Freeing seimclassical theory of the dreaded UV divergence

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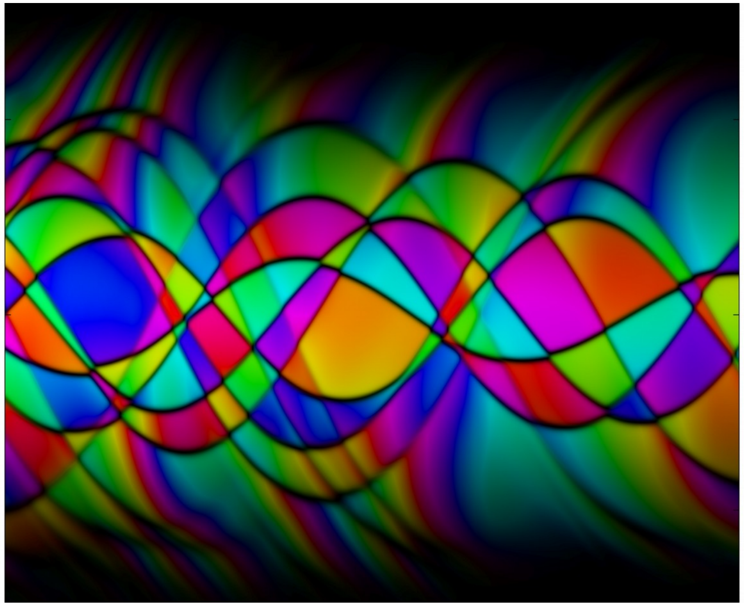
Outline

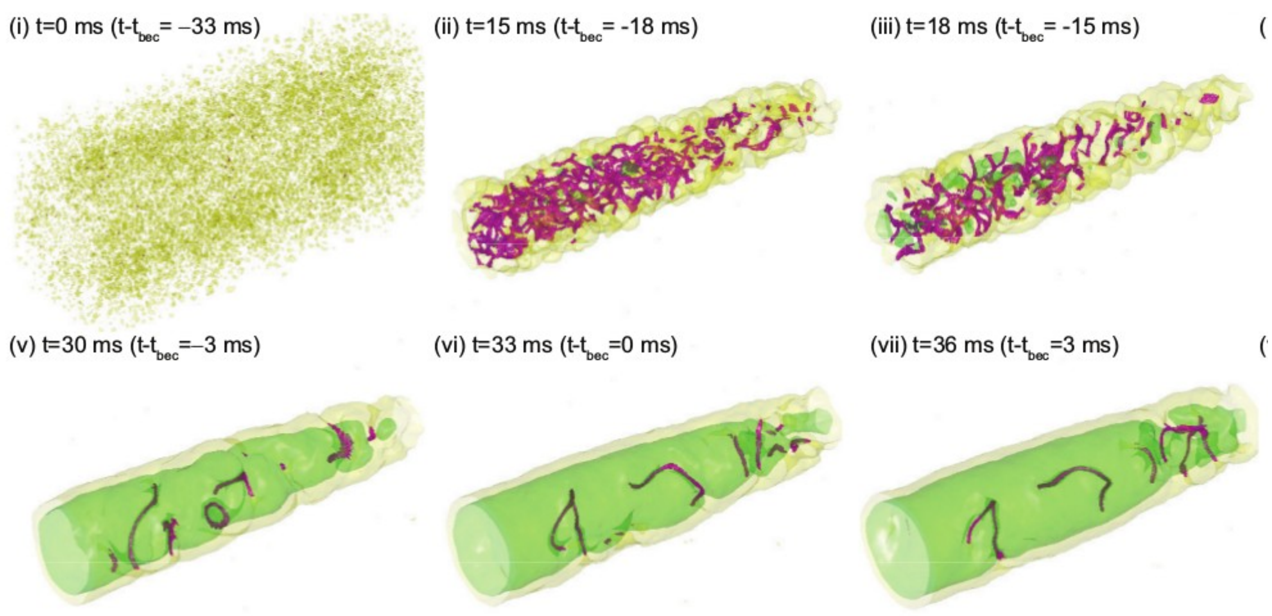
- Semiclassical wave fields for bosons (background)
- The UV divergence and cutoff issues
- Fixing it
- Simple example: 1d
  (~1000 modes)
- Serious example: collective breathing at high temperature in 3d
  (1000000s of modes)

The point of semiclassical field theory

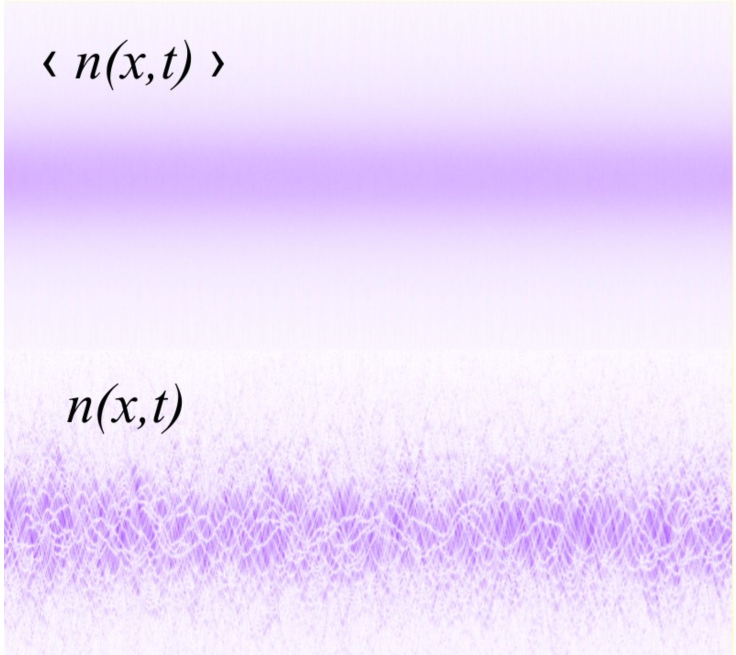
- Nonperturbative
- *T > 0*
- Single shots
- No special conditions, symmetries, geometries
- Scales very well with system size



1d gas – phase domains after cooling

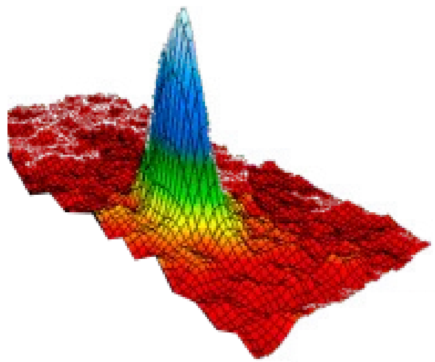


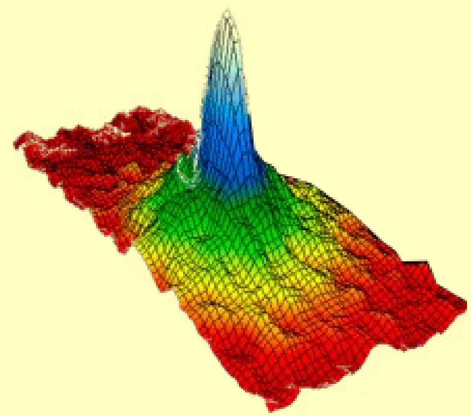
Liu, Donadello, Lamporesi, Ferrari, Gou, Dalfovo, Proukakis, Commun. Phys. **1**, 24 (2018)

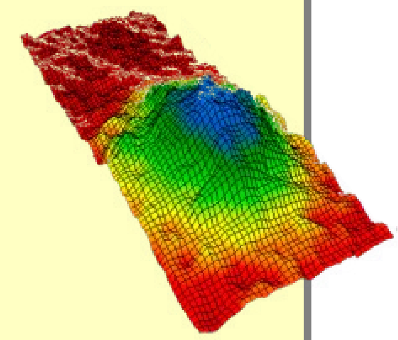


1d gas – thermal equilibrium

Thermal clouds - Classical fields essential







T=0

1 mode
GPE

Bogoliubov

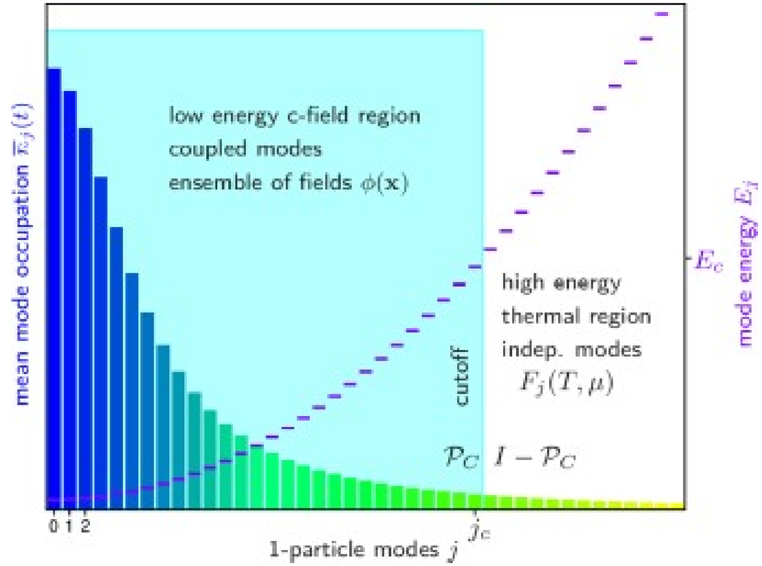
few modes
perturbative

Classical fields, ZNG

zillions of modes
non-perturbative

$T=T_c$

Simplest semiclassical method = "classical" wave fields



Bose field — semiclassical replacement

$$\widehat{\Psi}(\mathbf{x}) = \sum_j \widehat{a}_j \psi_j(\mathbf{x}) \longrightarrow \phi(\mathbf{x}) = \left\{ \sum_{j\in\mathcal{C}} \alpha_j \psi_j(\mathbf{x}) \right\}$$

Assuming high occupation:

$$\left[\widehat{a}_j, \widehat{a}_k^\dagger\right] = \delta_{jk}$$

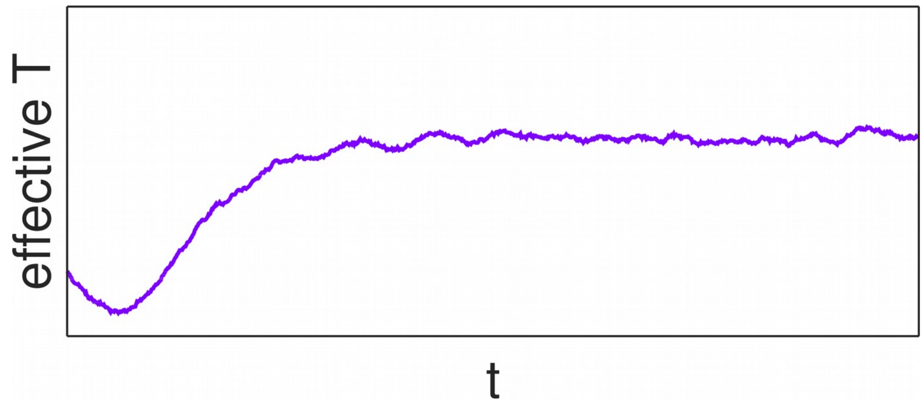
$$\widehat{a}_j \gg 1 \;\rightarrow \widehat{a}_j \approx \alpha_j$$

