

# A semiclassical field theory free of the ultraviolet catastrophe

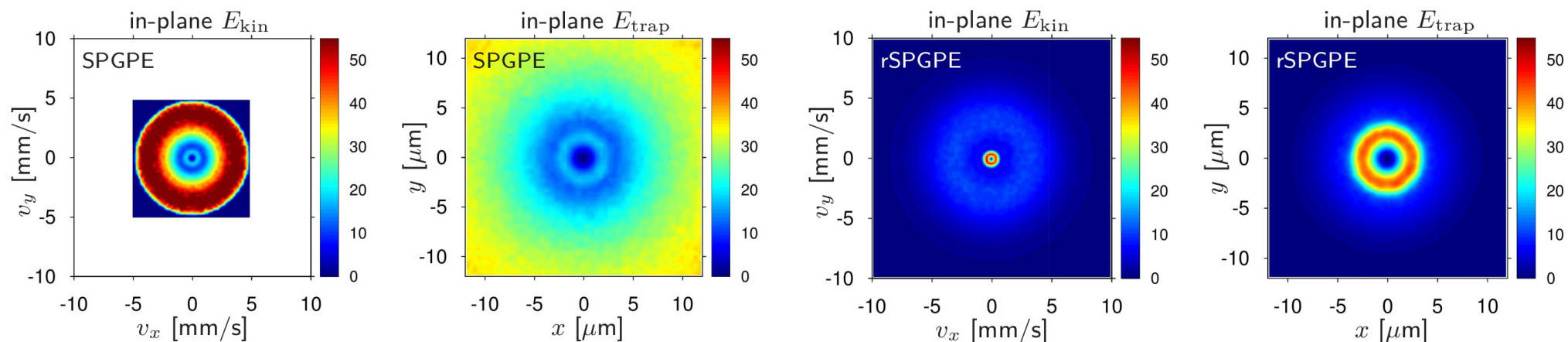
arXiv:1904.06266



Piotr Deuar

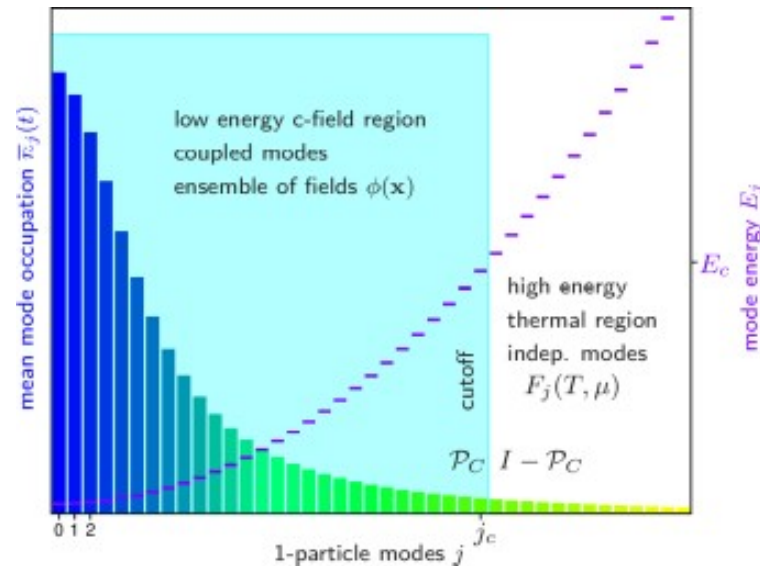
Joanna Pietraszewicz

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Warsaw, Poland*



- Background: semiclassical wave fields for ultracold atoms
- The UV divergence and cutoff issues
- Fixing it
- Simple example: 1d  
(~1000 modes)
- Serious example: 3d collective breathing mode near  $T_c$   
(1000000s of modes)

# Simplest semiclassical method = "classical" wave fields



Assuming high occupation:

Bose field semiclassical replacement

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

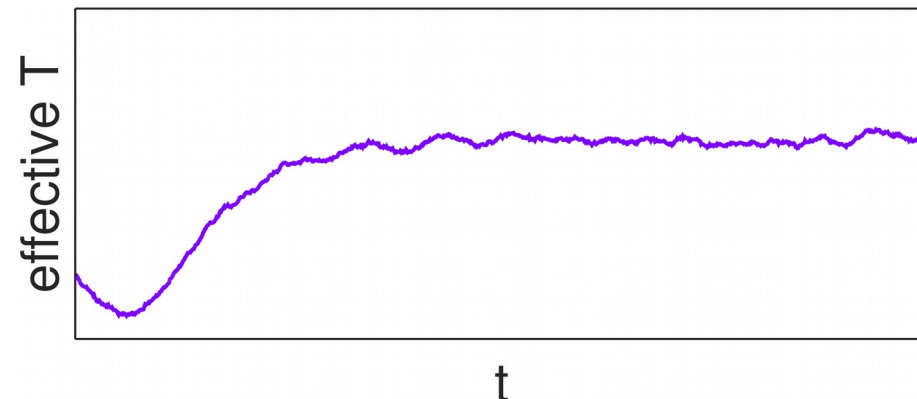
$$\begin{aligned} [\hat{a}_j, \hat{a}_k^\dagger] &= \delta_{jk} \\ \hat{a}_j \gg 1 &\rightarrow \hat{a}_j \approx \alpha_j \end{aligned}$$

Evolution: GPE

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

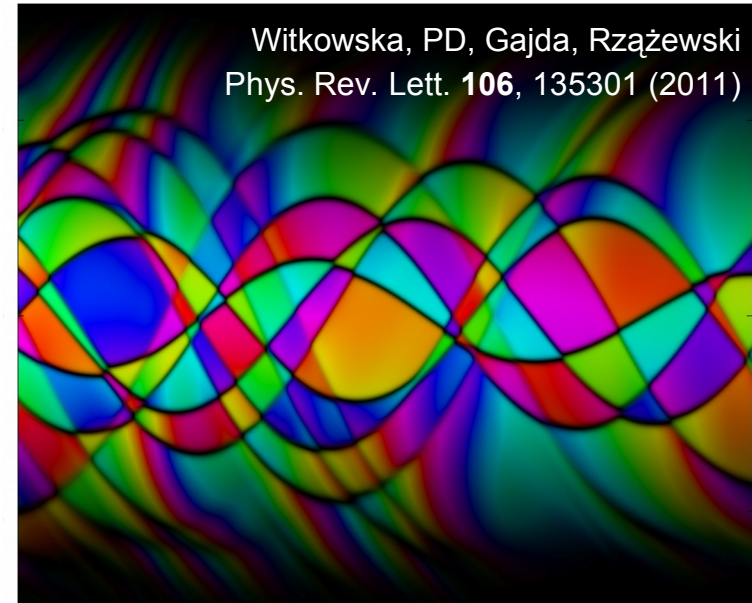
$$\mathcal{E}\phi(\mathbf{x}) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) + g|\phi(\mathbf{x})|^2 \right] \phi(\mathbf{x})$$

*Thermalised ensemble at long time*



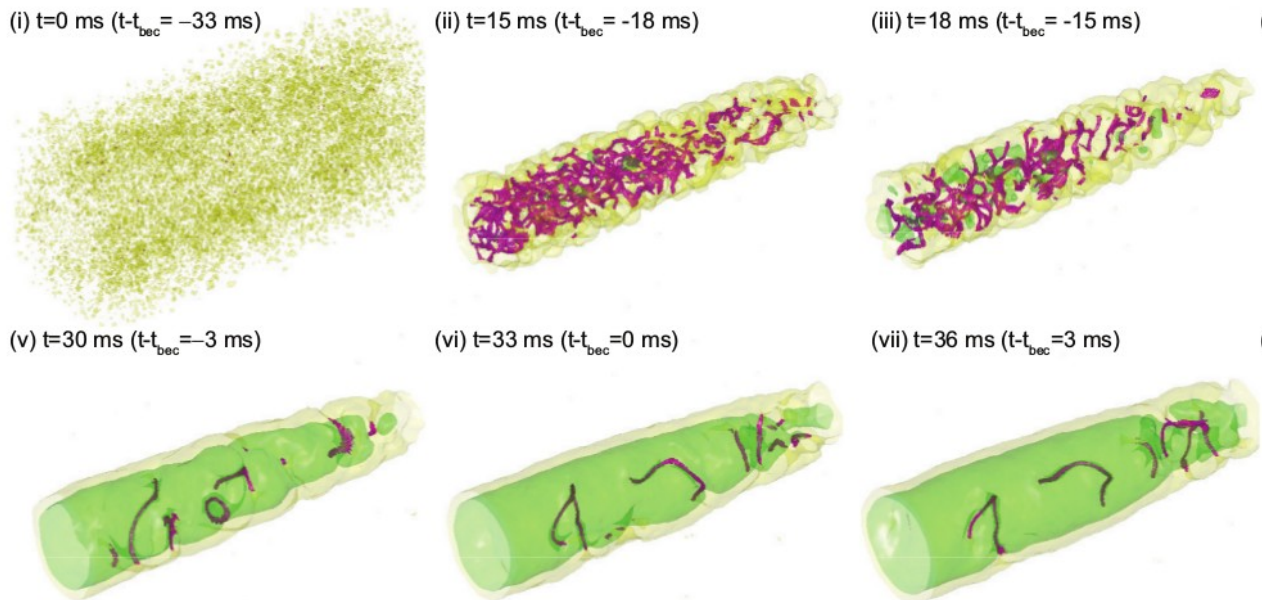
# Treatment of truly large systems

- Good scaling: makes  $10^7$  modes tractable
- Nonperturbative
- Makes  $T \gg 0$  possible
- Single shots = single realizations



