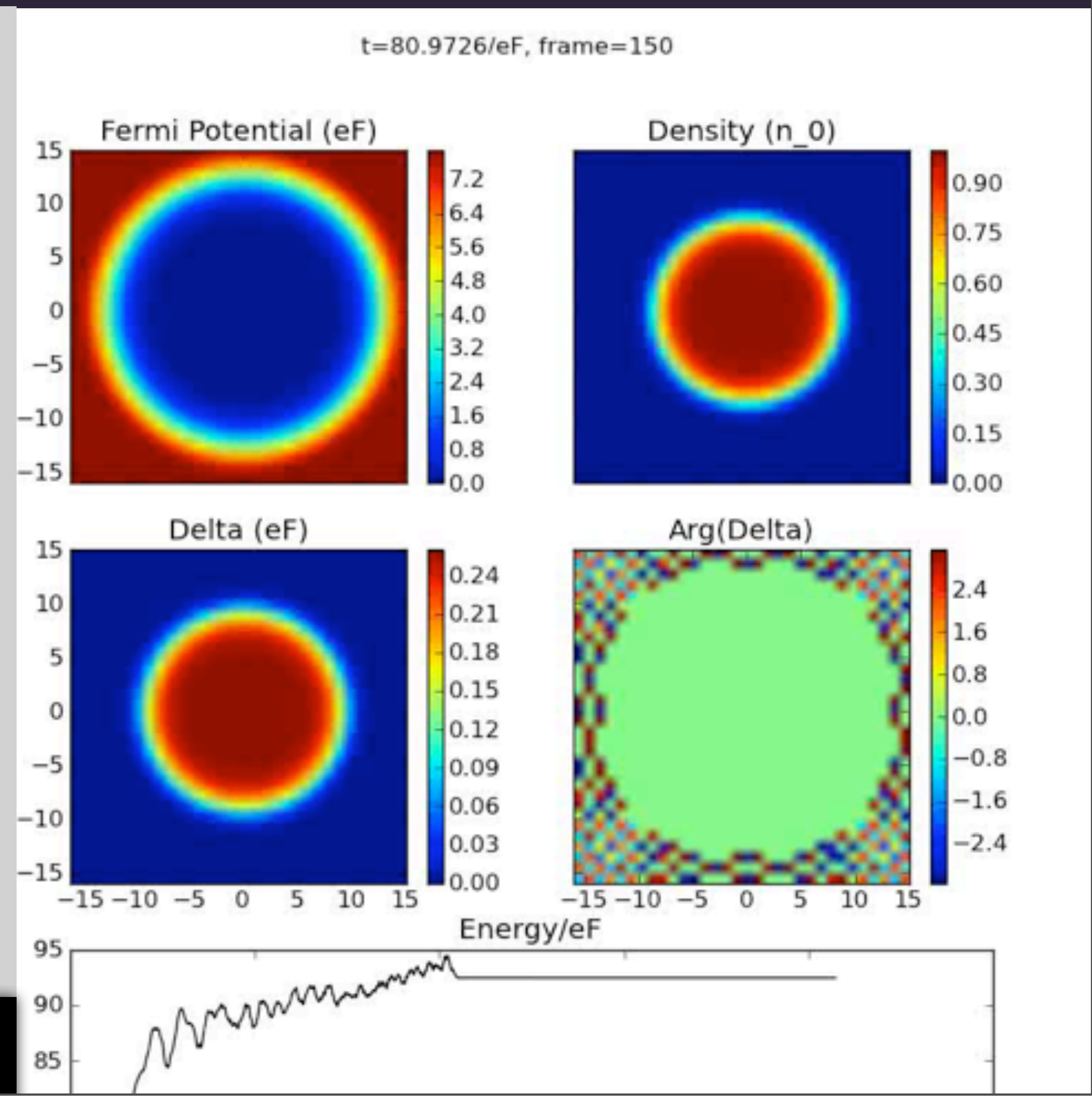
Comparison

Fermions
SLDA TDDFT

Gross Pitaevskii
model

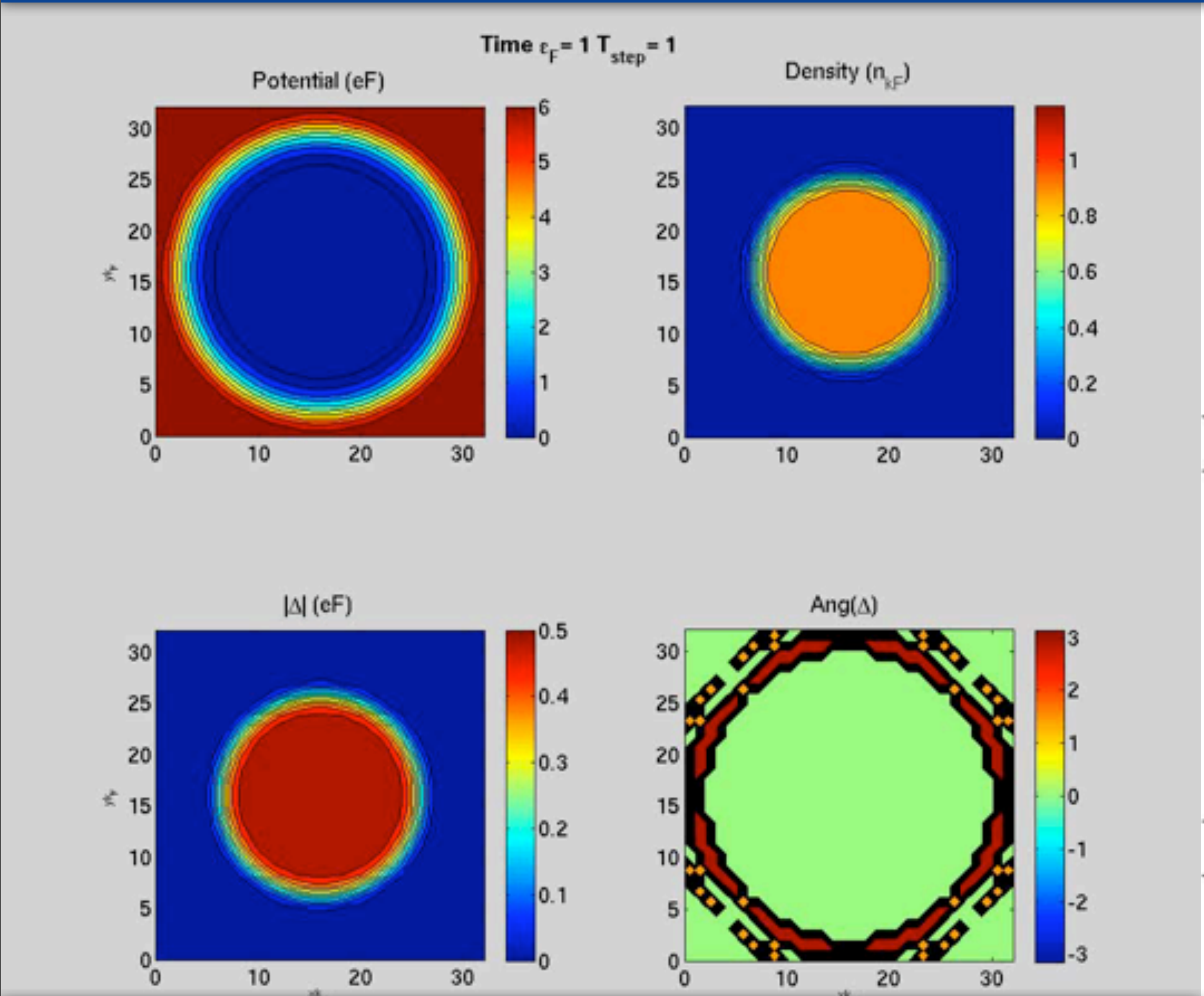


Bulgac et al. (Science 2011)