Evolution: GPE

$$\hbar \frac{d\phi(\mathbf{x})}{dt} = -i\mathcal{E}(\mathbf{x})\phi(\mathbf{x})$$

$$\mathcal{E}\phi(\mathbf{x}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + g\,|\phi(\mathbf{x})|^2\right]\phi(\mathbf{x})$$

Thermalised ensemble at long time



Methods for thermal bose gases

	ZNG	GPE (classical fields)	Projected GPE + Hartree-Fock	Stochastic GPE
nonperturbative low E modes	✓	✓	✓	✓
many modes at low E	✗	✓	✓	✓
High E modes	dynamic	✗	static	reservoir
temperature	?	extracted	extracted	set
Equilibrium ensemble	?	micro-canonical	micro-canonical	grand-canonical
UV divergence Cutoff dependence	no	STRONG	some	STRONG
numerical effort	LARGE	medium	medium	medium

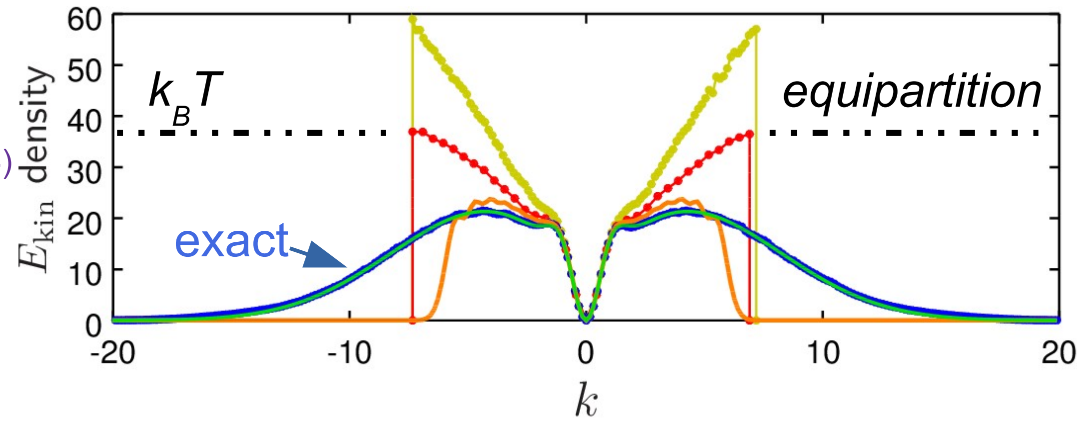
WANTED: a way to combine the good features of ZNG and classical fields

Age-old problem: cutoff dependence

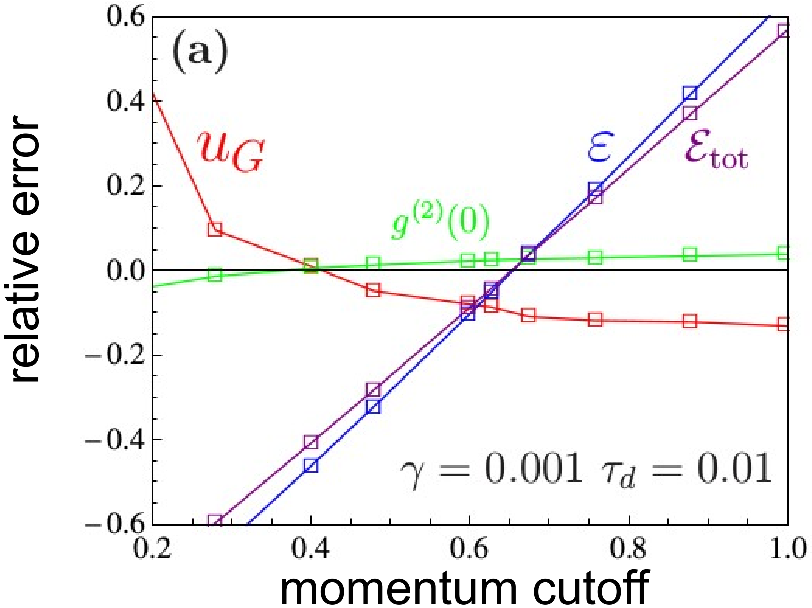
Studied by many:

Witkowska, Gajda, Rzążewski, PRA **79**, 033631 (2009)
Karpiuk, Brewczyk, Gajda, Rzążewski, PRA **81**, 013629 (2010)
Zawitkowski, Brewczyk, Gajda, Rzążewski, PRA **70**, 033614 (2004)
Bradley, Blakie, Gardiner, J Phys B **38**, 4259 (2005)
Cockburn, Proukakis, PRA **86**, 033610 (2010)
and the list goes on ...

Kinetic energy distribution, ideal gas in trap

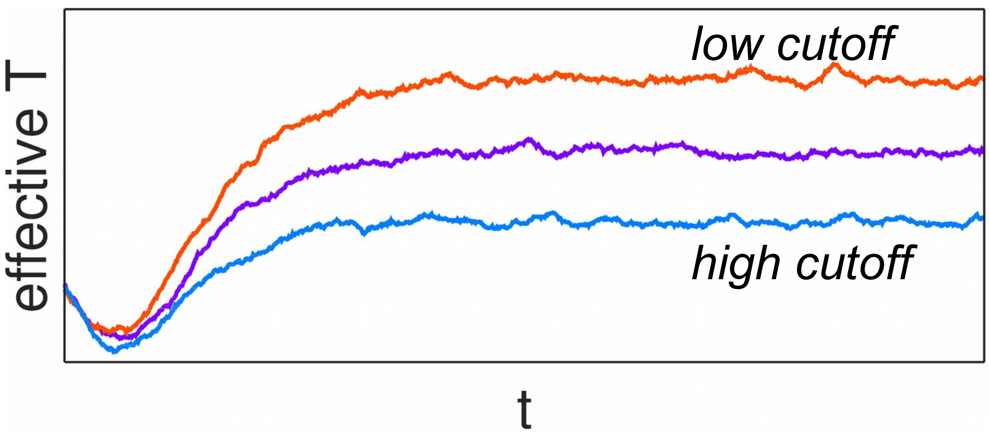


Most recent study: different observables



Pietraszewicz, PD, PRA **92**, 063620 (2015)
Pietraszewicz, PD, PRA **97**, 053607 (2018)
Pietraszewicz, PD, PRA **98**, 023622 (2018)

Equilibrium temperature depends on cutoff

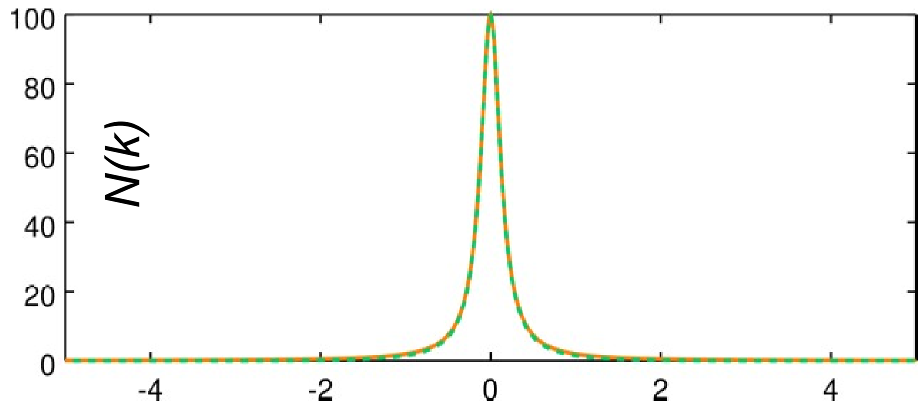


Ultraviolet catastrophe = nefarious equipartition

Quantum Bose-Einstein distribution ½$k_B T$ energy per *PARTICLE*

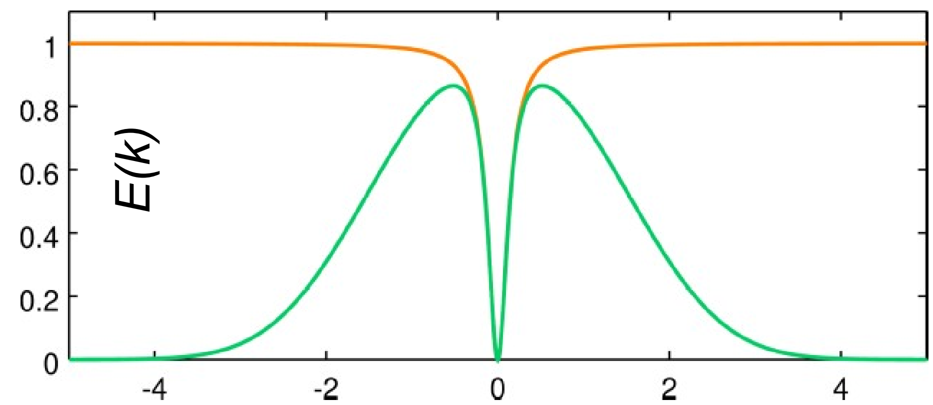
Classical field Rayleigh-Jeans distribution $k_B T$ energy per *MODE*

particles



momentum $k / \sqrt{(k_B T)}$

kinetic energy (ideal gas)



momentum $k / \sqrt{(k_B T)}$

Also applies to truncated Wigner at long times

Pietraszewicz, PD, PRA **98**, 023622 (2018)
PRA **97**, 053607 (2018)

