Classical matter wave fields in the interacting 1d Bose gas:
When do they apply and where to cut off?

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Aim: 1. To characterize the classical field description well enough that it can be trusted quantitatively
2. To determine in which physical regimes matter waves dominate the physics

How: (*) Determine error in many observables as a function of cutoff f_c
(**) Location of lowest $RMS(f_c)$ error gives optimal cutoff, magnitude of RMS gives a bound on accuracy

System parameters

$$\widehat{H} = \int d^3\mathbf{x}\,\left\{\widehat{\Psi}^\dagger(\mathbf{x})H_1\widehat{\Psi}(\mathbf{x}) + \frac{g}{2}\widehat{\Psi}^\dagger(\mathbf{x})^2\widehat{\Psi}(\mathbf{x})^2\right\}$$

$$H_1 = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})$$

Repulsive $g > 0$
Uniform
Open boundaries
→ grand canonical

Interaction strength

$$\gamma = \frac{m\,g}{\hbar^2\,n}$$

Relative temperature

$$\tau_d = \frac{T}{T_d} = \frac{m\,k_BT}{2\pi\hbar^2\,n^2}$$

High energy cutoff

$$f_c = k_c\frac{\Lambda_T}{2\pi} \qquad \hbar k_c = f_c\sqrt{2\pi m k_B T}$$

Observables

We studied the accuracy of:

- Density n (matched exactly)
- Temperature T (matched exactly)
- Energy per particle E
- Kinetic energy per particle $E_{\rm kin}$
- Interaction energy per particle $E_{\rm int}$
- $g^{(2)}(x\text{-}y)$ correlation (local density fluctuations)
- n_0 Occupation of lowest energy mode
- $g^{(1)}(x\text{-}y)$ correlation (phase coherence)
- Coarse-grained density fluctuations (e.g. imaging pixels)

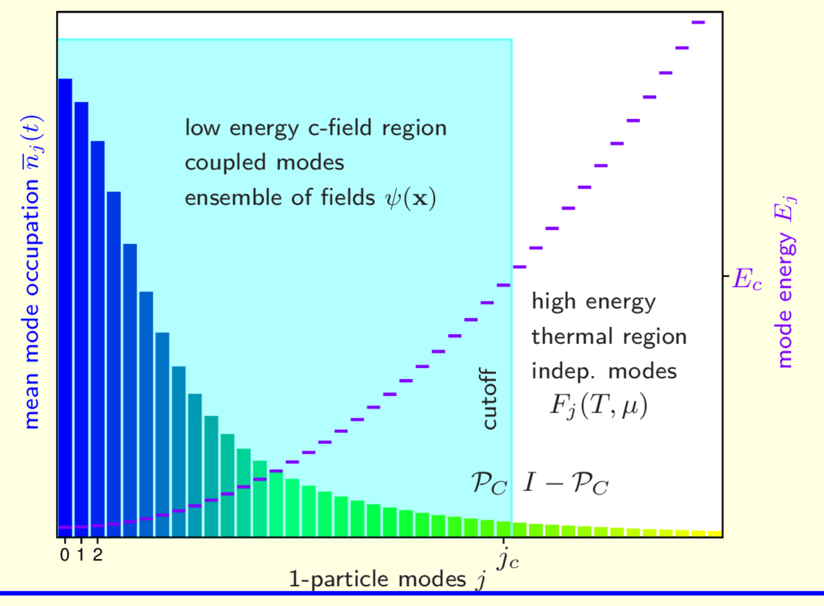
$$u_G = \lim_{L\to\infty}\frac{\mathrm{var}\,N}{\langle N\rangle} = 1 + \int dy\,\left[g^{(2)}(x,x+y) - 1\right]$$

The most sensitive observables

$$RMS = \sqrt{\max\left[\delta^{(E_{\rm kin})}_{\rm rel}, \delta^{(E_{\rm tot})}_{\rm rel}\right]^2 + \left(\delta^{(u_G)}_{\rm rel}\right)^2} \;\geq\; \max\left[\delta^{(\rm all)}\right]$$

Classical field model

Brewczyk, Gajda, Rzążewski, J. Phys. B **40**, R1 (2007)
Blakie et al. Adv. Phys. **57**, 363 (2008)