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

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



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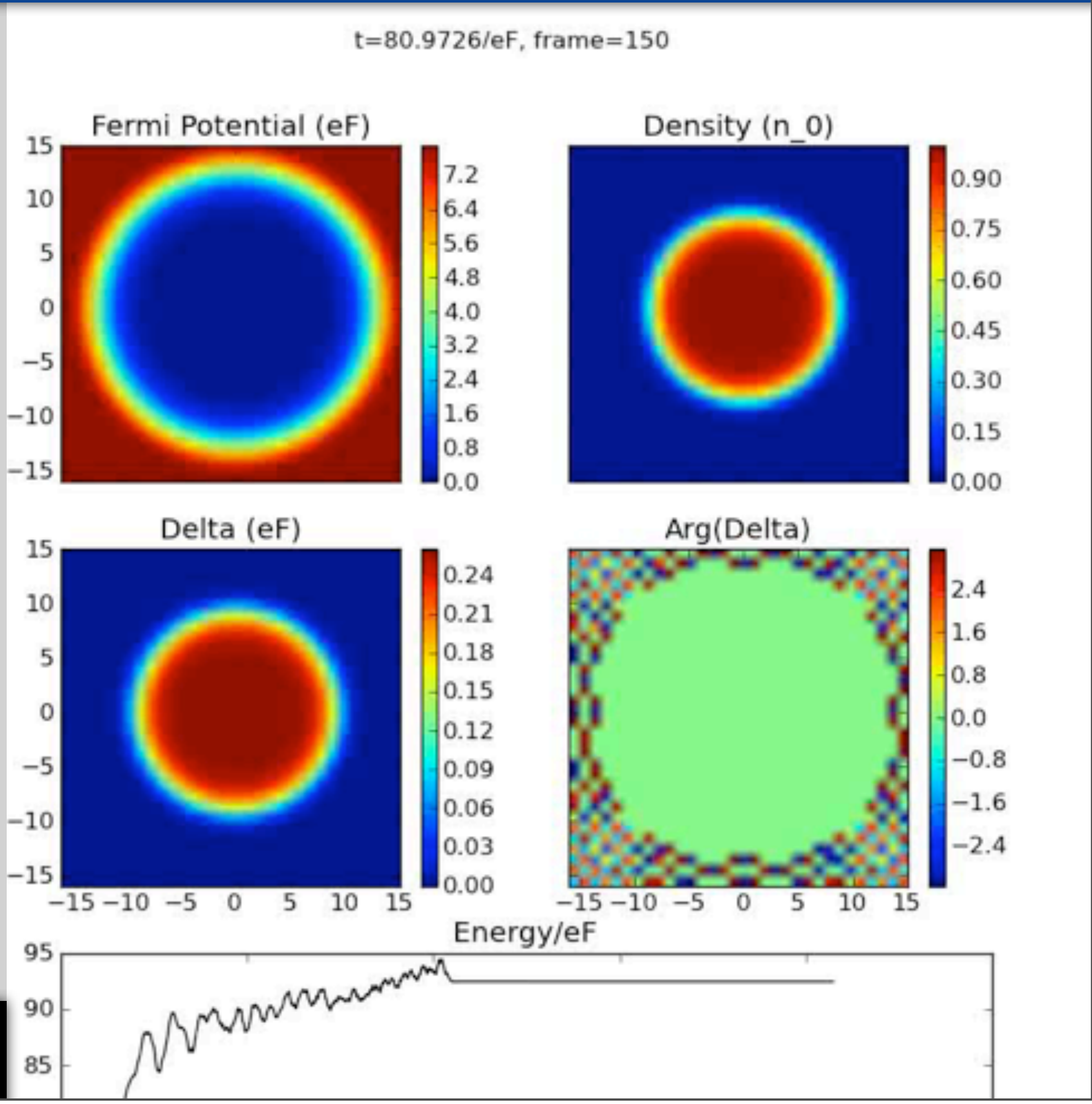
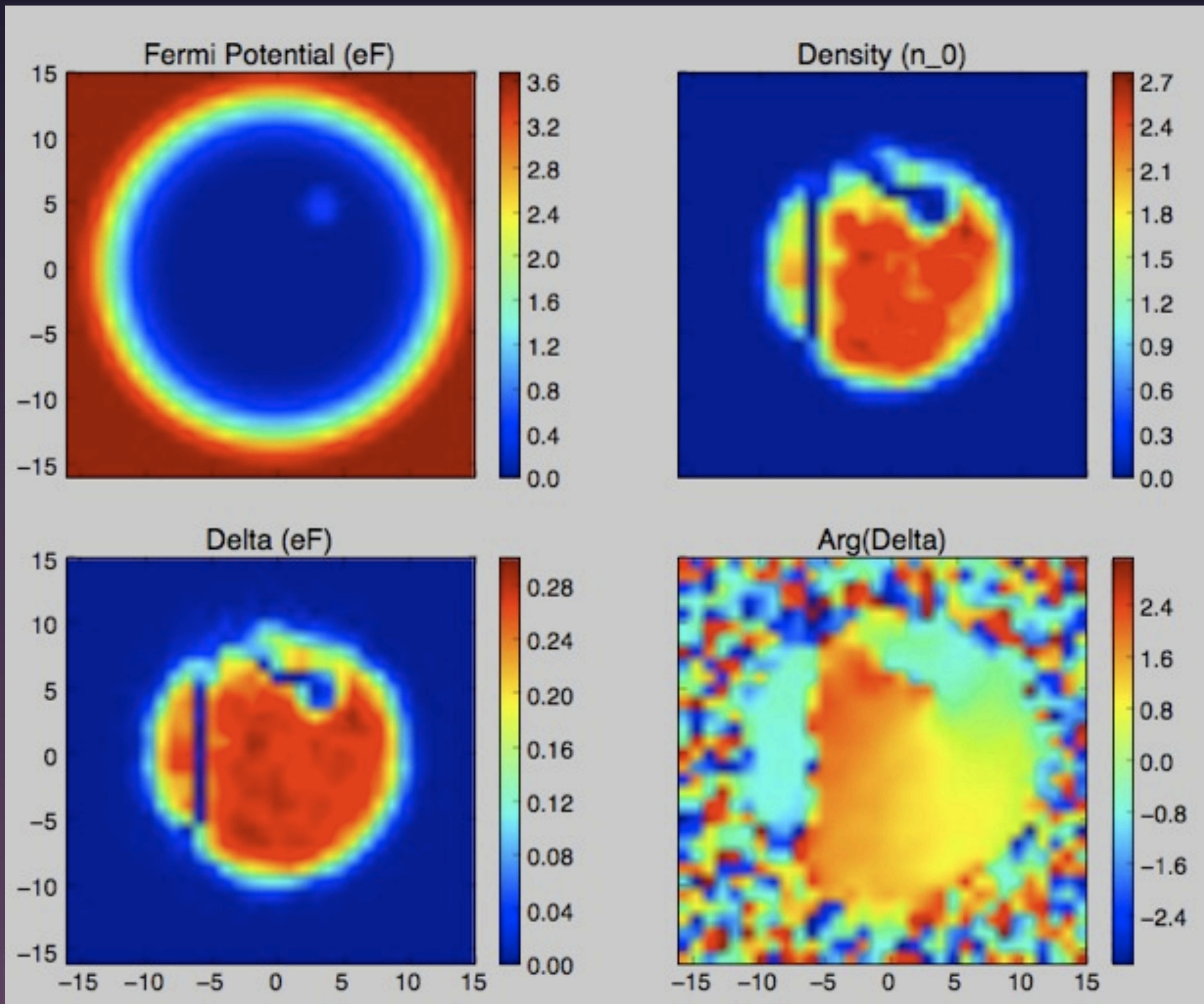


Weisäcker term bad?

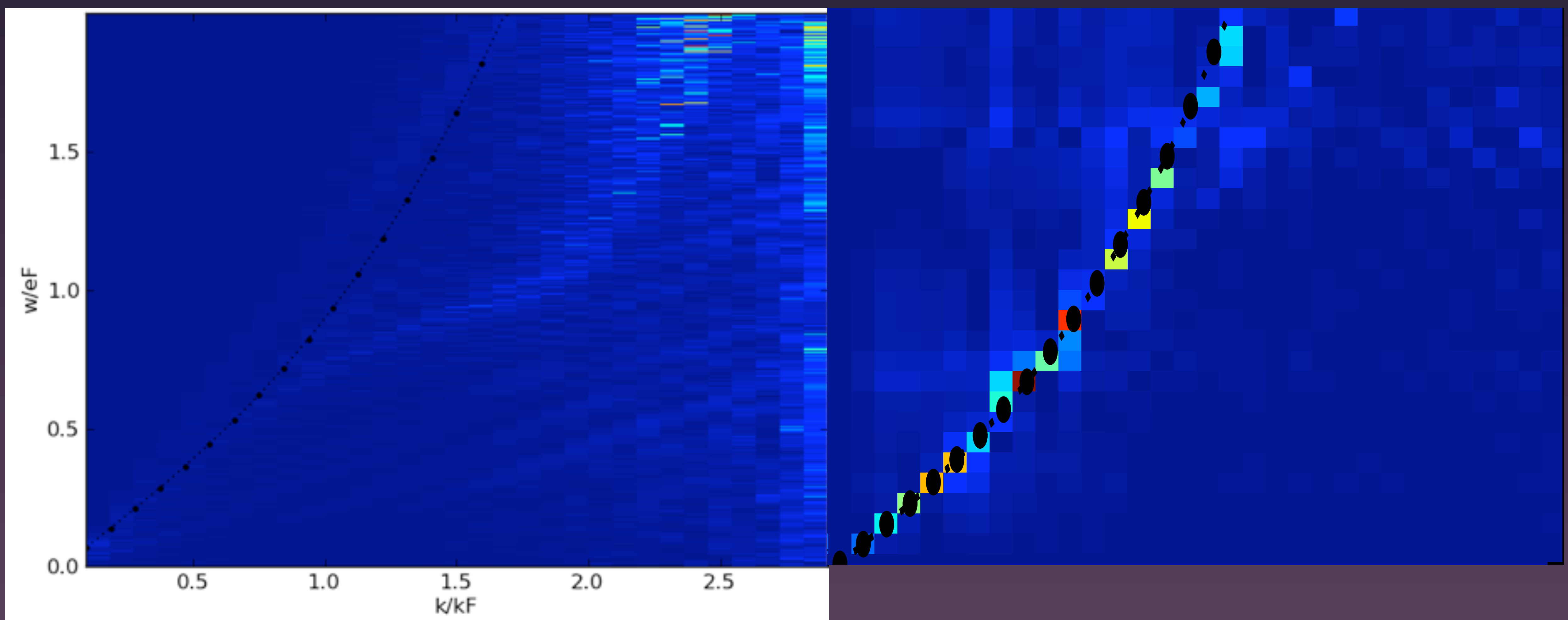


Small λ gives bad dynamics

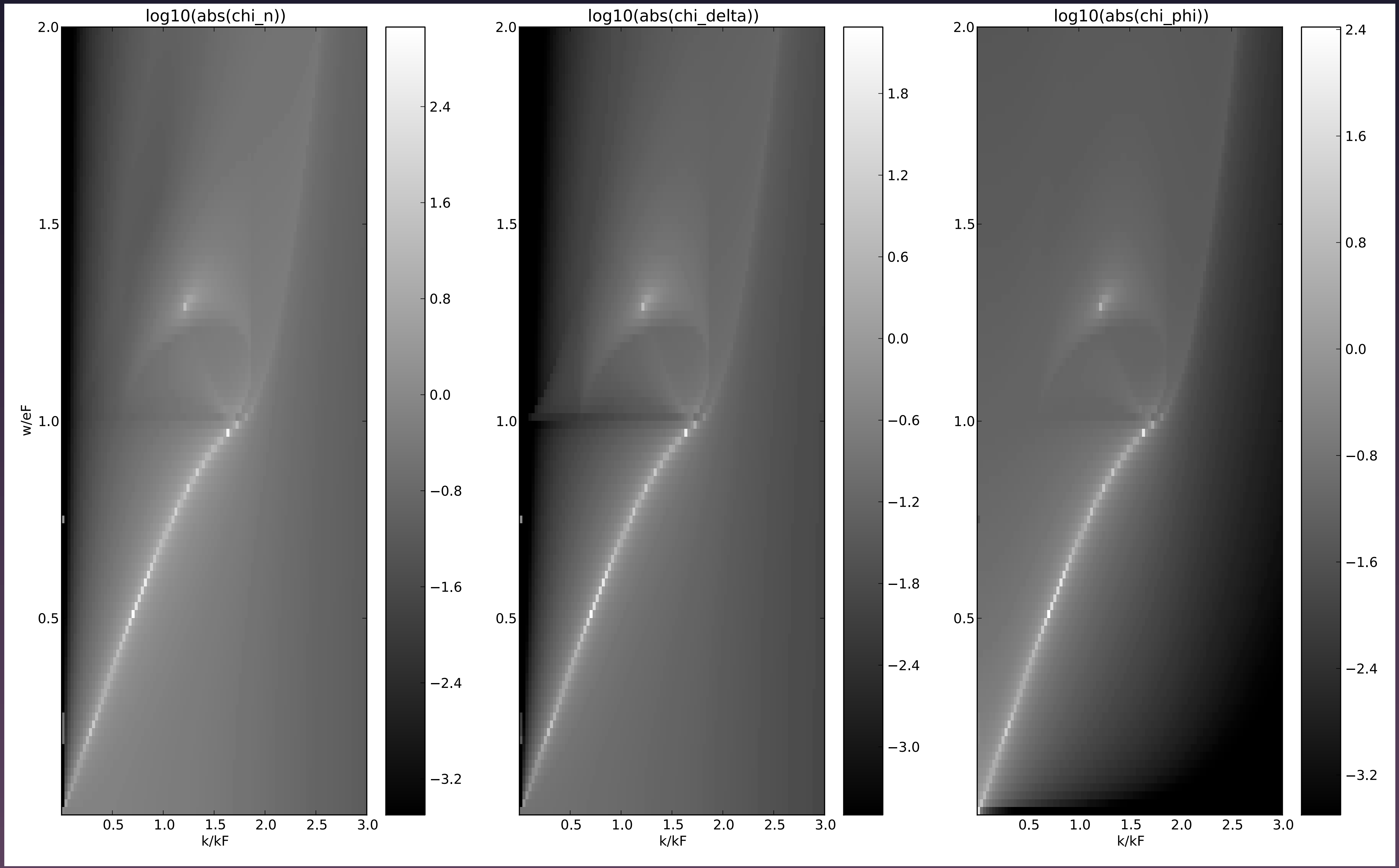
- Vortex lines “frozen”
- singular behaviour at core of vortex?