Witkowska, PD, Gajda, Rzażewski  
Phys. Rev. Lett. **106**, 135301 (2011)

1d gas – phase domains after cooling



$$\langle n(x, t) \rangle$$

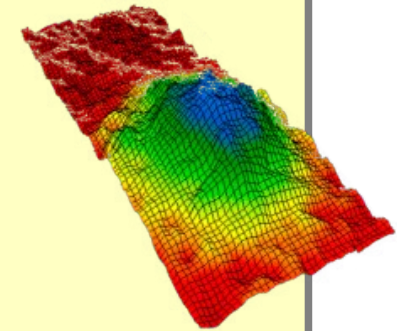
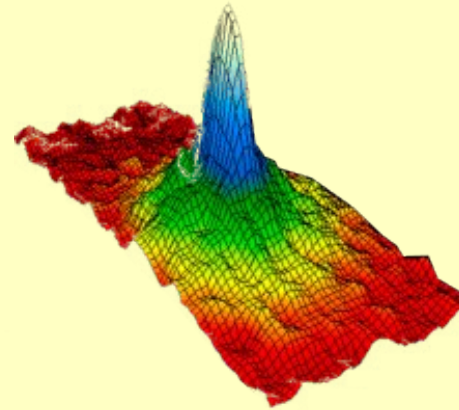
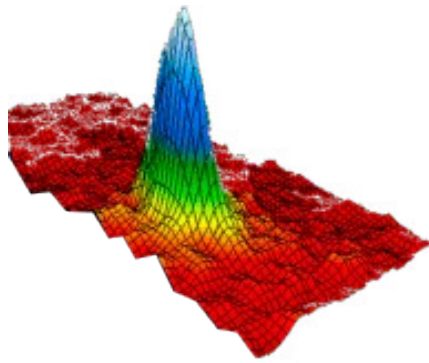
Karpiuk, PD, Bienias, Witkowska, Pawłowski,  
Gajda, Rzażewski, Brewczyk  
Phys. Rev. Lett. **109**, 205302 (2012)

$$n(x, t)$$

1d gas – thermal equilibrium

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

# Thermal clouds - Classical fields essential



$T=0$

1 mode  
GPE

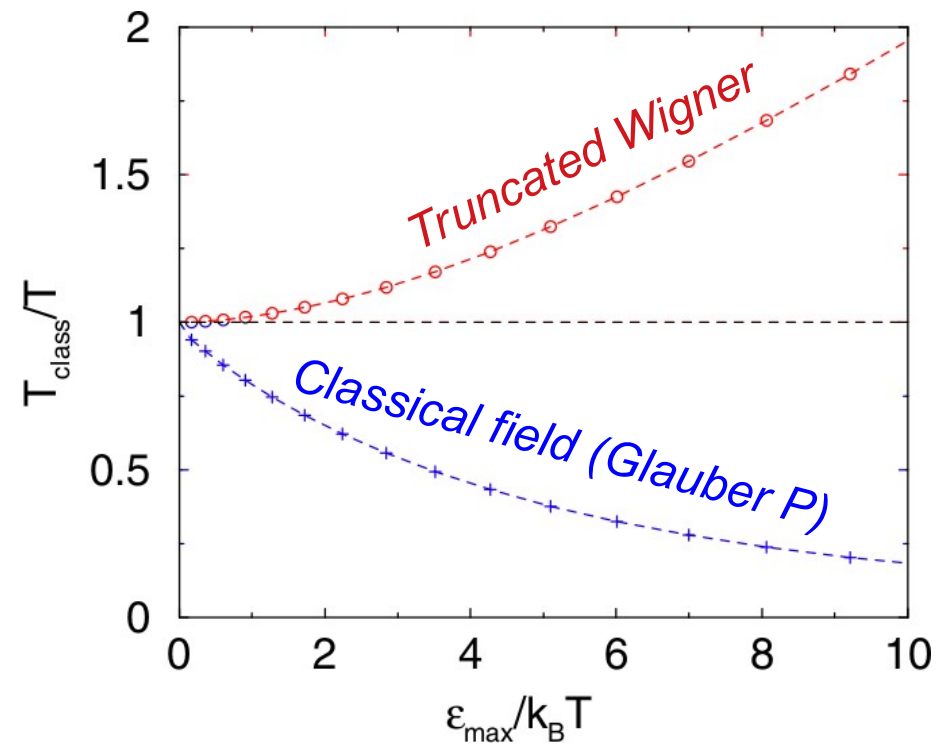
*Bogoliubov*  
few modes  
perturbative

*Classical fields, ZNG*  
zillions of modes  
non-perturbative

$T=T_c$

# However, problem 1: tainted thermalisation

*Annoyingly:  
Long time equilibrium temperature  
depends on cutoff*

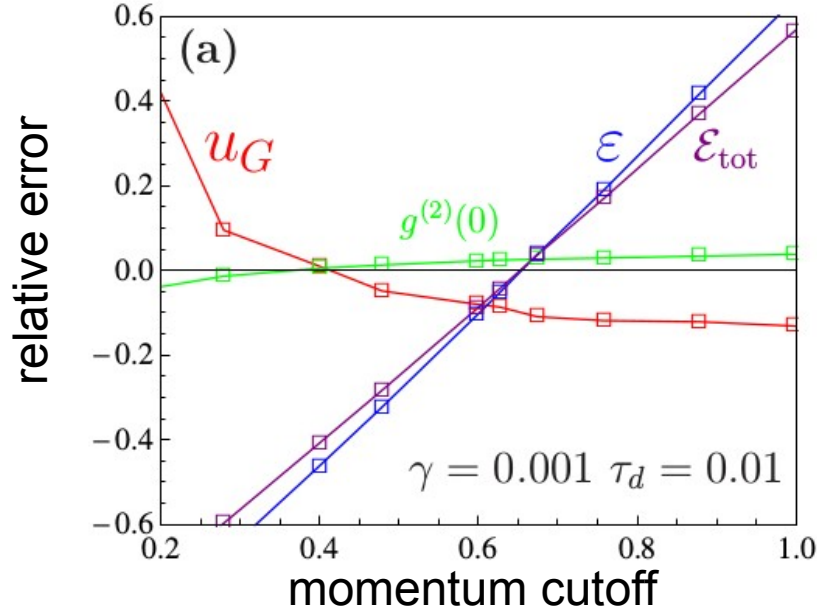


Sinatra, Lobo, Castin, J Phys B **35**, 3599 (2002)

- Stationary ensemble reached at long times can be bogus
- Will CERTAINLY be bogus if lattice is too fine (momentum cutoff too high)

# Problem 2: Cutoff dependence

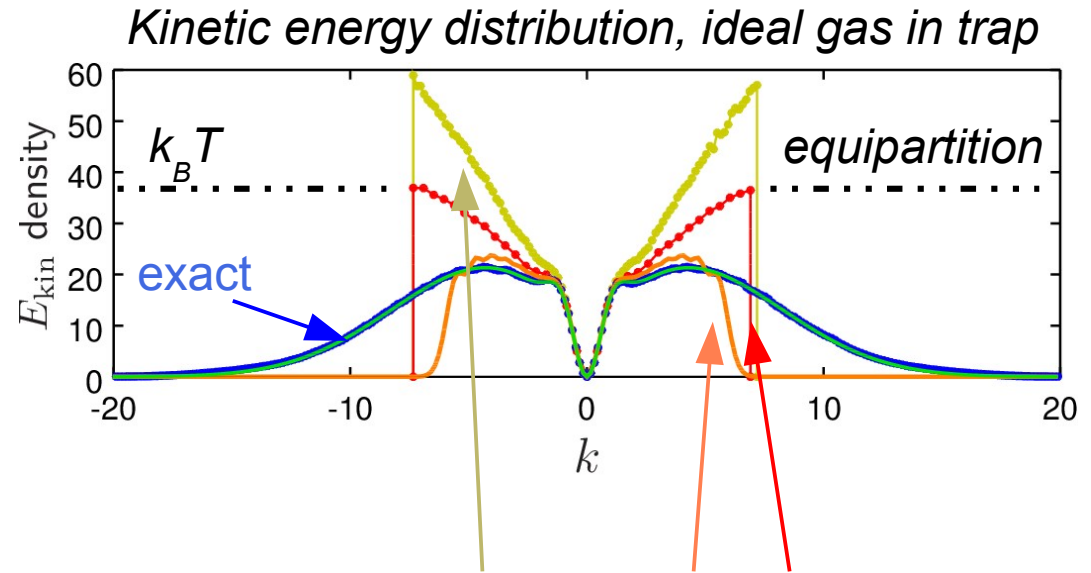
*Different observables depend differently on cutoff*



PRA **92**, 063620 (2015)

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

PRA **98**, 023622 (2018)



Various bases with "optimal" cutoff

The end result: results tend to be qualitative only :-)

Studied by many:

Witkowska, Gajda, Rzażewski, PRA **79**, 033631 (2009)

Karpiuk, Brewczyk, Gajda, Rzażewski, PRA **81**, 013629 (2010)

Zawitkowski, Brewczyk, Gajda, Rzażewski, PRA **70**, 033614 (2004)

Bradley, Blakie, Gardiner, J Phys B **38**, 4259 (2005)

Cockburn, Proukakis, PRA **86**, 033610 (2010)

and the list goes on ...