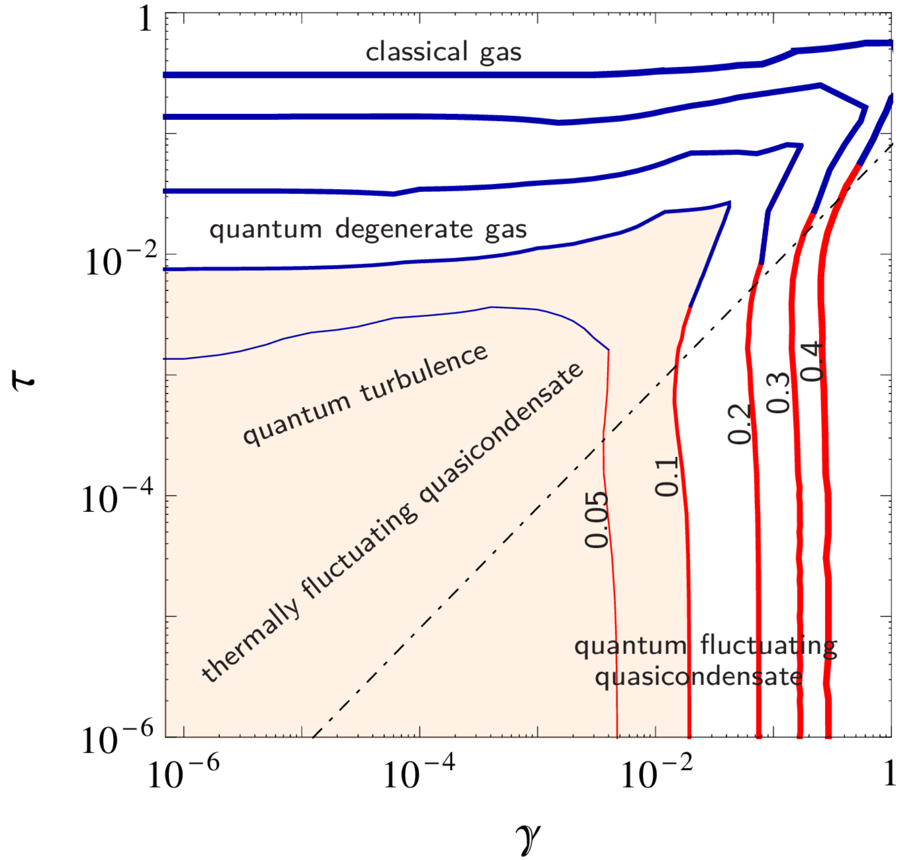
- Uniform 1d Bose gas: comparison to exact results

$$\gamma = \frac{mg}{\hbar^2 n}; \qquad \tau_d = \frac{T}{T_d}$$

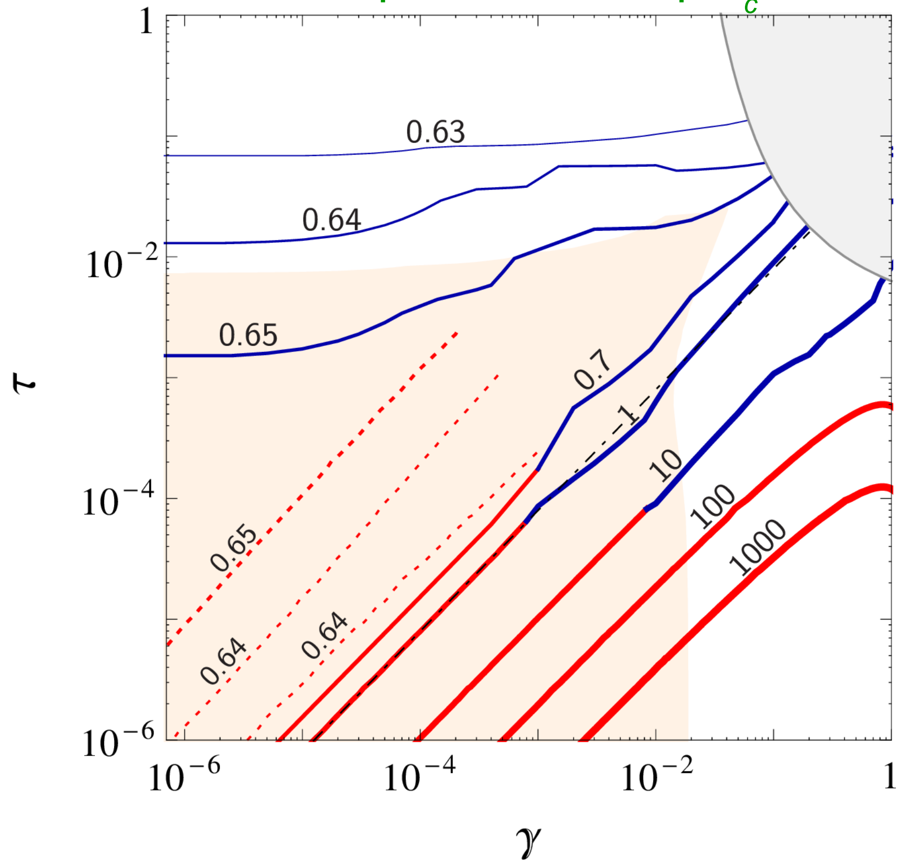
Relative error $$\delta_\Omega(\gamma,\tau_d,f_c) := \frac{\Delta\Omega}{\Omega} = \left(\frac{\Omega^{(\mathrm{cf})}(\gamma,\tau_d,f_c)}{\Omega(\gamma,\tau_d)} - 1\right)$$

Global error bound $$RMS(\gamma,\tau_d,f_c) = \sqrt{\left(\delta_{u_G}\right)^2 + \max\left[\delta_\varepsilon^2, \delta_{\mathcal{E}_{\mathrm{tot}}}^2\right]}$$

Global accuracy of observables min *RMS*

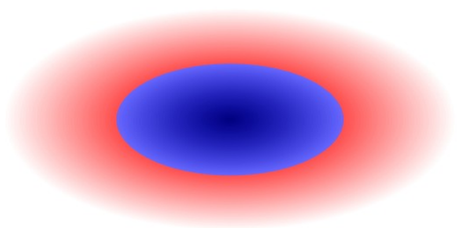


Optimal cutoff opt f_c

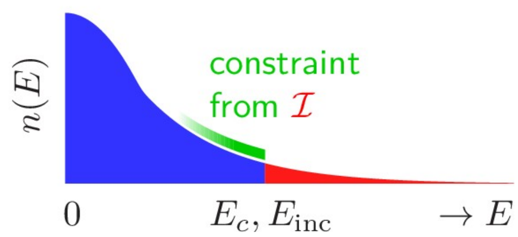


Stochastic Gross-Pitaevskii equation (SGPE)

real space



occupations



complex noise

$$\hbar \frac{\partial \phi(\mathbf{x})}{\partial t} = -i\mathcal{E}(\mathbf{x})\phi(\mathbf{x}) - \gamma\left[\mathcal{E}(\mathbf{x}) - \mu\right]\phi(\mathbf{x}) + \sqrt{2\hbar\gamma k_B T}\,\eta(\mathbf{x},t)$$

Loss rate to "incoherent" tails

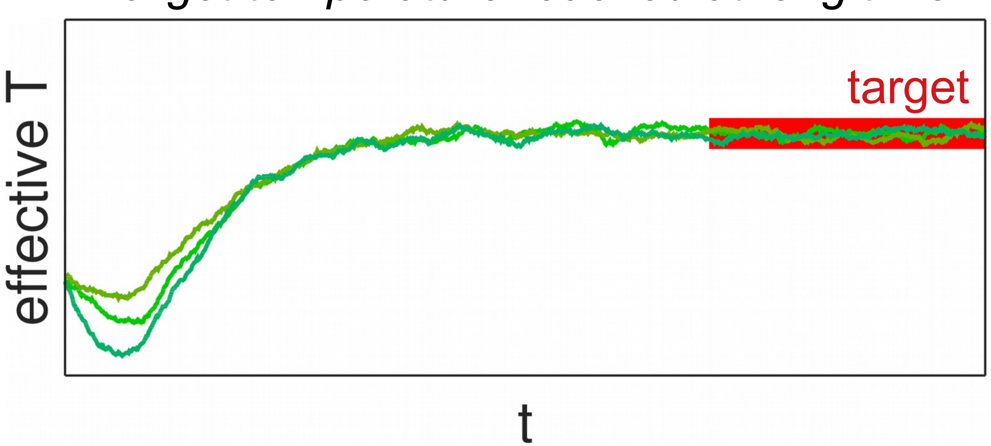
Incoherent growth from tails

Hamiltonian evolution of "coherent" field

$$\mathcal{E}\phi(\mathbf{x}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + g\,|\phi(\mathbf{x})|^2\right]\phi(\mathbf{x})$$

BUT, still UV divergent

Target temperature reached at long time

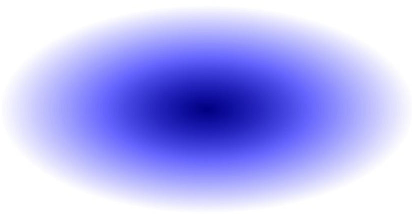


Invokes a "classical field" linearisation of occupation in tails (correct when $\overline{N}(\omega) \gg 1$)

$$\overline{N}(\omega) \to \frac{k_B T}{\omega(\mathbf{x}) - \mu}$$

$\to$ equipartition strikes again :(

real space



occupations

Use proper quantum occupations

$$\overline{N}(\omega) = N_{BE} = \left[e^{\frac{\omega(\mathbf{x})-\mu}{k_B T}} - 1 \right]^{-1}$$

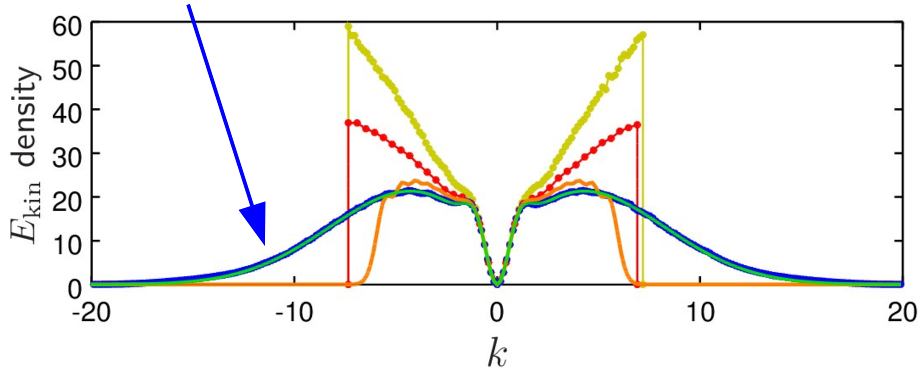
Obtain *regularised* SGPE

$$\hbar \frac{\partial \phi(\mathbf{x})}{\partial t} = -i\mathcal{E}(\mathbf{x})\phi(\mathbf{x}) - \gamma k_B T \left[e^{\frac{\mathcal{E}(\mathbf{x})-\mu}{k_B T}} - 1 \right] \phi(\mathbf{x}) + \sqrt{2\hbar\gamma k_B T}\, \eta(\mathbf{x}, t)$$