Best match with SLDA for λ≈0.21

Response from real-time dynamics



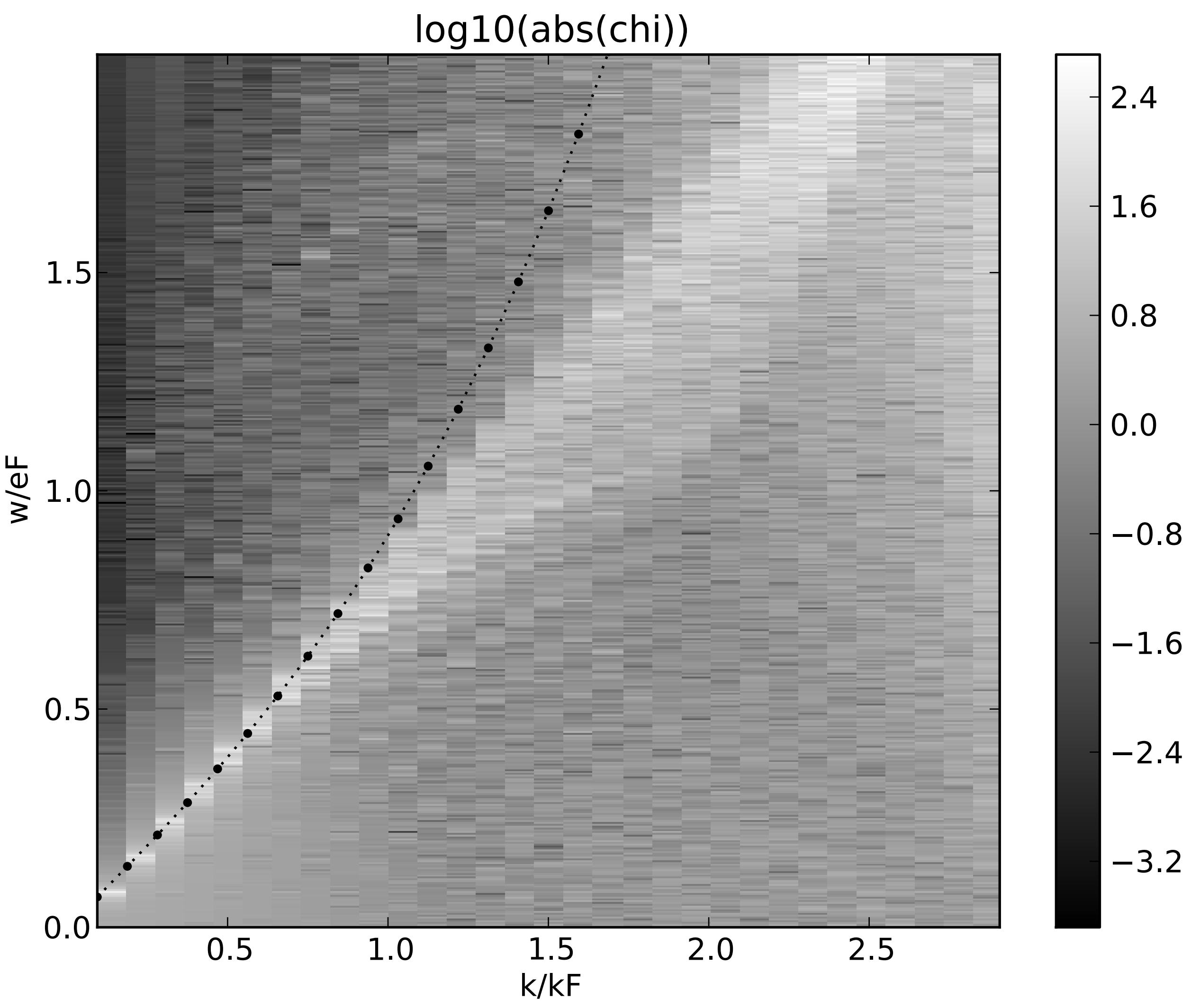
Linear Response



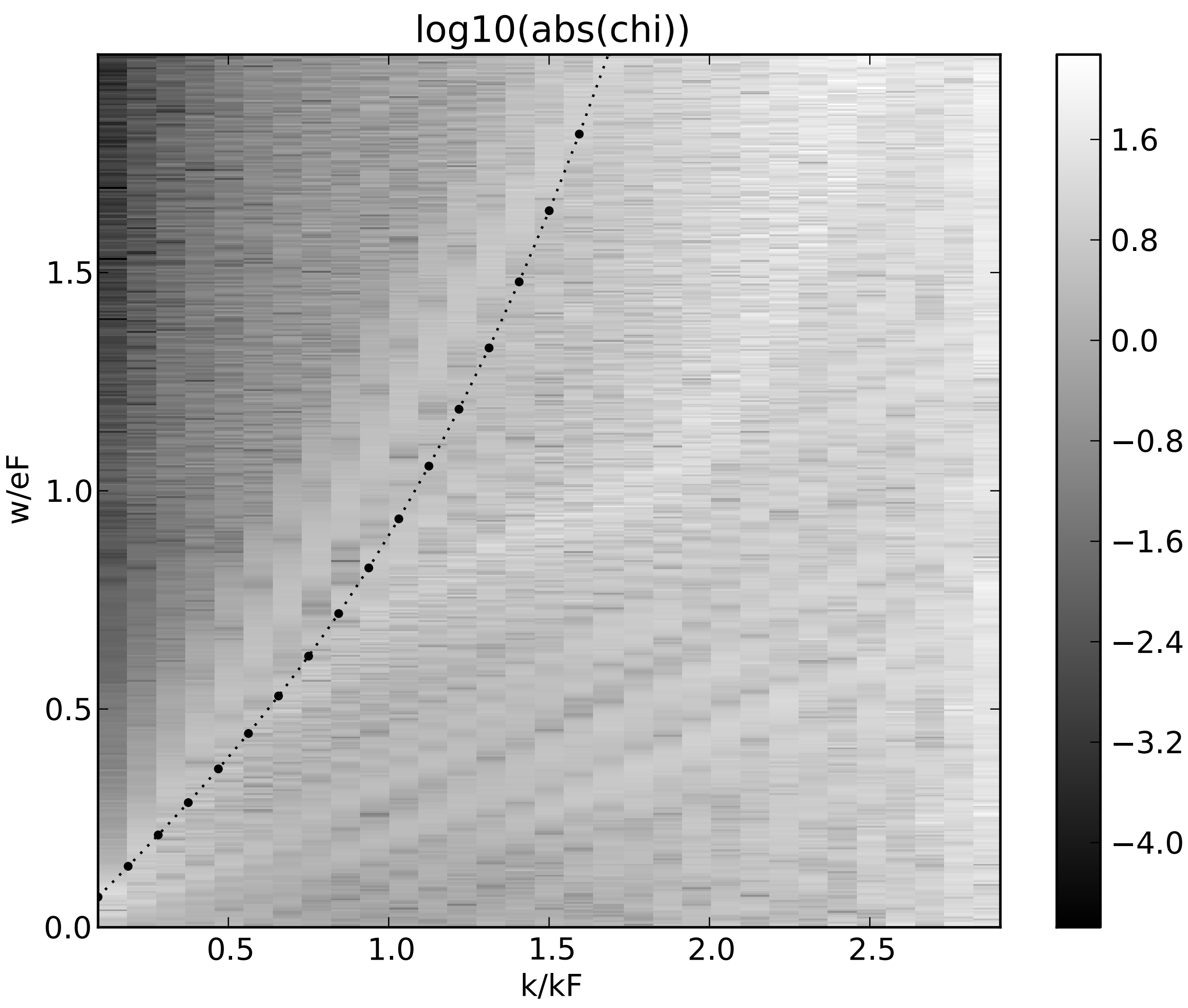
Work with Rishi Sharma (TRIUMF)

Non-Linear Response?