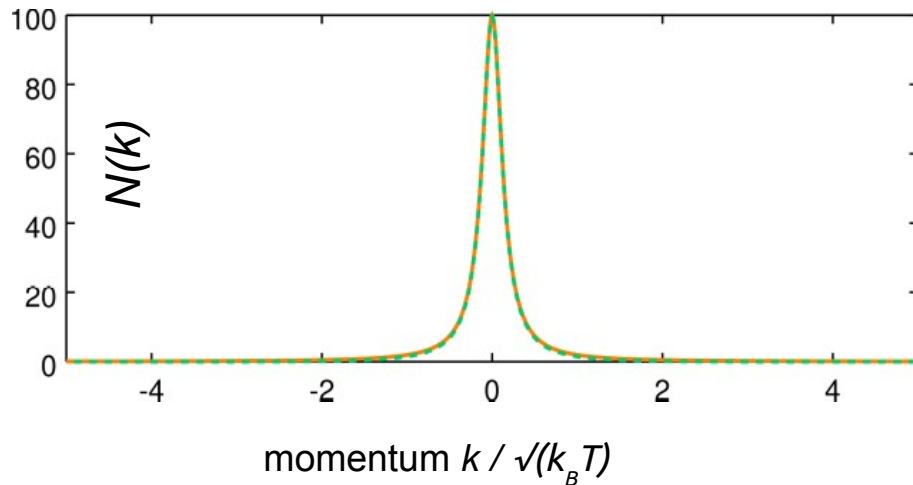
# Cause: wrong degrees of freedom = UV catastrophe

Quantum Bose-Einstein distribution  $\frac{1}{2}k_B T$  energy per *PARTICLE*

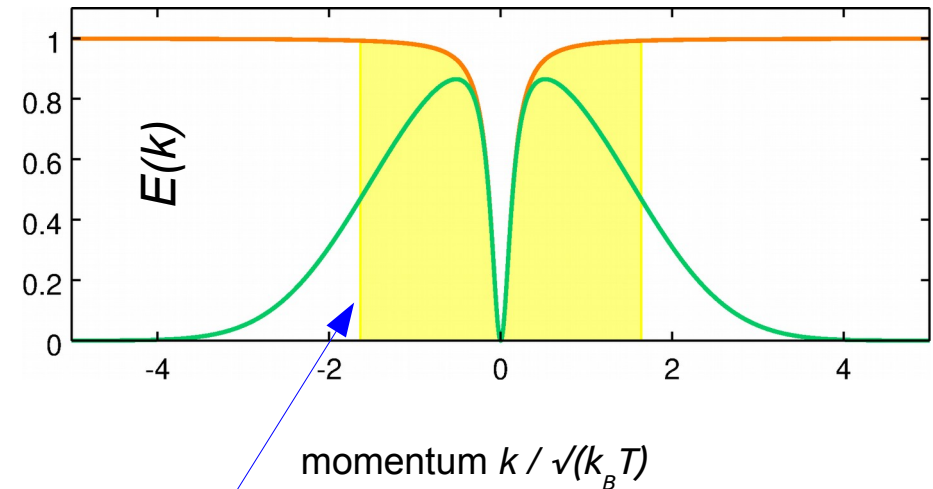
Classical field Rayleigh-Jeans distribution  $k_B T$  energy per *MODE*

→ *too many particles at high energy*

Mode occupations



kinetic energy (ideal gas)

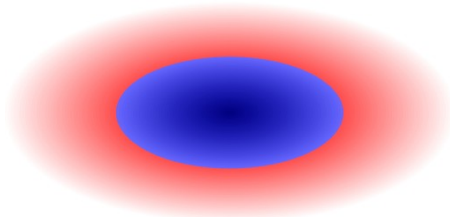


Typical cutoff choice

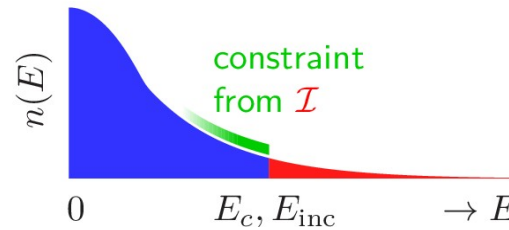


# Start of fix: stochastic Gross-Pitaevskii equation (SGPE)

real space



occupations



Commonly used alternative to plain GPE

complex noise

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

GPE

Hamiltonian evolution of  
“coherent” field

Loss rate to “incoherent” tails

Incoherent growth from tails

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

**Temperature is tamed,  
but occupation of tails is  
still UV divergent.**

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

$$\bar{N}(\omega) \rightarrow \frac{k_B T}{\omega(\mathbf{x}) - \mu}$$

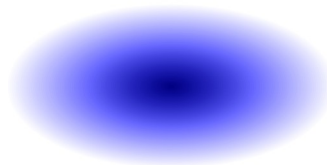
→ equipartition znówu :(

# A regularized SGPE

Preserve proper quantum occupations in master equation

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

real space



occupations

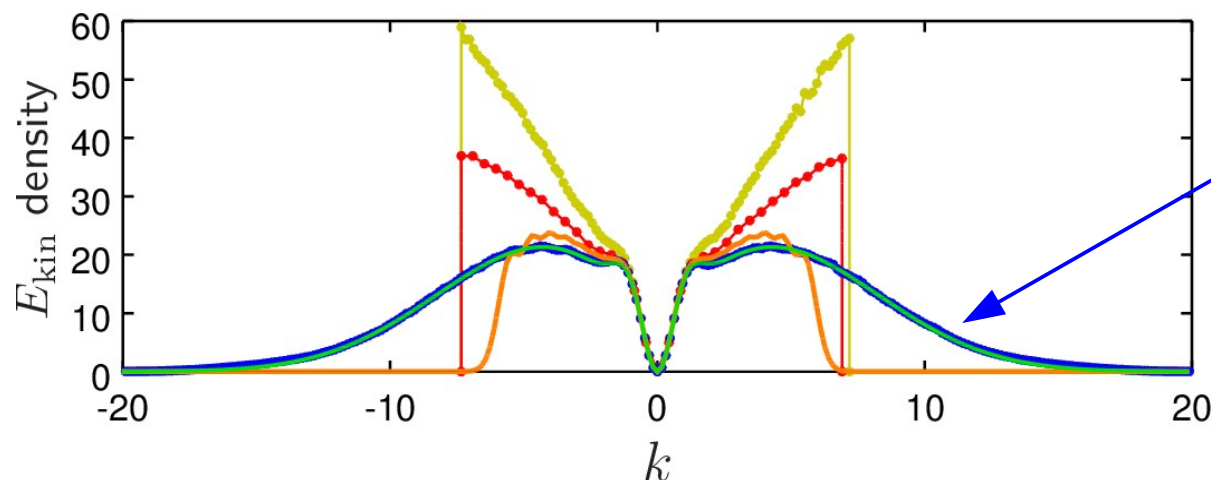


Obtain *regularised* SGPE

Details: [arXiv:1904.06266](https://arxiv.org/abs/1904.06266)

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

*Crucial development: an algorithm that keeps tractable MlogM scaling*

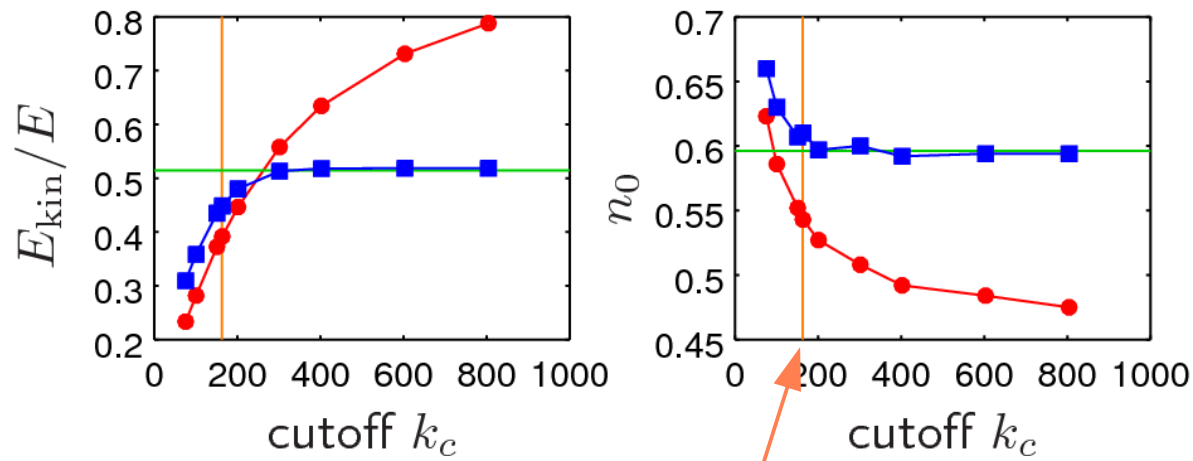
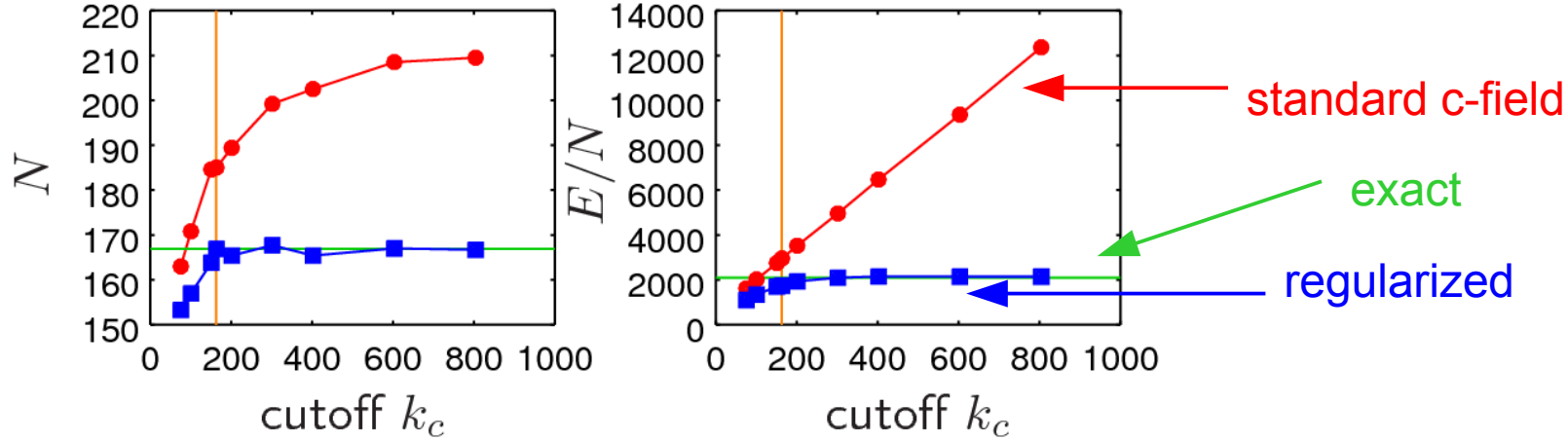