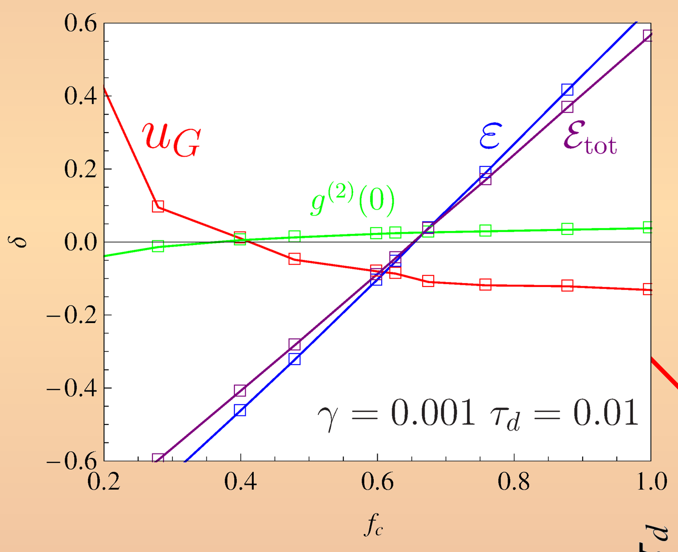
$$\widehat{\Psi}(\mathbf{x}) = \sum_j \widehat{a}_j\phi_j(\mathbf{x}) \to \Psi_C(\mathbf{x}) = \left\{\sum_{j\in\mathcal{C}}\alpha_j\phi_j(\mathbf{x})\right\}$$

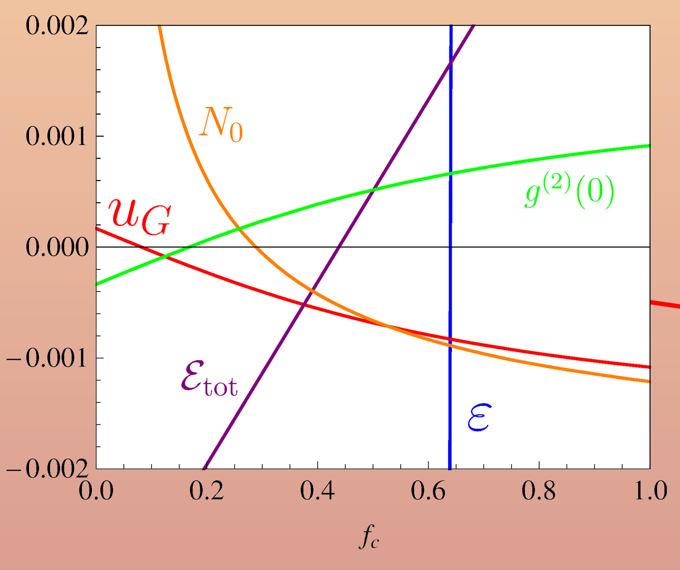
= matter waves: $i\hbar\dfrac{d\psi_C(\mathbf{x})}{dt} = \left(H_1 + g\,|\psi_C(\mathbf{x})|^2\right)\psi_C(\mathbf{x})$