V=0.05

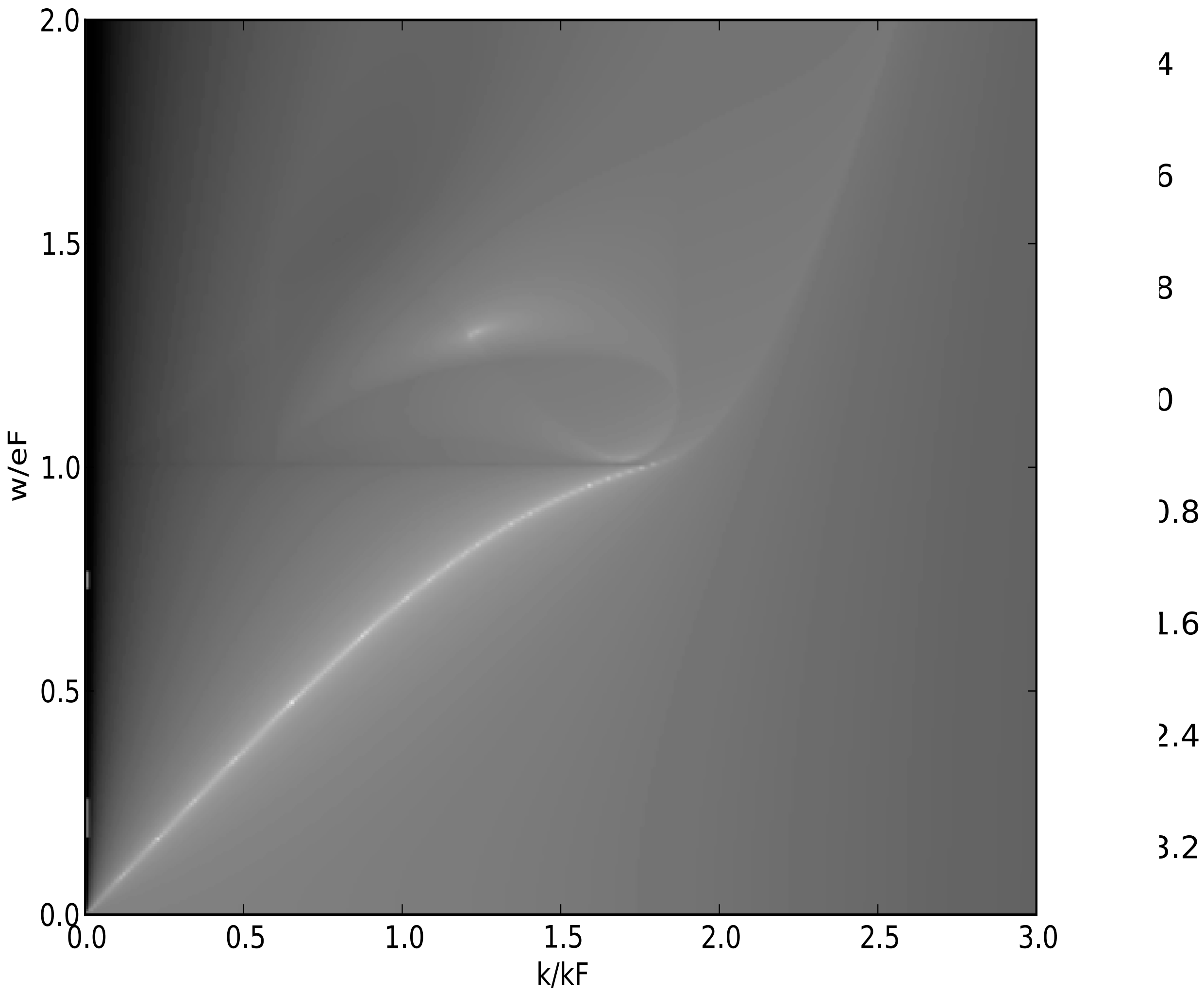


V=0.5

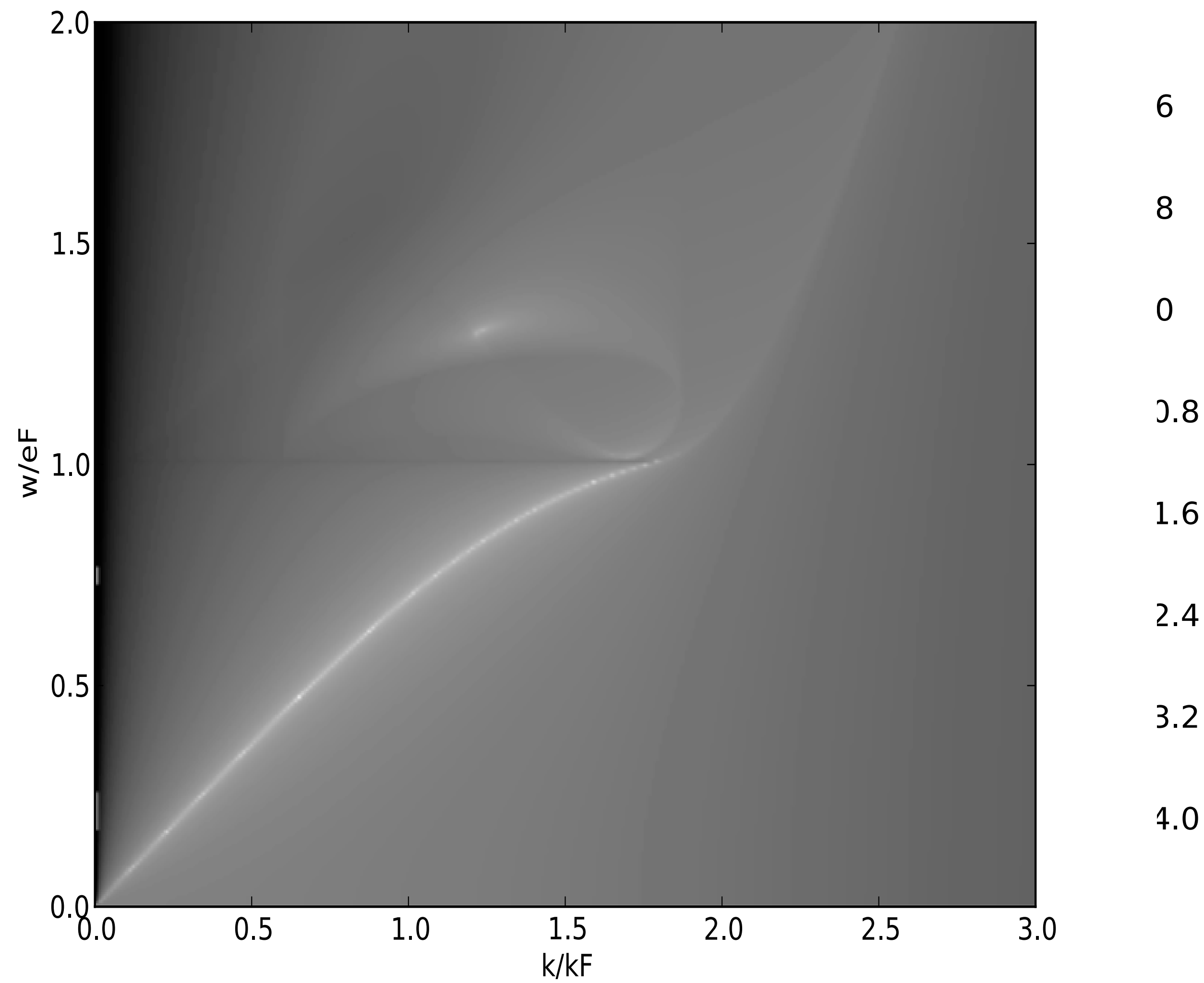


Non-Linear Response?

V=0.05

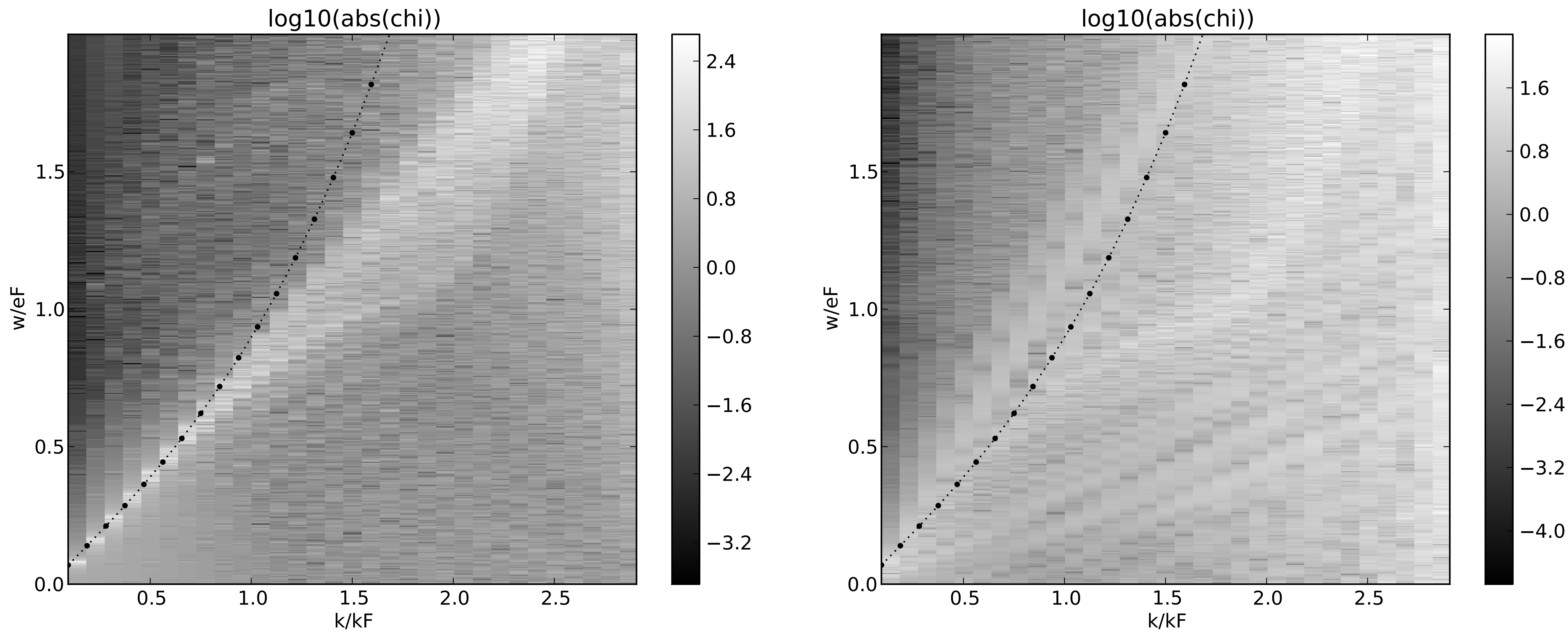


V=0.5



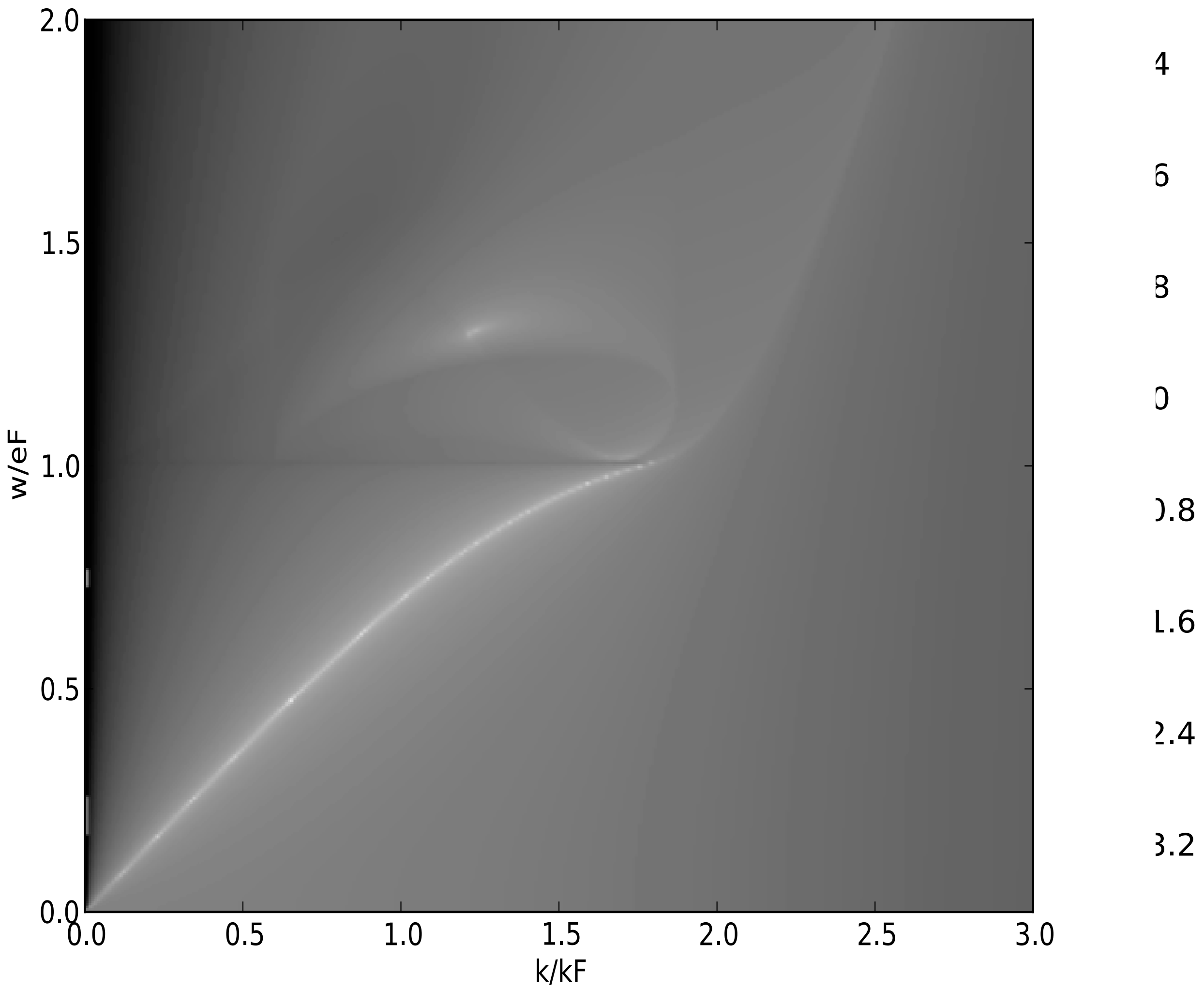
Non-Linear Response?

