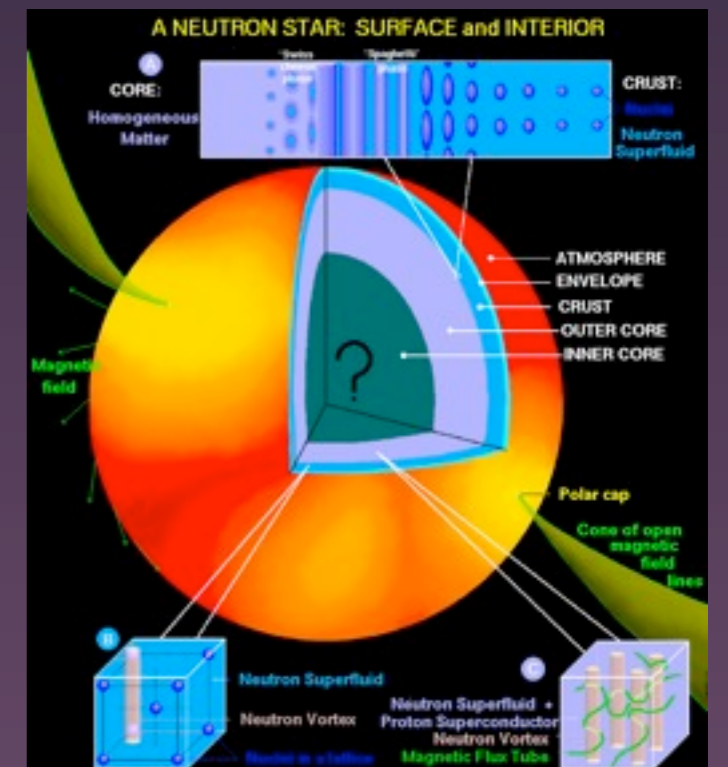
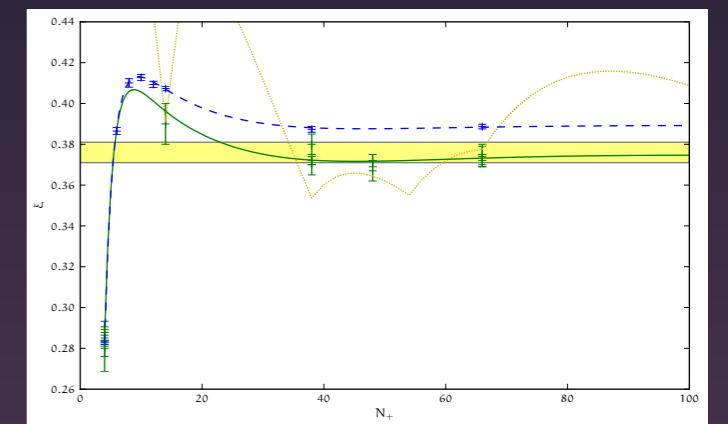
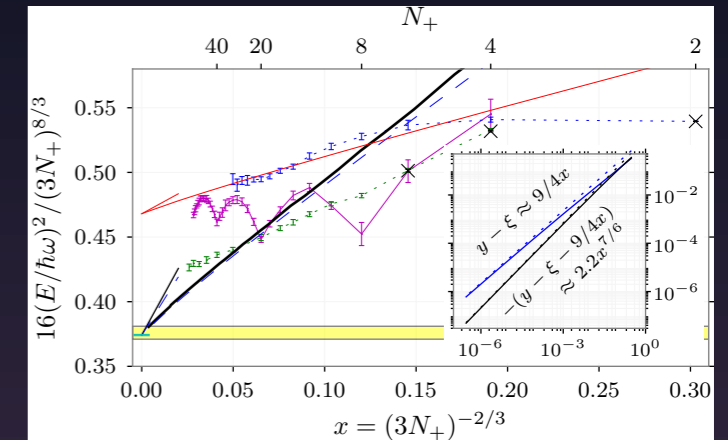


# Static and Dynamic Properties near Unitary from DFT

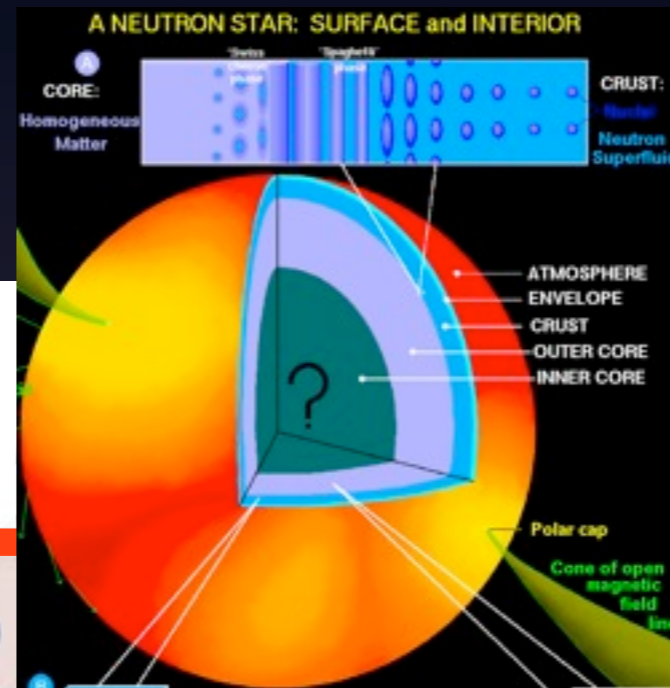
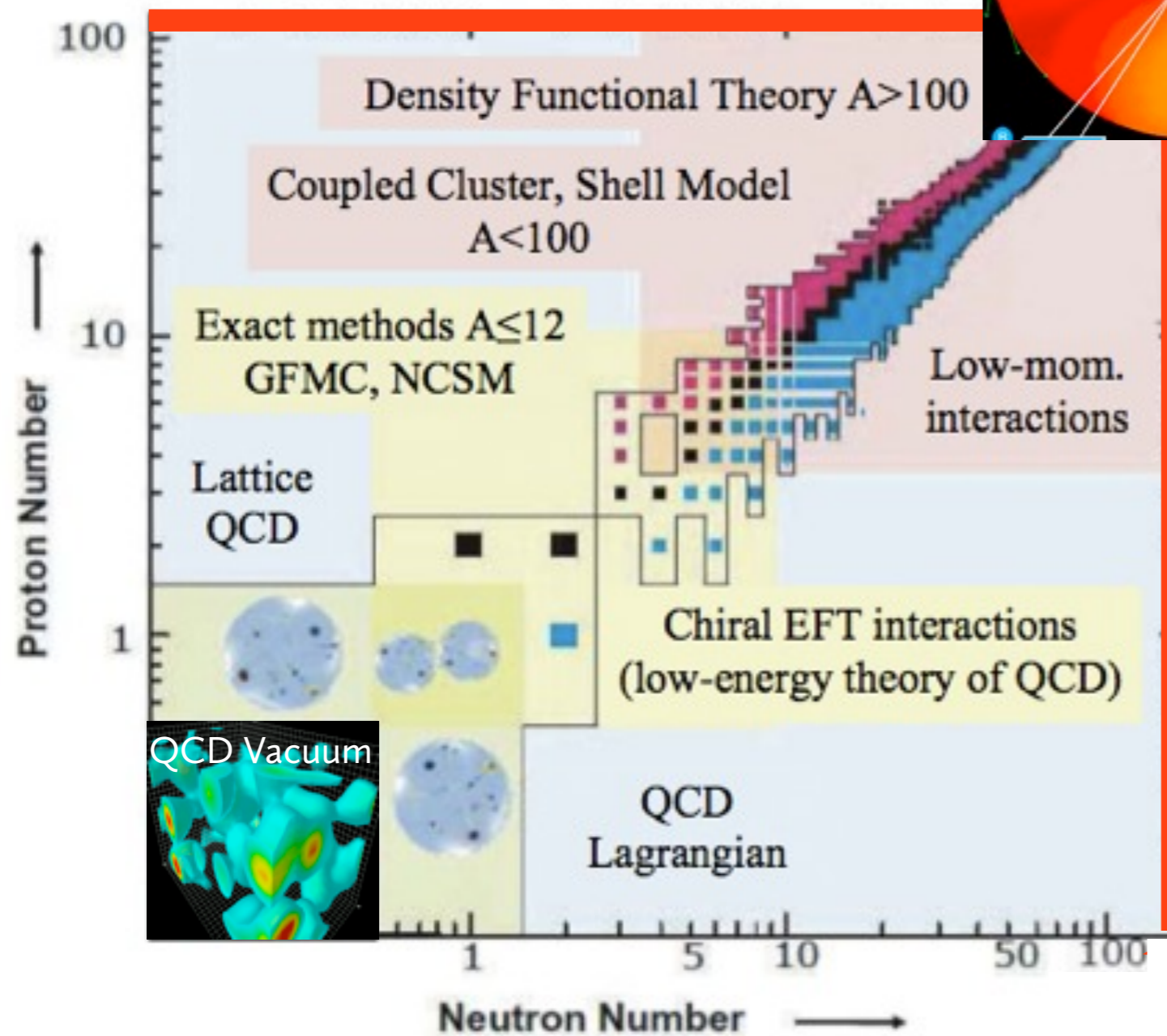
Michael McNeil Forbes  
Institute for Nuclear Theory (INT)  
University of Washington, Seattle, WA

# Outline

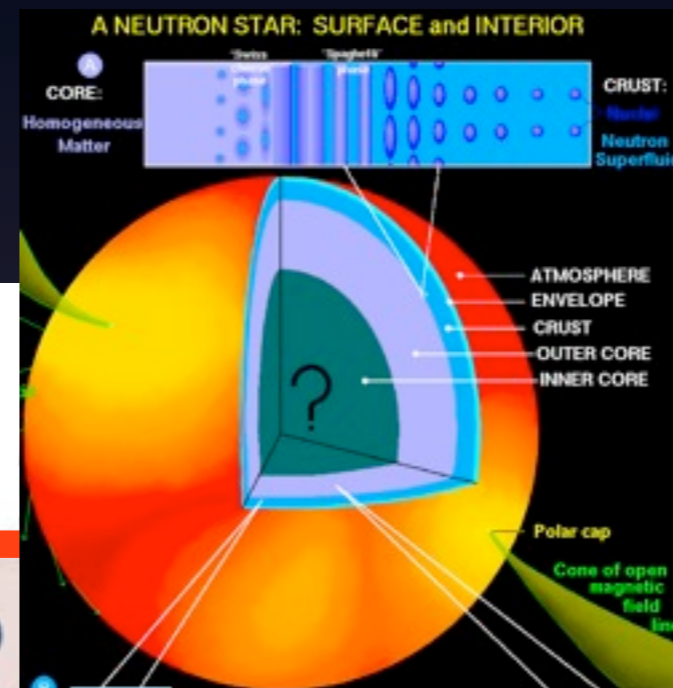
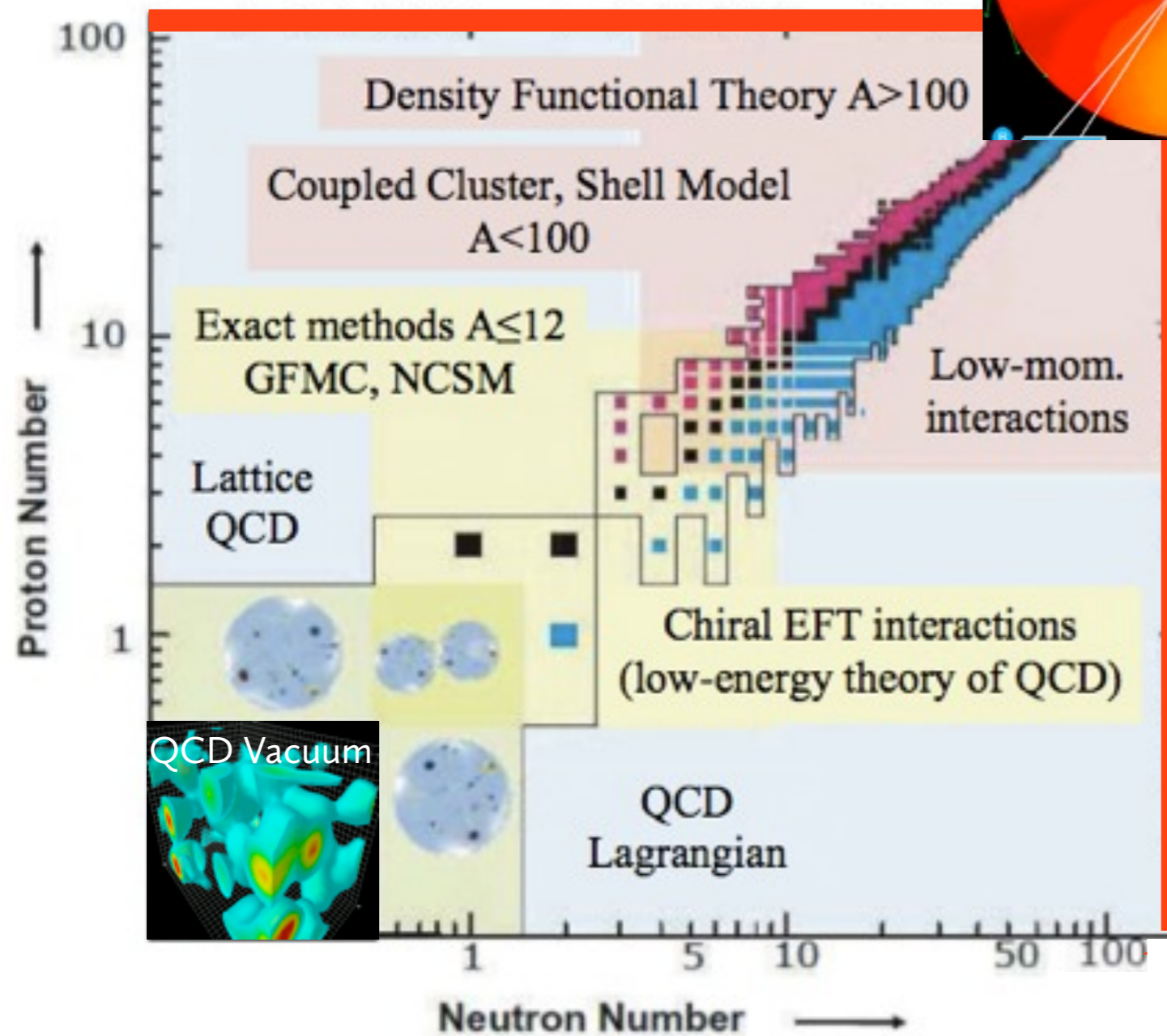
- DFT for Unitary Fermi Gas
  - Static: boxes and traps
  - Gradient corrections
- Gross-Pitaevskii–Equation (GPE)
  - Works for low-energy Unitary Fermi Gas!
  - “Laboratory on your Laptop”
  - scale up to neutron stars (glitching)



# 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

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)

# 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)

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

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

- Take regulator  $\lambda \rightarrow \infty$  and coupling  $g \rightarrow 0$  to fix s-wave scattering length  $a^{-1} \propto (\lambda - g^{-1}) = 0$  (unitary limit)
- Universal physics:
  - $\mathcal{E}(\rho) = \xi \mathcal{E}_{\text{FG}}(\rho) \propto \rho^{5/3}$ ,  $\xi = 0.376(5)$
- Good model of dilute neutron matter in neutron stars

# Statics

# Density Functional Theory (DFT)

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

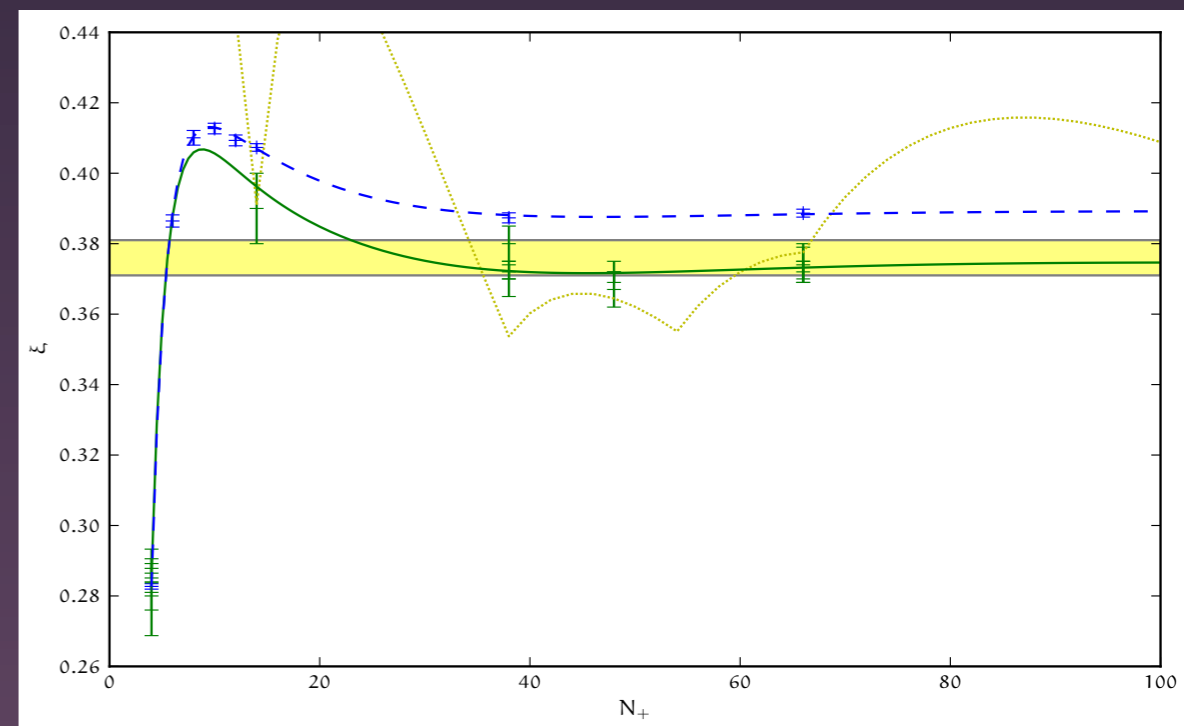
$$\int d^3\mathbf{x} \{ \mathcal{E}[n(\mathbf{x})] + V(\mathbf{x})n(\mathbf{x}) \}$$

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

# SLDA: Superfluid Local Density Approximation

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

- Three densities:  
 $n \approx \langle a^\dagger a \rangle$ ,  $\tau \approx \langle \nabla a^\dagger \nabla a \rangle$ ,  $v \approx \langle ab \rangle$
- Three parameters:
  - Effective mass ( $m/\alpha$ )
  - Hartree ( $\beta$ ), Pairing ( $g$ )



Forbes, Gandolfi, Gezerlis (2012)

# BdG: contained in SLDA

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

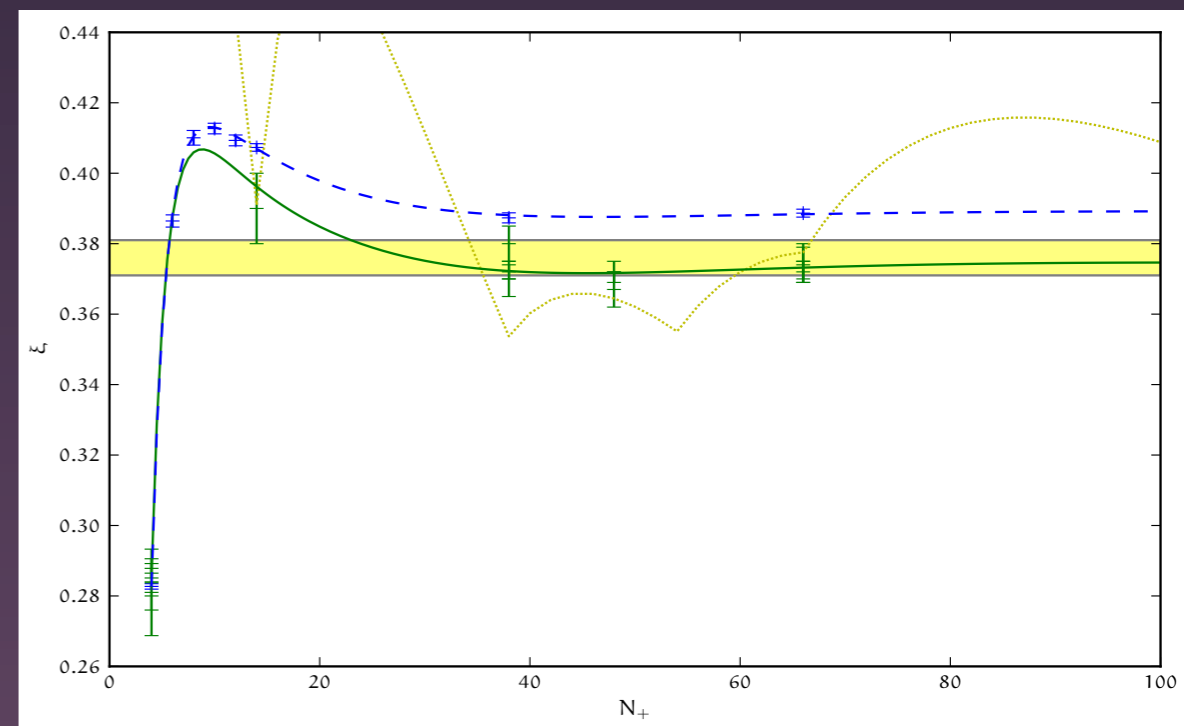
$\langle \nabla \hat{a}^\dagger \nabla \hat{a} \rangle + \langle \nabla \hat{b}^\dagger \nabla \hat{b} \rangle$ 
 $\langle \hat{a}^\dagger \hat{b}^\dagger \rangle \langle \hat{b} \hat{a} \rangle$