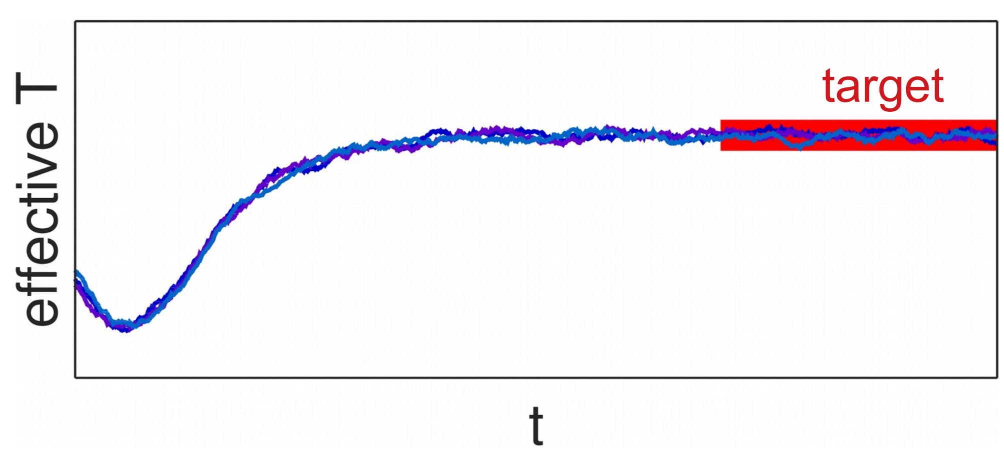
"Only" real difference

$$\mathcal{E}\phi(\mathbf{x}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + g\,|\phi(\mathbf{x})|^2 \right] \phi(\mathbf{x})$$

UV divergence is gone



Evolution well controlled



Derivation (rather abridged)

$$\overline{N}(\omega) \to \frac{k_B T}{\omega(\mathbf{x}) - \mu}$$

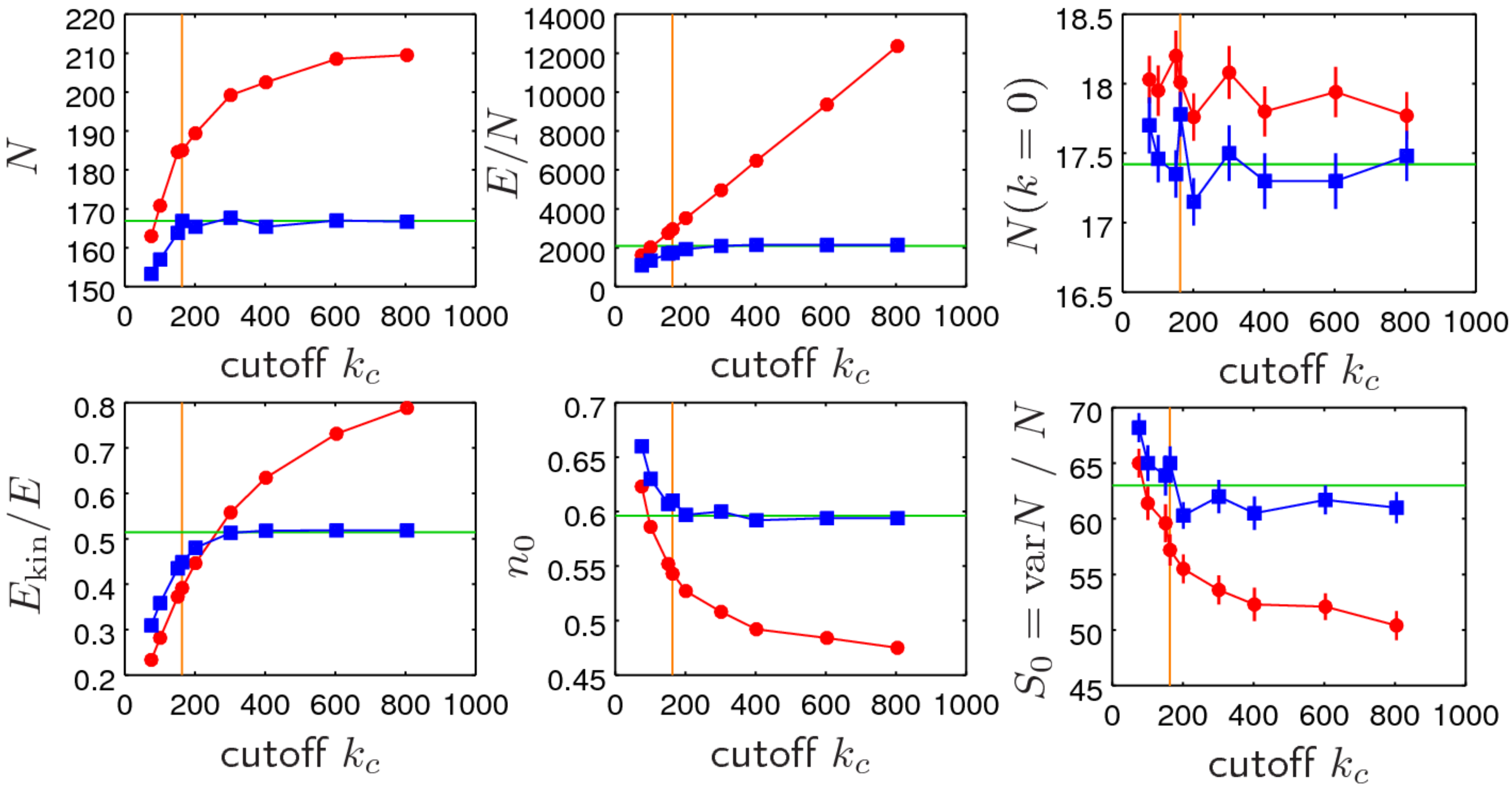
- Start with master equation for stochastic GPE model
  - ***BUT DO NOT linearize bath***
- Keep only one-particle exchange terms with reservoir
  - Like in SGPE derivation
- Reduce reservoir coupling to a localised form
  - Happened automatically in SGPE, need to take care here
- Represent master equation using positive-P distribution
  - Needed to pinpoint how to properly remove quantum noise (problem didn't occur in SGPE)
- Convert to Fokker-Planck equation
- Convert to stochastic equation
- Remove quantum noise terms which cause instability (noise amplification)
- Obtain regularised SGPE:

Stubborn term. Not diagonal; and likes to be huge.

$$\hbar\frac{\partial\phi(\mathbf{x})}{\partial t} = -i\mathcal{E}(\mathbf{x})\phi(\mathbf{x}) - \gamma k_B T\left[e^{\frac{\mathcal{E}-\mu}{k_B T}} - 1\right]\phi(\mathbf{x}) + \sqrt{2\hbar\gamma k_B T}\,\eta(\mathbf{x},t)$$

- Implement timestep in a special way to preserve the tractable computational cost of plain SGPE
  - Was not needed in SGPE, there was no exponential.
  - This is tricky. Probably the reason the equation was not tried earlier.

Ideal 1d trapped gas (cutoff dependence)



exact

plain SGPE

modified SGPE

cutoff from arXiv:1707.01776

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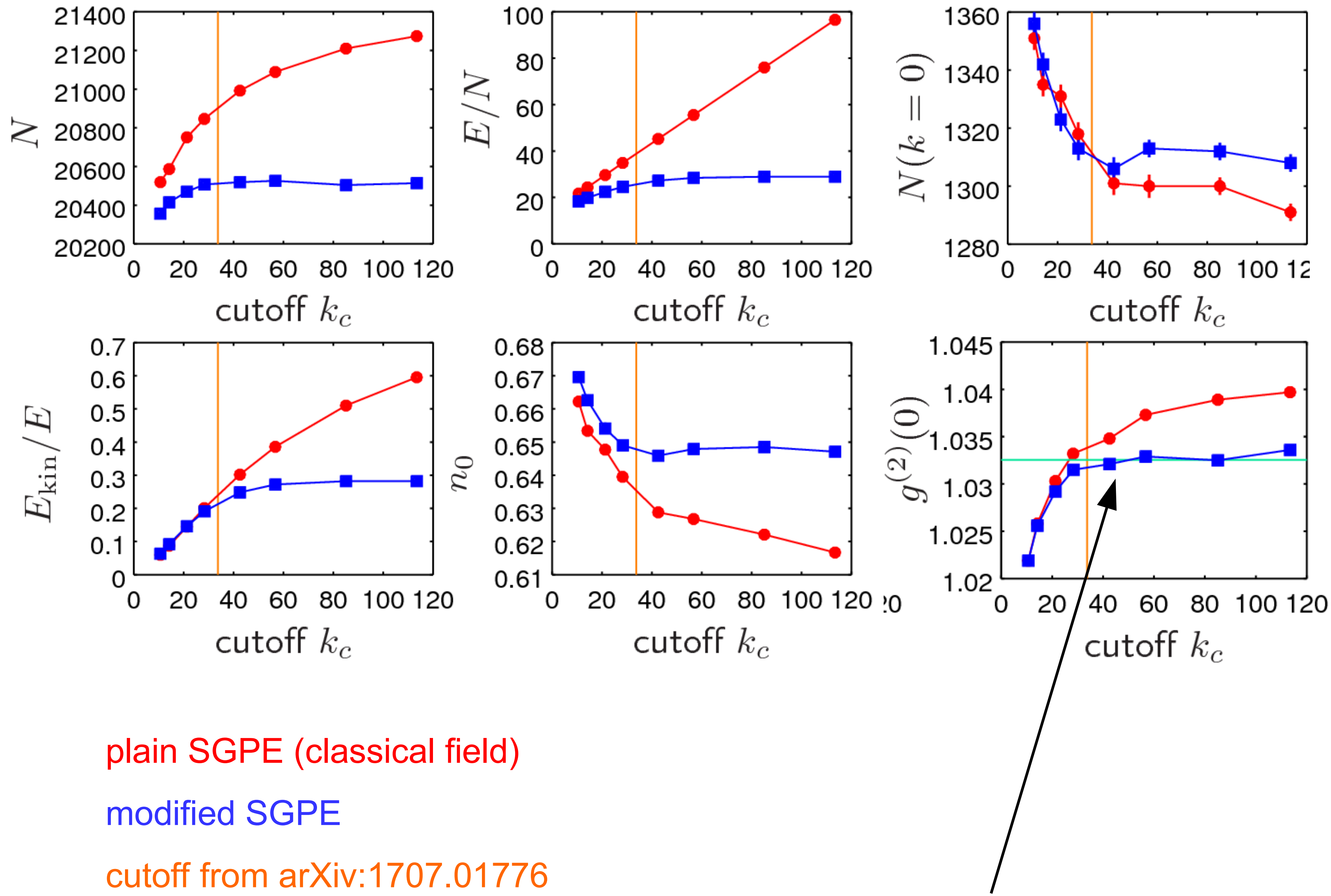
Interacting 1d trapped gas



plain SGPE (classical field)