V=0.05 V=0.5

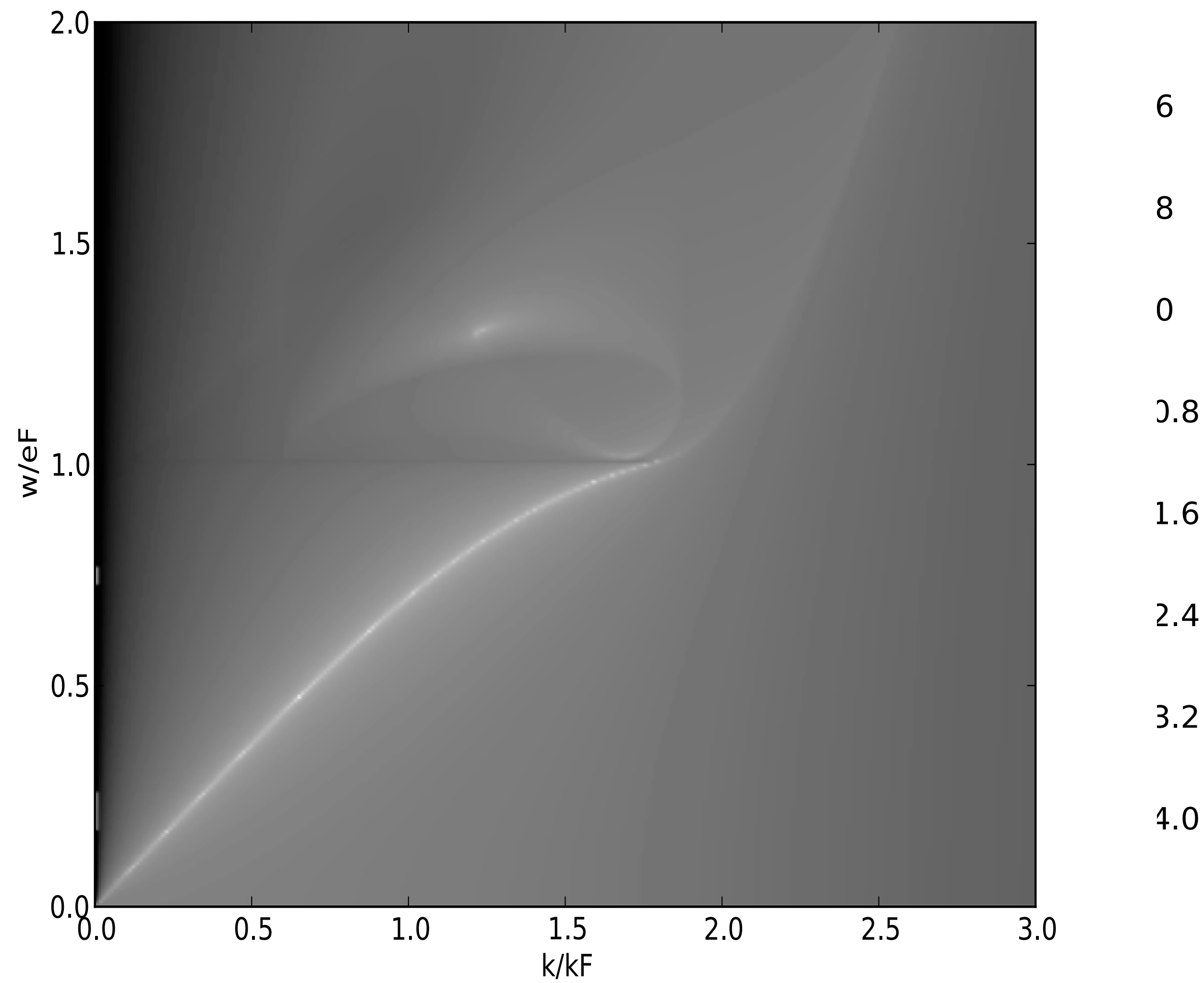


Non-Linear Response?

V=0.05

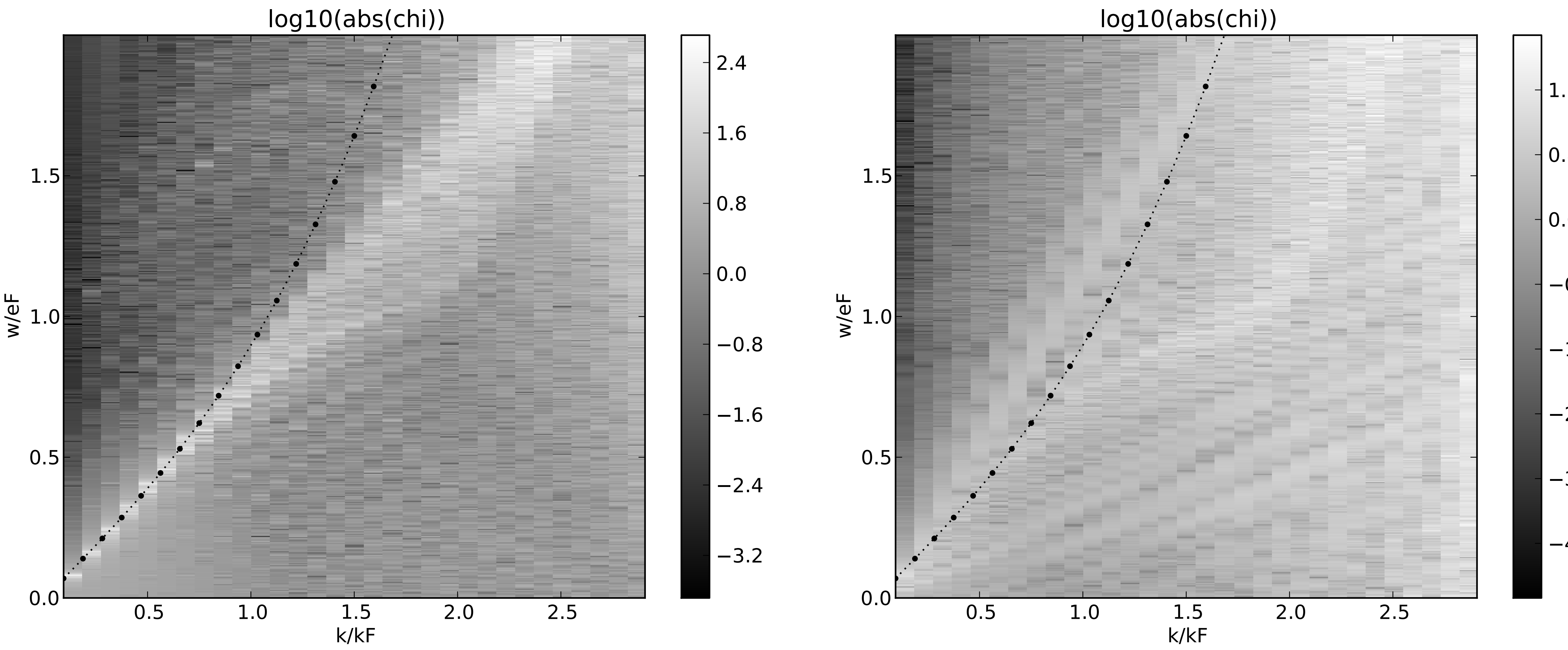


V=0.5



Non-Linear Response?