- 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

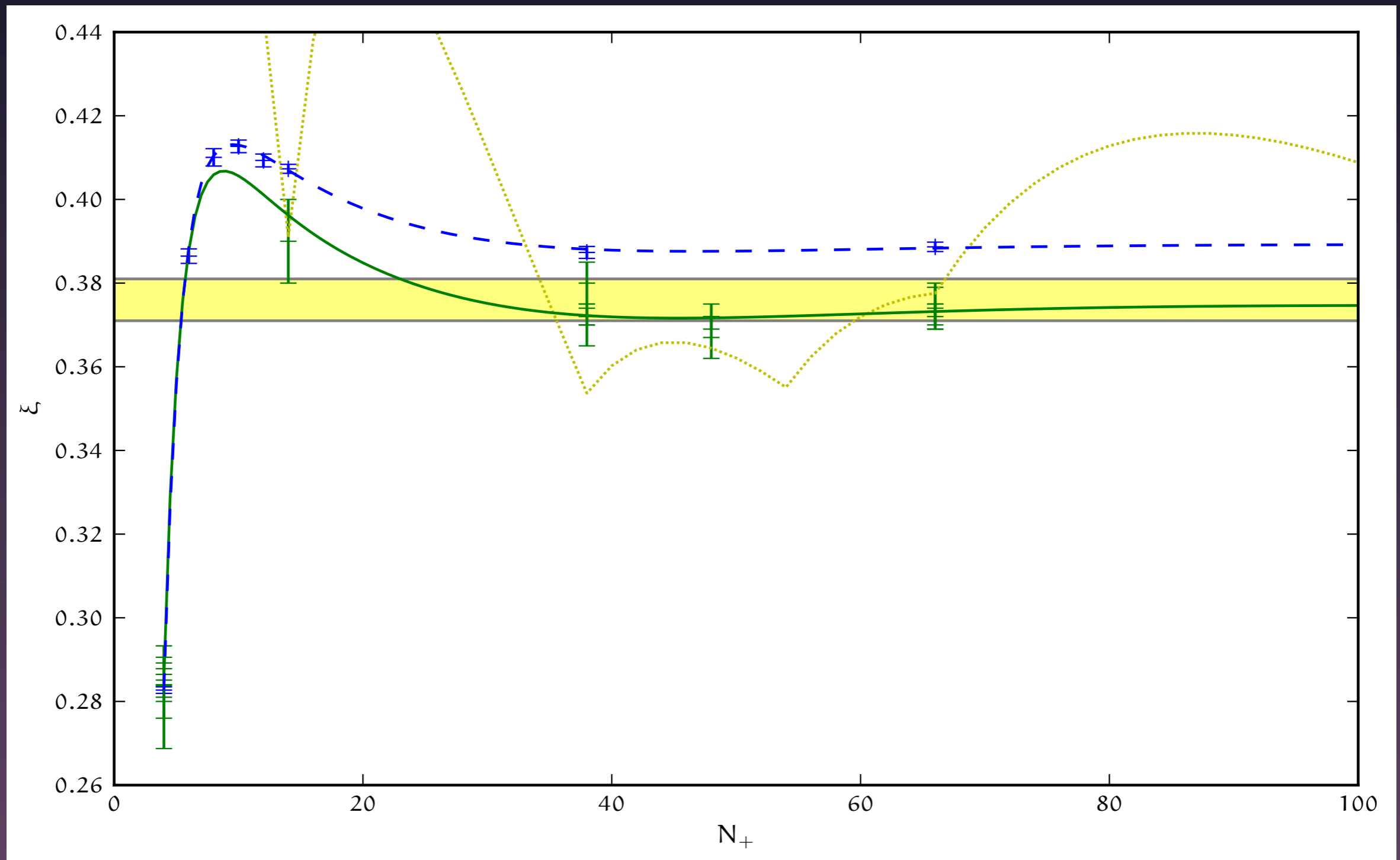
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 $n \approx \langle a^\dagger a \rangle$ ,  $\tau \approx \langle \nabla a^\dagger \nabla a \rangle$ ,  $v \approx \langle ab \rangle$
- Three parameters:
  - Effective mass ( $m/\alpha$ )
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Forbes, Gandolfi, Gezerlis (2012)

# SLDA: Superfluid Local

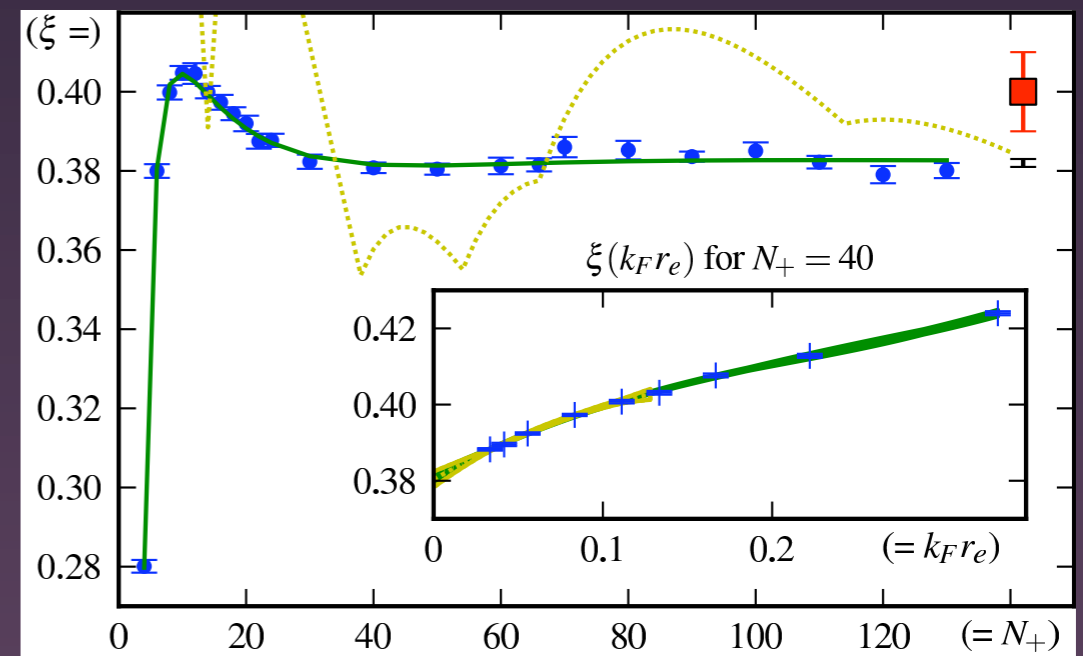


Forbes, Gandolfi, Gezerlis (2012)

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

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

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



Forbes, Gandolfi, Gezerlis (2011, 2012)

# Fit directly to QMC

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

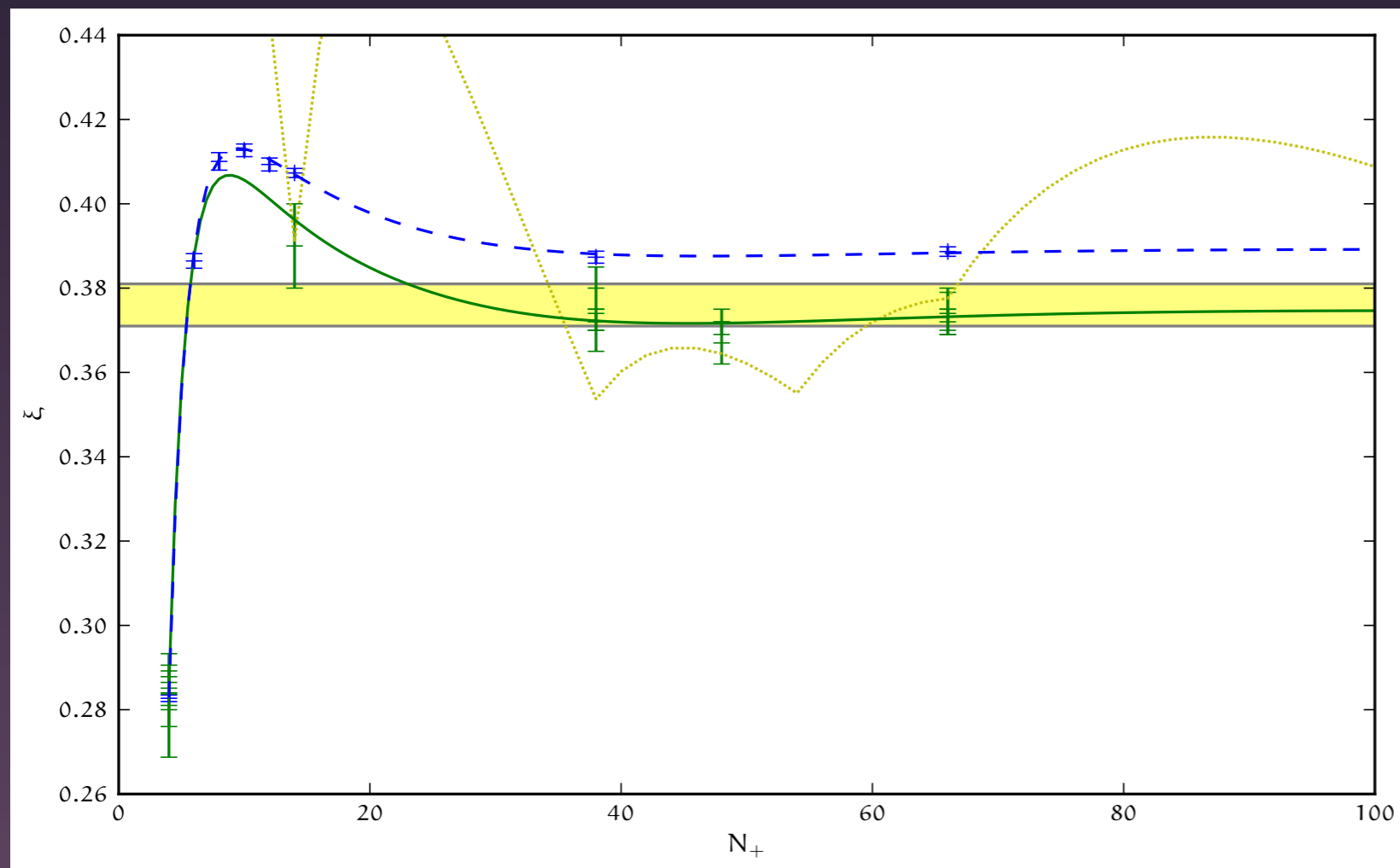
- Each parameter becomes a quadratic polynomial:
  - $\alpha(k_{\text{F}r_e})$ ,  $\beta(k_{\text{F}r_e})$ ,  $\gamma(k_{\text{F}r_e})$
- we actually use physical parameters  
 $\xi(k_{\text{F}r_e})$ ,  $\Delta(k_{\text{F}r_e})$ ,  $\alpha(k_{\text{F}r_e})$
- 9 total parameters for all N

# Fit directly to QMC

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

- Not complete story for modeling range:
  - Does not regulate theory
  - No structure for gap ( $\Delta_p$ )  
probably requires non-local functional

# Fit SLDA to box QMC

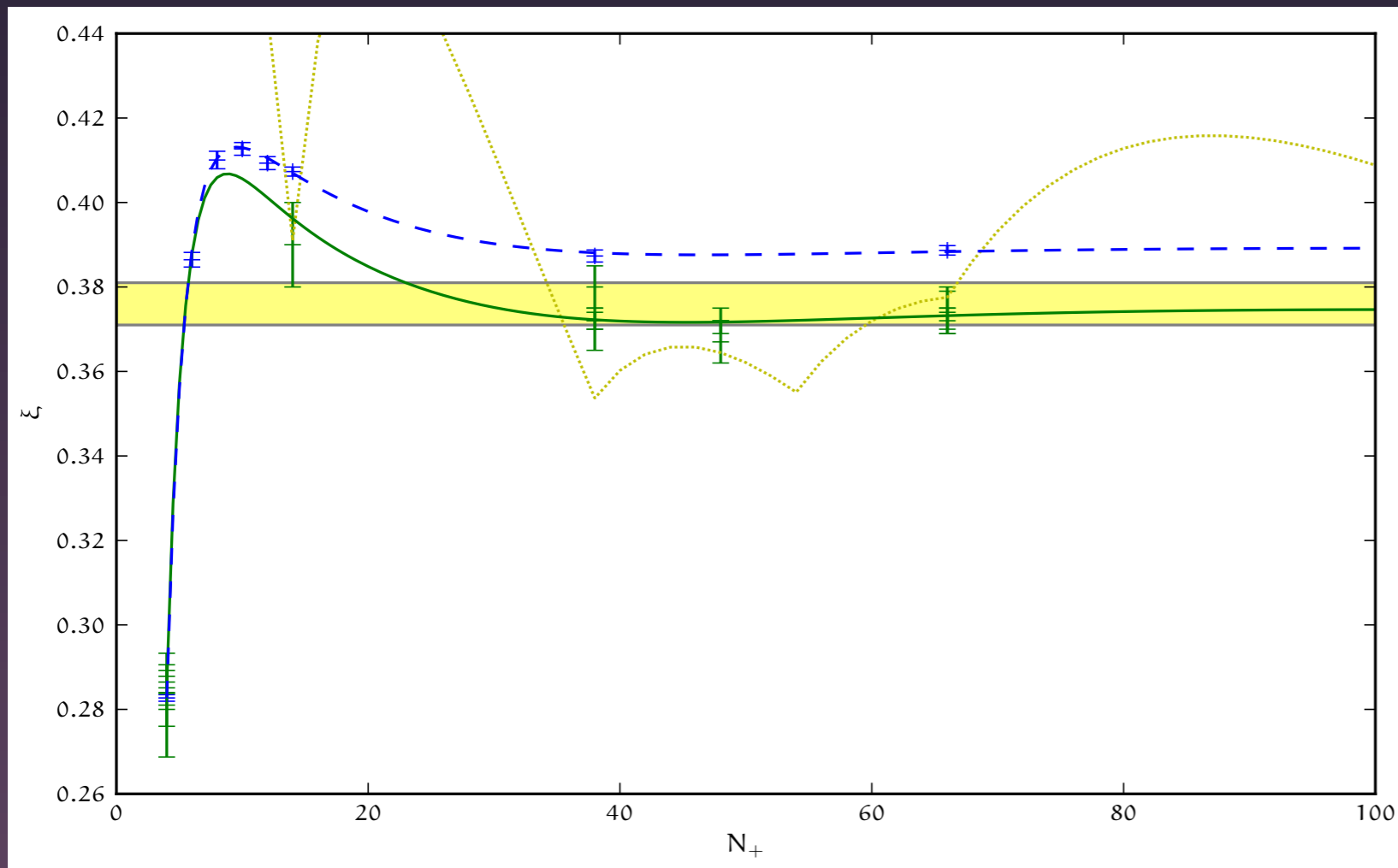


- Fit 60 QMC with 9 parameter model
- Directly use QMC with sub-percent errors
  - reduced  $\chi^2 = 6$

Forbes, Gandolfi, Gezerlis PRL (2011)

# SLDA parameters

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



Forbes, Gandolfi, Gezerlis (2012)

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

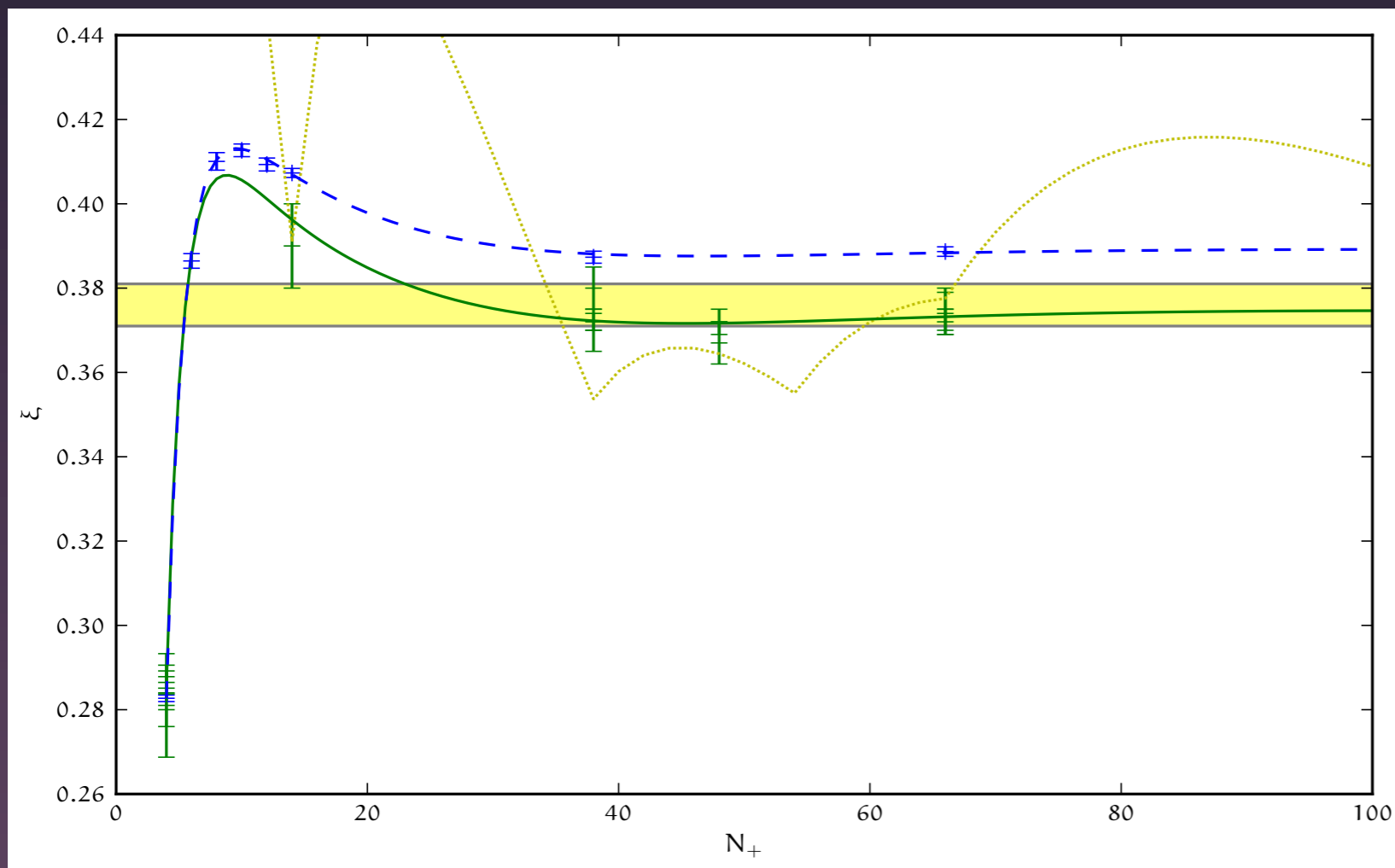
Universal slope

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

$$S=0.12(1)$$

# SLDA parameters

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



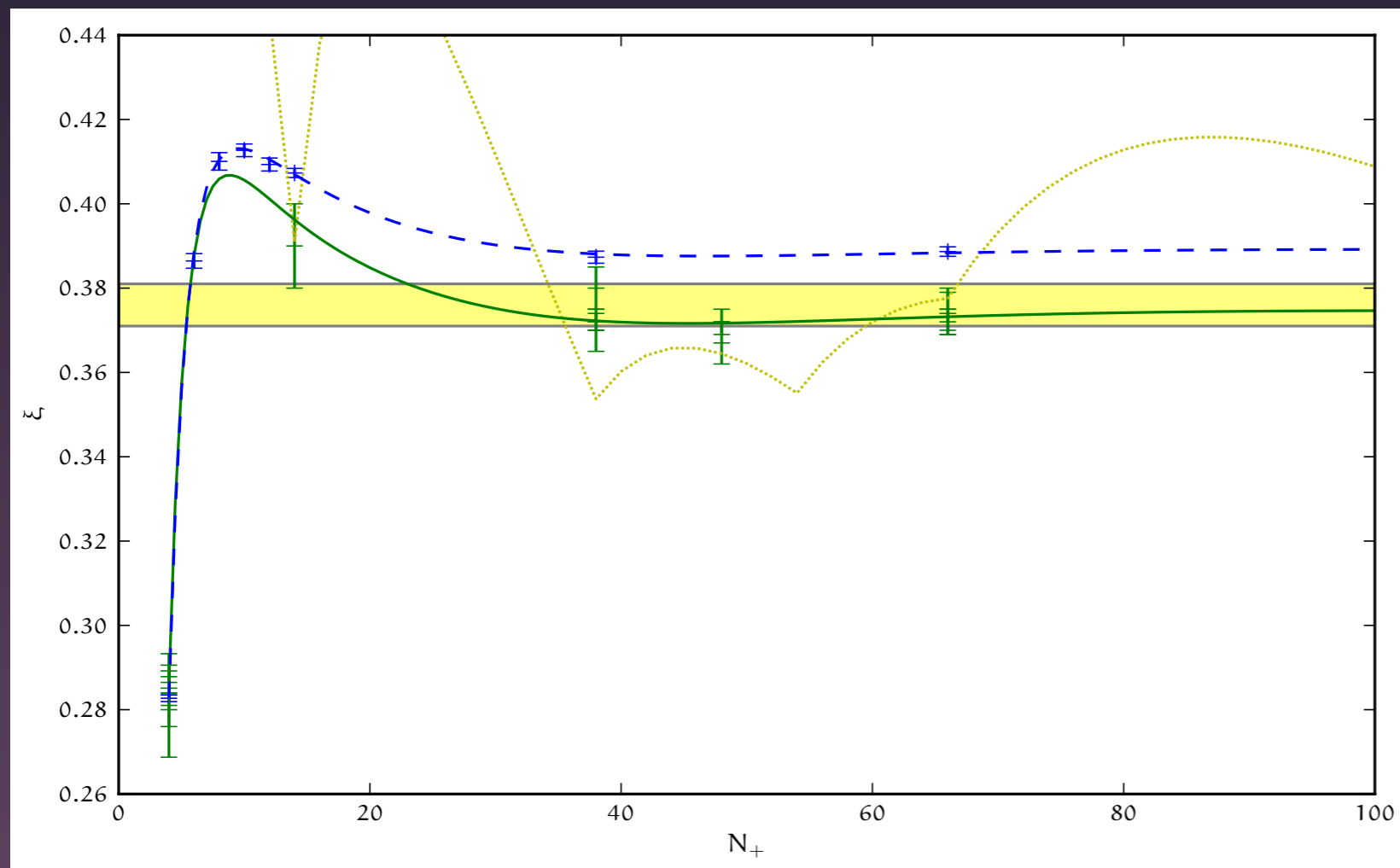
Forbes, Gandolfi, Gezerlis (2012)

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	1.289(7)	-0.69(3)	

Gap and inverse mass  
seem too large

Limitation of fixed  
node approximation?