*UV divergence is gone*

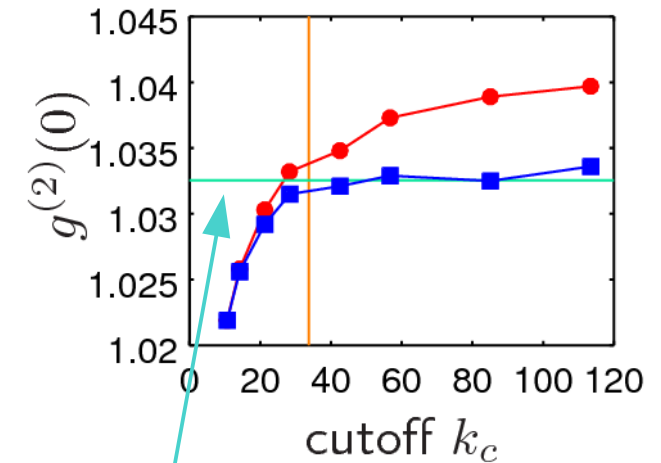
*Matches Bose-Einstein*

# Testing: 1d trapped gas (cutoff dependence)

## Ideal gas



## Interacting gas

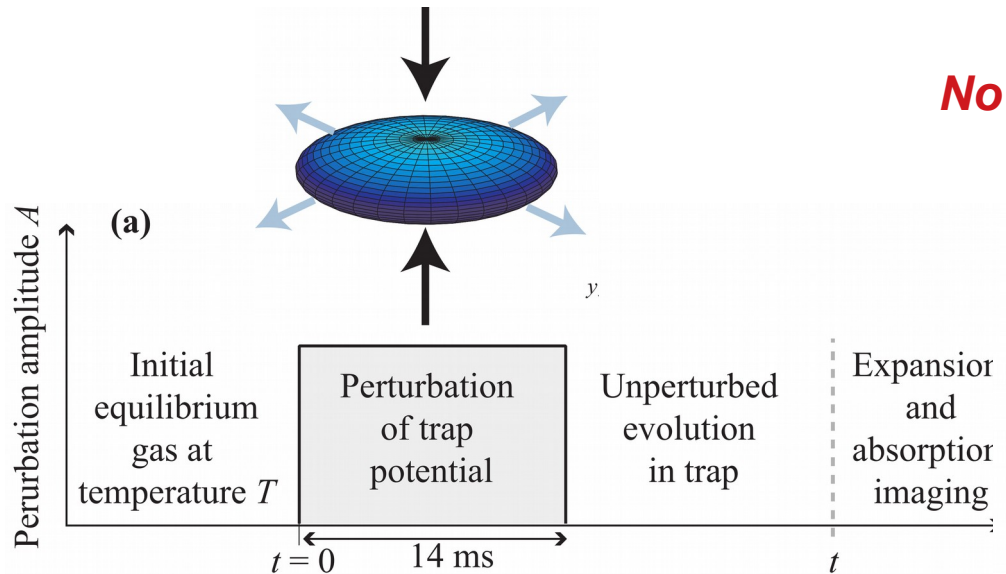


cutoff from PRA 97, 053607 (2018)

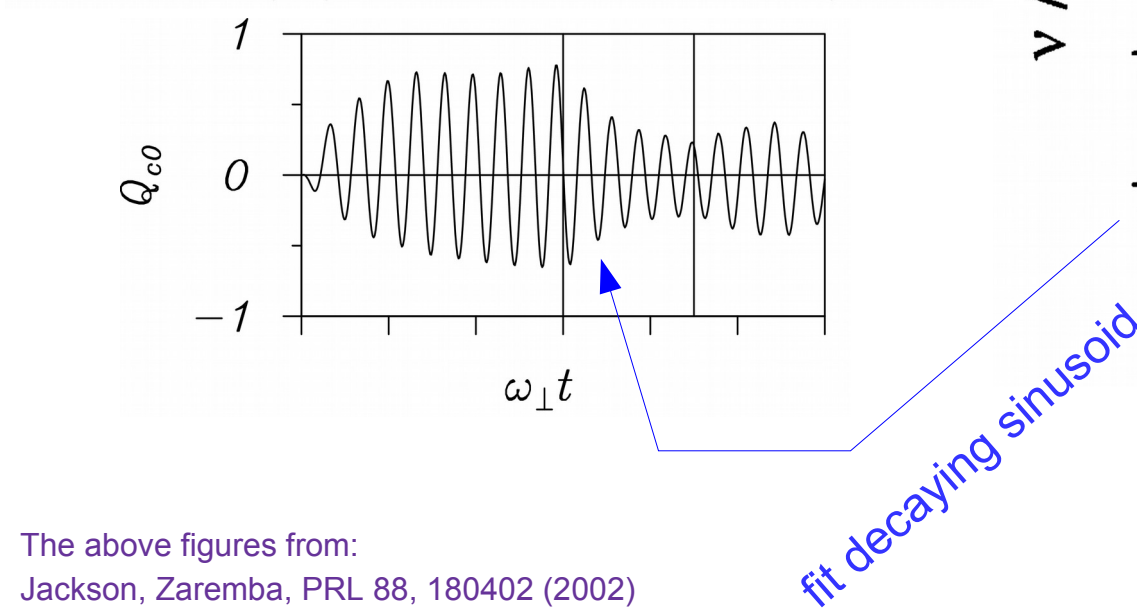
extended Bogoliubov as per Mora+Castin PRA 67, 053615 (2003)

# Litmus test for thermal cloud: $m=0$ collective mode

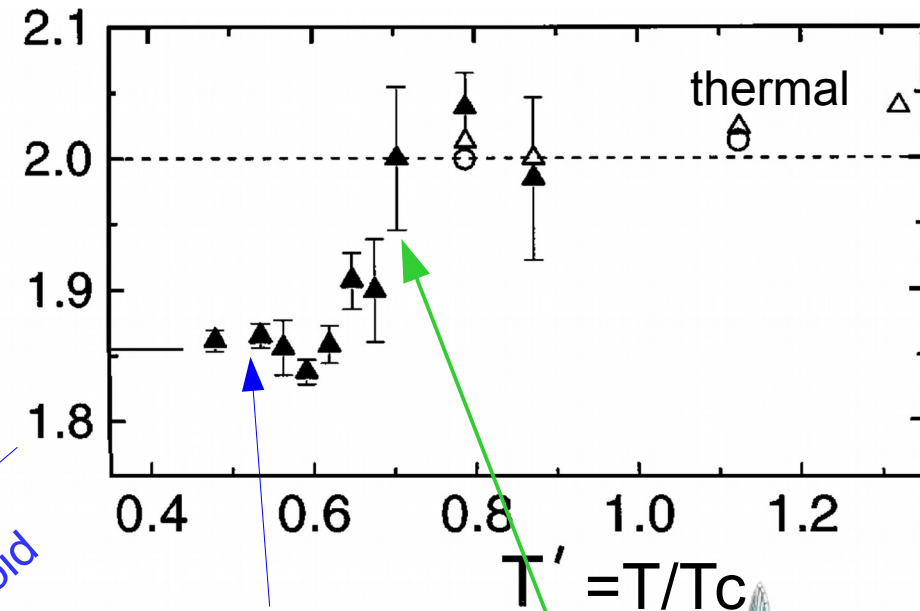
*Famous experiment:* Jin, Matthews, Ensher, Wieman, Cornell, PRL 78, 764 (1997)