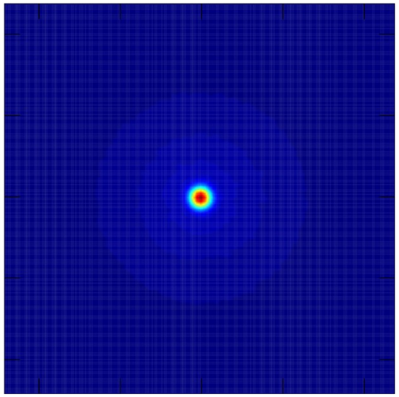
modified SGPE

cutoff from arXiv:1707.01776

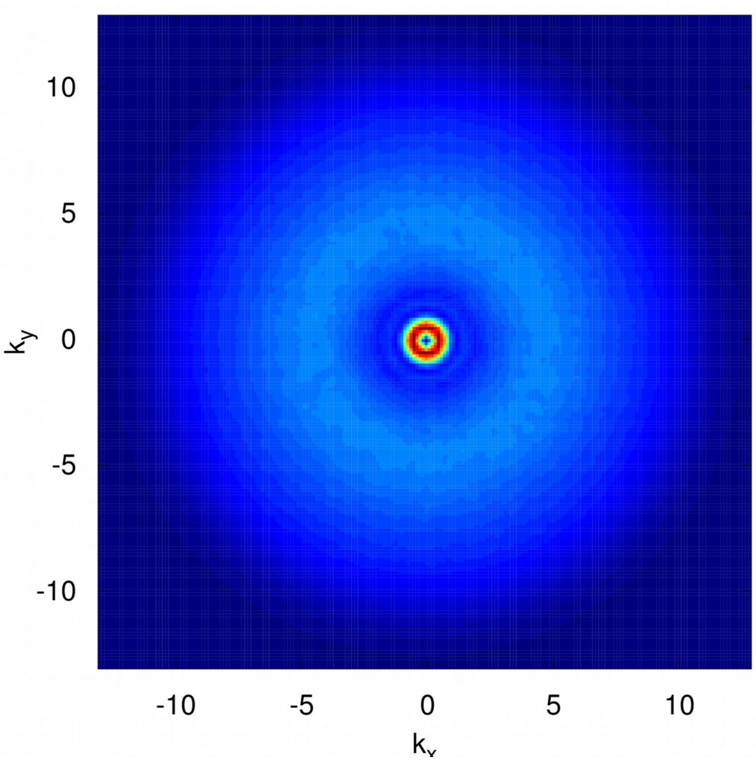
extended Bogoliubov as per Mora+Castin PRA 67, 053615 (2003)

Interacting 3d trapped gas

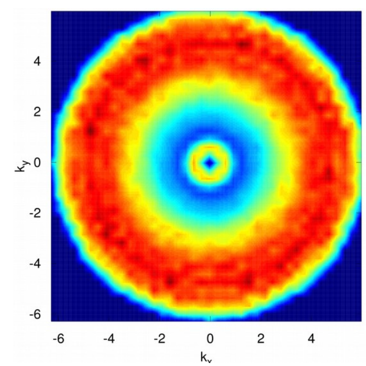
density in momentum space



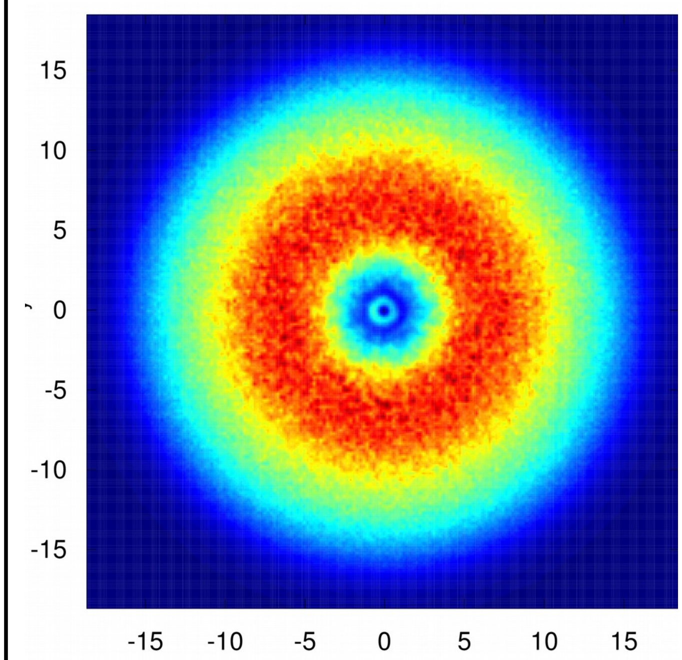
kinetic energy density



plain SGPE – to scale

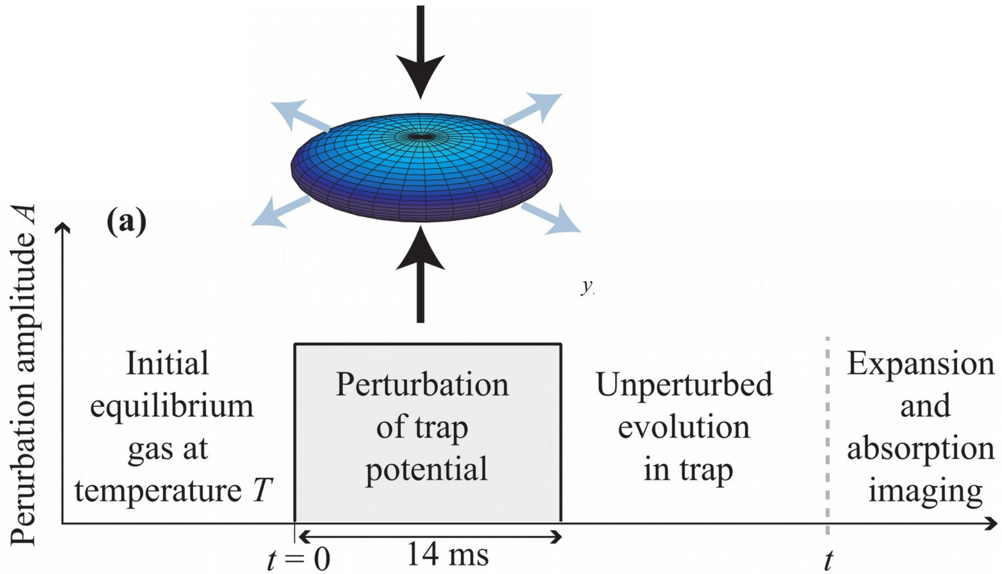


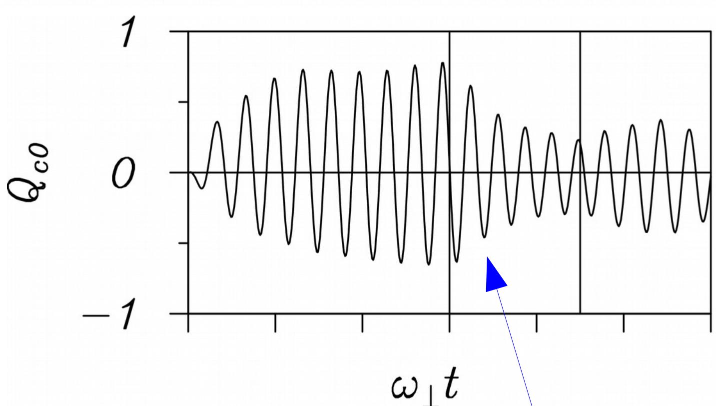
higher temperature



Litmus test for thermal cloud: *m=0* collective mode

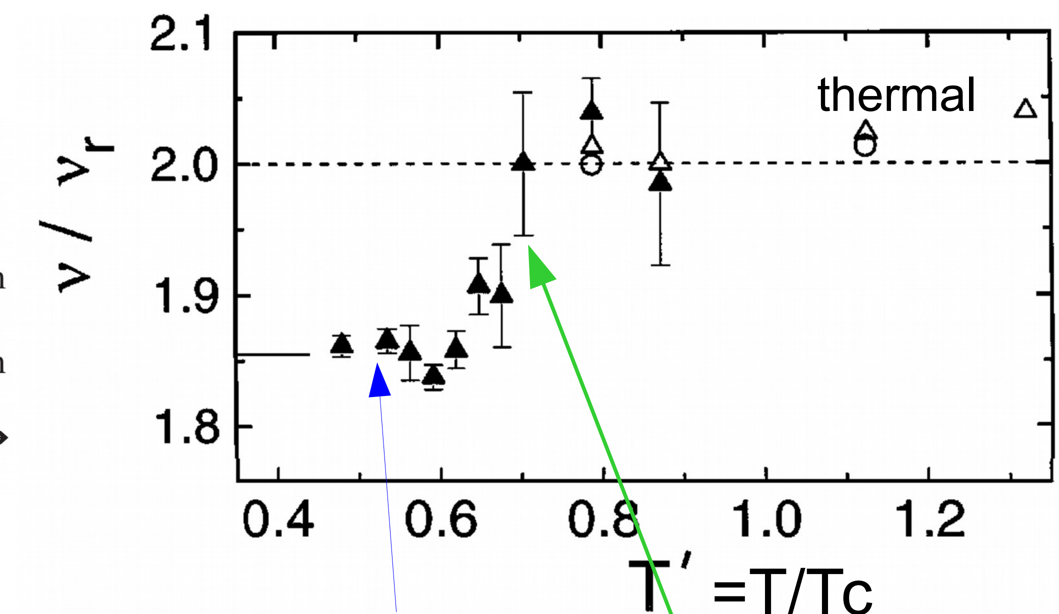
Ancient evil experiment: Jin, Matthews, Ensher, Wieman, Cornell, PRL 78, 764 (1997)





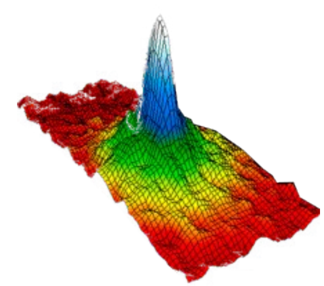
fit decaying sinusoid

adapted from: Jin *et al*, PRL 78, 764 (1997)



condensate oscillations

shift due to drag of thermal cloud on condensate



The above figures from:
Jackson, Zaremba, PRL 88, 180402 (2002)
Bezett, Blakie, PRA 79, 023602 (2009)

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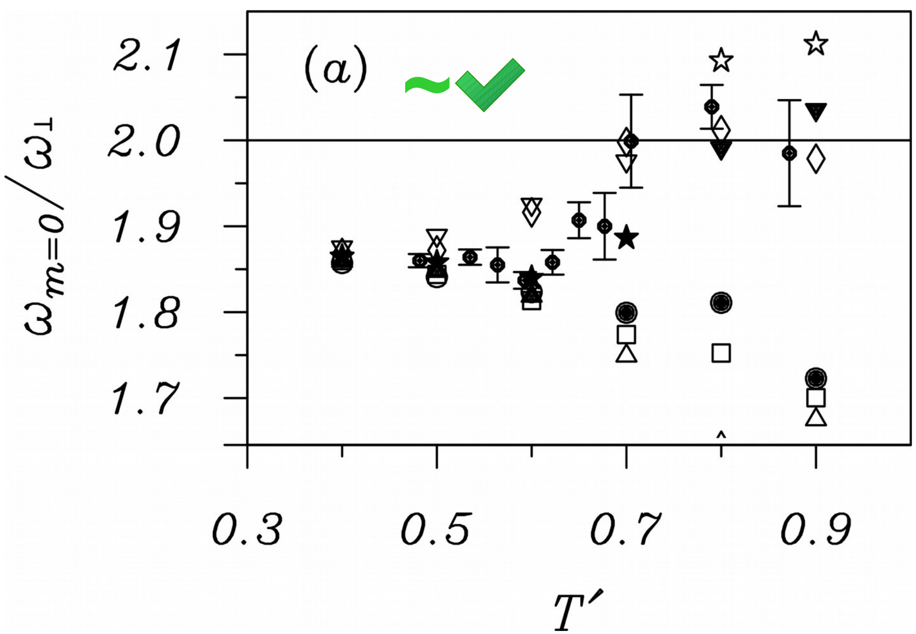
Results of *m=0* mode tests in the past