# Unbiased SLDA fit at $r_{\text{eff}}=0$



$N_+$	$\xi_{N_+}$	Method
2	$-0.415332919\dots$	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 unbiased results

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

Forbes, Gandolfi, Gezerlis (2012)

# Generalizations?

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

- In principle, could have functions of the dimensionless quantity:

$$\frac{\alpha \frac{\tau}{m} + g \nu^\dagger \nu}{n^{5/3}}$$

- No evidence that this complication is needed yet

# Gradient Corrections?

$$\mathcal{E}(n, \tau, \nu) = \left( \alpha \frac{\tau}{m} + g \nu^\dagger \nu \right) + \beta \mathcal{E}_{FG}(n) + \frac{\delta \lambda}{8m} \frac{(\nabla n)^2}{n}$$

- Leading order gradient corrections (Weizäcker term)
  - Has no effect (unconstrained by) previous box results

# Low Energy Theory

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

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

- 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:
  - $\xi, c_1, c_2$  (I prefer  $c_\chi = -6\pi^2(2\xi)^{3/2}(2c_1 - 9c_2)$ ,  $c_\omega = -6\pi^2(2\xi)^{3/2}(2c_1 + 3c_2)$ )

# Low Energy Theory

$$\chi(q) = \frac{-mk_F}{\hbar^2 \pi^2 \xi} \left[ 1 - \frac{c_\chi}{12\xi} \frac{q^2}{k_F^2} \right] \quad \omega_q = q \underbrace{\frac{\hbar k_F \sqrt{\xi}}{m\sqrt{3}}}_{c_s} \left[ 1 + \frac{c_\omega}{24\xi} \frac{q^2}{k_F^2} \right]$$

$$c_\chi = -6\pi^2(2\xi)^{3/2}(2c_1 - 9c_2), \quad c_\omega = -6\pi^2(2\xi)^{3/2}(2c_1 + 3c_2)$$

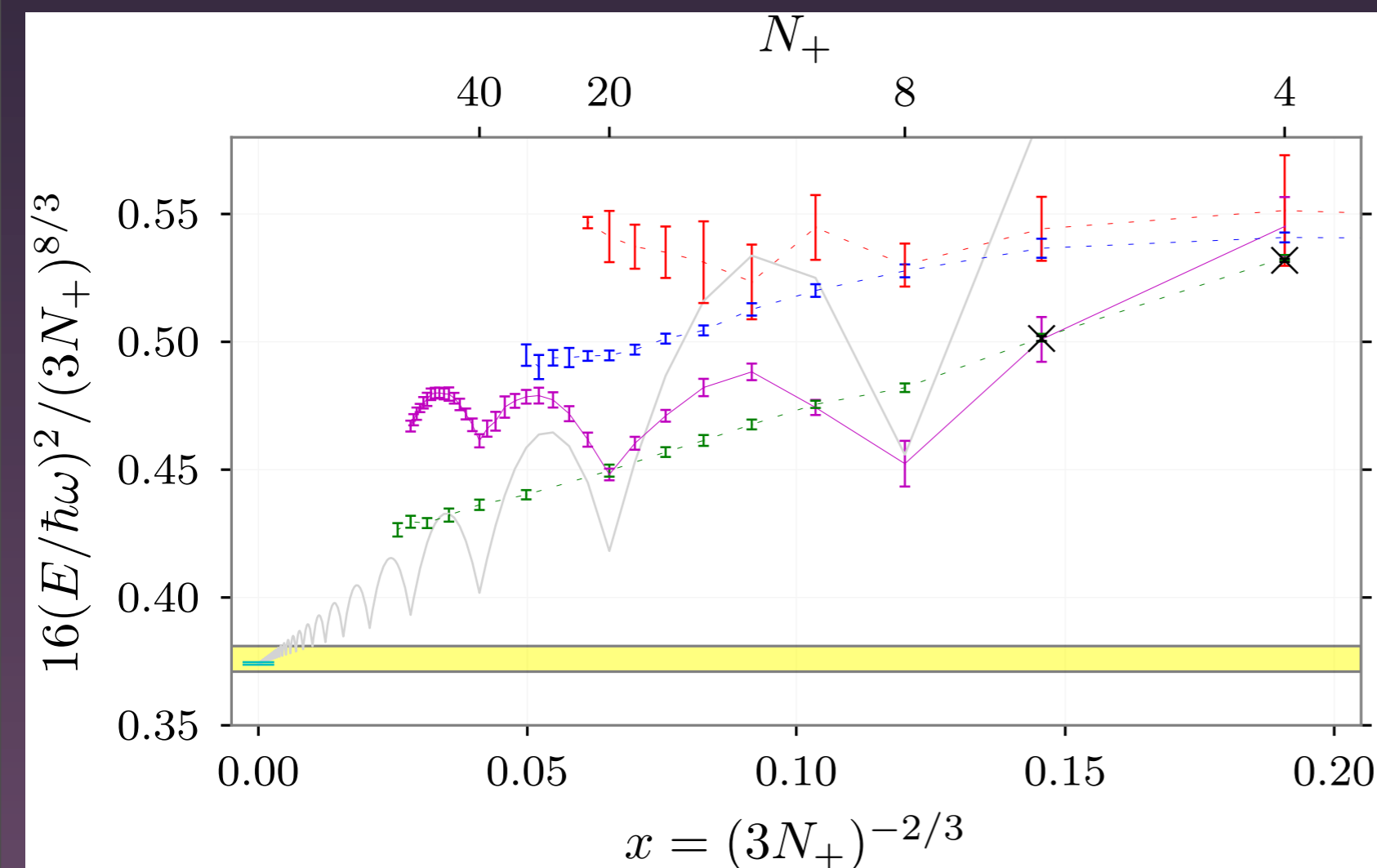
- Leading order: one parameter  $\xi=0.3742(5)$
- Two new universal constants at NLO:
  - Static:  $c_\chi=1.5(3)$  (Forbes 2013: not a proper 1-sigma error)
    - (BdG  $c_\chi=7/3=2.33$ ;  $\epsilon$ -expansion  $c_\chi=1.6+O(\epsilon^2)$ ; GPE  $c_\chi=2.25$ )
  - Dynamic:  $c_\omega=?$ 
    - (BdG  $c_\omega=0.7539$ ;  $\epsilon$ -expansion  $c_\omega=c_\chi+O(\epsilon^2)$ ; GPE  $c_\omega=c_\chi$ )

BdG Juan and Valle 2009;  $\epsilon$ -expansion Rupak and Schäfer 2007

# Harmonic Traps

$$E(N_+) = \frac{\sqrt{\xi}}{4} \hbar \omega \left[ \overbrace{(3N_+)^{4/3}}^{\text{LDA}} - \frac{c_x}{6\xi} (3N_+)^{2/3} + \mathcal{O}(N_+^{5/9}) \right],$$

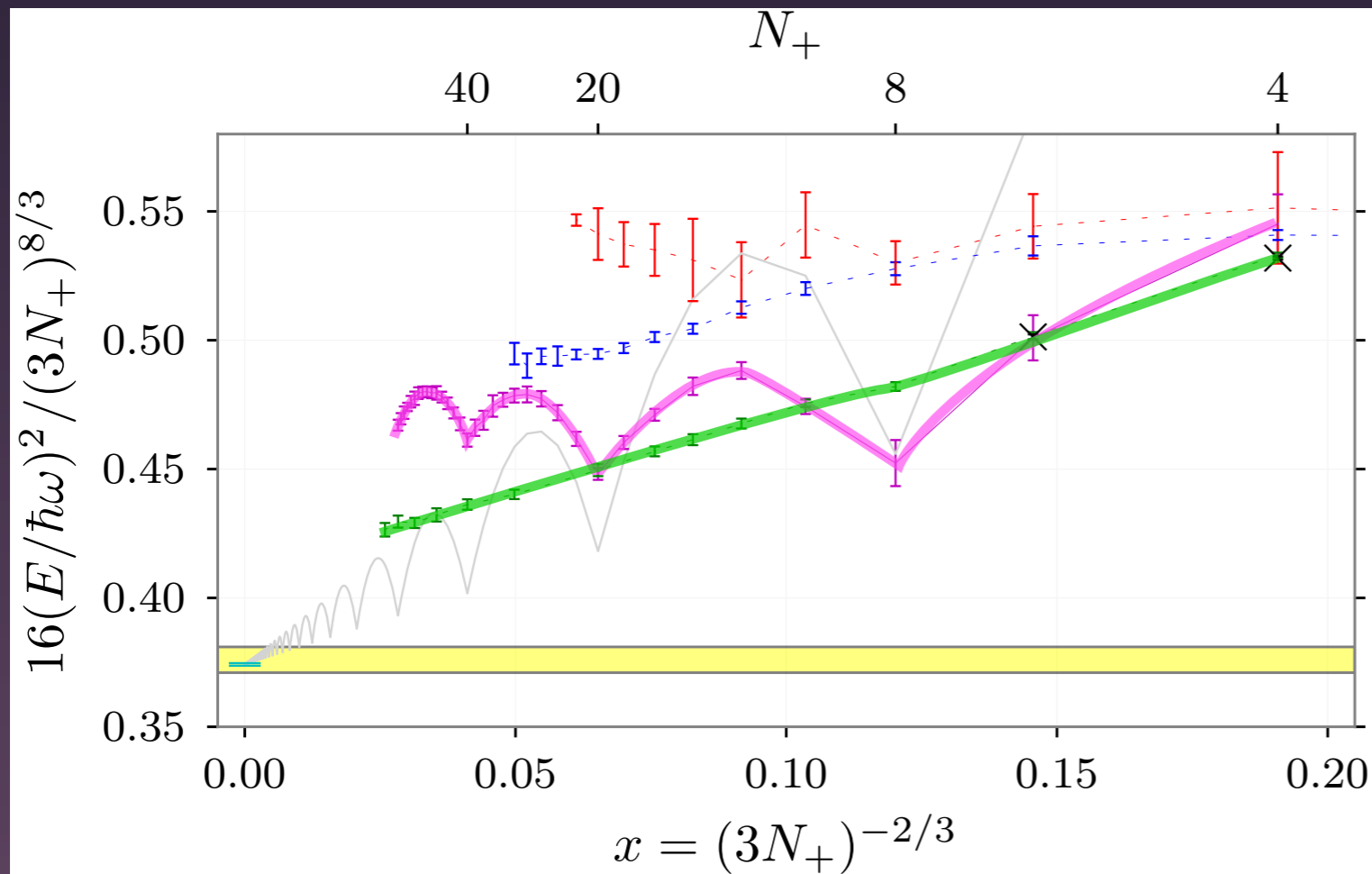
$$\frac{16E^2}{\xi \hbar^2 \omega^2 (3N_+)^{8/3}} = \xi + c_x x + \mathcal{O}(x^{7/6}), \quad x = \frac{1}{(3N_+)^{2/3}}$$



- Static structure factor describes slope

Forbes 2013

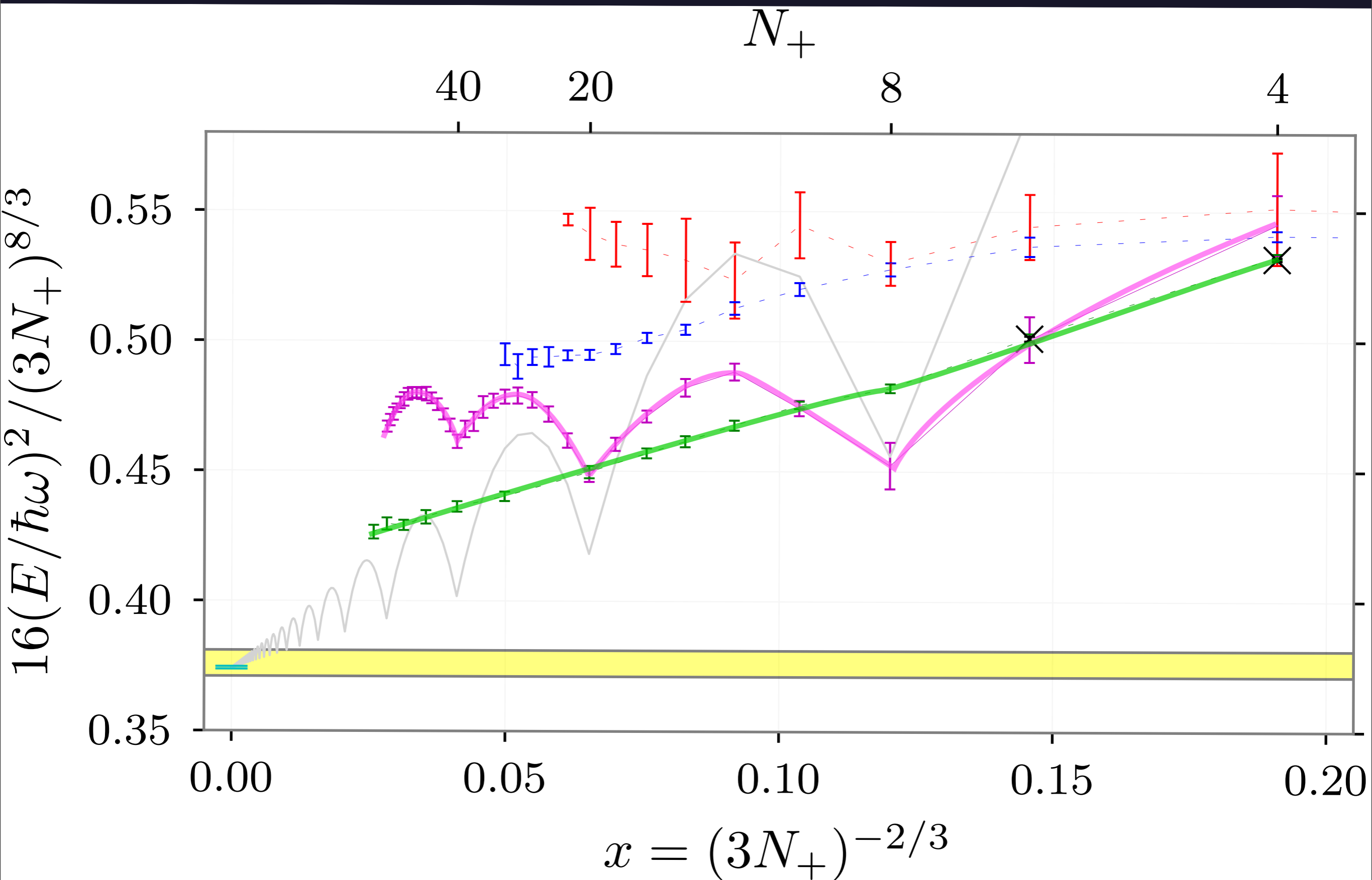
# QMC Disagreements



Variational QMC  
bound (green) not  
consistent with QMC  
results

Still need resolution:  
Are there shell effects?

Blume and Daily 2011;  
Endres, Kaplan, Lee, Nicholson 2011;  
Forbes, Gandalfi, Gezerlis 2012; Forbes 2013

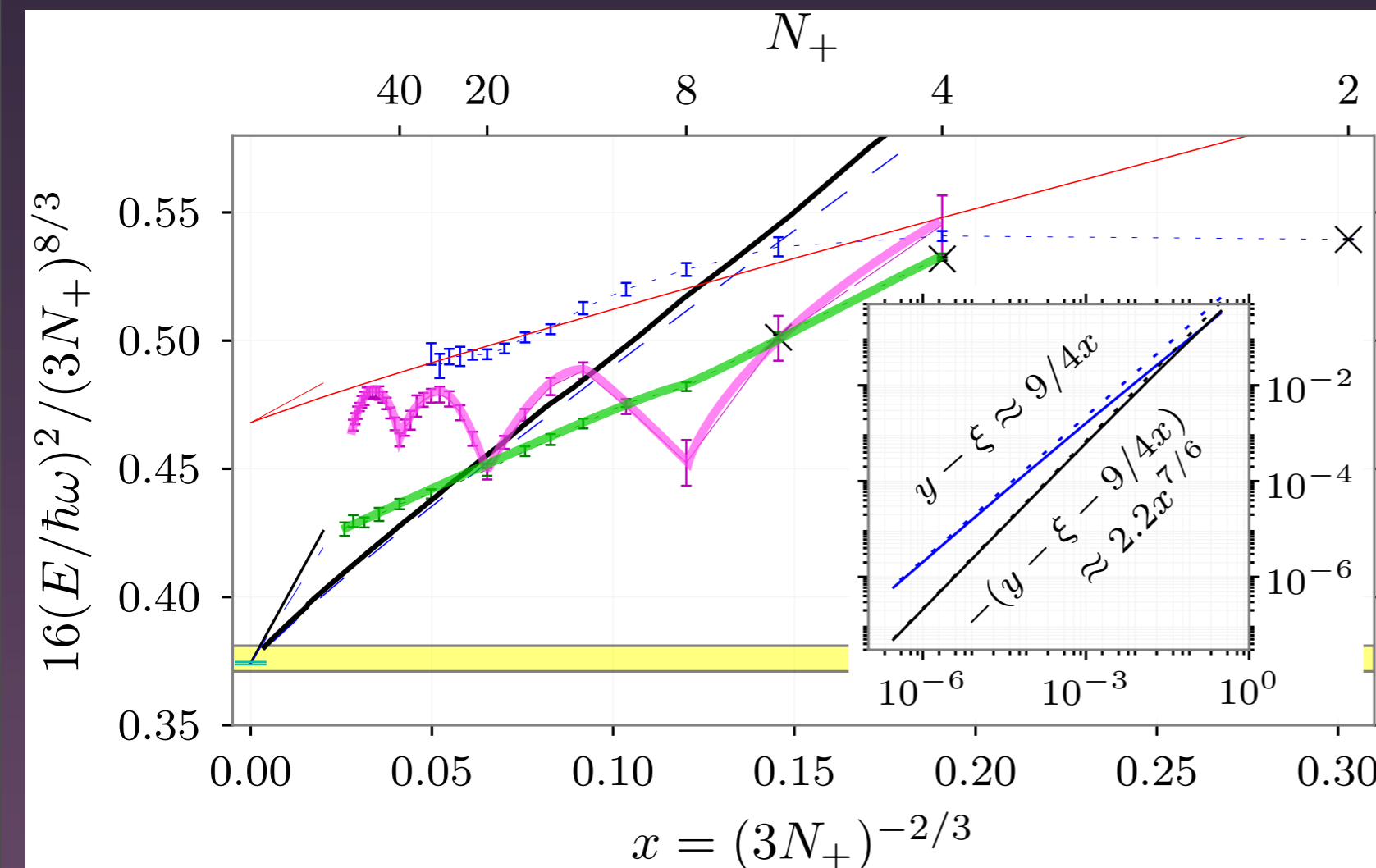


# Thermodynamic Limit

$$E(N_+) = \frac{\sqrt{\xi}}{4} \hbar \omega \left[ \overbrace{(3N_+)^{4/3}}^{\text{LDA}} - \frac{c_x}{6\xi} (3N_+)^{2/3} + O(N_+^{5/9}) \right],$$

$$\frac{16E^2}{\xi \hbar^2 \omega^2 (3N_+)^{8/3}} = \xi + c_x x + O(x^{7/6}), \quad x = \frac{1}{(3N_+)^{2/3}}$$

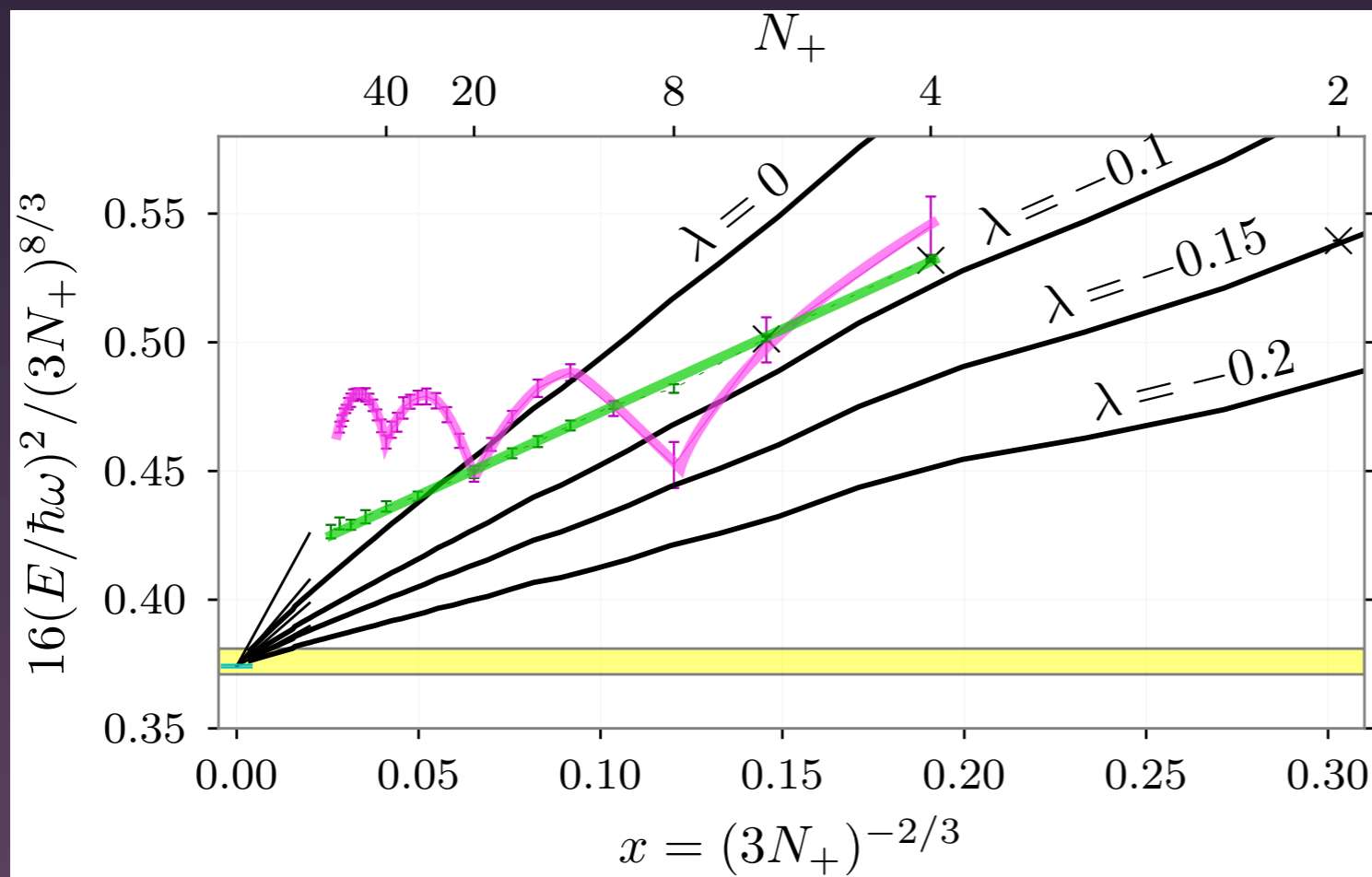
- Thermodynamic limit is far away!
- Hard to see asymptotic behaviour ( $N \sim 10^8$ )
- Validity of LDA?