**No dynamical theory has been successful in replicating this – over 20 years**



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



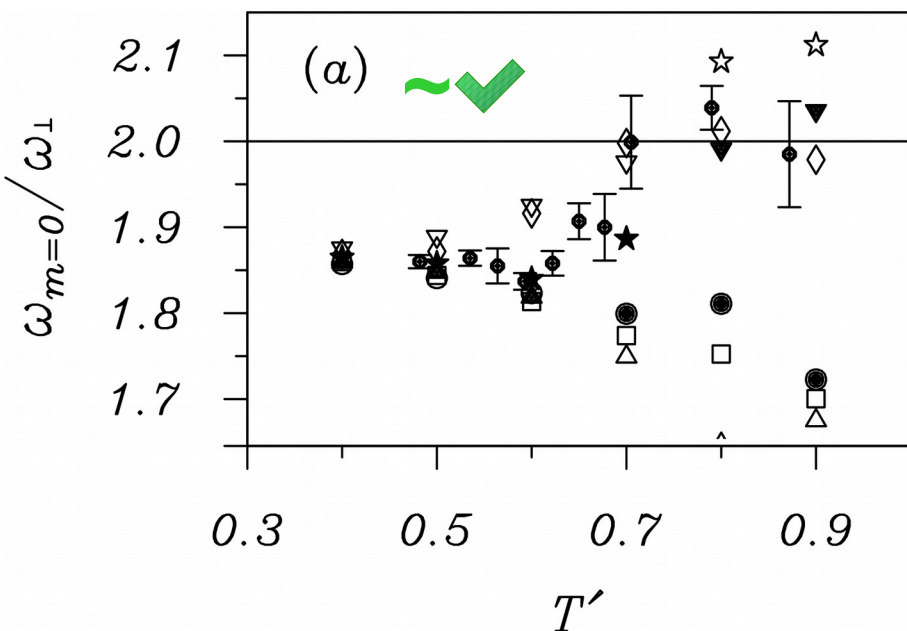
The above figures from:  
 Jackson, Zaremba, PRL 88, 180402 (2002)  
 Bezett, Blakie, PRA 79, 023602 (2009)

# Results of $m=0$ mode tests in the past

## Targeted approaches

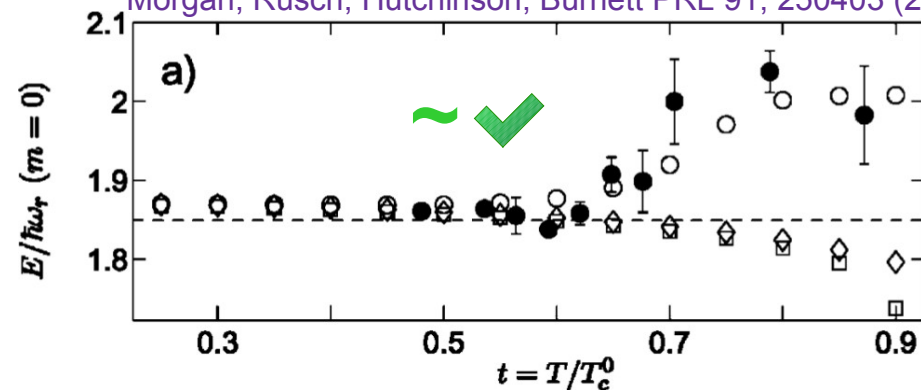
### ZNG

Jackson, Zaremba, PRL 88, 180402 (2002)



### Frequencies from “2<sup>nd</sup> order Bogoliubov”

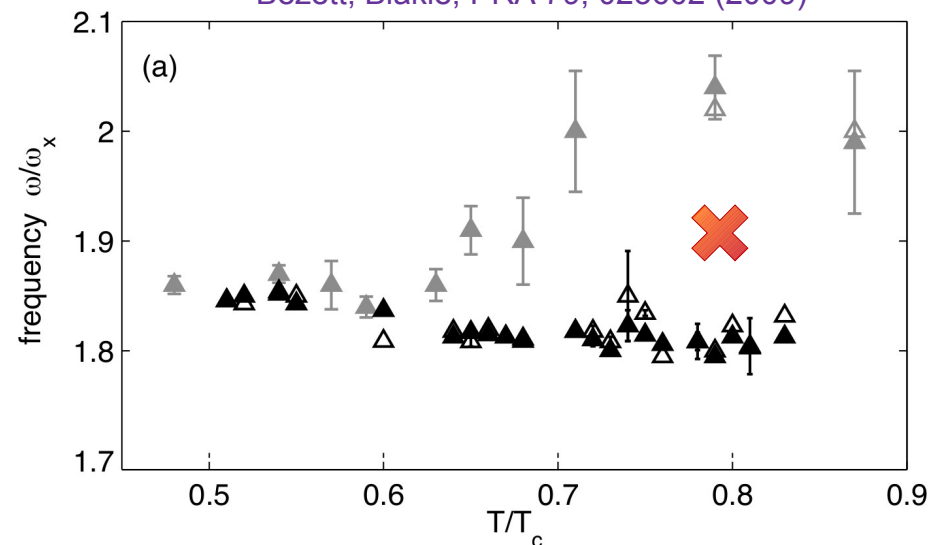
Morgan, Rusch, Hutchinson, Burnett PRL 91, 250403 (2003)



## Flexible simulations

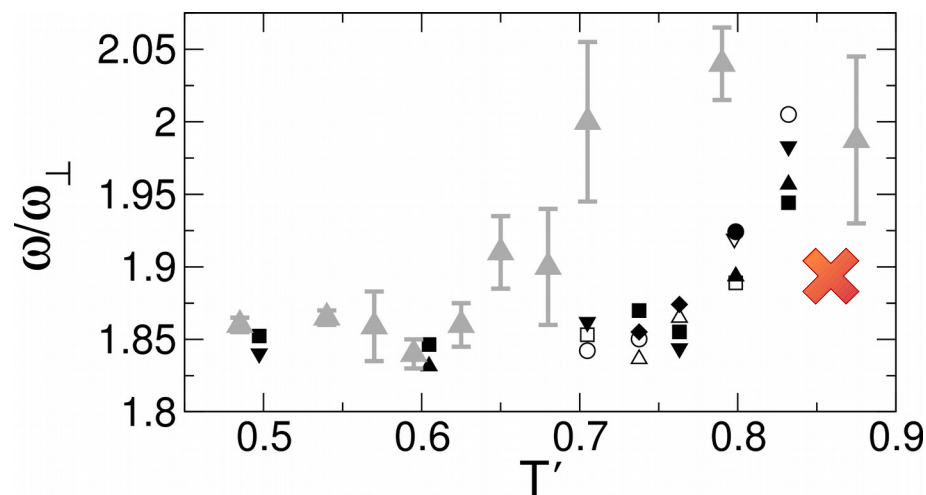
### Classical fields + HF

Bezett, Blakie, PRA 79, 023602 (2009)



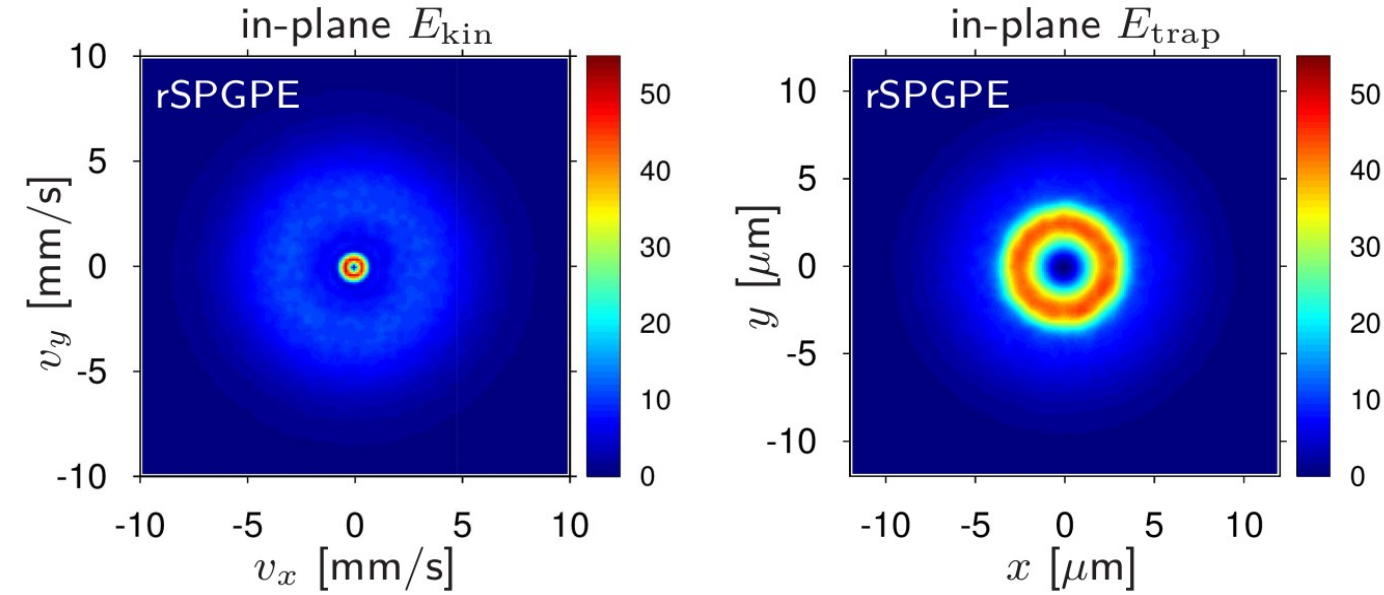
### Classical fields (higher cutoff)