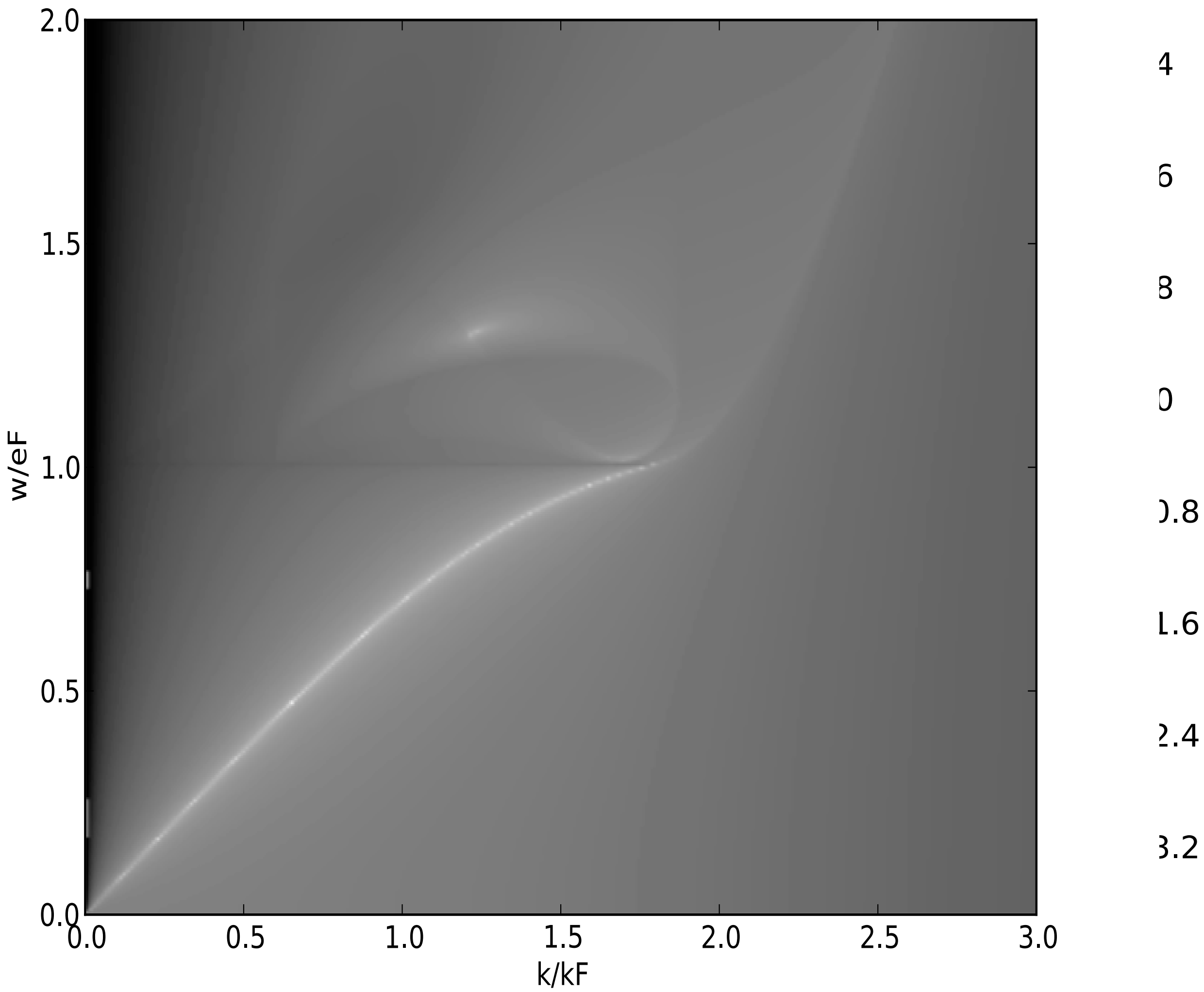
V=0.05 V=0.5

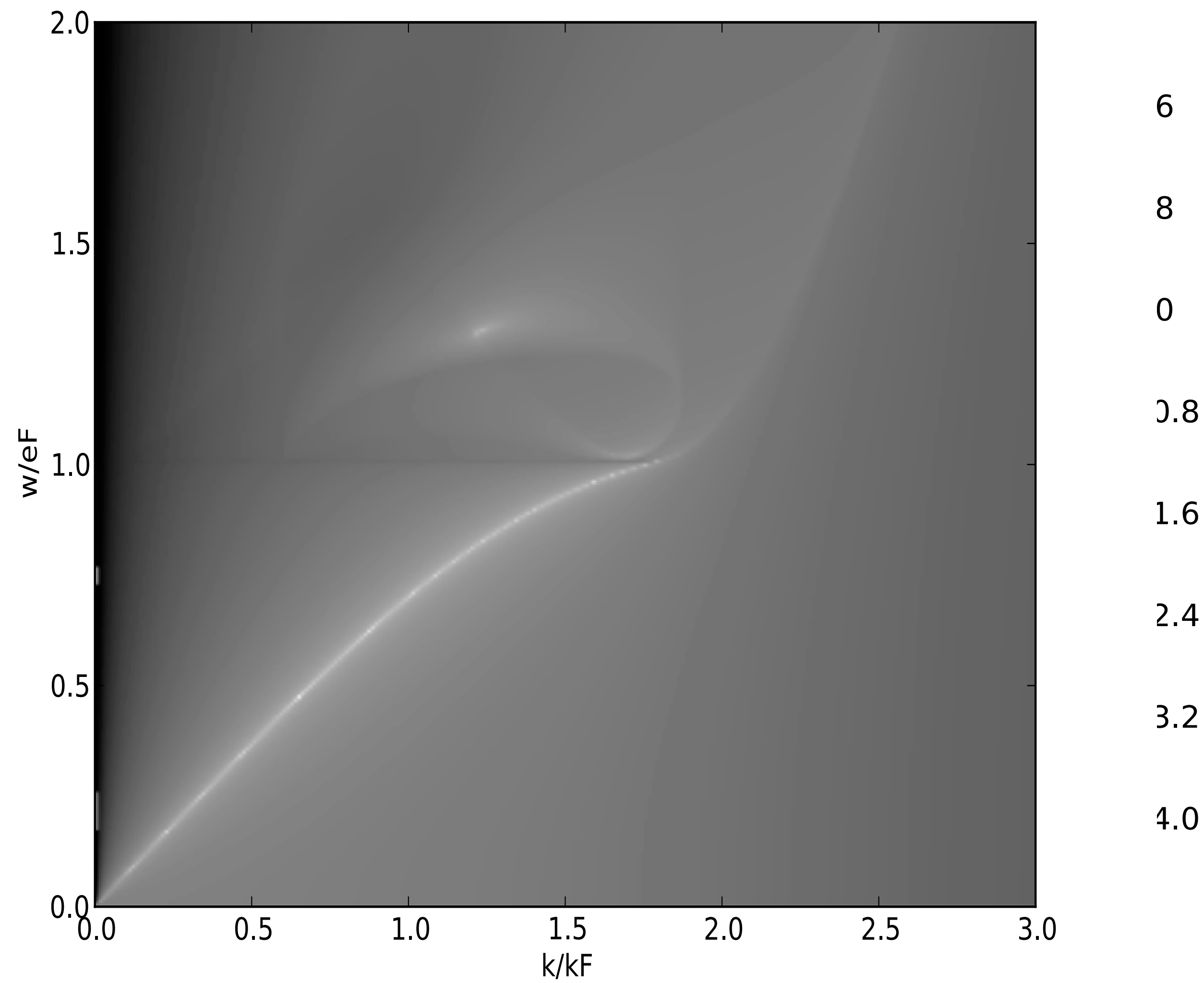


Non-Linear Response?

V=0.05

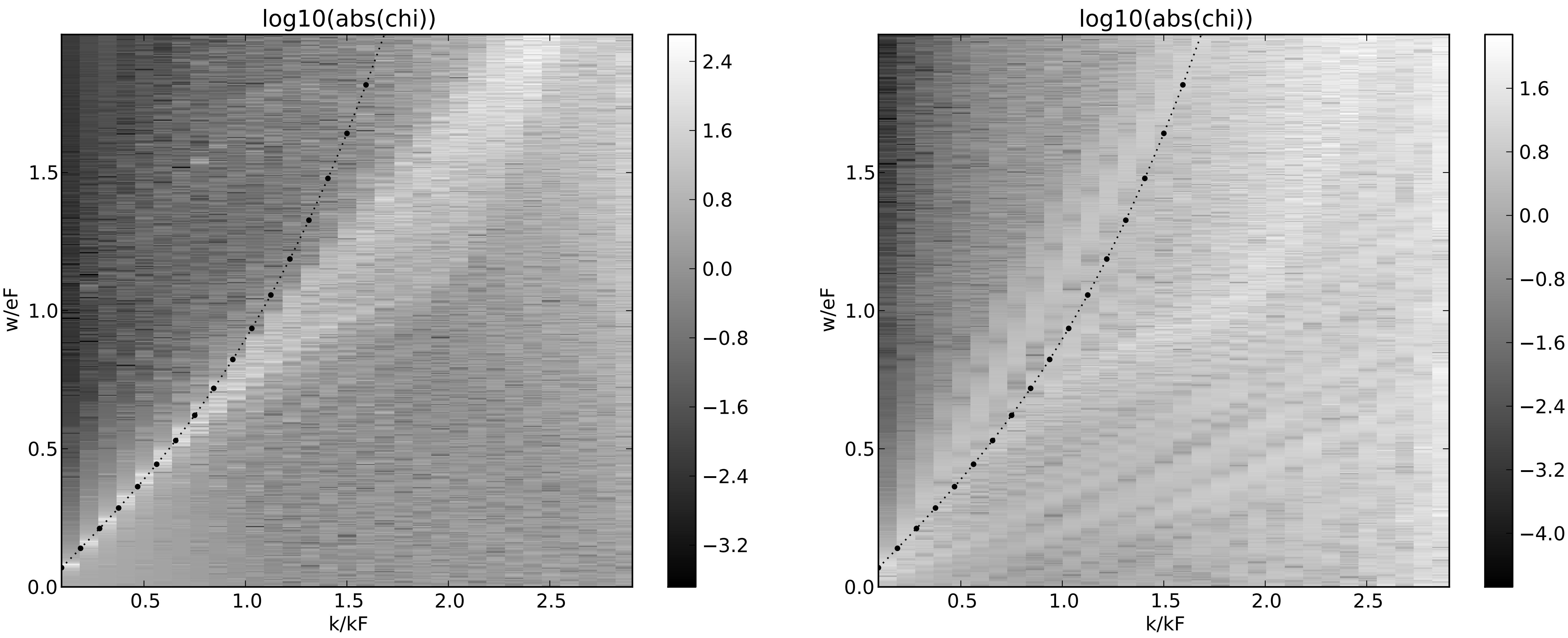
V=0.5





Non-Linear Response?

V=0.05 V=0.5



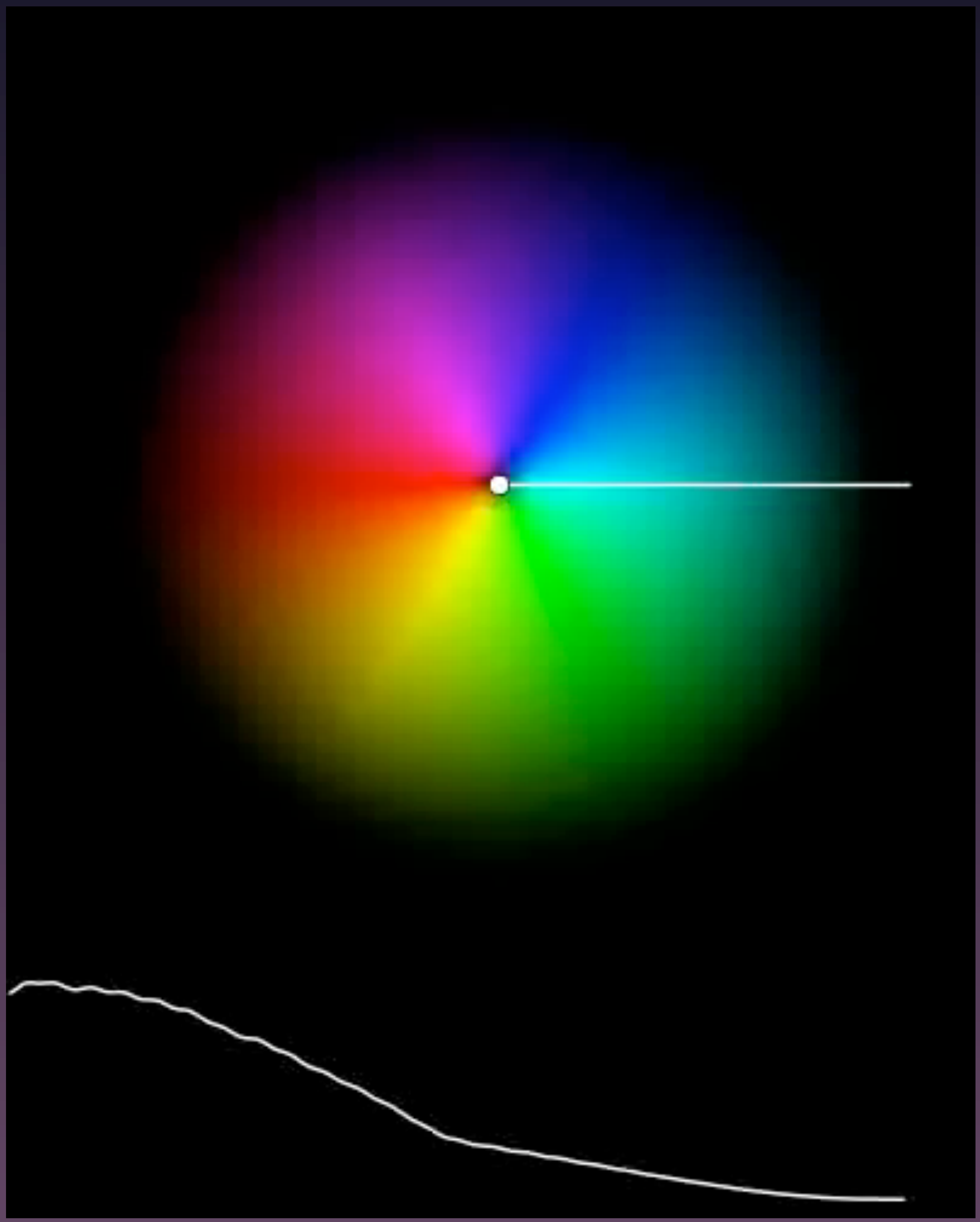
Application: Vortex Pinning

- Pulsar glitching (neutron stars)
  - Massive vortex unpinning events?