Forbes 2013

# Gradient Corrections?

$$\mathcal{E}(n, \tau, v) = \left( \alpha \frac{\tau}{m} + g v^\dagger v \right) + \beta \mathcal{E}_{FG}(n) + \frac{\lambda}{8m} \frac{(\nabla n)^2}{n}$$

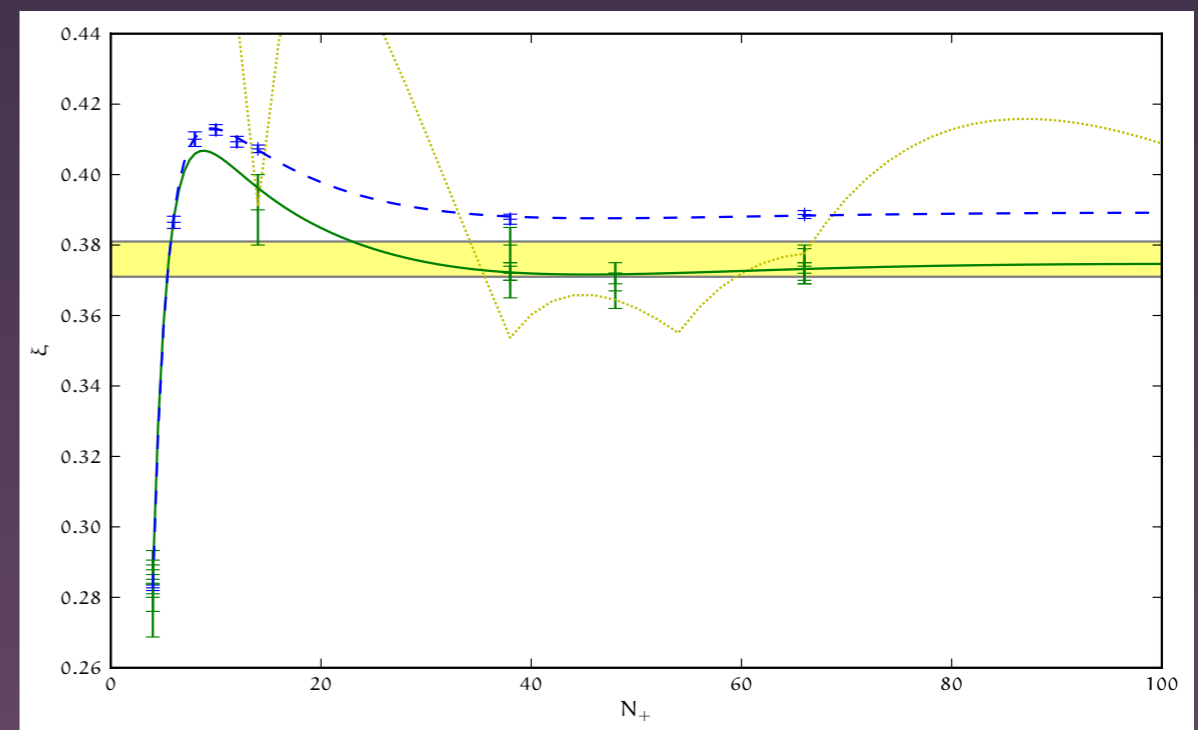
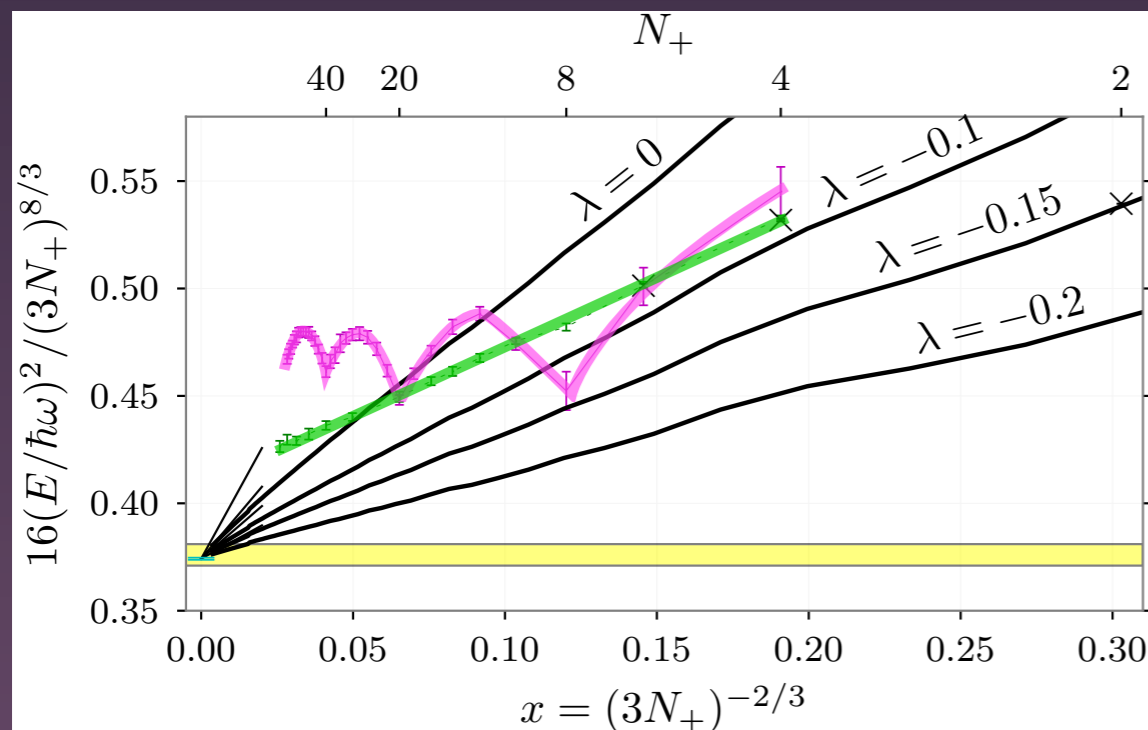


- Negative!
- $c_\chi = 1.5(3)$
- Only LO gradient affects  $c_\chi$
- Still a “small” effect ( $\sim 10\%$ )

# SLDA Summary

$$\mathcal{E}(n, \tau, \nu) = \left( \alpha \frac{\tau}{m} + g \nu^\dagger \nu \right) + \beta \mathcal{E}_{FG}(n) + \frac{\lambda}{8m} \frac{(\nabla n)^2}{n}$$

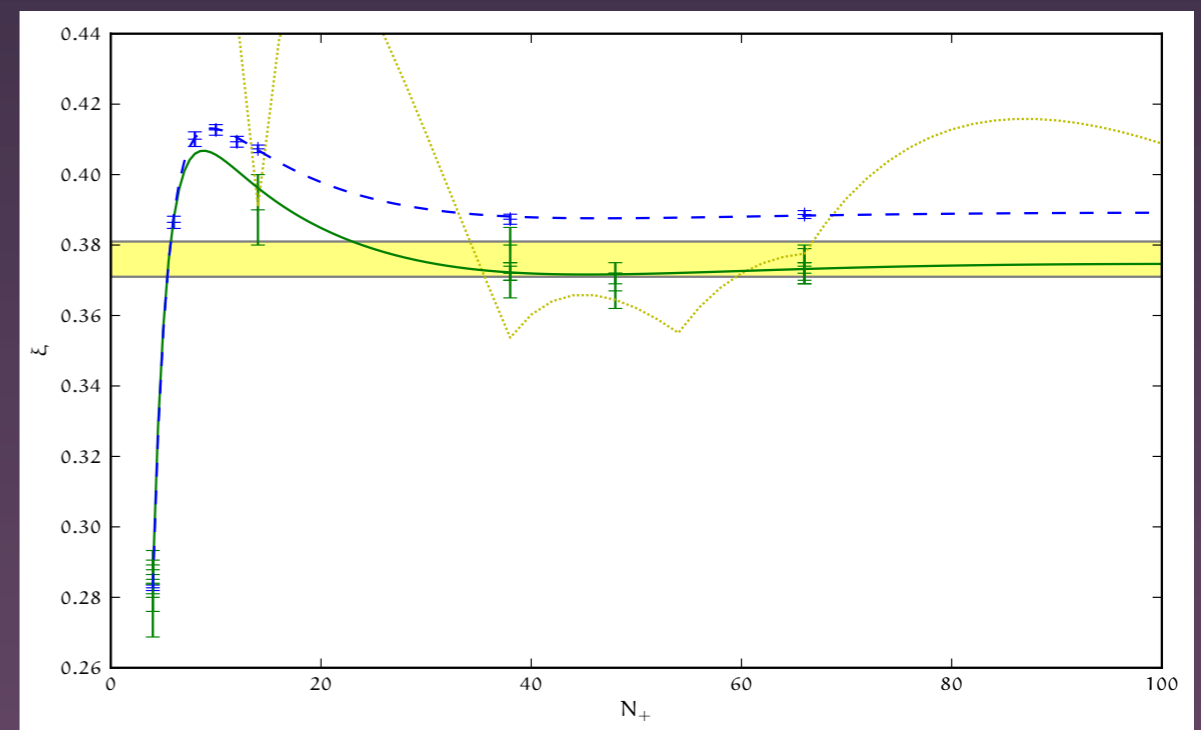
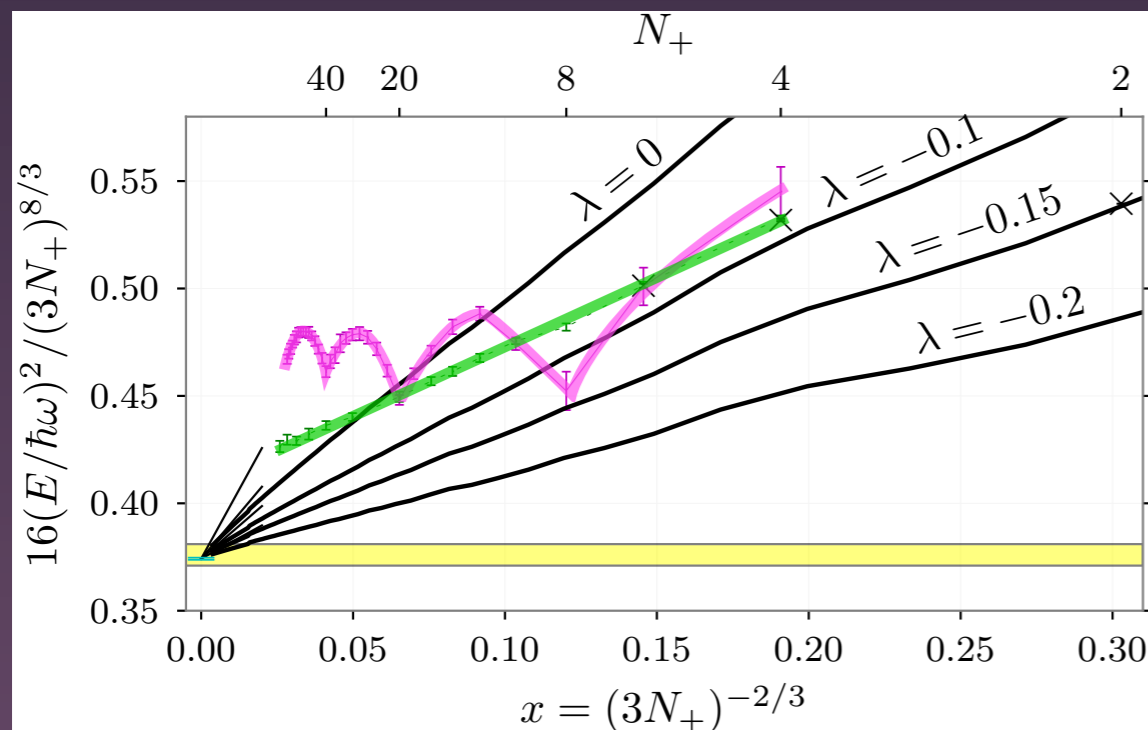
- Works remarkably well



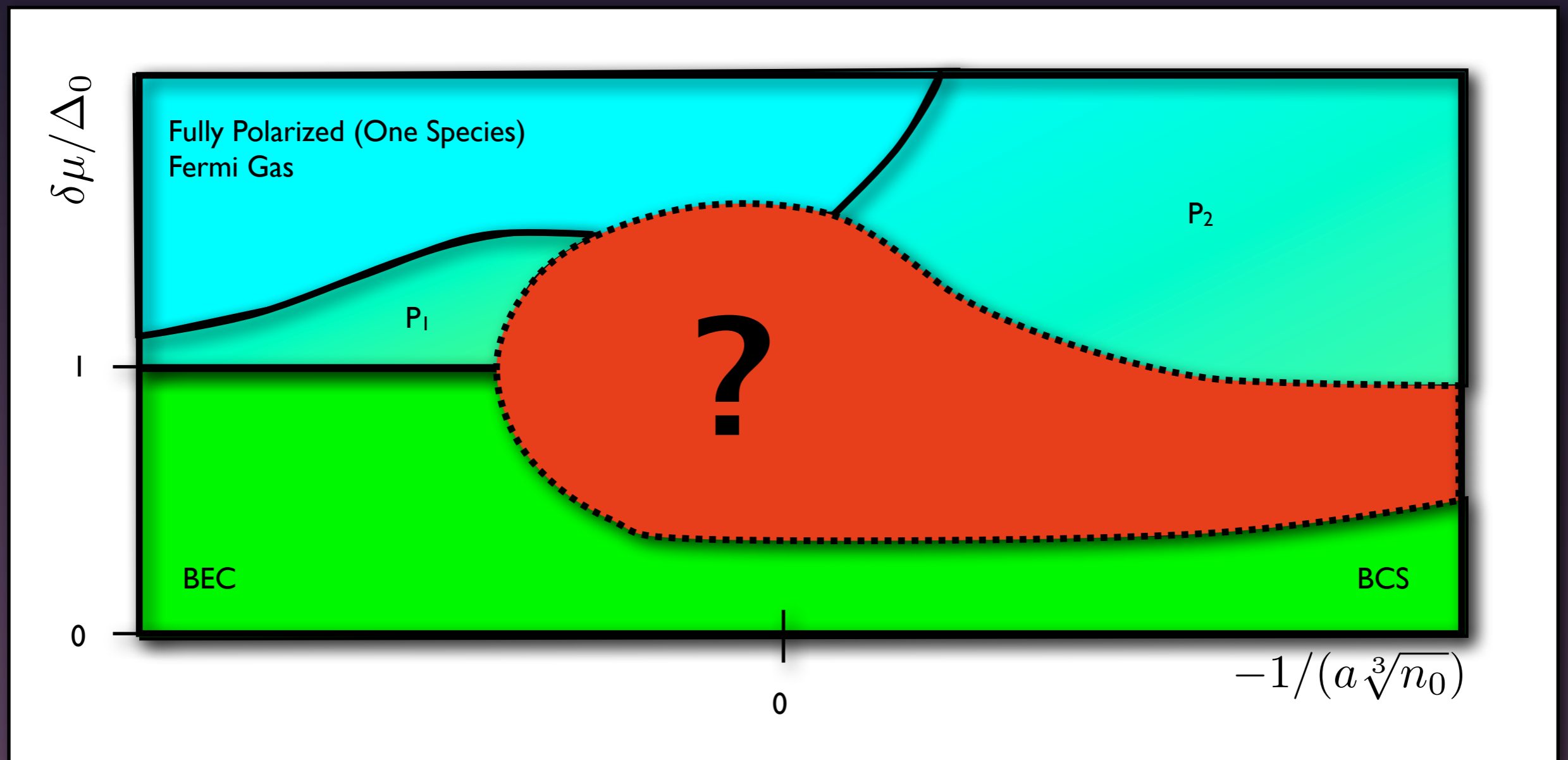
# SLDA Summary

$$\mathcal{E}(n, \tau, v) = \left( \alpha \frac{\tau}{m} + g v^\dagger v \right) + \beta \mathcal{E}_{FG}(n) + \frac{\lambda}{8m} \frac{(\nabla n)^2}{n}$$

- Extrapolation: small to large systems (IR convergence)

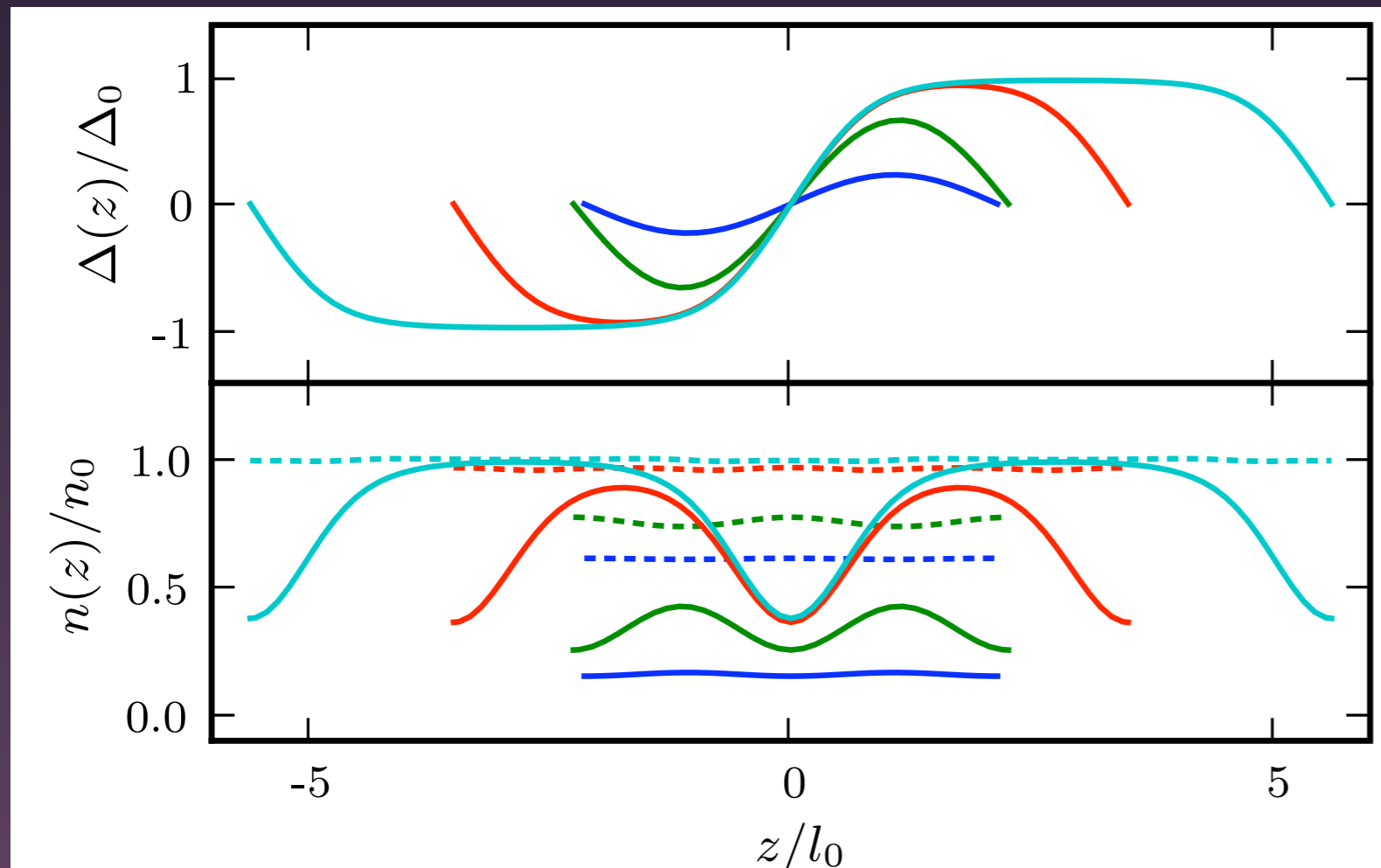


# Phase Structure



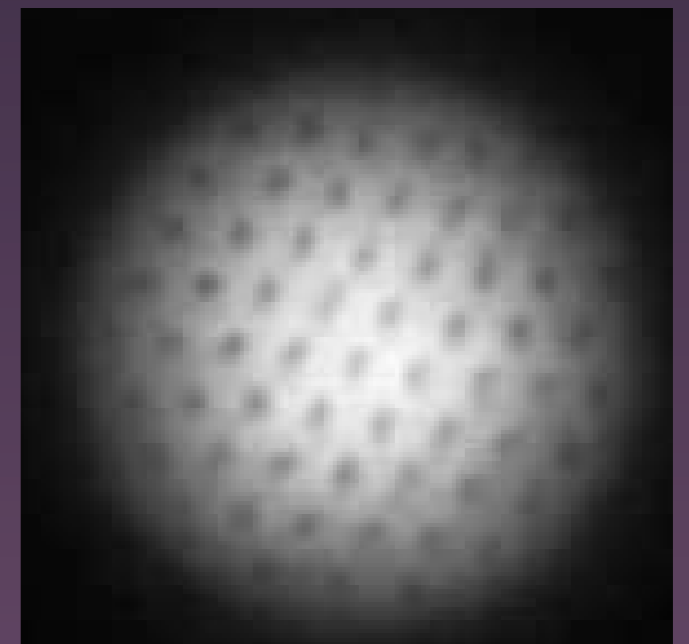
Based on D.T. Son and M. Stephanov (2005)  
P-wave states by A.Bulgac, M.M.Forbes, A.Schwenk PRL 97 020402 (2006)

# ASLDA DFT predicts (FF)LO at Unitarity: Supersolid!



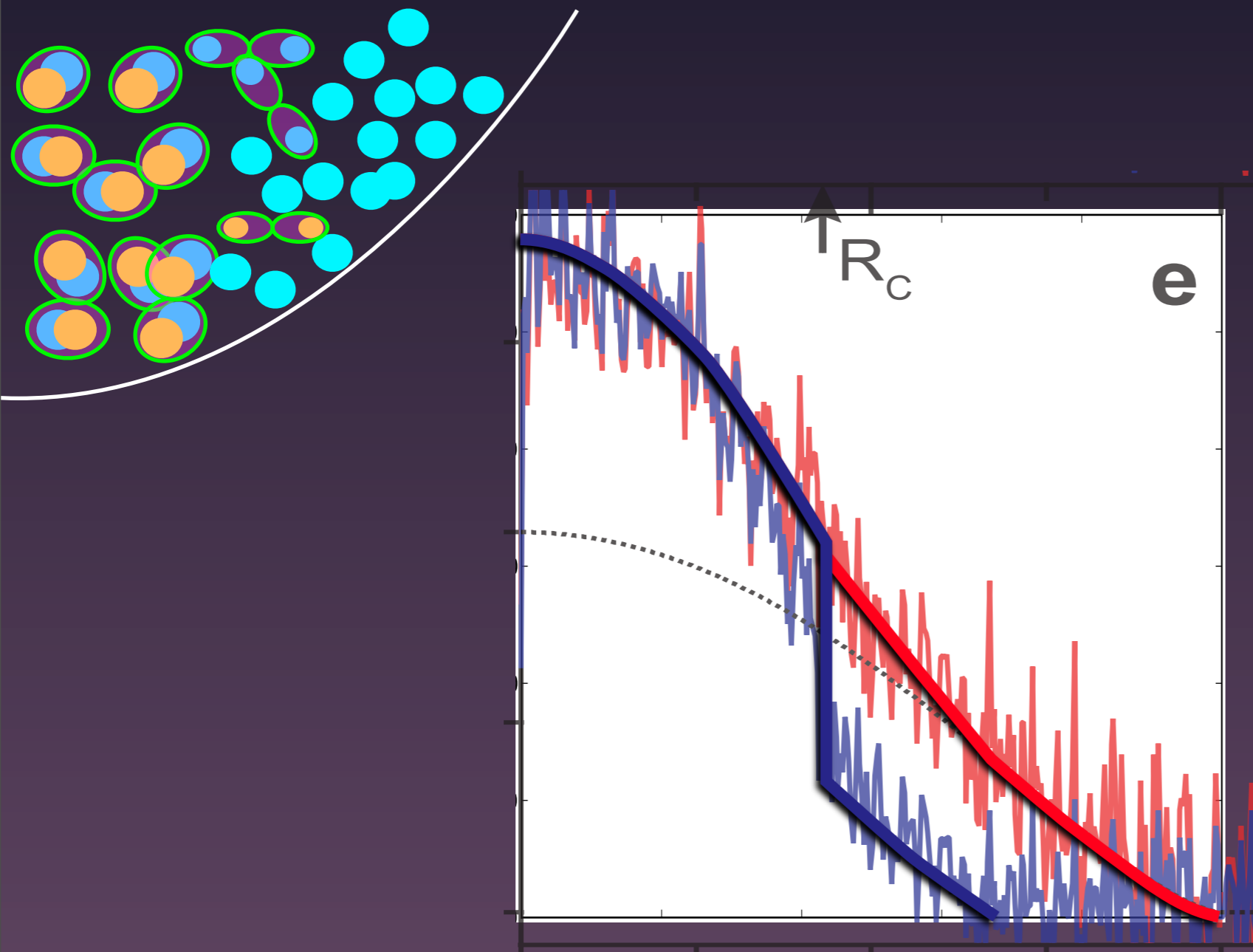
Large density contrast  
(factor of 2)

Similar to contrast of  
vortex core



Bulgac and Forbes PRL 101 (2008) 215301

# Observations: Nothing?



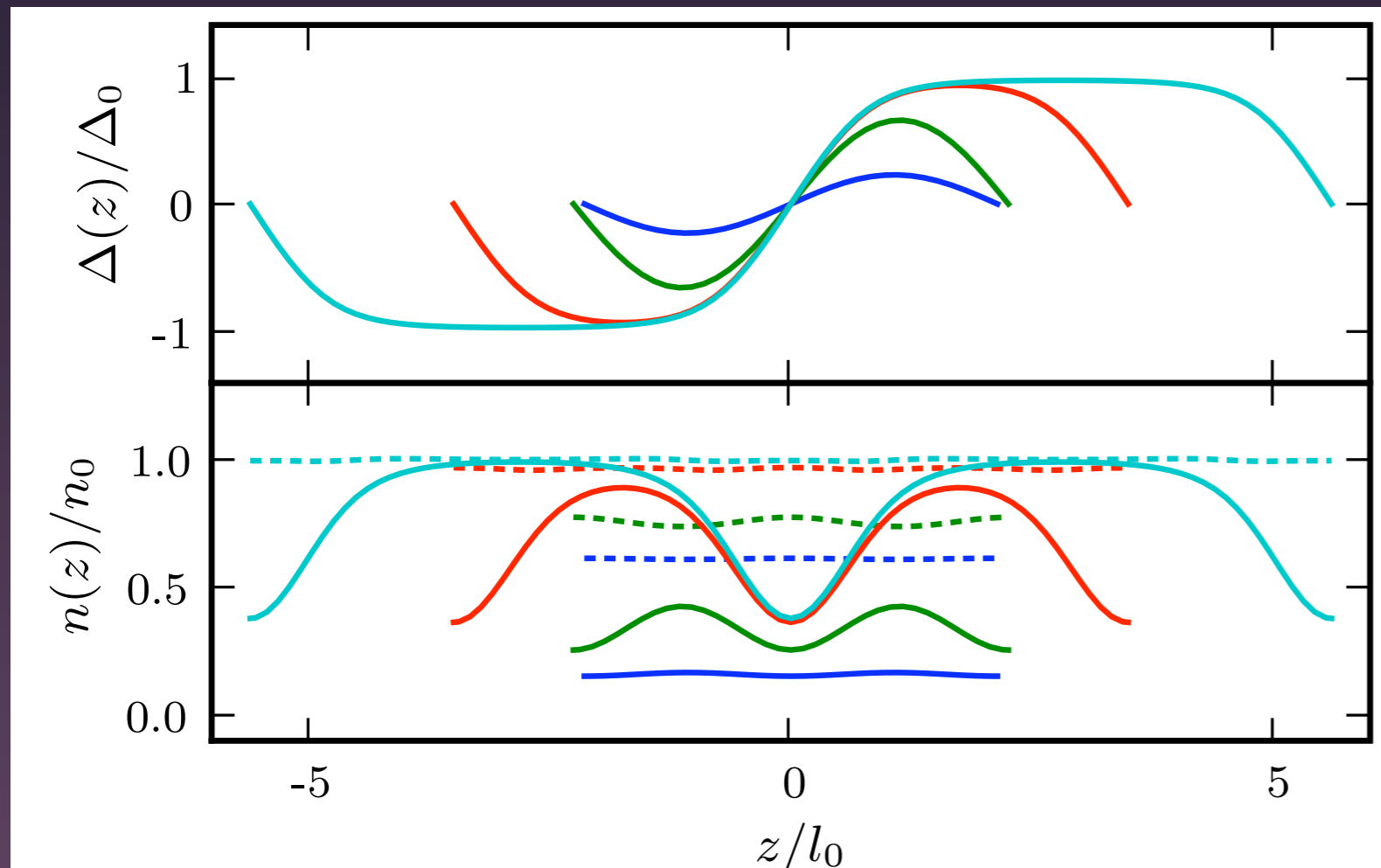
Paired core

Polarized wings

Maybe there are no  
interesting polarized  
superfluid phases?