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

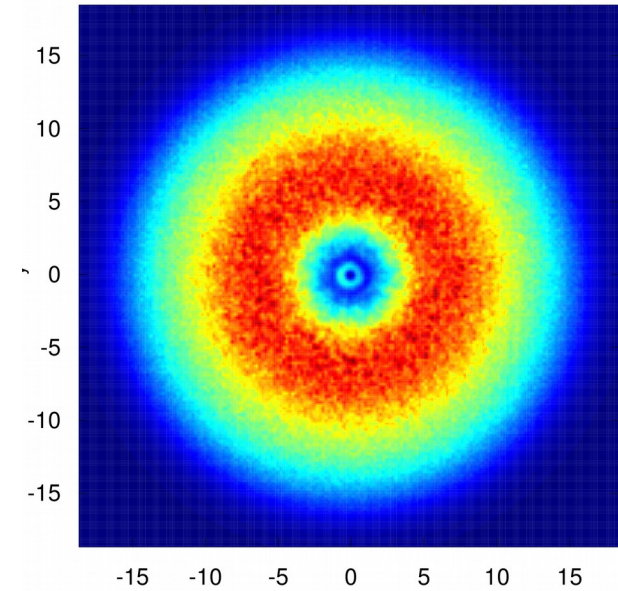


# Interacting 3d trapped gas: equilibrium ensemble

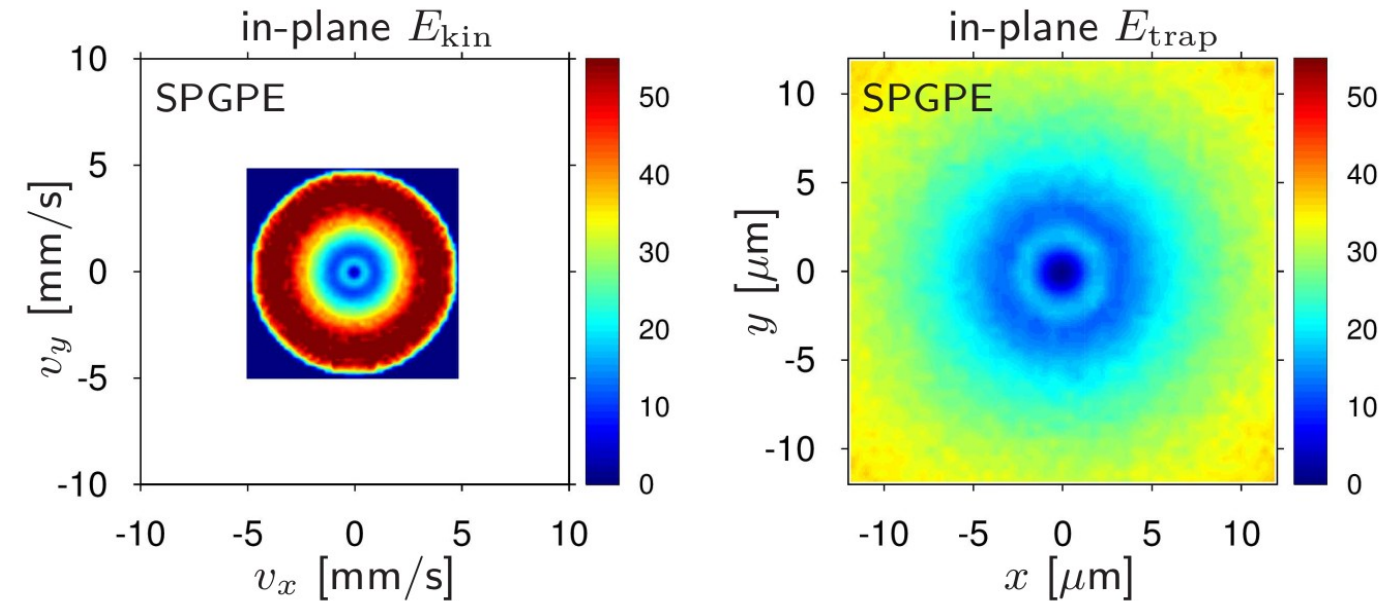
## ENERGY DENSITIES



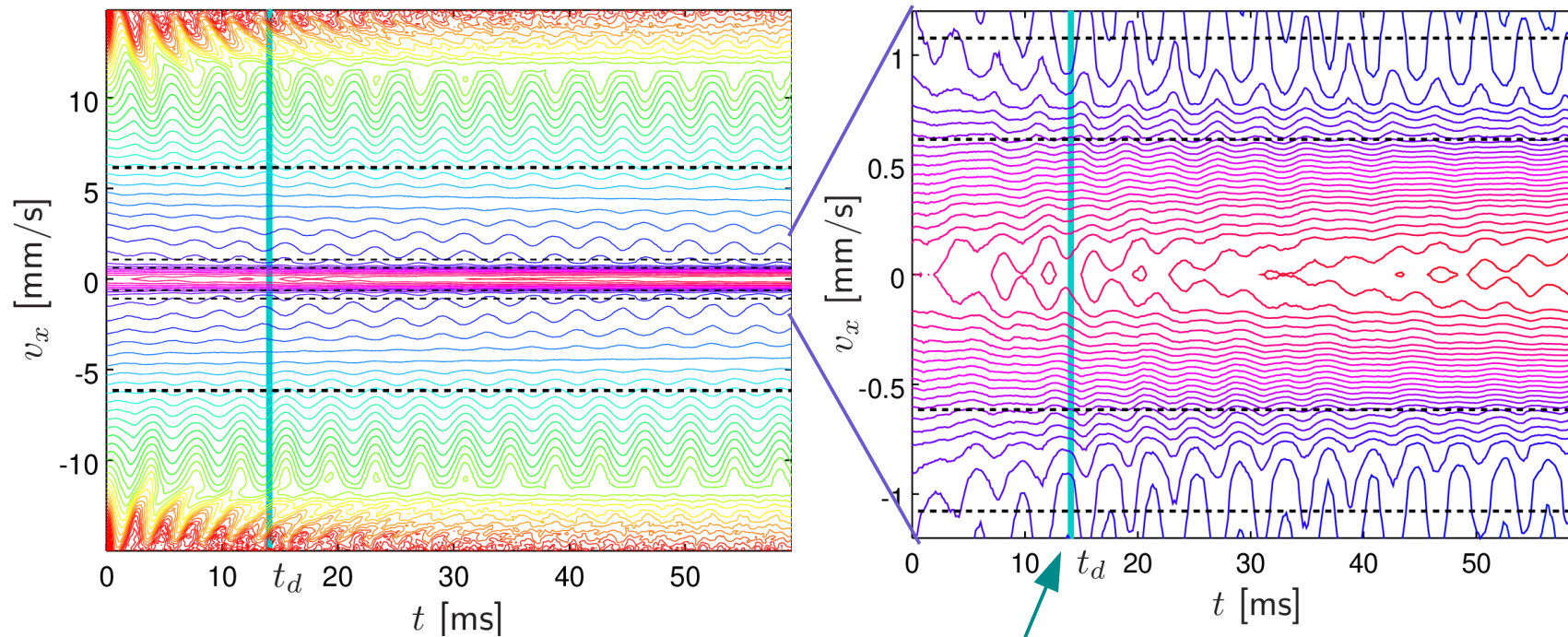
## higher temperature



## plain classical field (to scale):

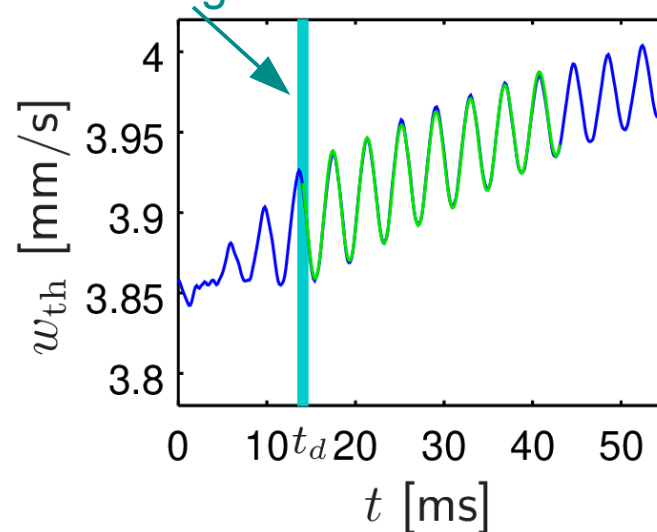
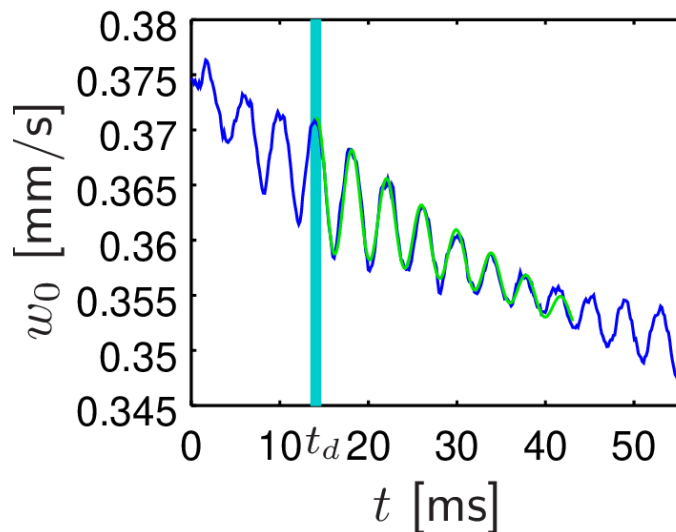