Targeted approaches

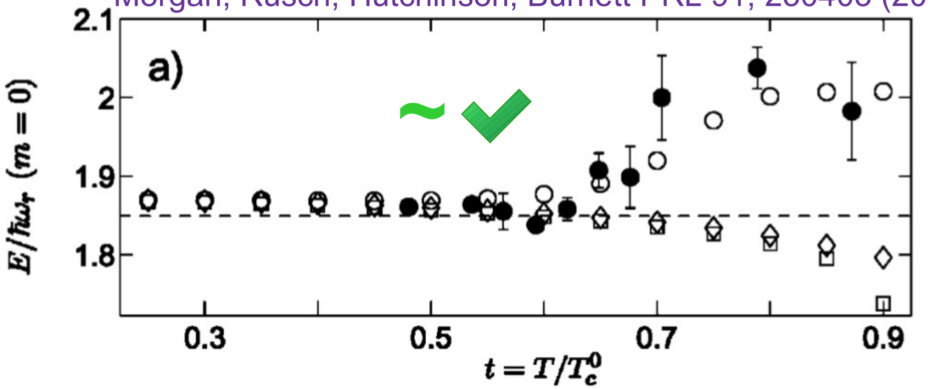
ZNG

Jackson, Zaremba, PRL 88, 180402 (2002)



Frequencies from "2nd order Bogoliubov"

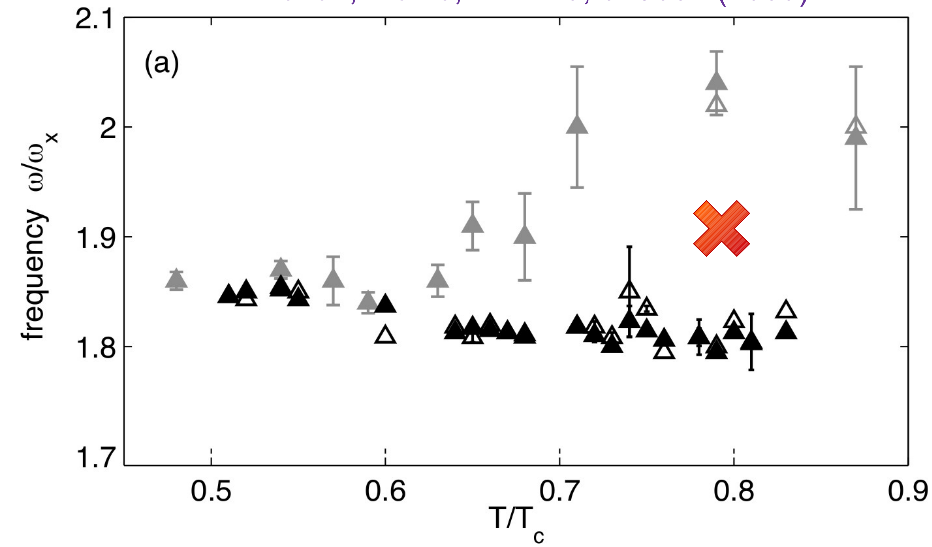
Morgan, Rusch, Hutchinson, Burnett PRL 91, 250403 (2003)



Flexible simulations

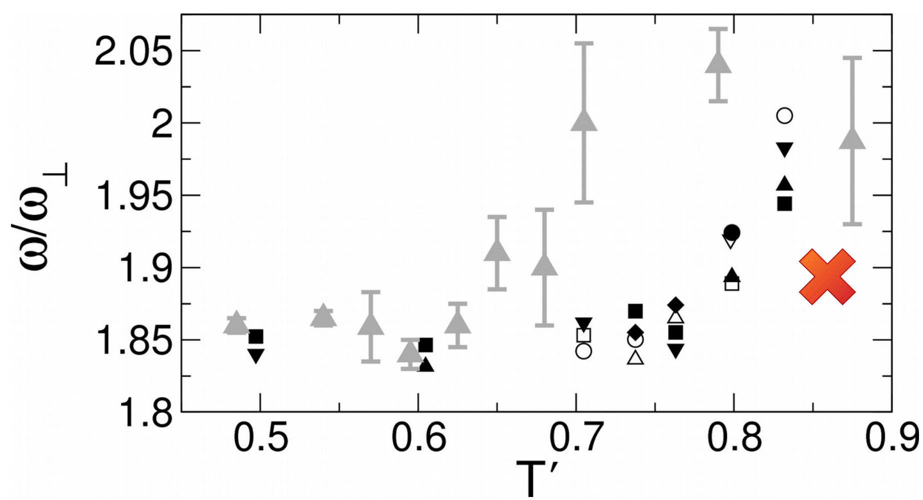
Classical fields + HF

Bezett, Blakie, PRA 79, 023602 (2009)

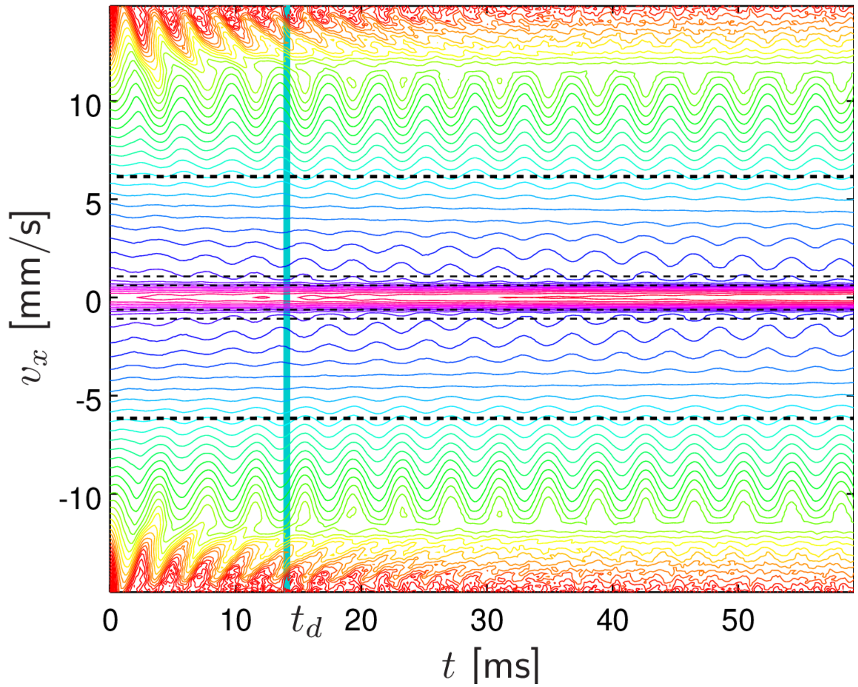


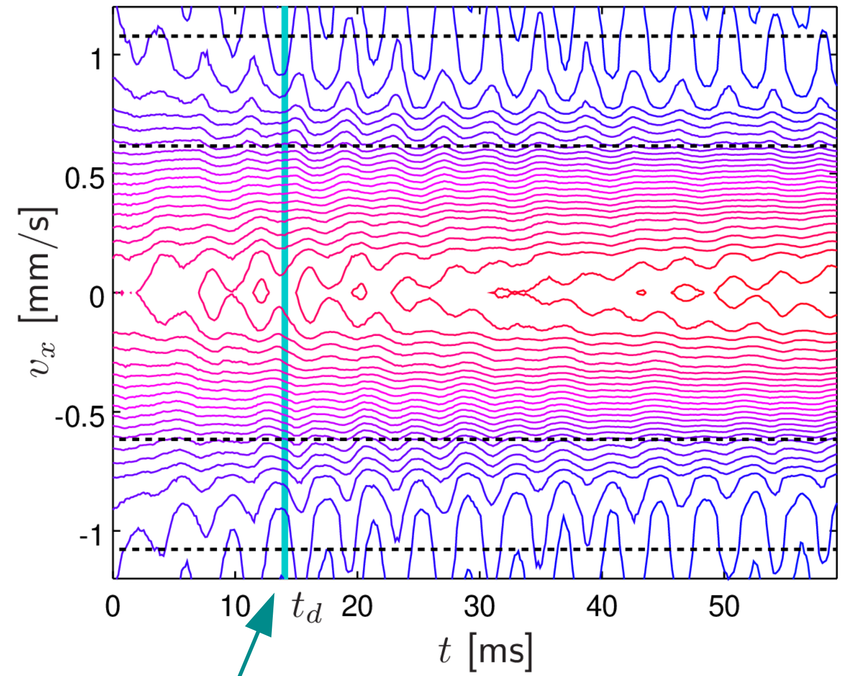
Classical fields (higher cutoff)

Karpiuk, Brewczyk, Gajda, Rzążewski, PRA 81, 013629 (2010)



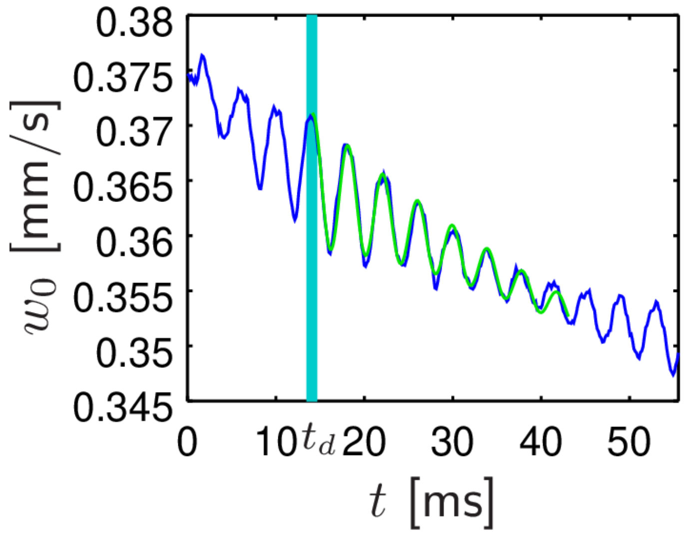
Contours of log density during evolution:

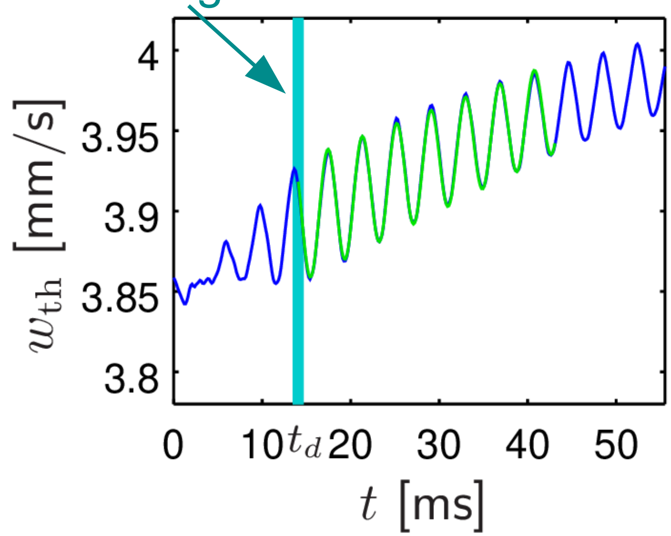




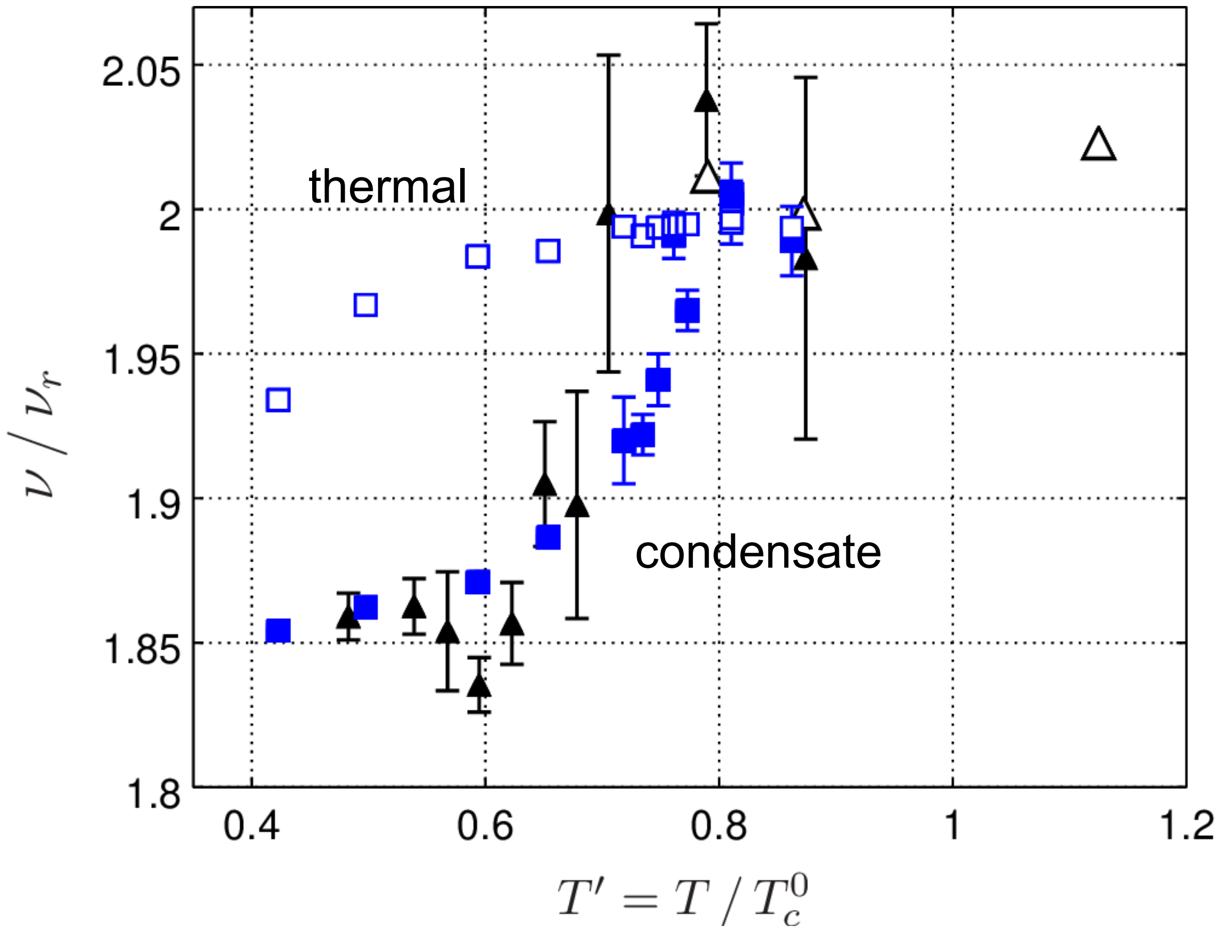
End of driving:

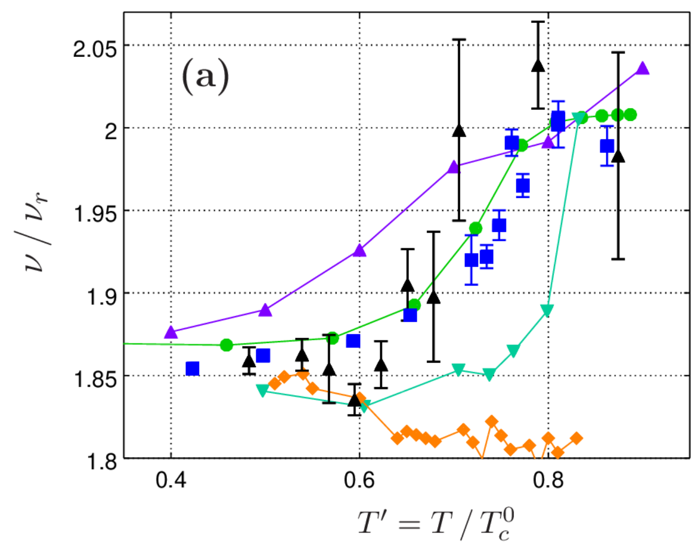
Fitting of width:

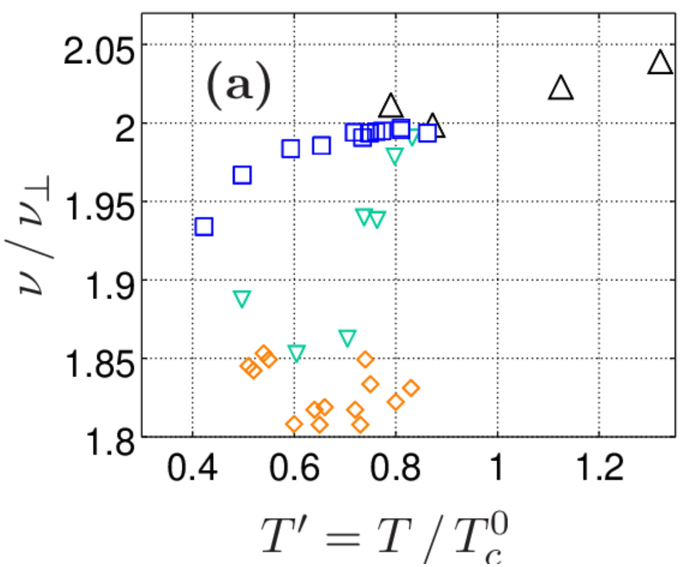




Results: *m=0* mode frequency







Experiment: Jin, Matthews, Ensher, Wieman, Cornell, PRL 78, 764 (1997)

This work (2018)

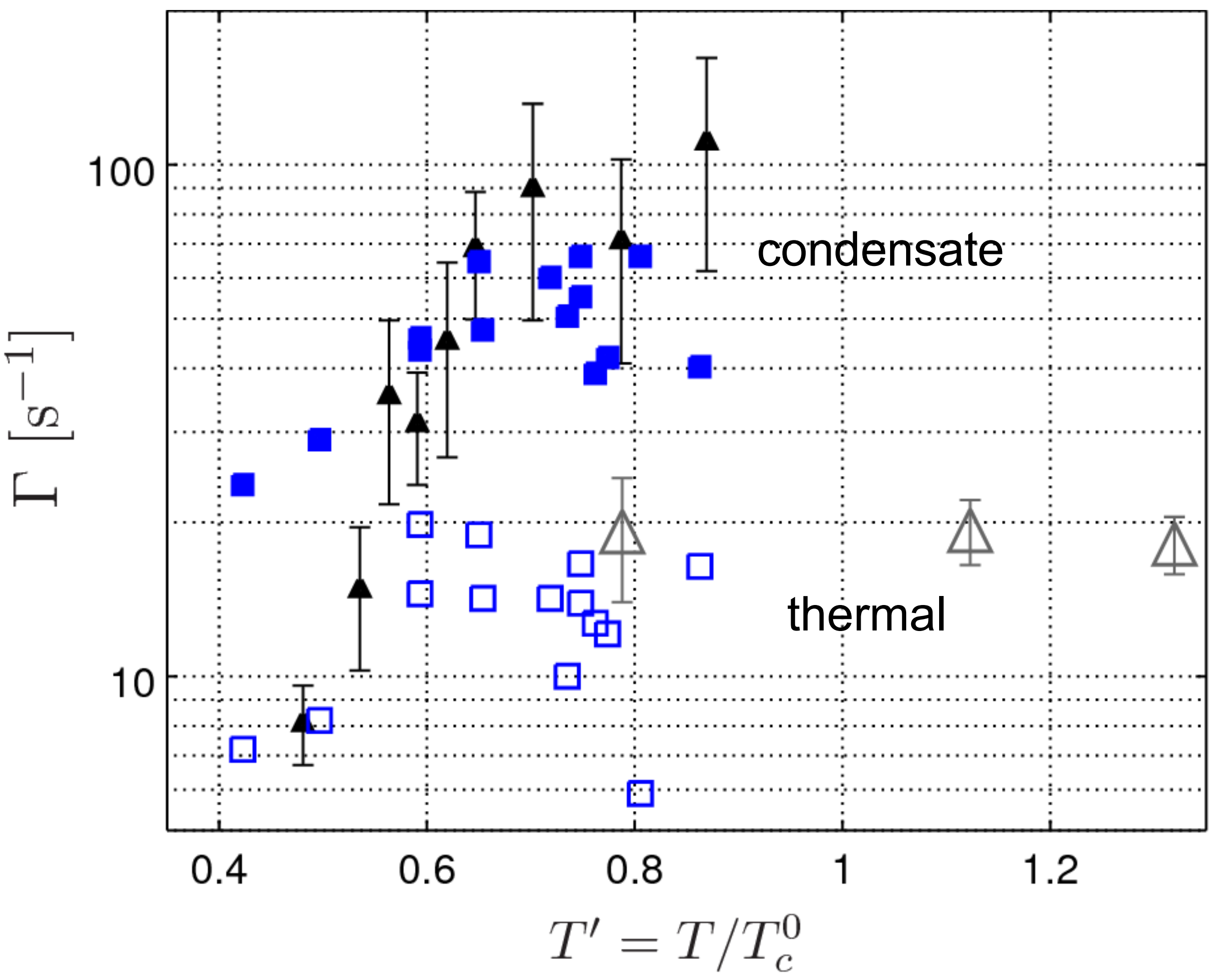
ZNG: Jackson, Zaremba, PRL 88, 180402 (2002)