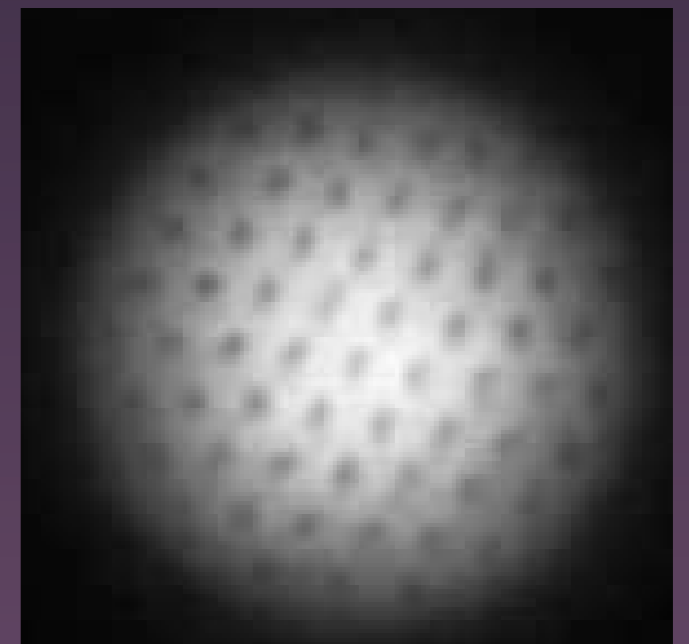
MIT Experimental data from Shin et. al (2008)

# DFT predicts (FF)LO at Unitarity: Supersolid!



Large density contrast  
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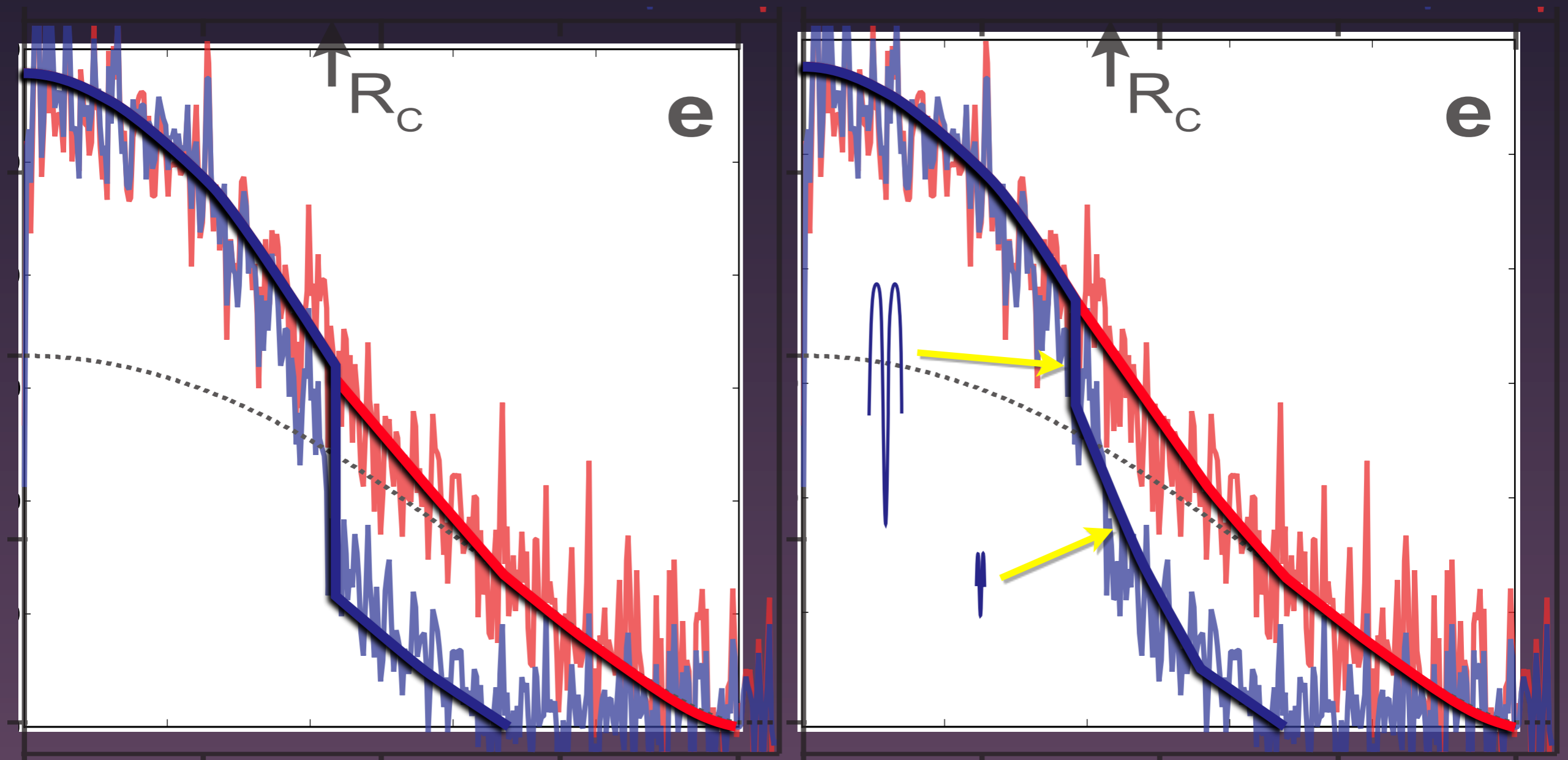
Similar to contrast of  
vortex core



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?

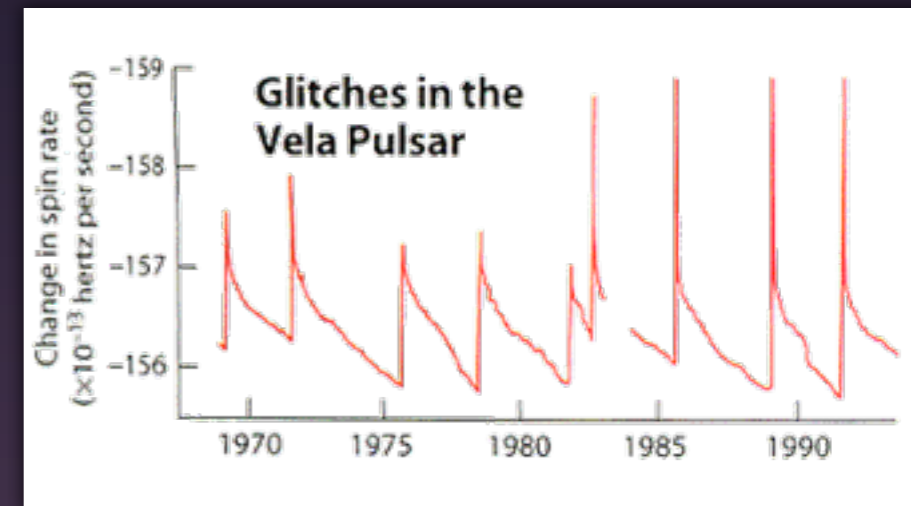
- It is not there:
  - Other homogenous phases might be better.
  - $T$  might be too high (fluctuations kill 1D FFLO).
  - Trap frustrates formation (traps are not flat enough).
- It is not seen:
  - Noise washes out signature.
  - Small physical volume for FFLO.
- Need a nice flat trap: Large physical volume of FFLO

# Dynamics

# Application: Vortex Pinning

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

Anderson and Itoh (1975)



Pulsar Astronomy by Andrew G. Lyne and Francis

- 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

# TDDFT (TDSLDA)

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

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

# GPE model for UFG

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

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

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

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

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

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

# GPE model = Extended Thomas Fermi (ETF)

$$E[\Psi] = \int d^3\vec{x} \left( \frac{|\nabla \sqrt{\rho_F}|^2}{8m_F} + V_F(\vec{x})\rho_F + \xi \mathcal{E}_{FG}(\rho_F) + \frac{4\lambda - 1}{8m_F} (\nabla \sqrt{\rho_F})^2 \right)$$

- In the absence of currents (i.e. no vortices), kinetic and Weizsäcker terms behave the same  
Vortices etc. appear as kinks in  $\sqrt{\rho_F}$
- See Salasnich for a discussion

# GPE model = Extended Thomas Fermi (ETF)

$$E[\Psi] = \int d^3\vec{x} \left( \frac{|\nabla \sqrt{\rho_F}|^2}{8m_F} + V_F(\vec{x})\rho_F + \xi \mathcal{E}_{FG}(\rho_F) + \frac{4\lambda + 1}{8m_F} (\nabla \sqrt{\rho_F})^2 \right)$$

- Weizsäcker term “breaks” vortices
- (Also does not match experiment)