Contours of log density during evolution:

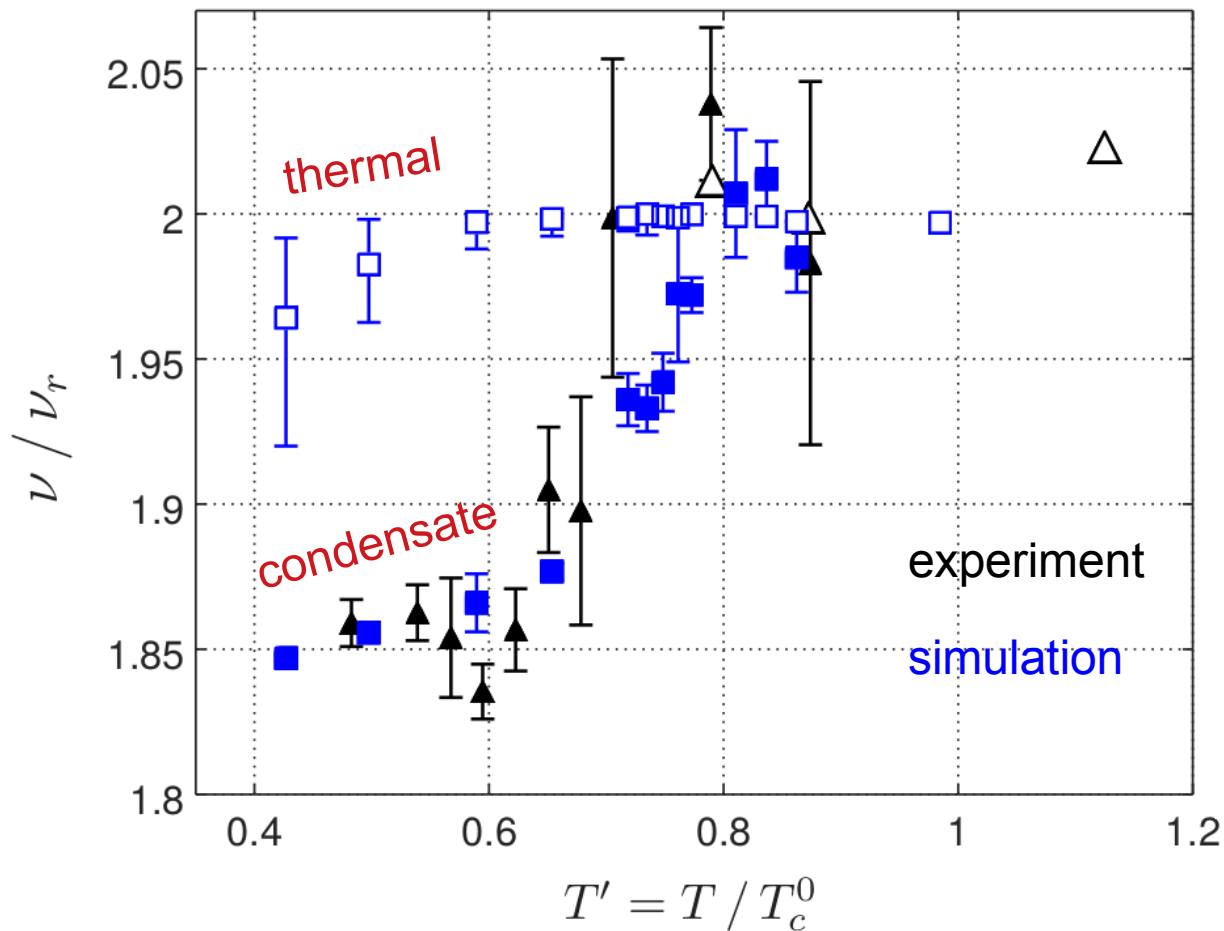


End of driving:

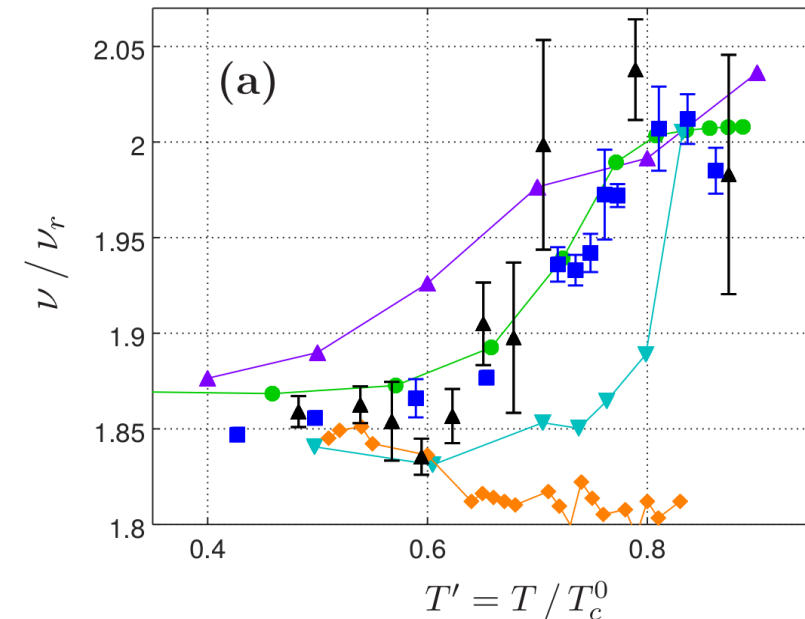
Fitting of width:



# Results: $m=0$ mode frequency



Compared to past results:



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

[This work \(2018\)](#)

[ZNG: Jackson, Zaremba, PRL 88, 180402 \(2002\)](#)

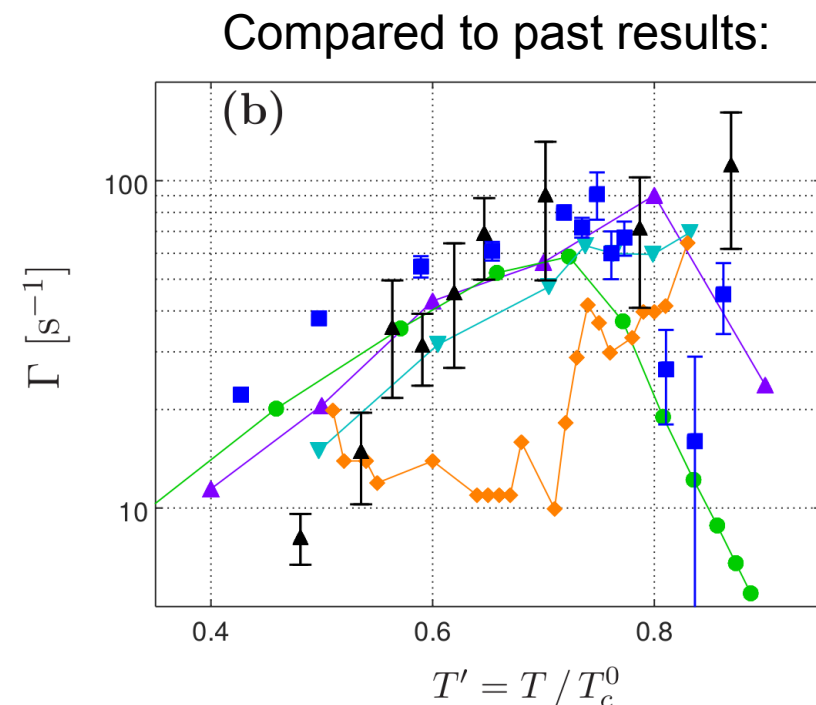
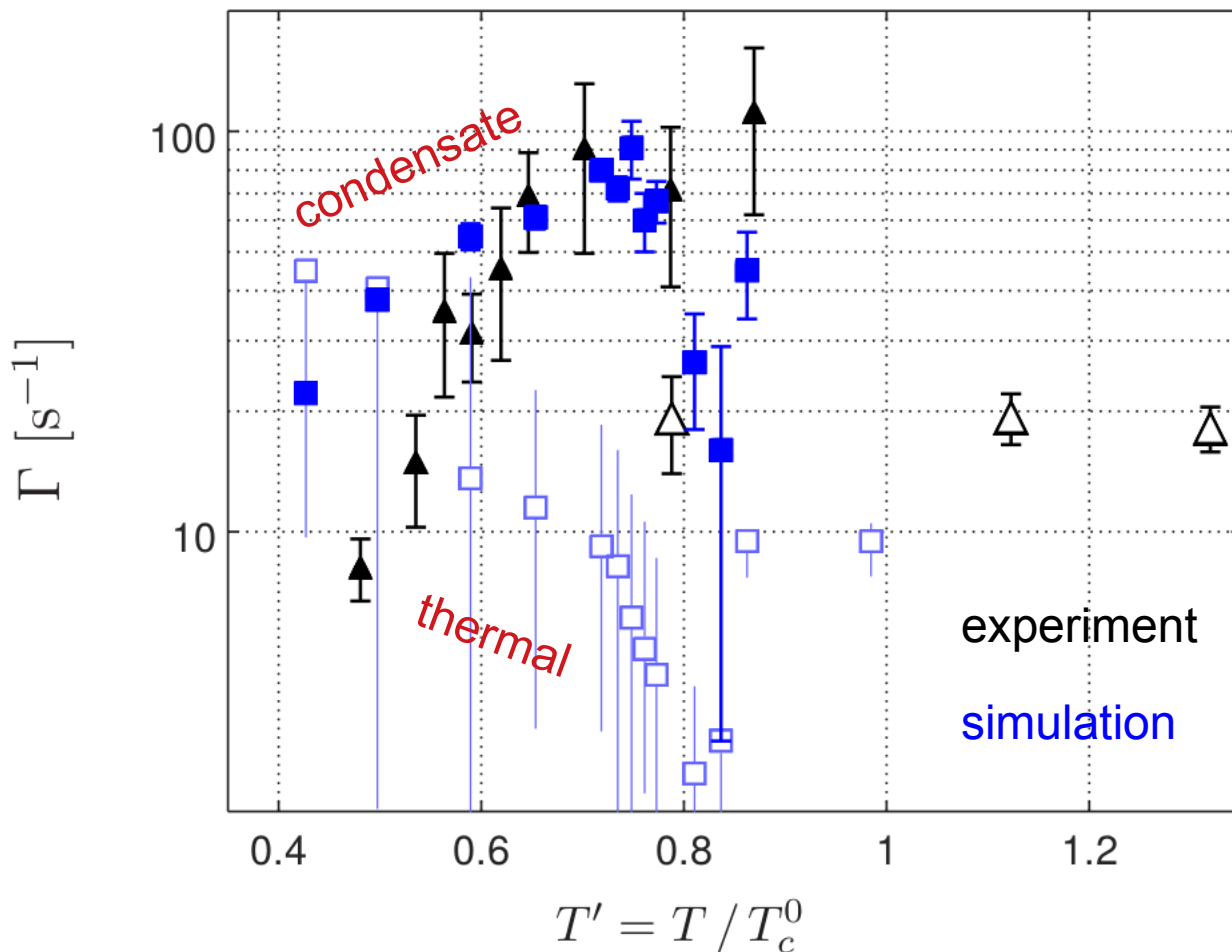
[2nd order Bogoliubov: Morgan, Rusch, Hutchinson, Burnett PRL 91, 250403 \(2003\)](#) [not a simulation]