    (Anderson and Itoh (1975)
- Need Vortex-Defect interactions (force)

Pinning Force

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

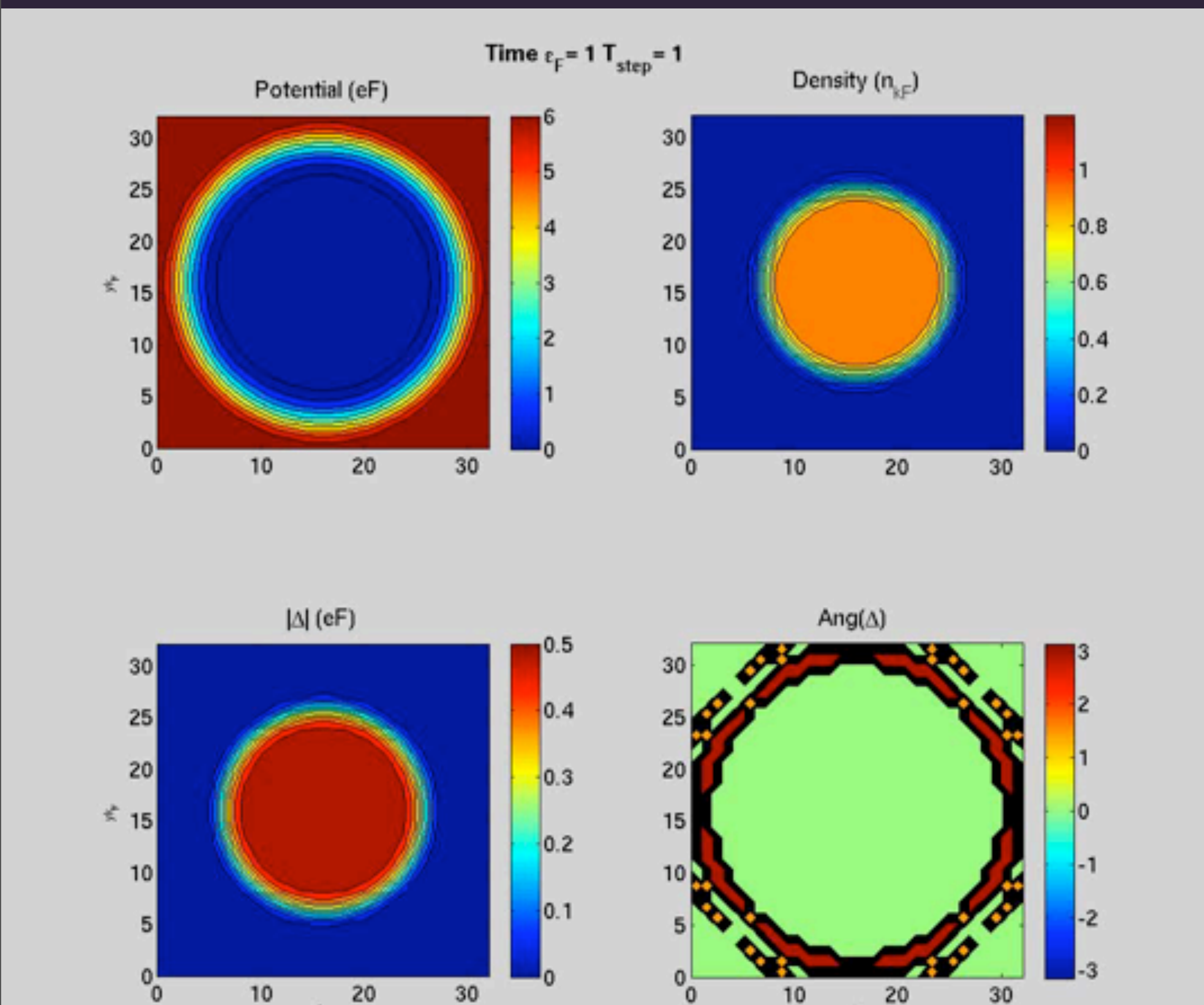


Thermodynamics

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

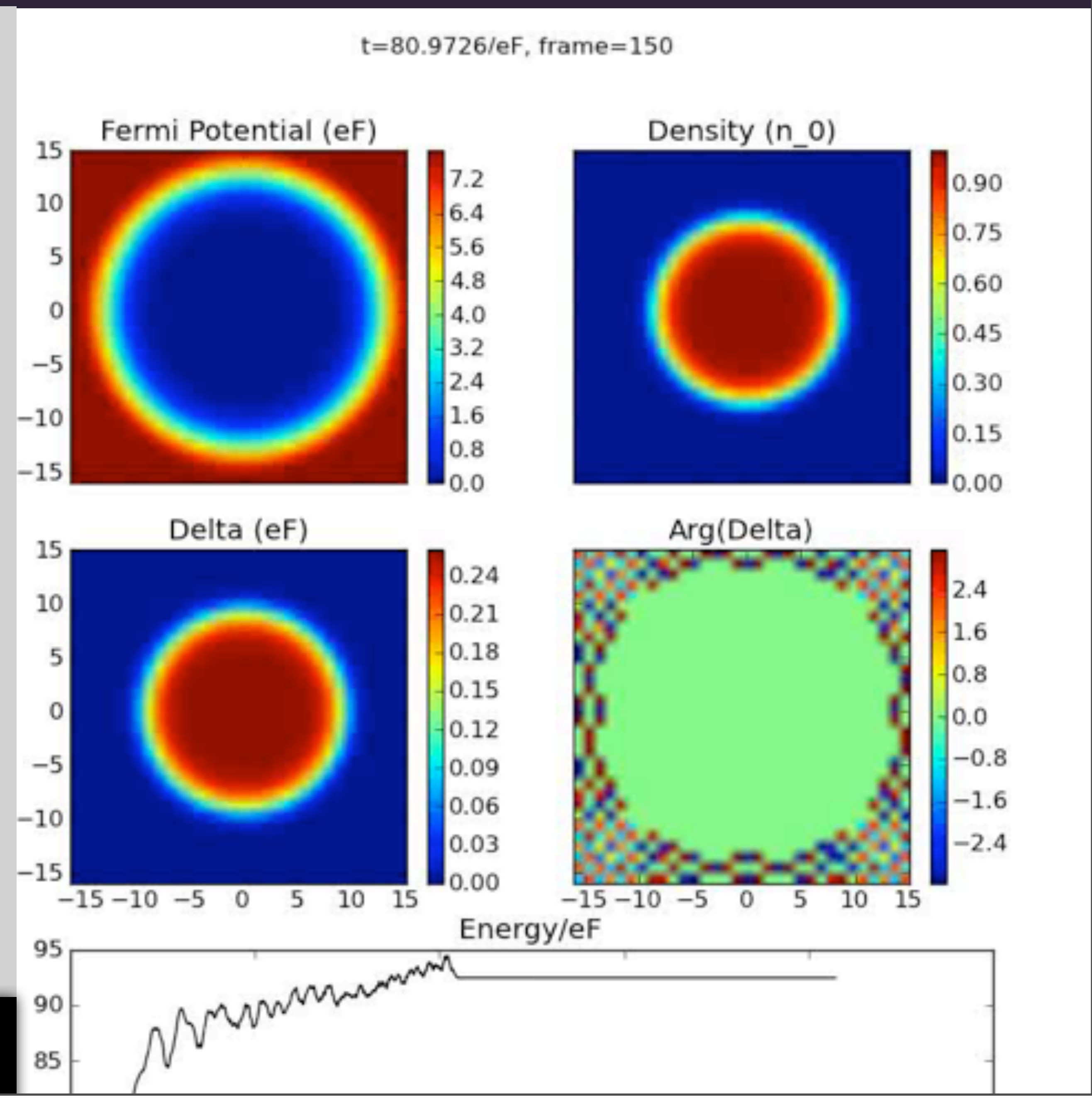
Comparison

Fermions
SLDA TDDFT



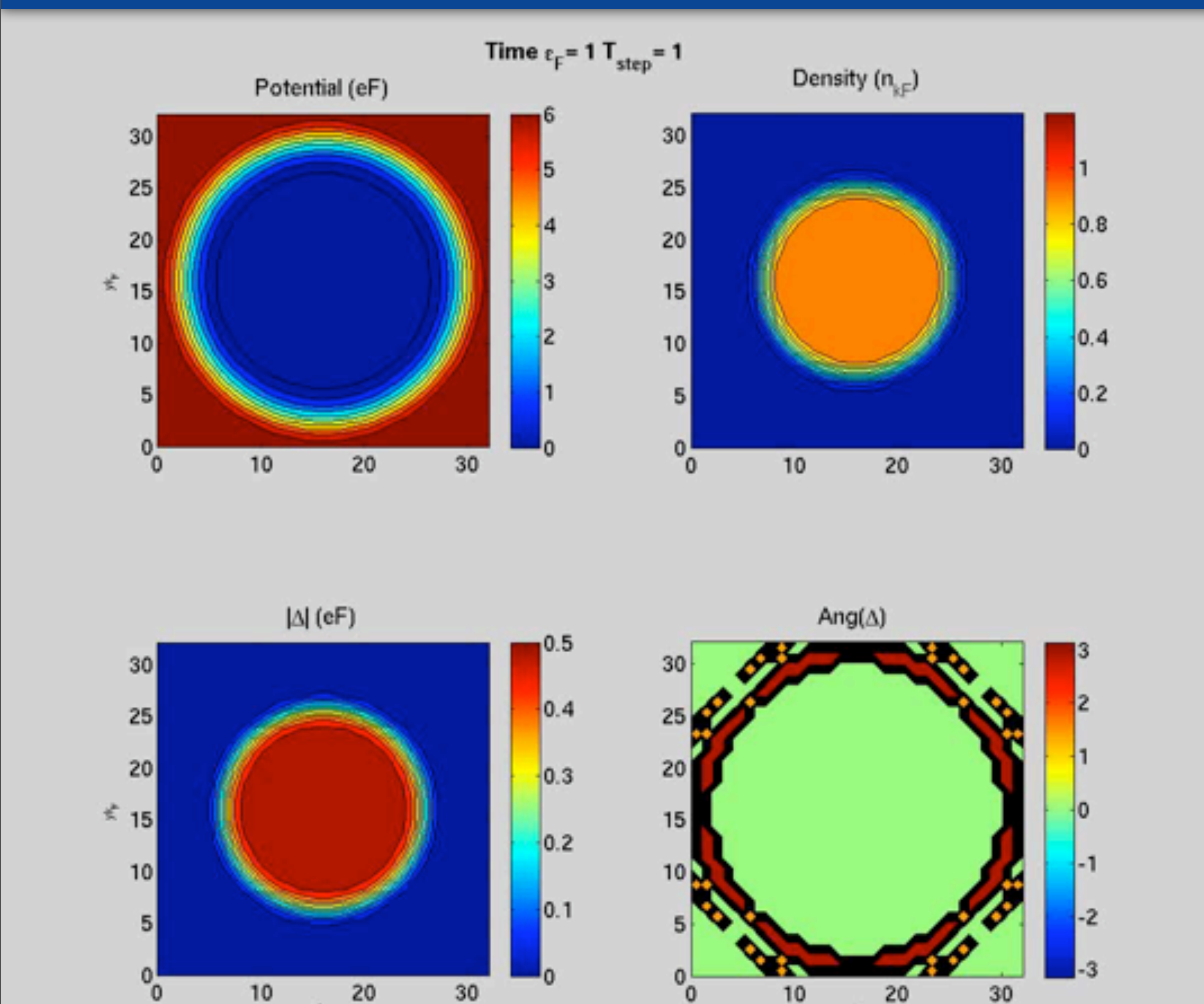
Bulgac et al. (Science 2011)

Gross Pitaevskii
model

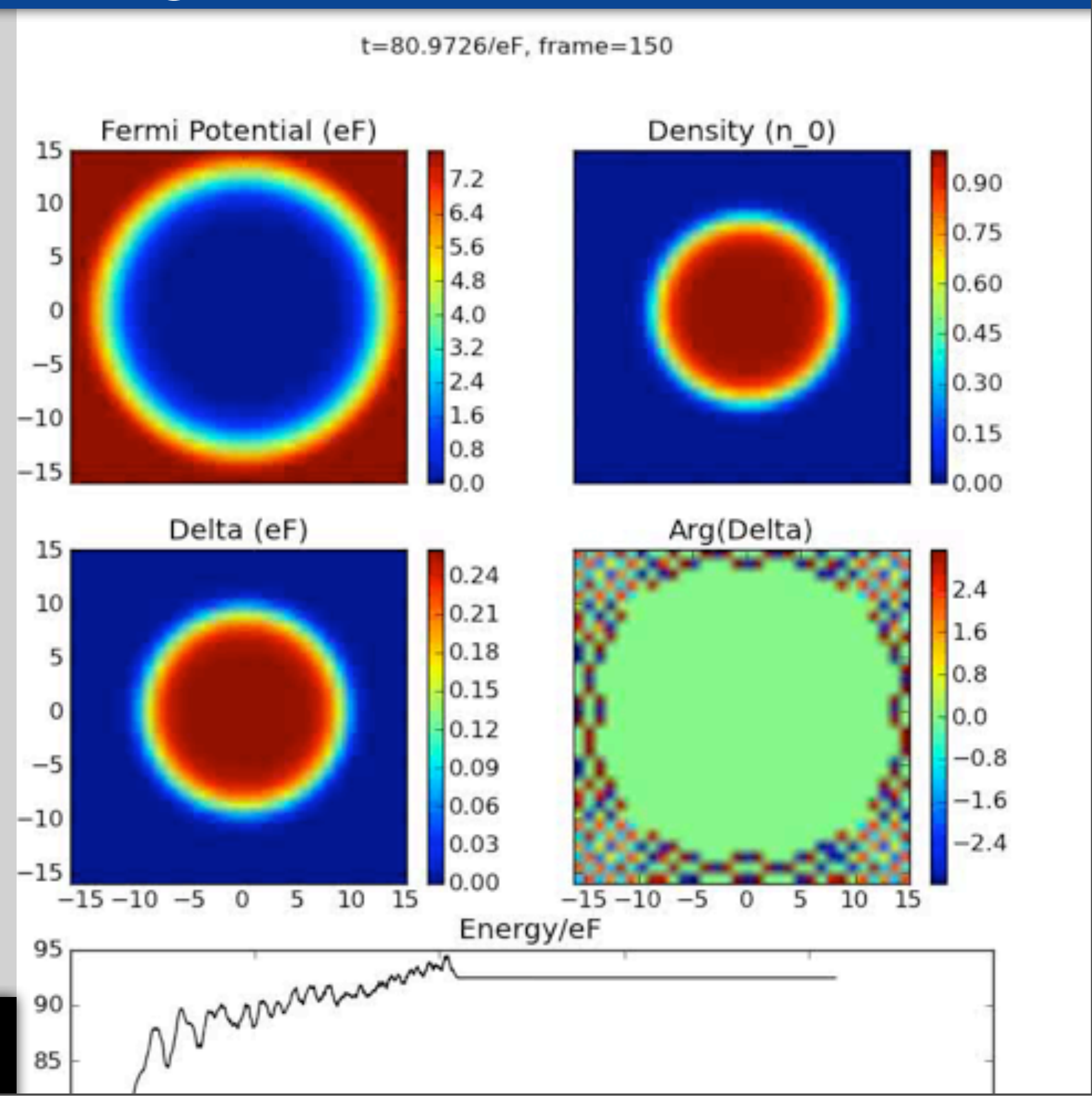


- Fermions:
- Simulation hard!
- Evolve 10^4–10^6 wavefunctions
- Requires supercomputers

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



Bulgac et al. (Science 2011)



Applications

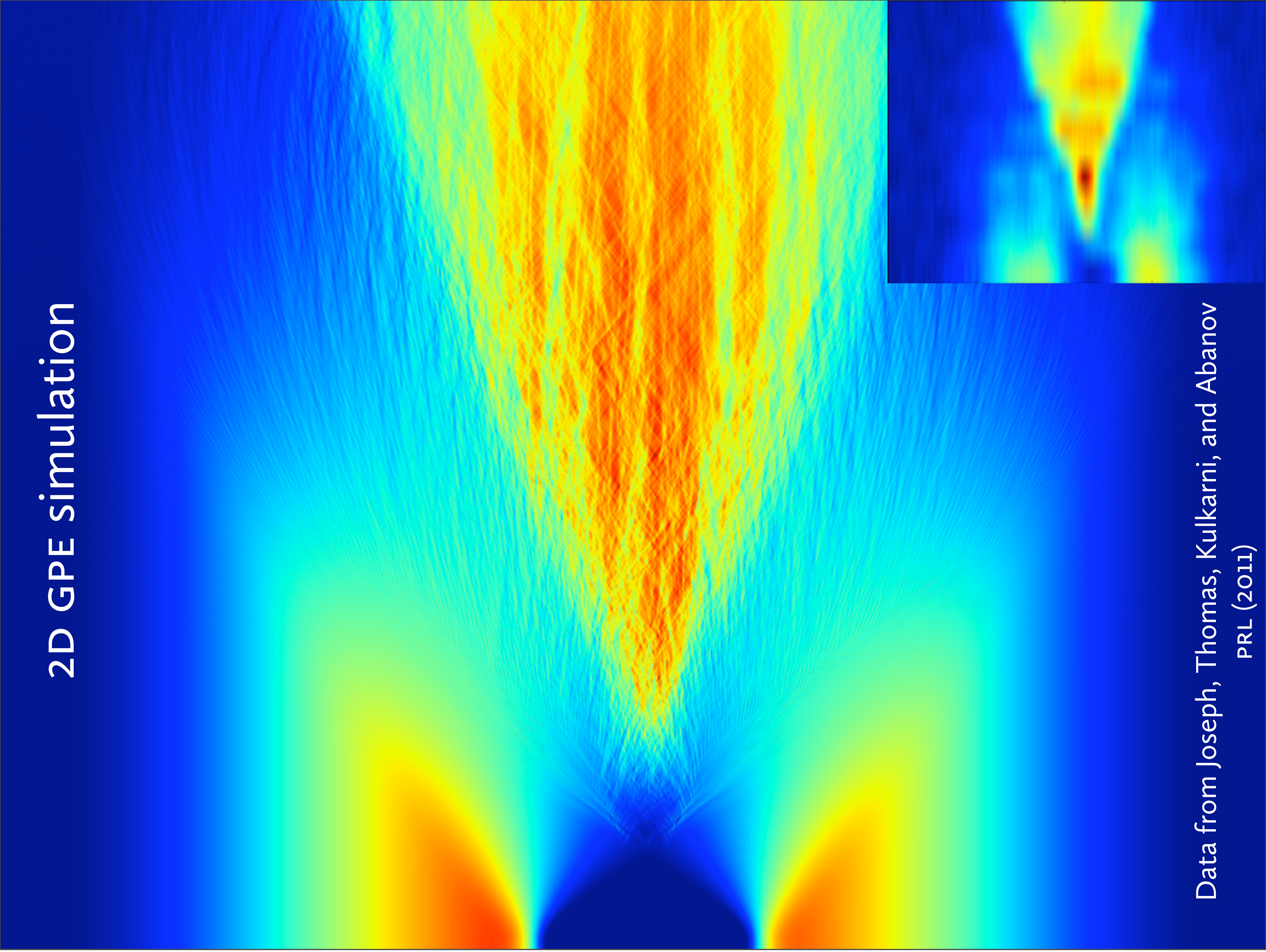
- Fast qualitatively accurate simulation:
  - Design initial conditions and $V(t)$ for experiment and expensive fermion DFT calculations
  - Develop intuition for quantum hydrodynamics
- Framework to attack large-scale simulations
  - Neutron star glitches (vortex depinning?)
  - Multi-scale simulations

Future Work

- Deal with pair-breaking
  - Two fluid model: transfer energy and mass to a normal component
  - Stochastic extensions?
- More flexible model
  - How to get past Galilean invariance?
- Multiscale model - matching
  - Is GPE enough?
    - database of vortex/vortex interactions?
    - spawn small fermionic solvers to deal with collisions?

Conclusion

- GPE-like models simply simulate qualitative dynamics of Fermi superfluids
- A feasible solution to model bulk superfluids?


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