# GPE model for UFG

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

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

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

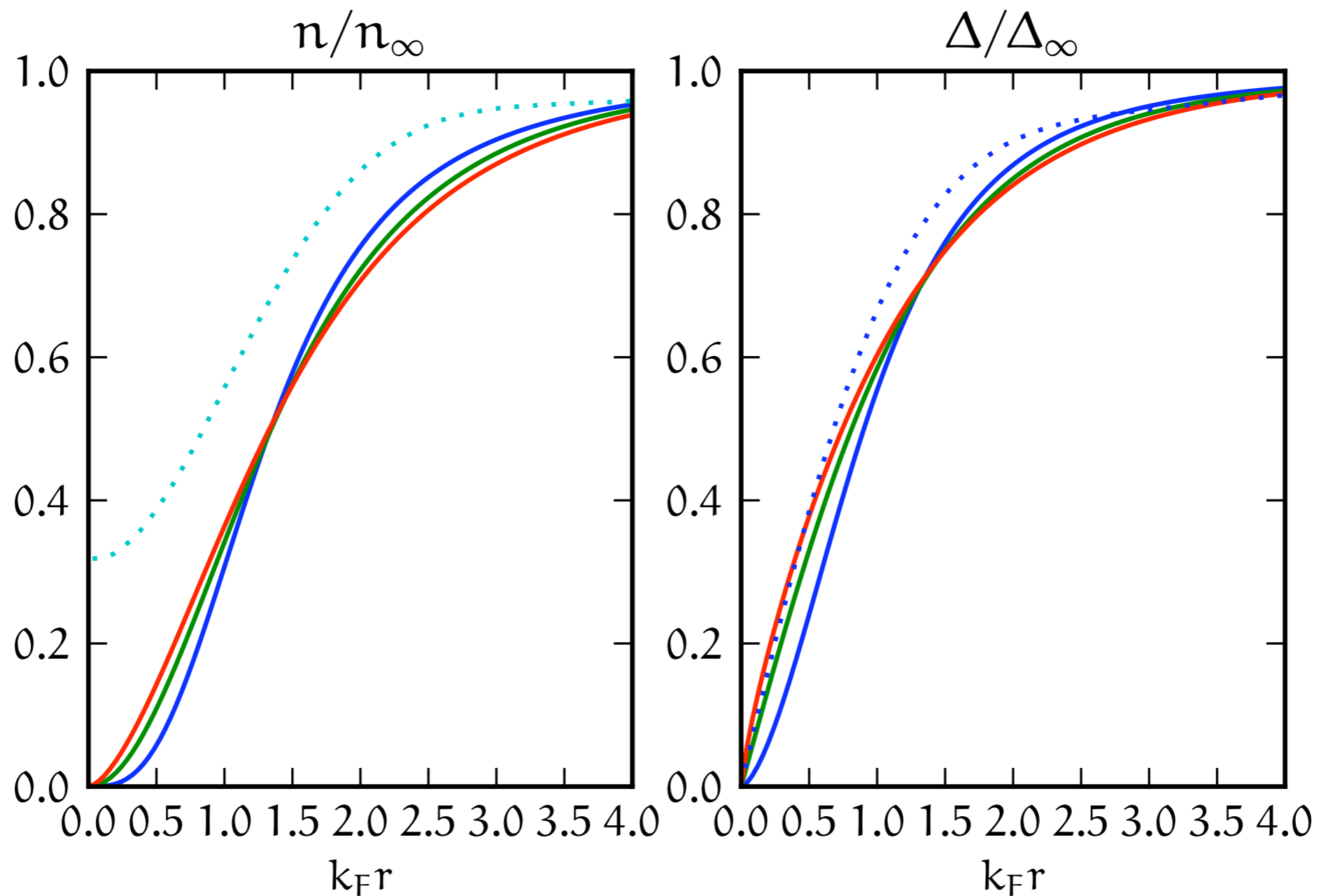
# Matching Theories: The Good

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

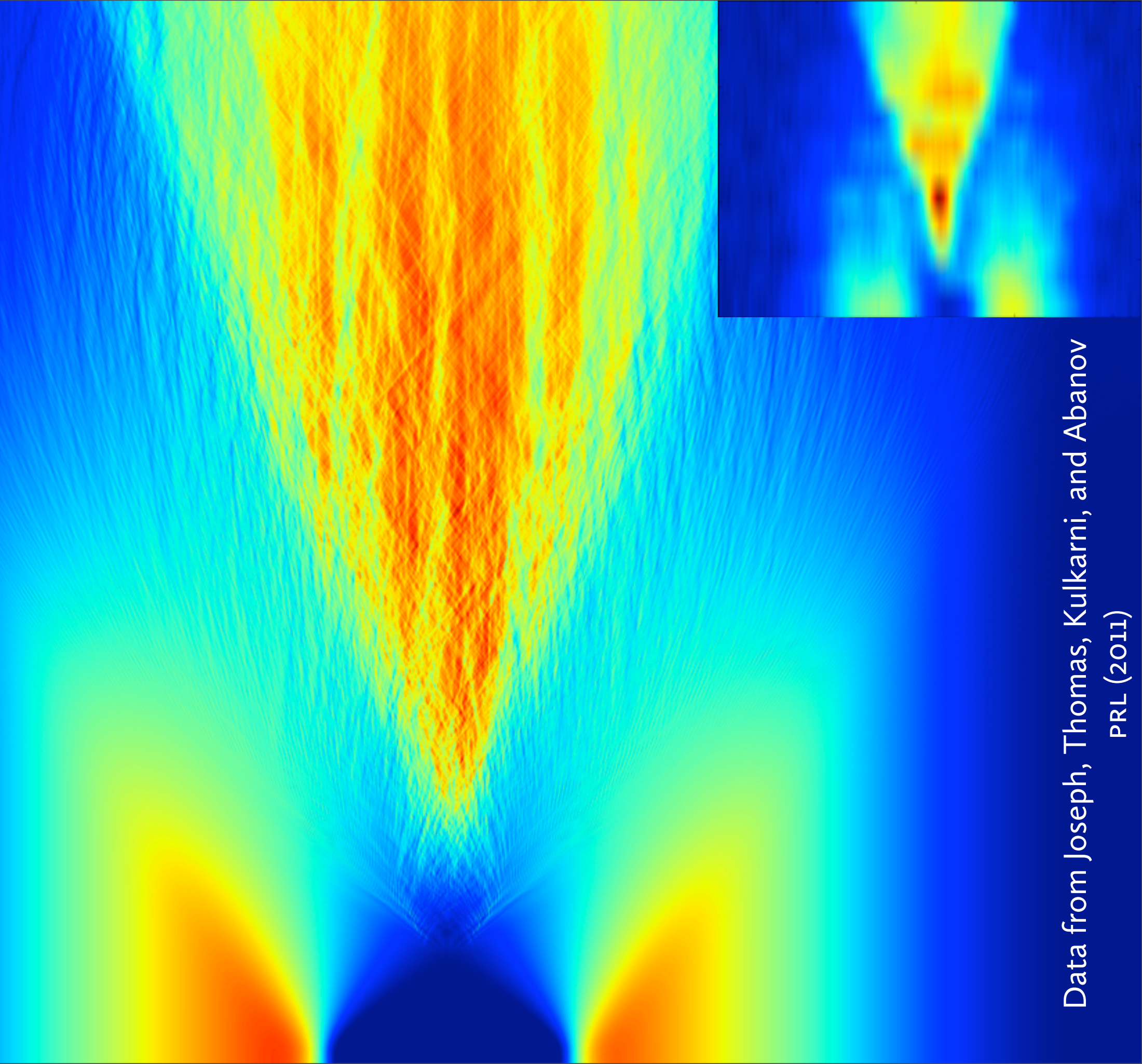
# Matching Theories: The Bad

- 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

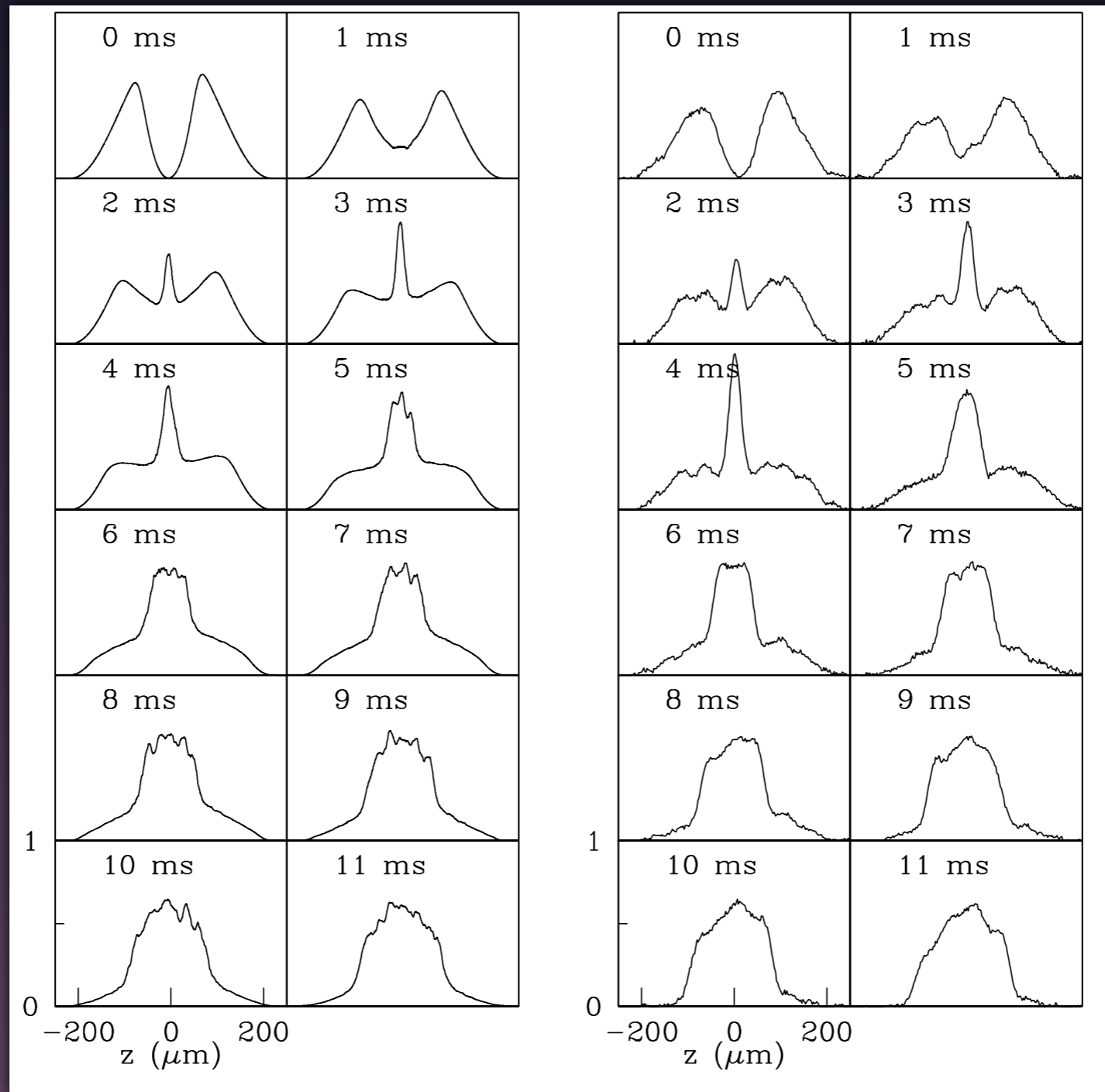


# 2D GPE simulation



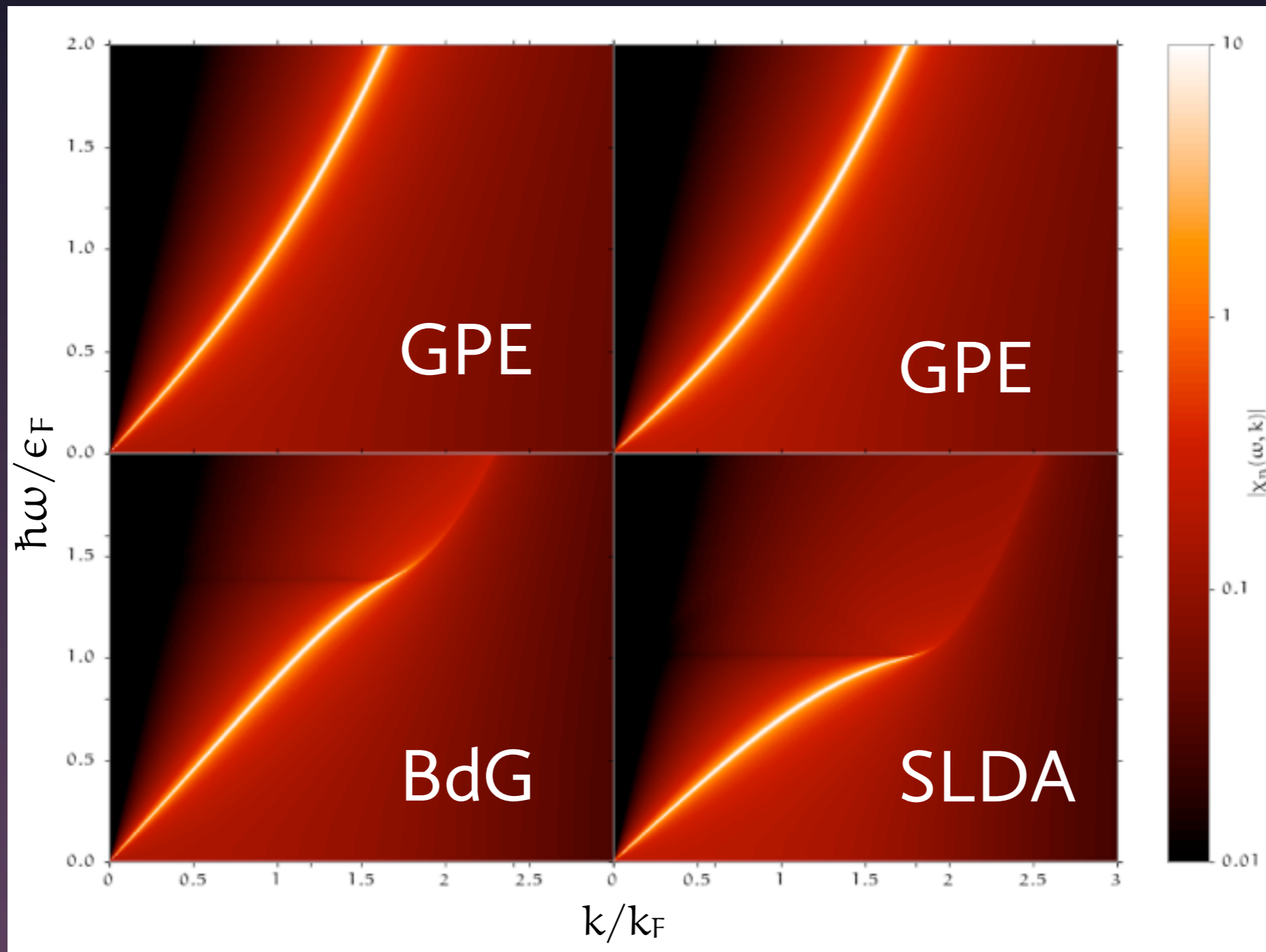
Data from Joseph, Thomas, Kulkarni, and Abanov  
PRL (2011)

# GPE vs. Experiment



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

# Linear Response

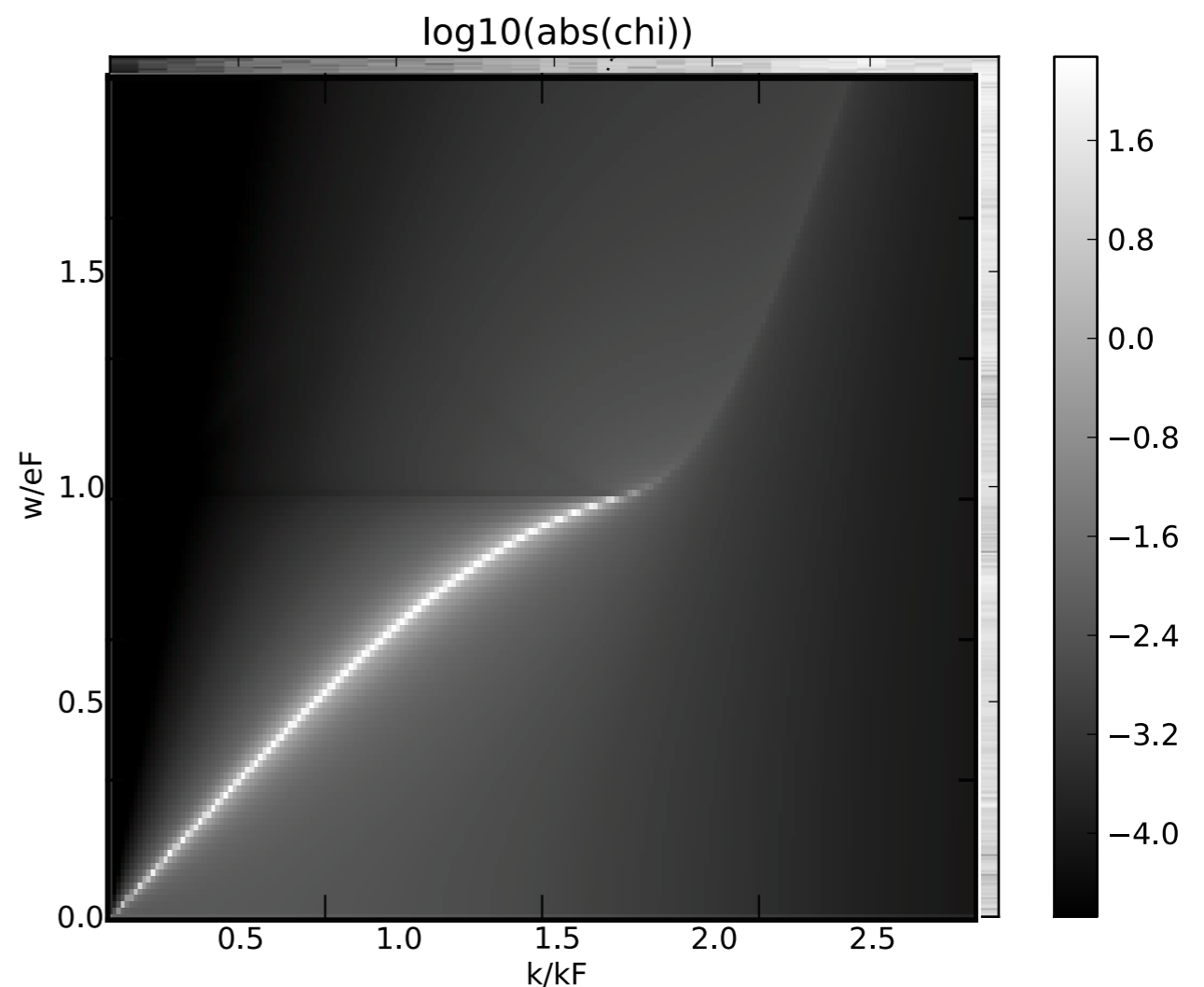
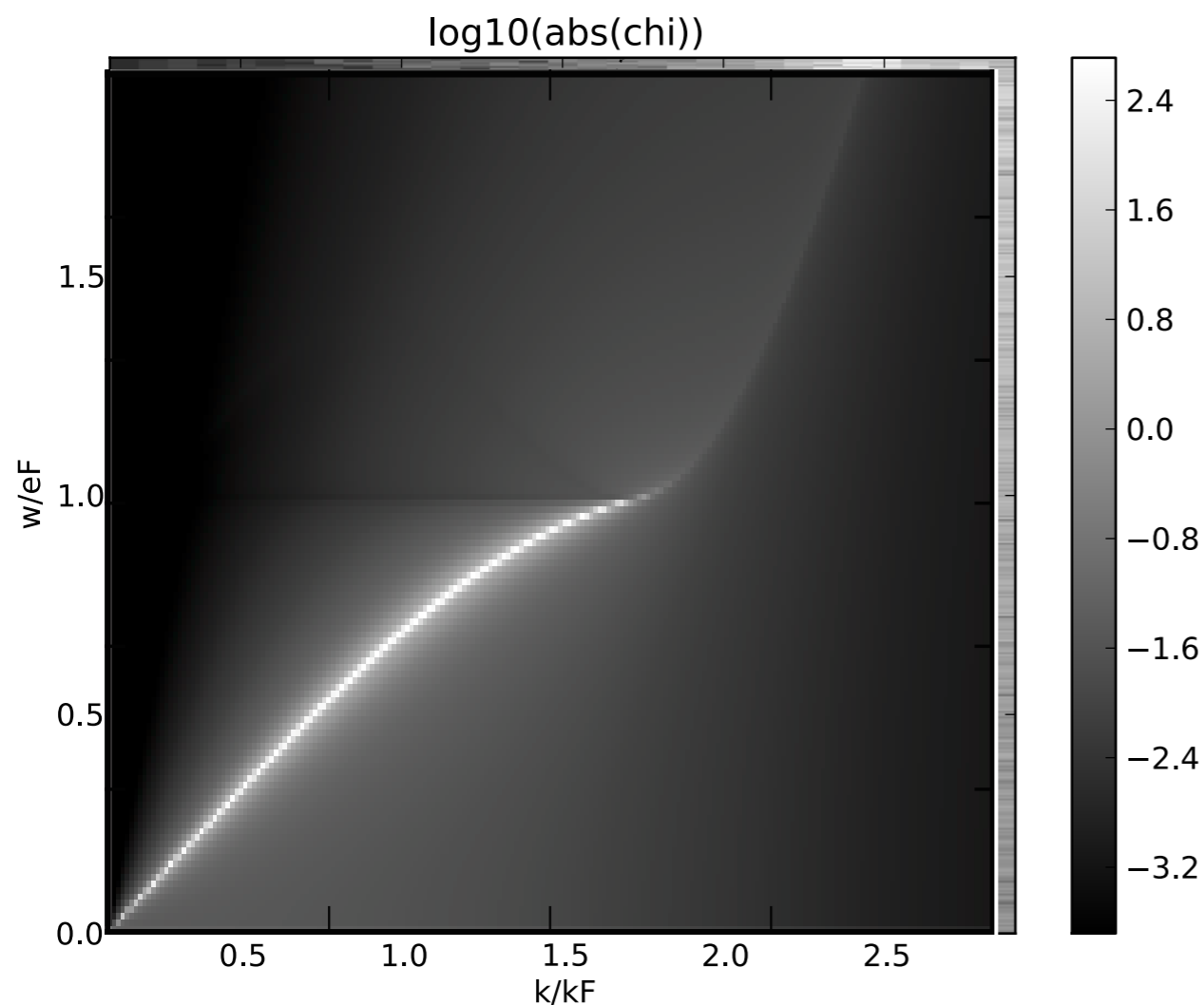


Work with Rishi Sharma (TRIUMF)

# Non-Linear Response?

$V=0.05$

$V=0.5$

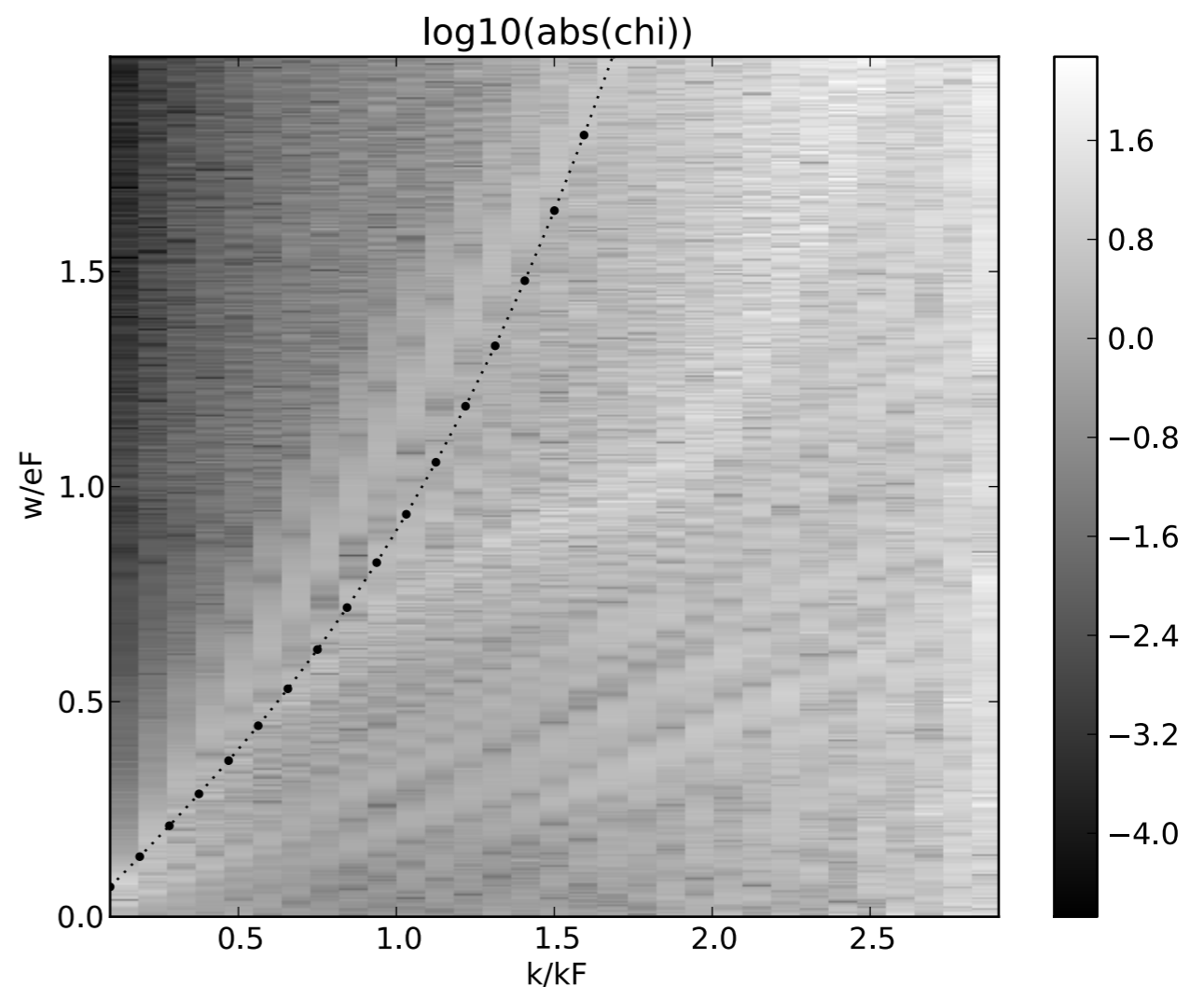
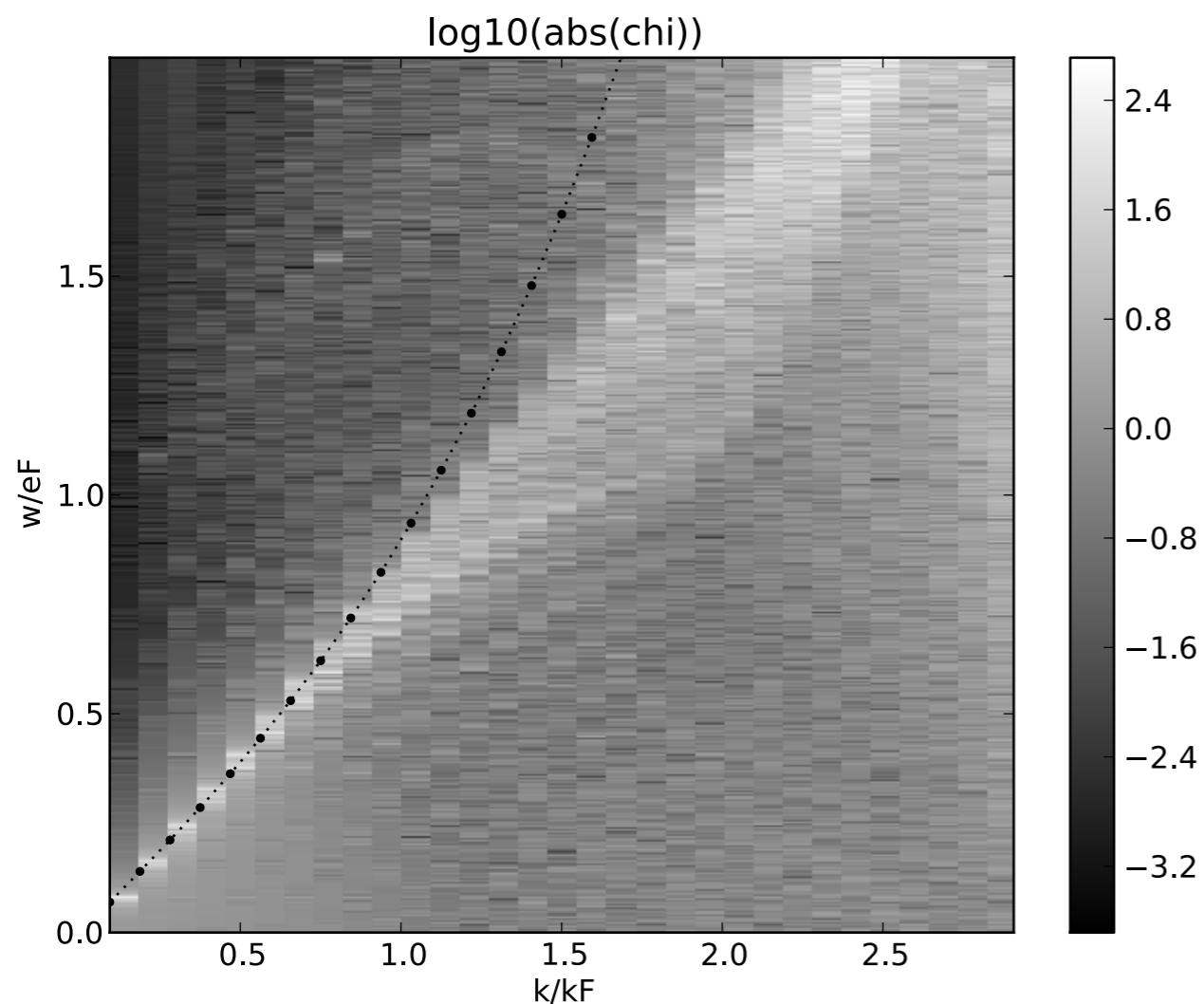


Work with Alan Luo and Rishi Sharma

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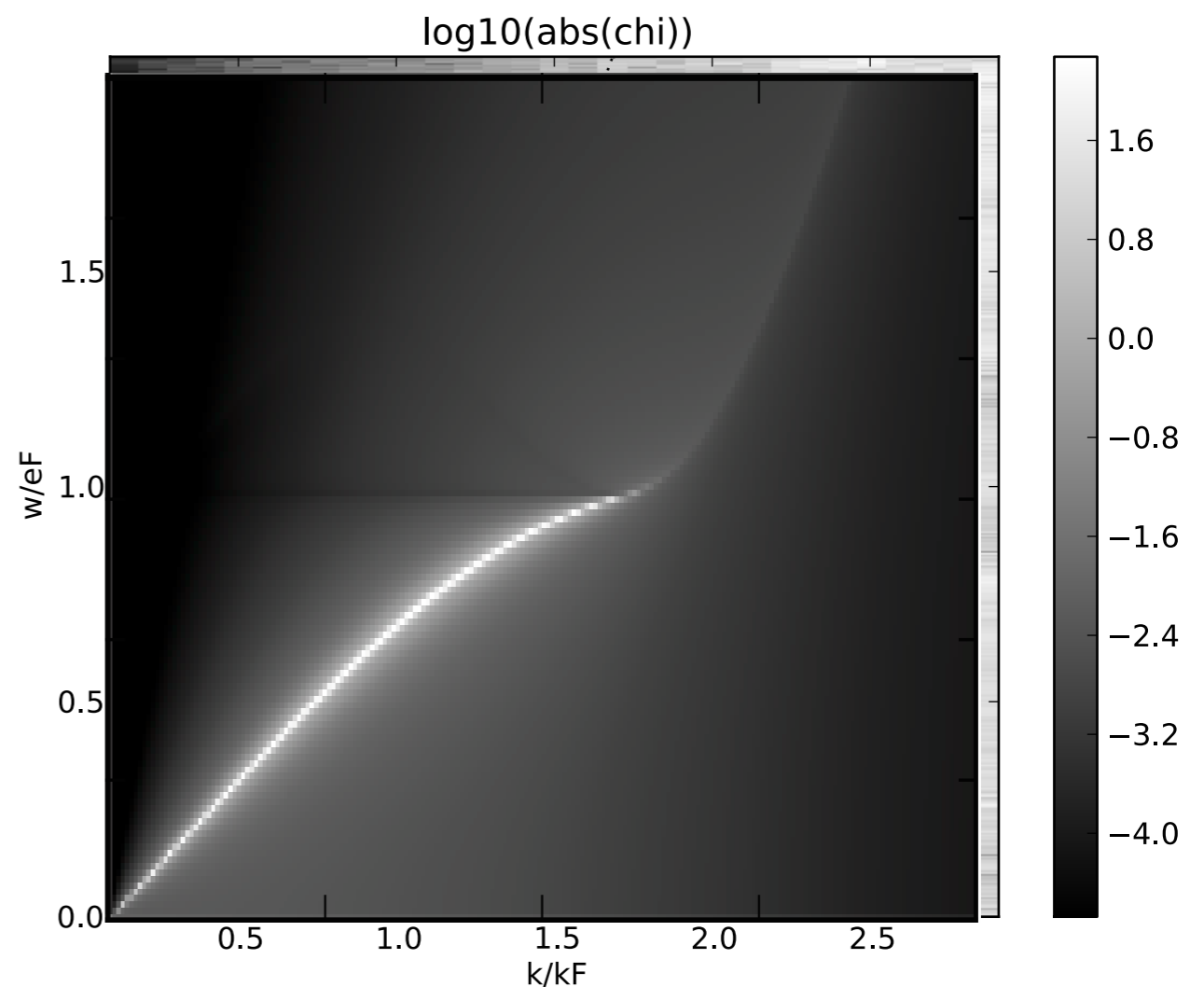
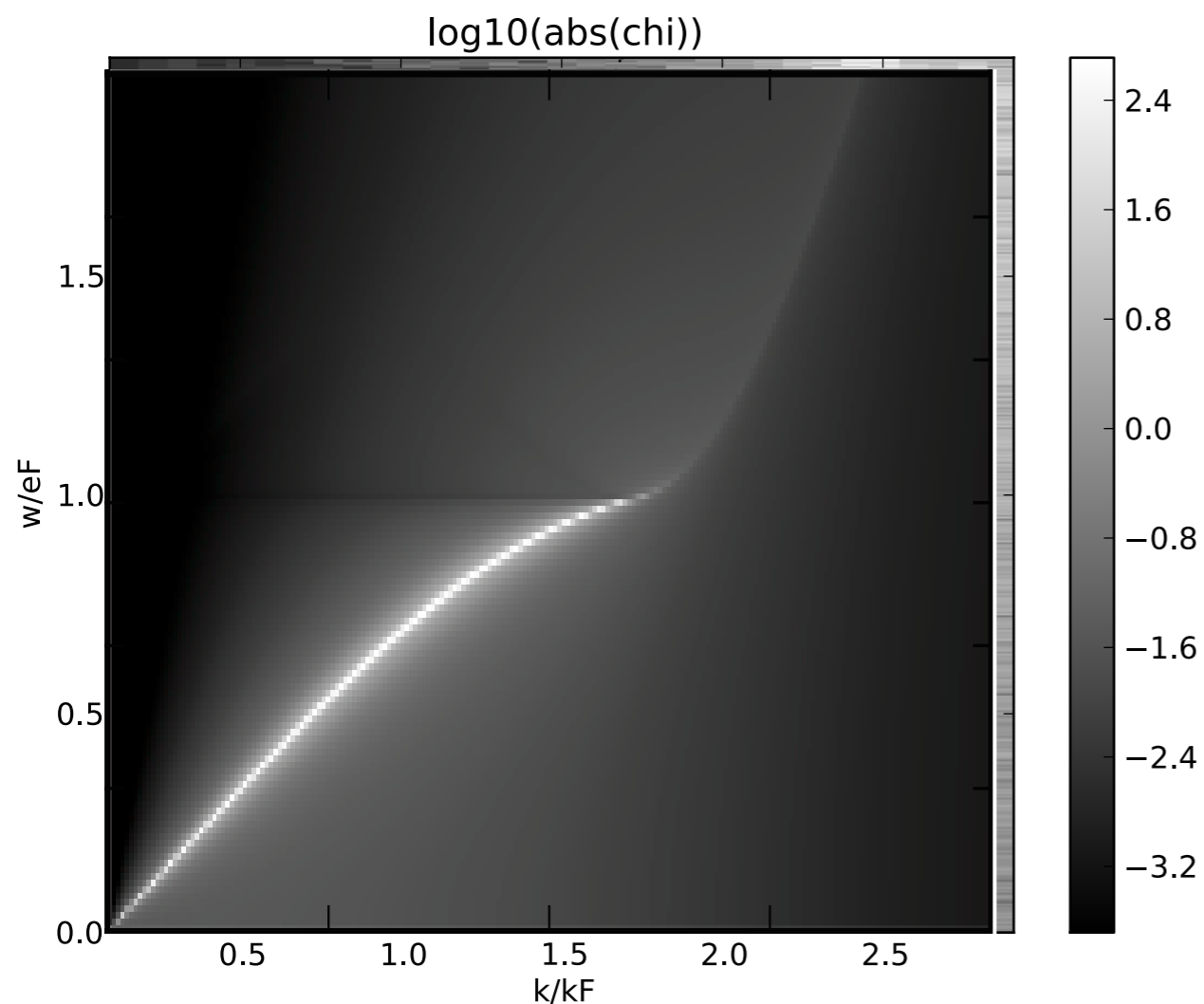