2nd order Bogoliubov: Morgan, Rusch, Hutchinson, Burnett PRL 91, 250403 (2003)

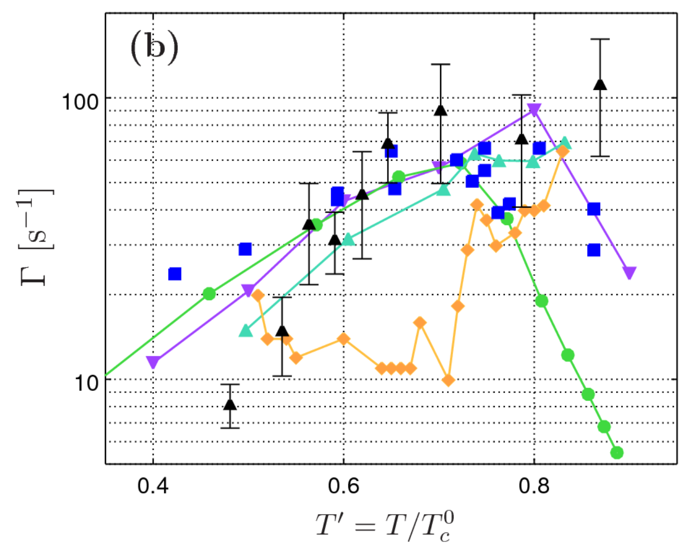
PGPE+HF: Bezettt, Blakie, PRA 79, 023602 (2009)

PGPE: Karpiuk, Brewczyk, Gajda, Rzążewski, PRA 81, 013629 (2010)

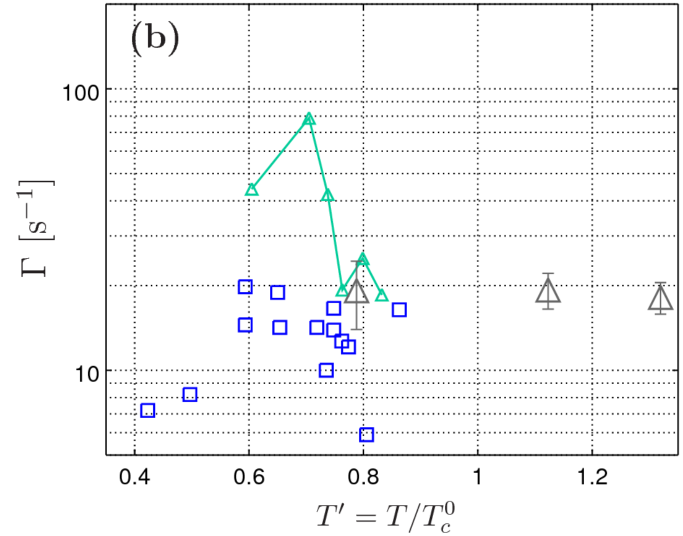
m=0 mode damping



condensate



thermal



Experiment: Jin, Matthews, Ensher, Wieman, Cornell, PRL 78, 764 *(*1997)

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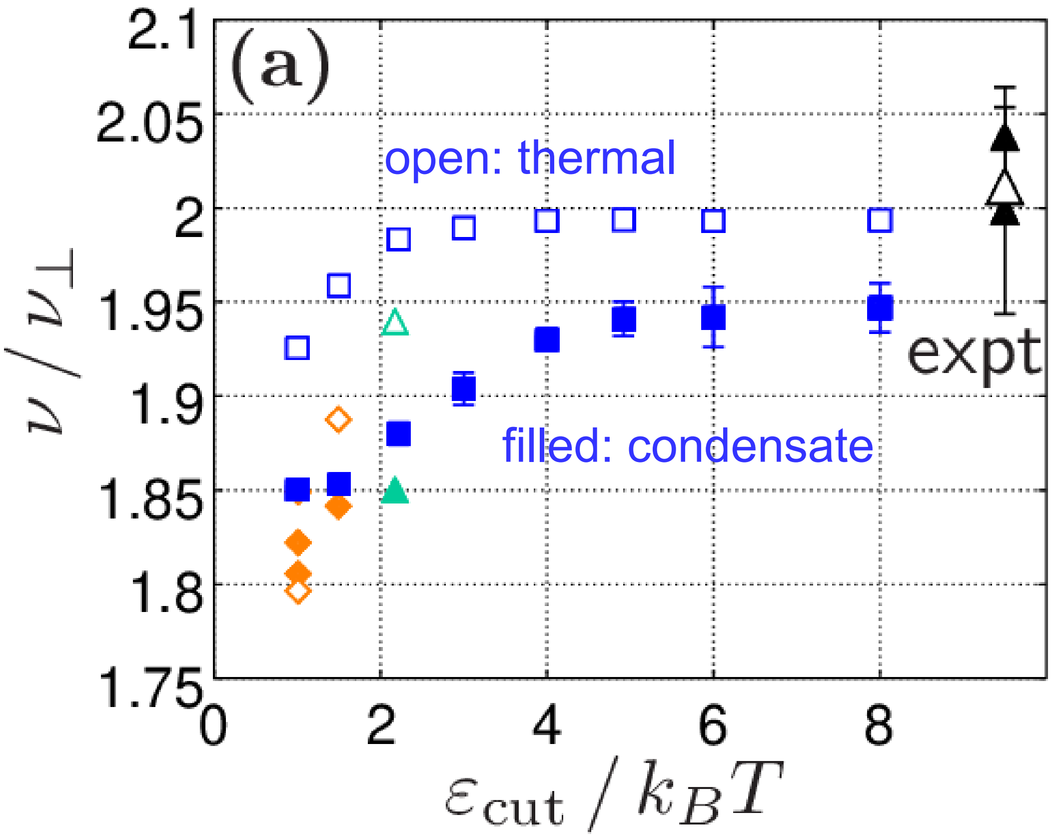
Cutoff dependence

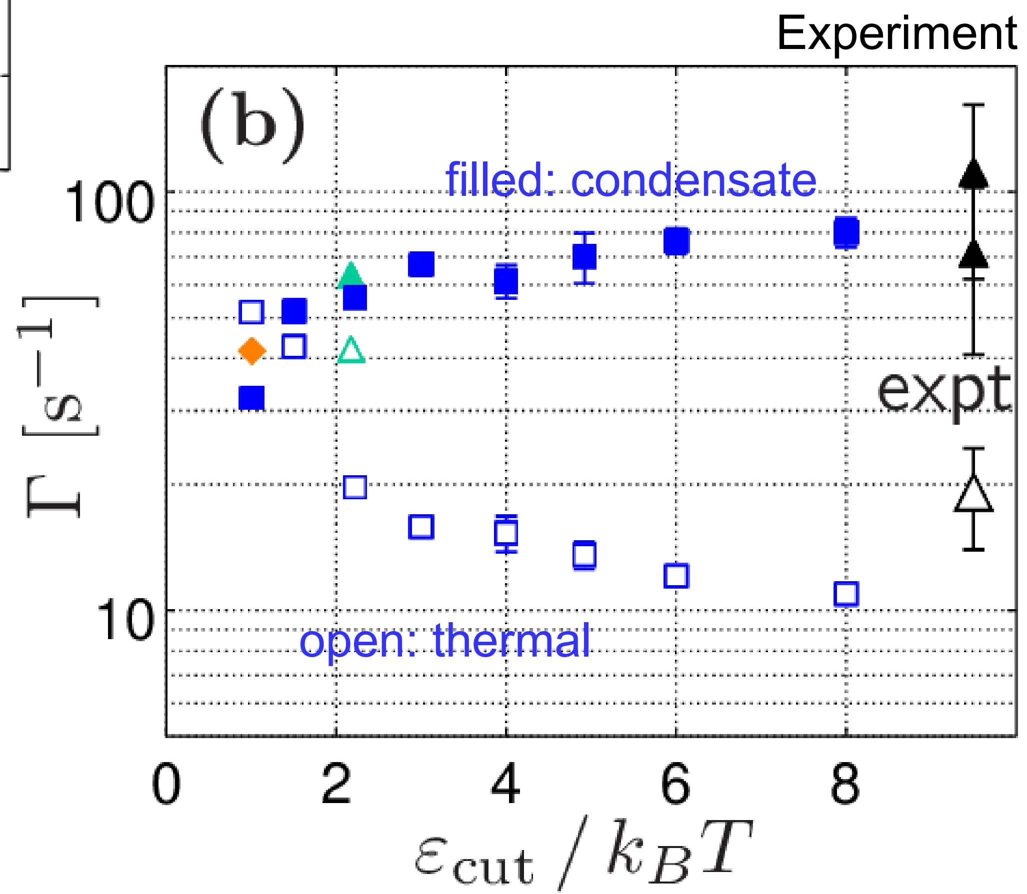


Experiment Jin *et al* 1997

Bezett + Blakie 2009

Karpiuk, Brewczyk, Gajda, Rzążewski 2010

This work



Outlook

- Quantitative results with classical fields

  Robust because no fitting of technical parameters such as cutoff

- Numerical effort comparable to SGPE

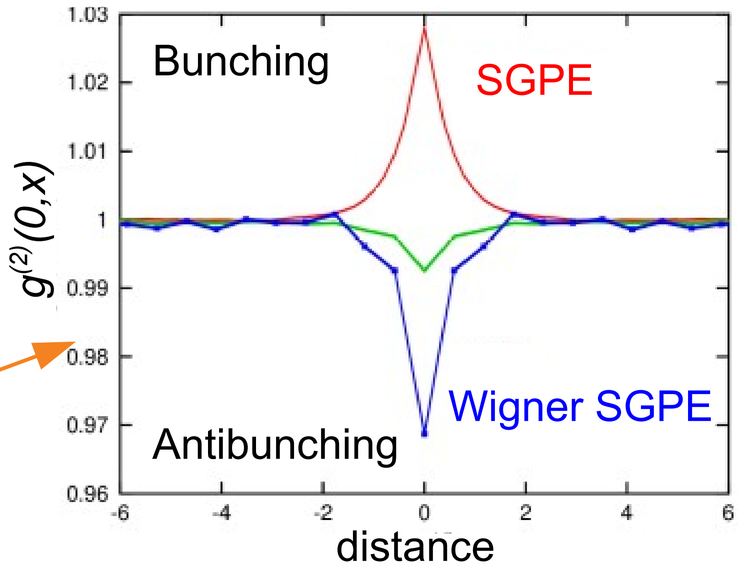
  though, lattice may need to be larger

- Still lacks wave-particle duality

  but this is harder to spot than expected

- NEXT: Wigner representation version

  to include quantum fluctuations



Thanks to discussions with

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Emilia Witkowska

Simon Gardiner
Crispin Gardiner
Matt Davis
Ashton Bradley
Blair Blakie

Krzysztof Gawryluk
Tomasz Karpiuk
Thomas Gasenzer
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