[PGPE+HF: Bezettl, Blakie, PRA 79, 023602 \(2009\)](#)

[PGPE: Karpiuk, Brewczyk, Gajda, Rzażewski, PRA 81, 013629 \(2010\)](#)



# $m=0$ mode damping



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) **[not a simulation]**

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

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

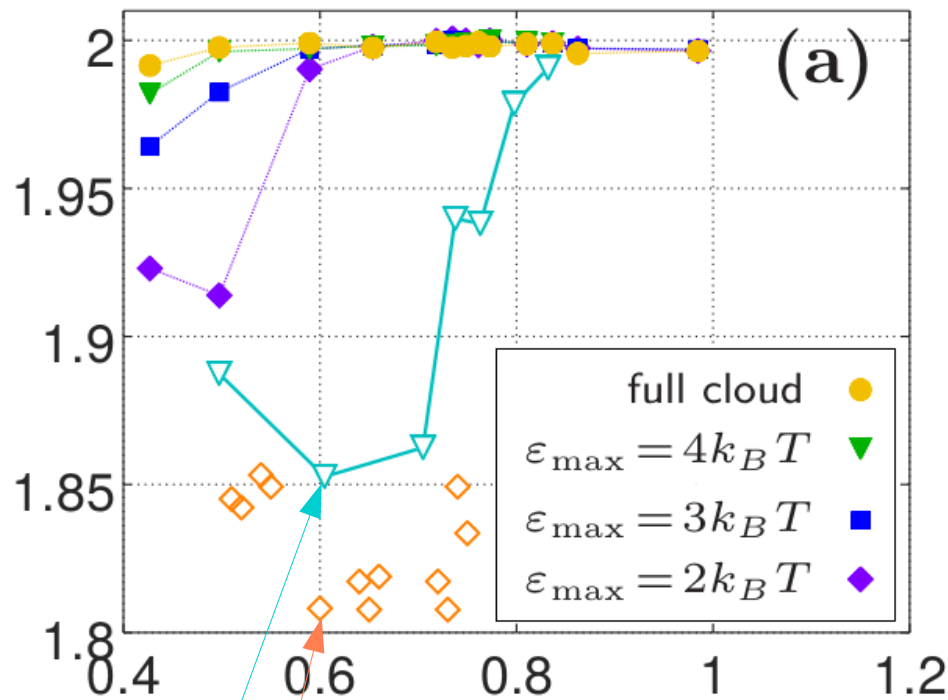
# Thermal cloud

- Since there are no artificial cutoffs, energies of  $k_B T$  and more can be investigated

e.g. it can be seen that the thermal cloud does not move as a coherent body

Frequency and damping depend on distance from the condensate

Frequency dependence on energy



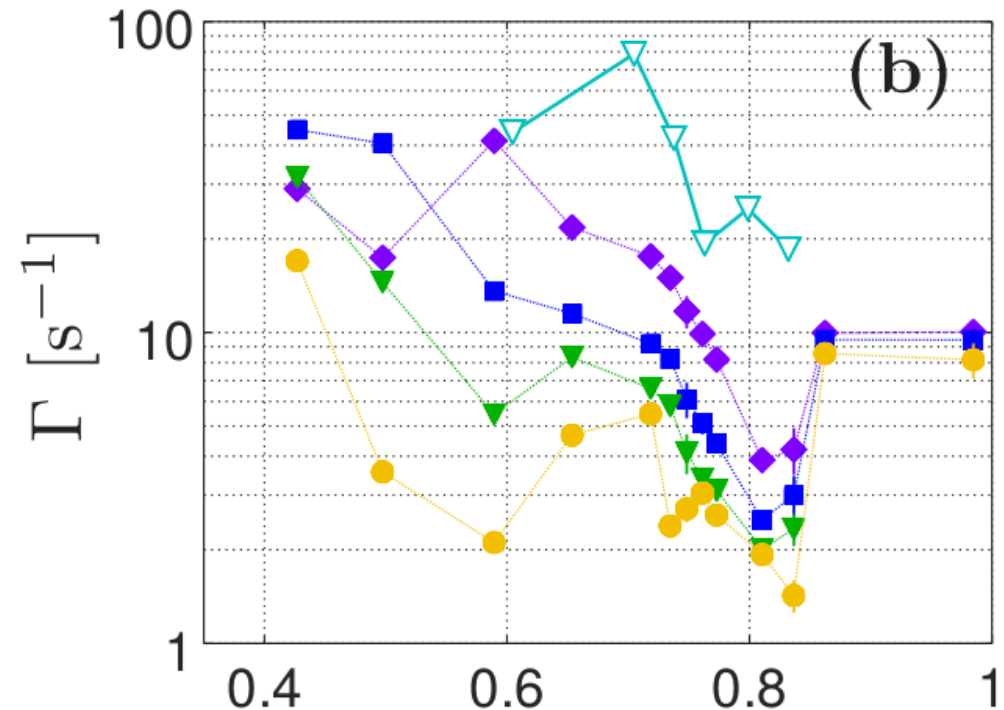
$$T' = T / T_c^0$$

Karpiuk, Brewczyk, Gajda, Rzążewski 2010

Bezett + Blakie 2009

cutoff  $1 k_B T$

Damping rate dependence on energy

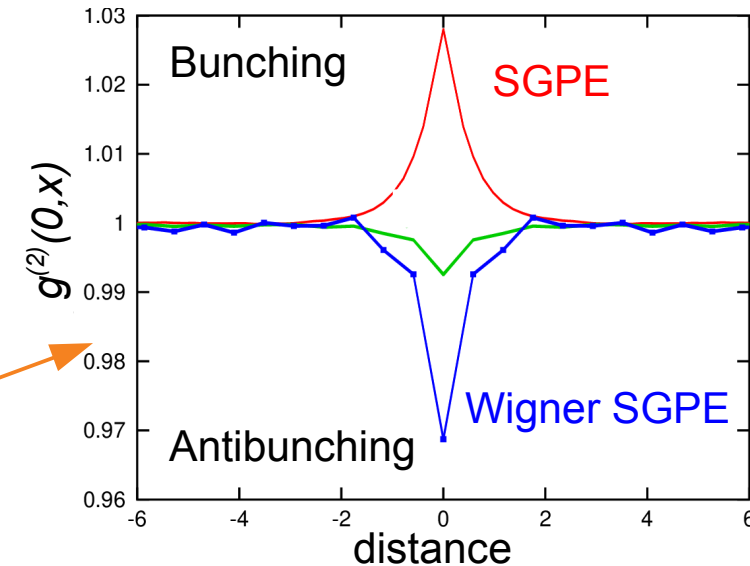


$$T' = T / T_c^0$$

cutoff  $2 k_B T$

- Accurate results with classical fields, also above  $k_B T$   
*no UV divergence, no cutoff dependence*
- 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*

arXiv:1904.06266



Thanks to many people for discussions over the years:

Nick Proukakis  
Mariusz Gajda  
Mirosław Brewczyk  
Kazimierz Rzążewski  
Emilia Witkowska

Simon Gardiner  
Crispin Gardiner  
Matt Davis  
Ashton Bradley  
Blair Blakie

Krzysztof Gawryluk  
Tomasz Karpiuk  
Thomas Gasenzer  
Andrew Daley  
Igor Nowicki