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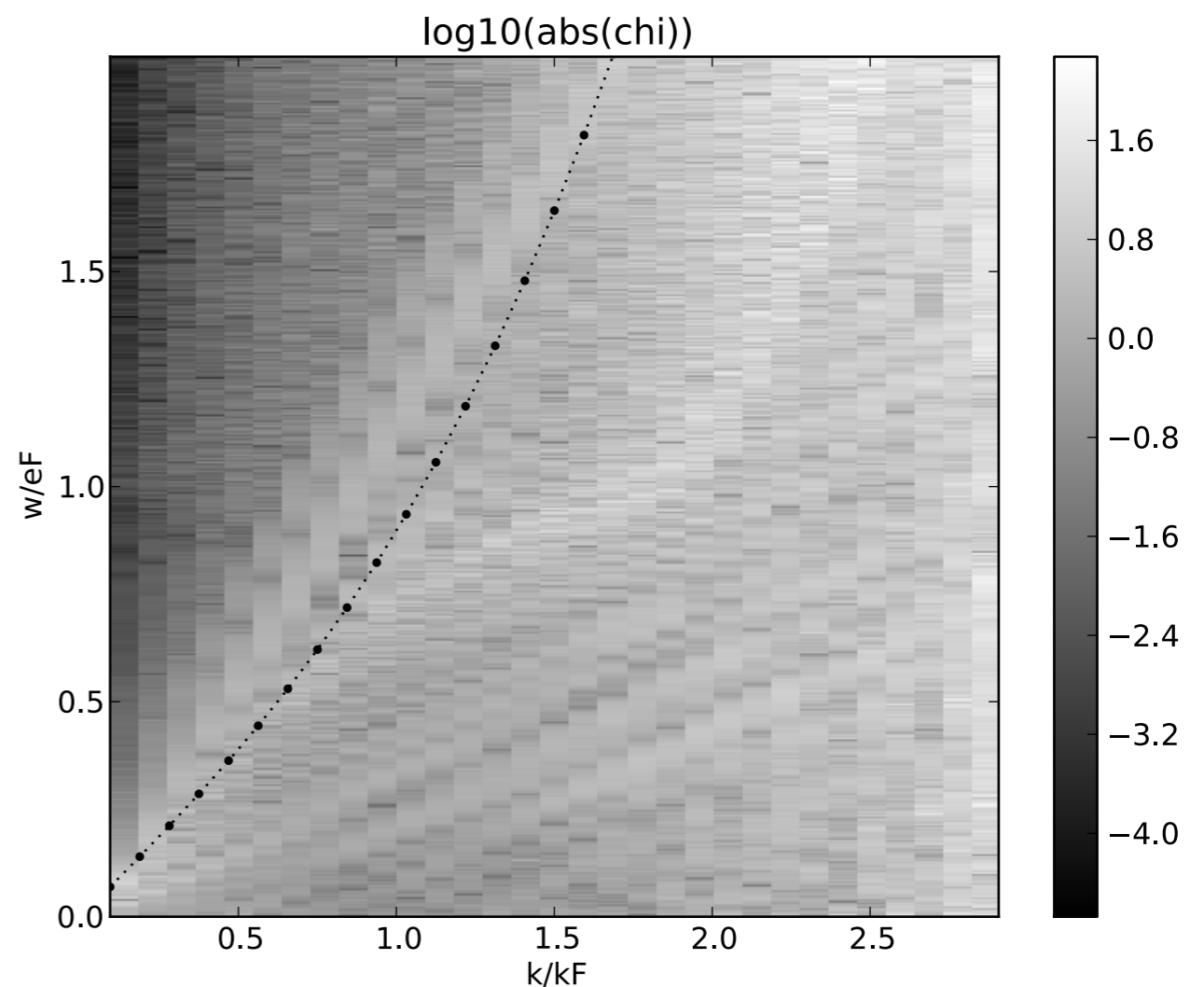
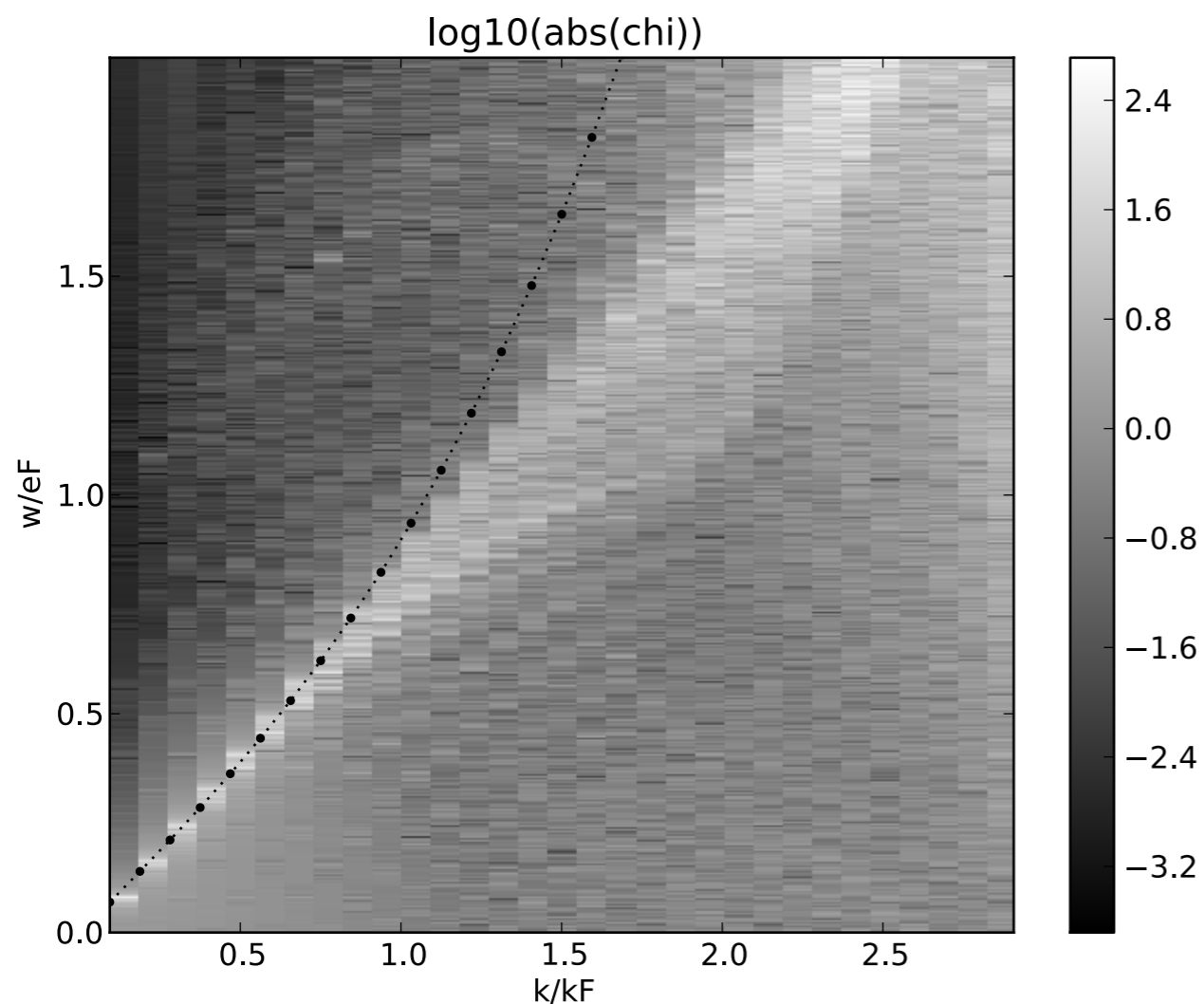


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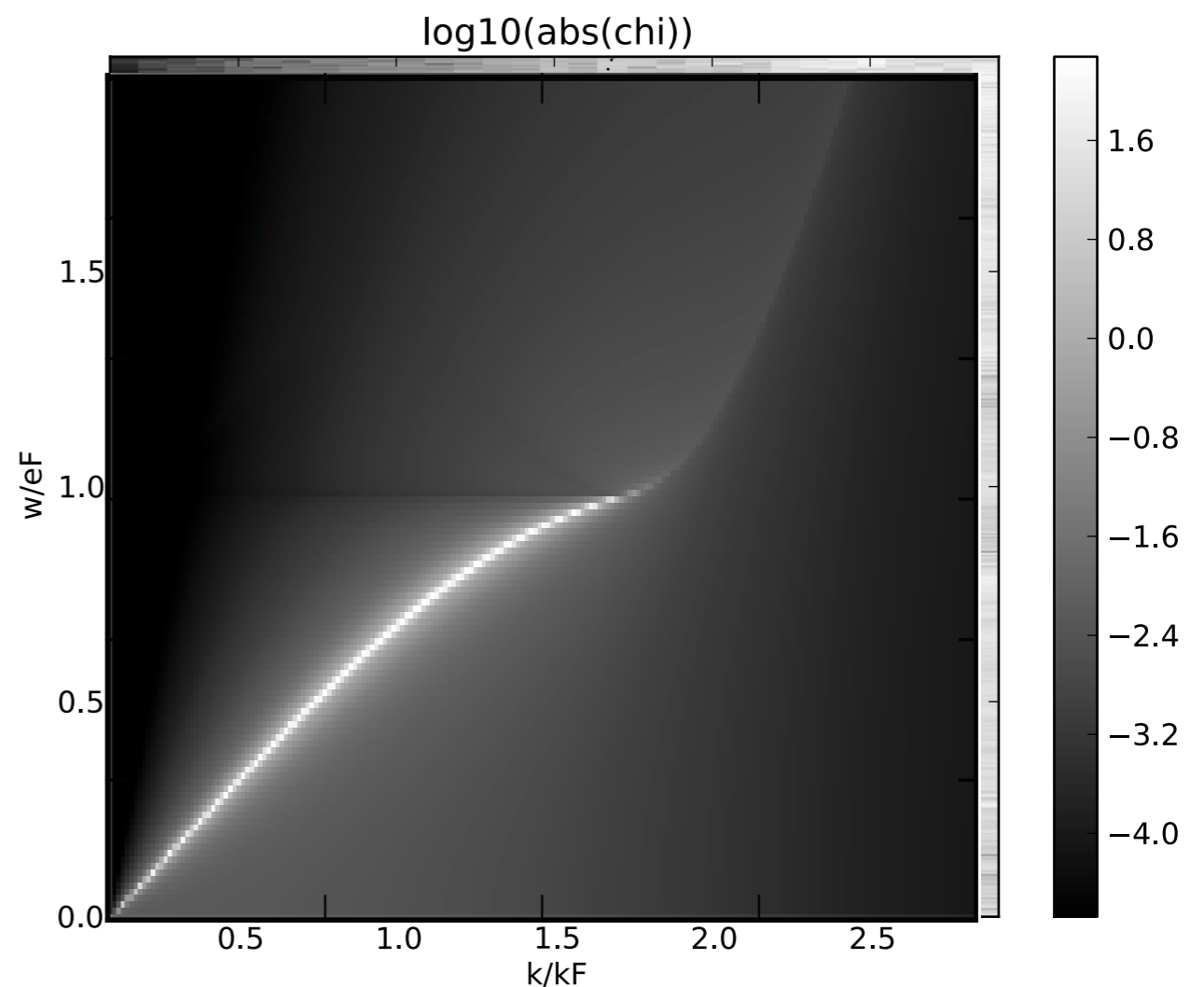
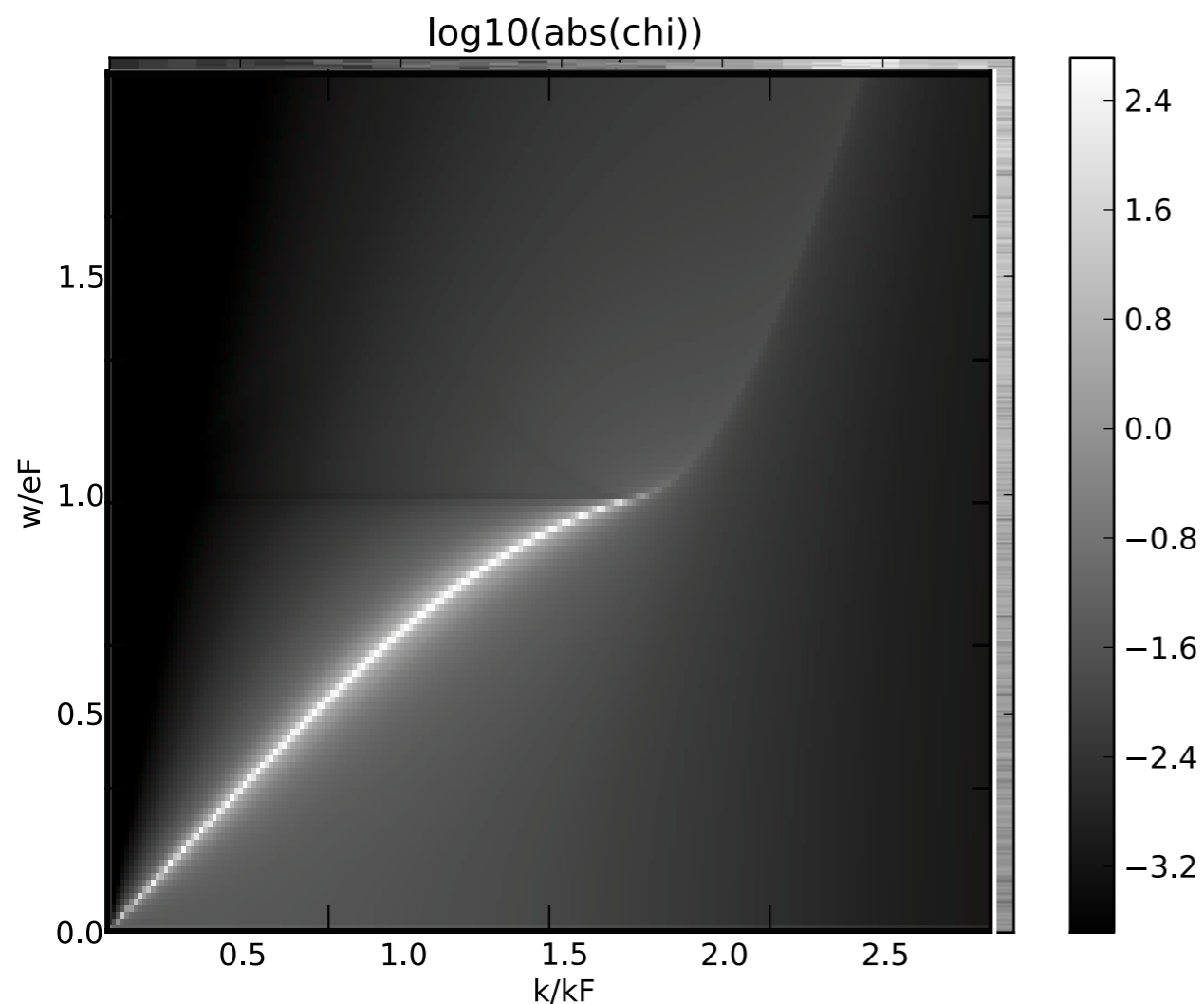


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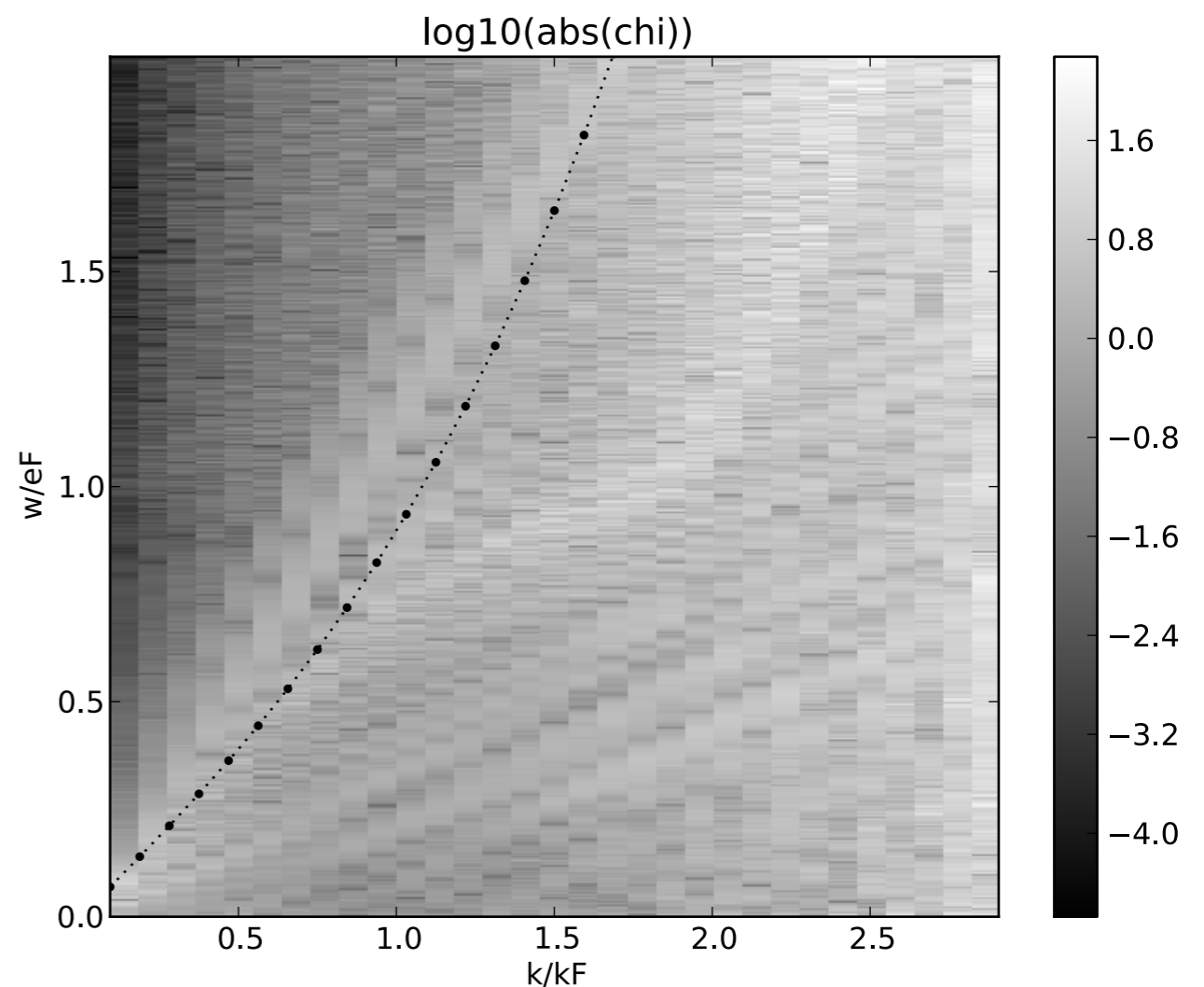
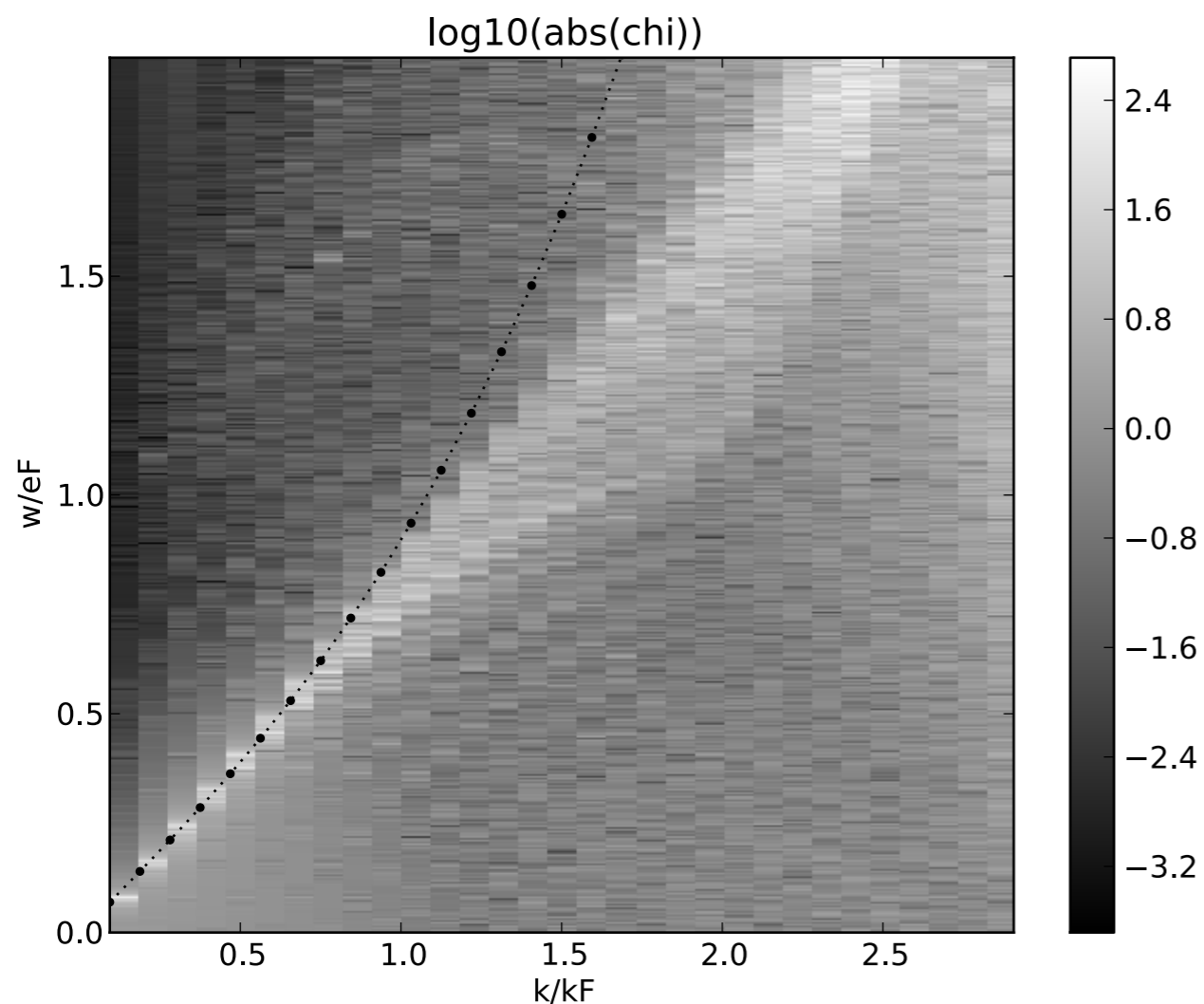


Work with Alan Luo and Rishi Sharma

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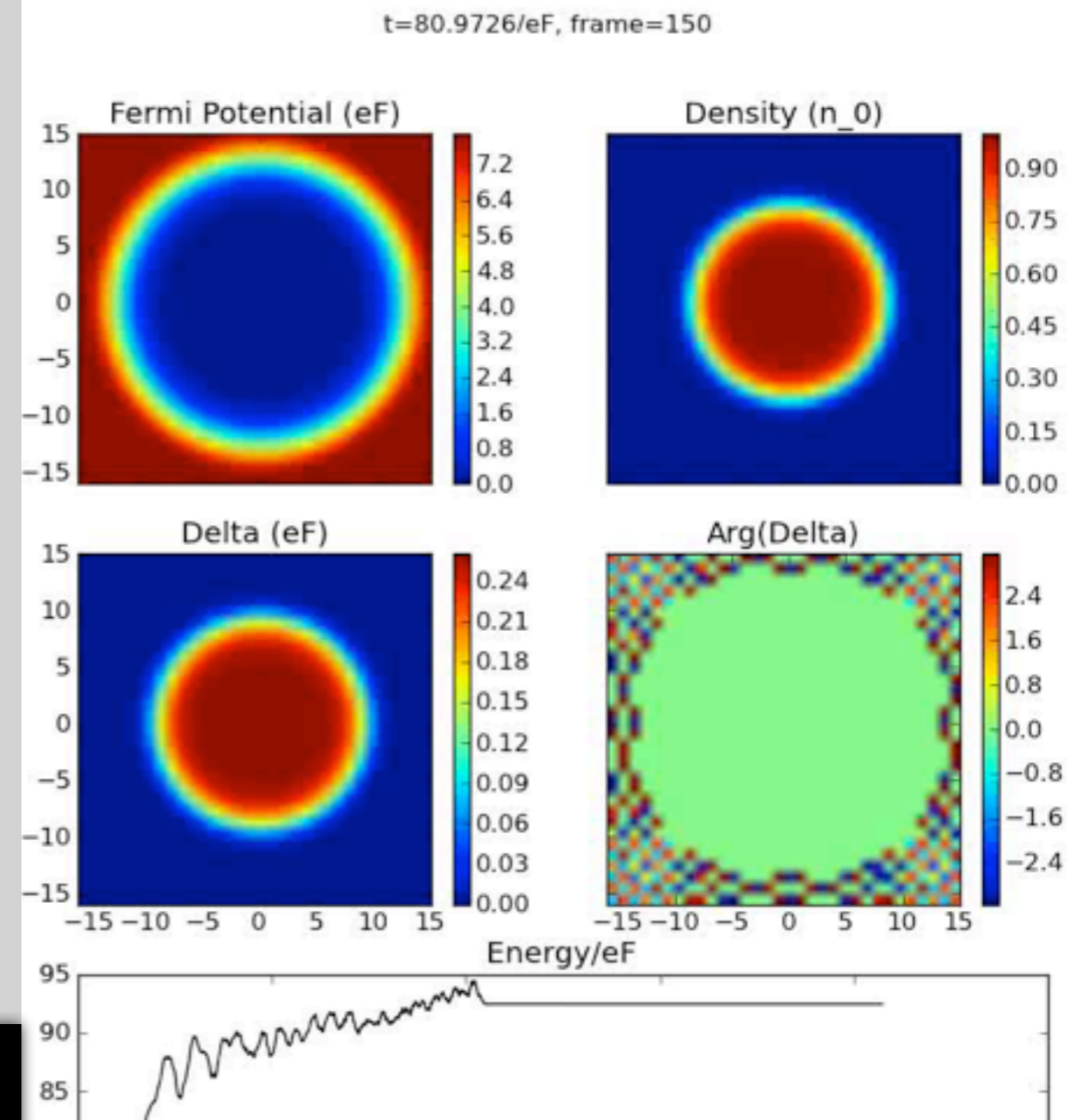
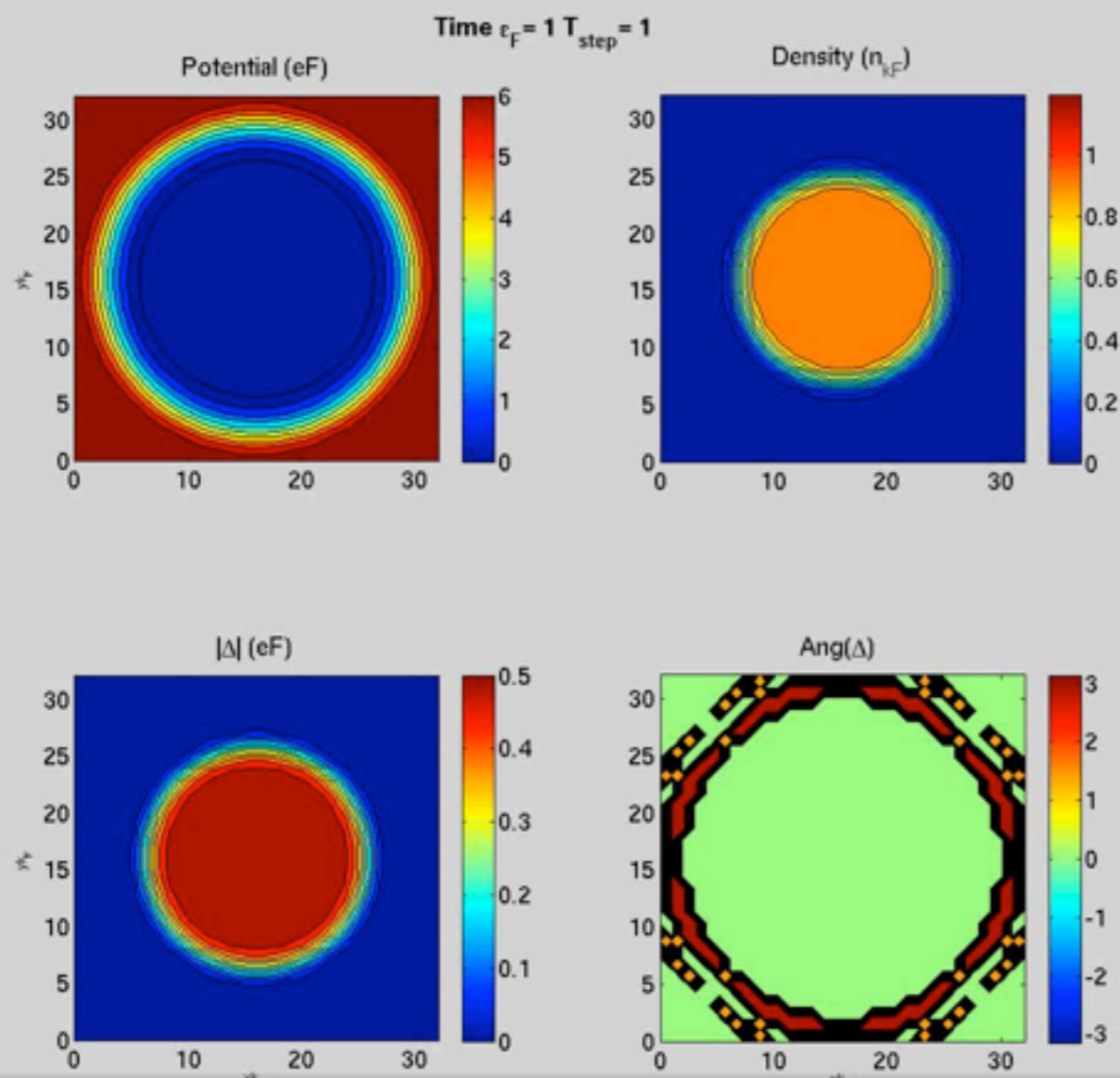


Work with Alan Luo and Rishi Sharma

# Comparison

Fermions  
SLDA TDDFT

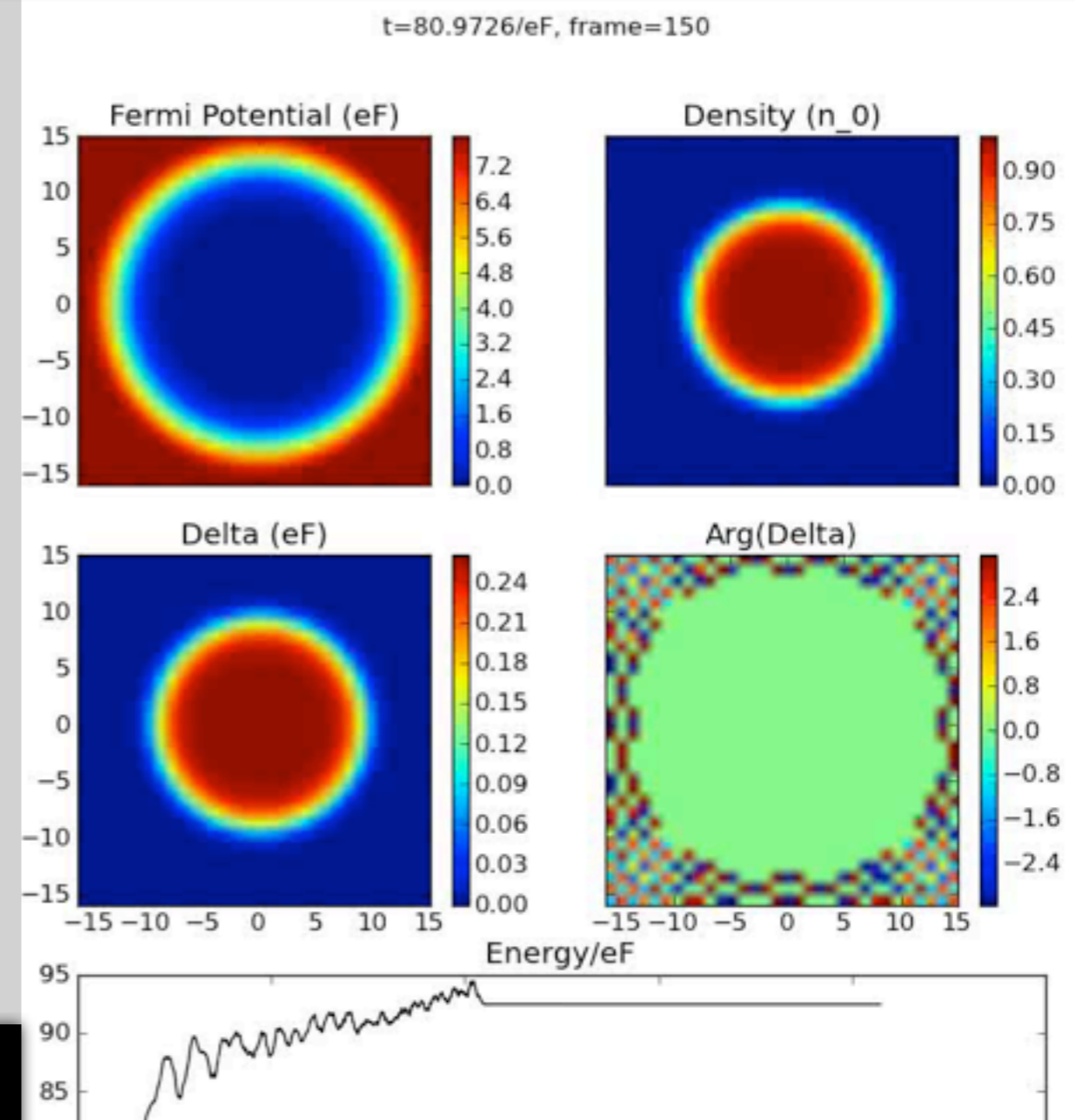
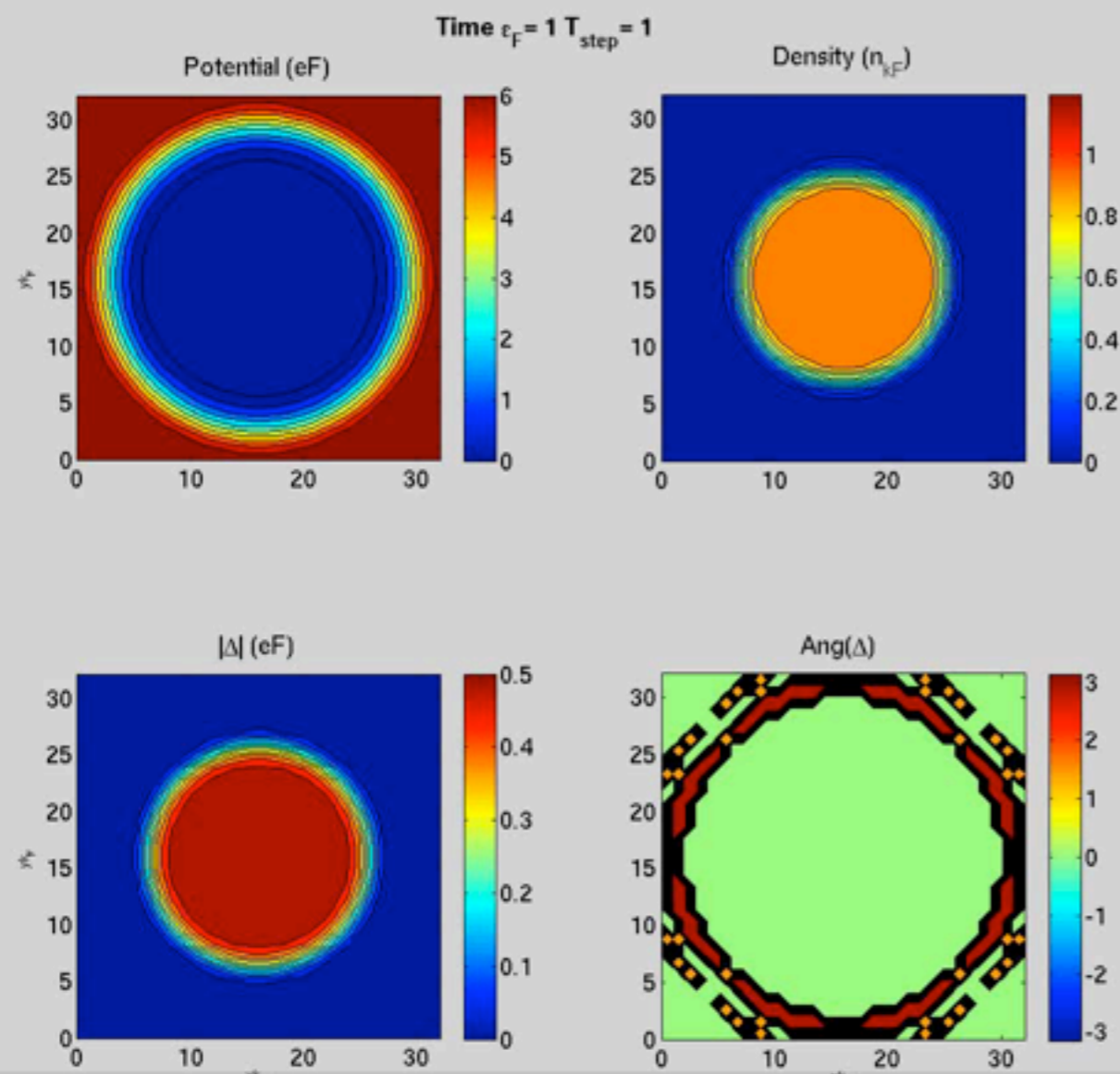
Gross Pitaevskii  
model



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)

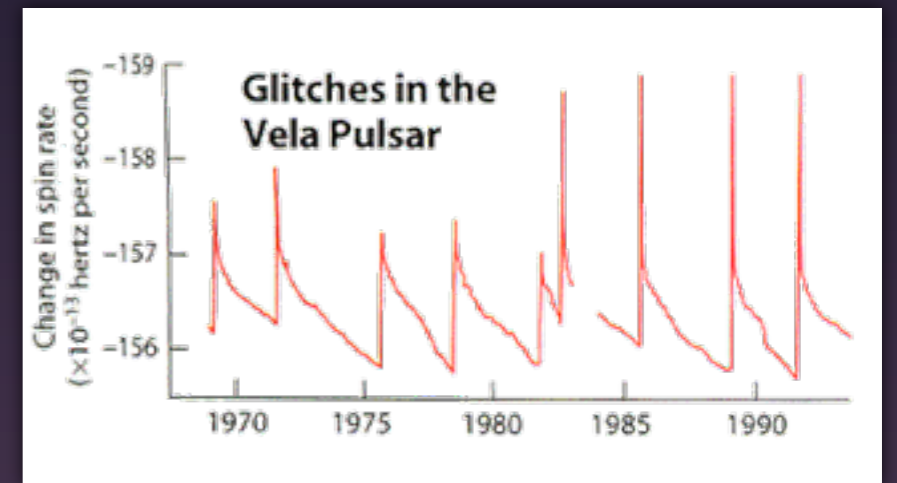
# GPE Simulations of Unitary Fermi Gas

“A Laboratory on your Laptop”

# Application: Vortex Pinning

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

Anderson and Itoh (1975)

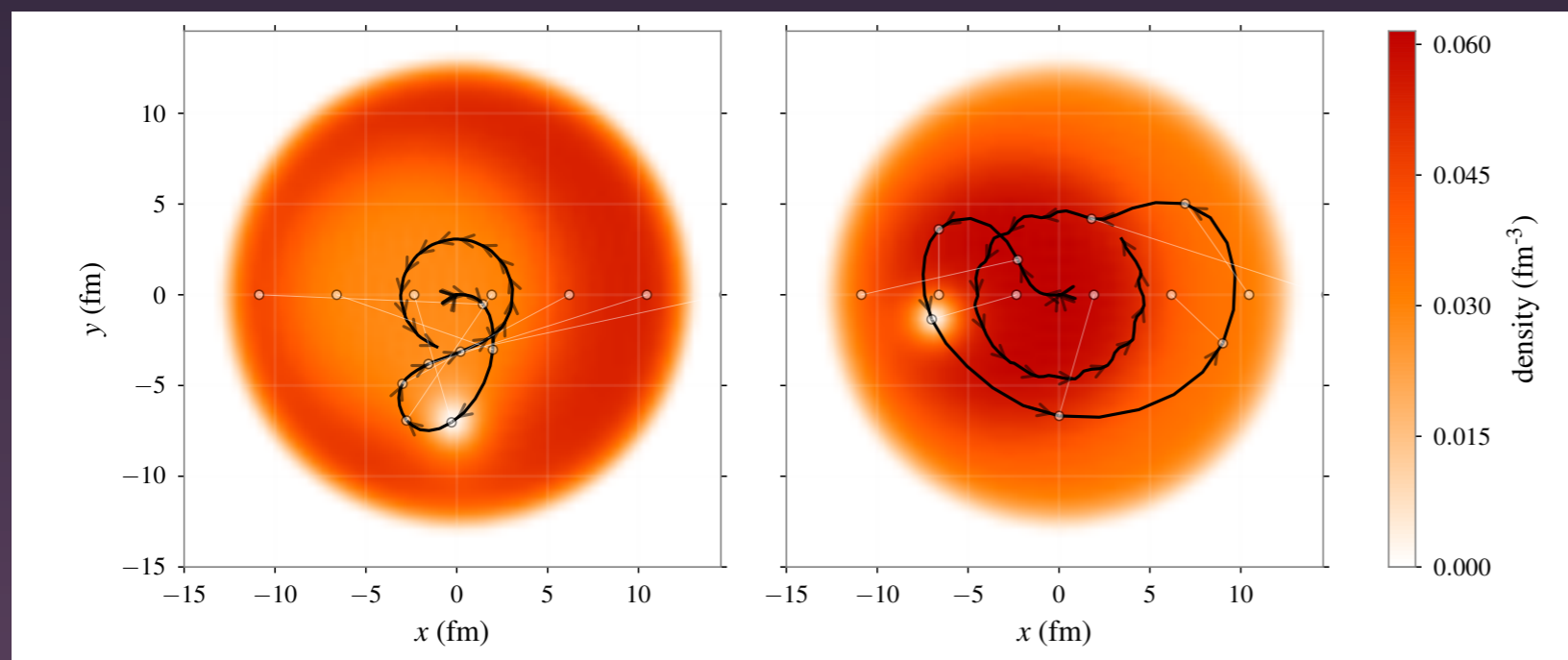


Pulsar Astronomy by Andrew G. Lyne and Francis

- 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

# Pinning Force

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



## Thermodynamics

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

Bulgac, Forbes, Sharma 2013

# 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

- SLDA DFT: Excellent agreement with expt. and QMC
  - Tool for extrapolating from small to large  
(Generalize to aid with IR convergence?)
- GPE models works quite well for low energy dynamics
  - Quantitative agreement at unitarity  
(Can their domain of validity be expanded?)
- “A Laboratory on your Laptop”
  - A feasible solution for bulk superfluid dynamics?
  - Neutron star glitches?