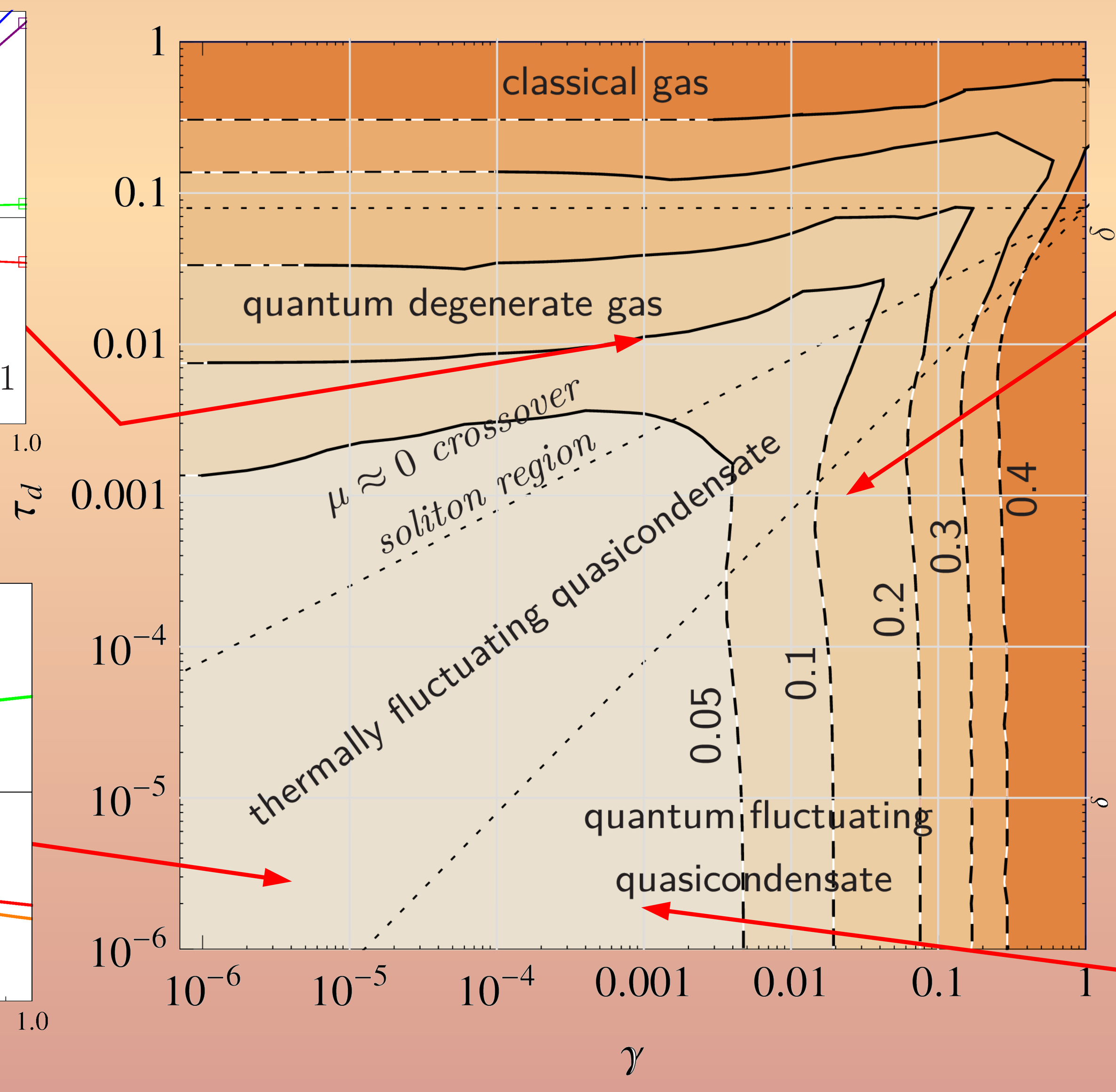
The matter wave regime

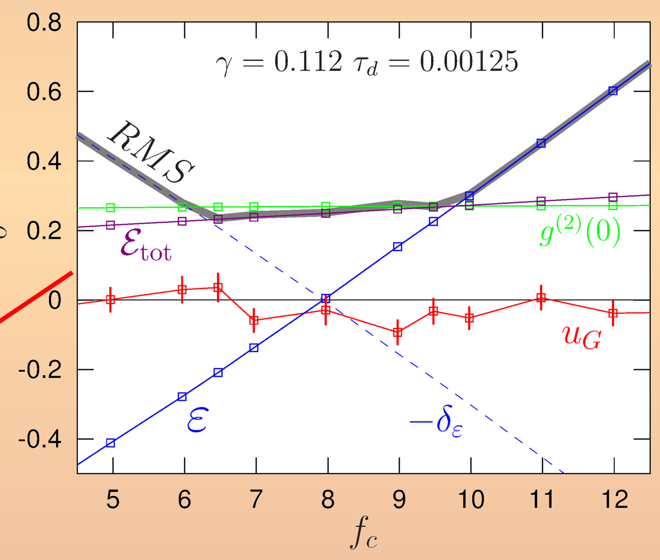
Bound on relative error:

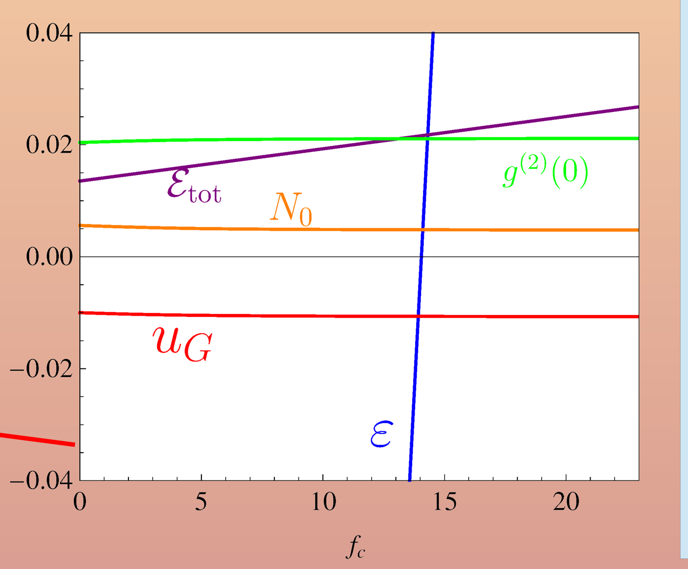
δ = relative error of c-field







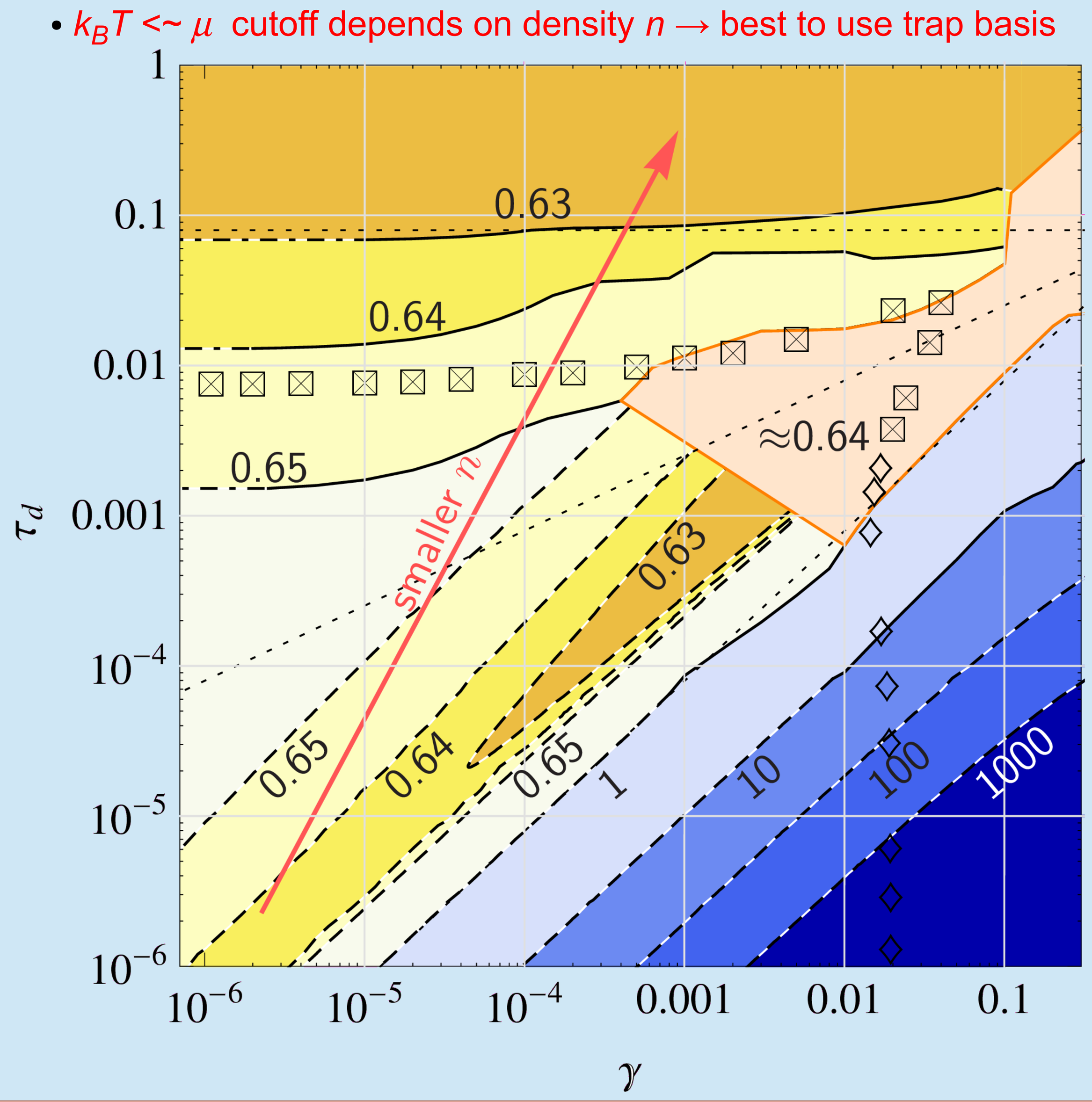




Globally optimum cutoff

Two behaviours

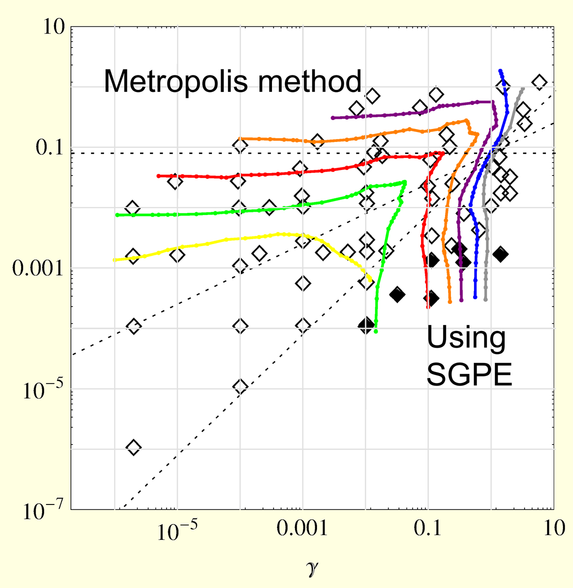
- k_BT >~ μ universal cutoff f_c ~ 0.64 → basis mostly irrelevant
- k_BT <~ μ cutoff depends on density n → best to use trap basis

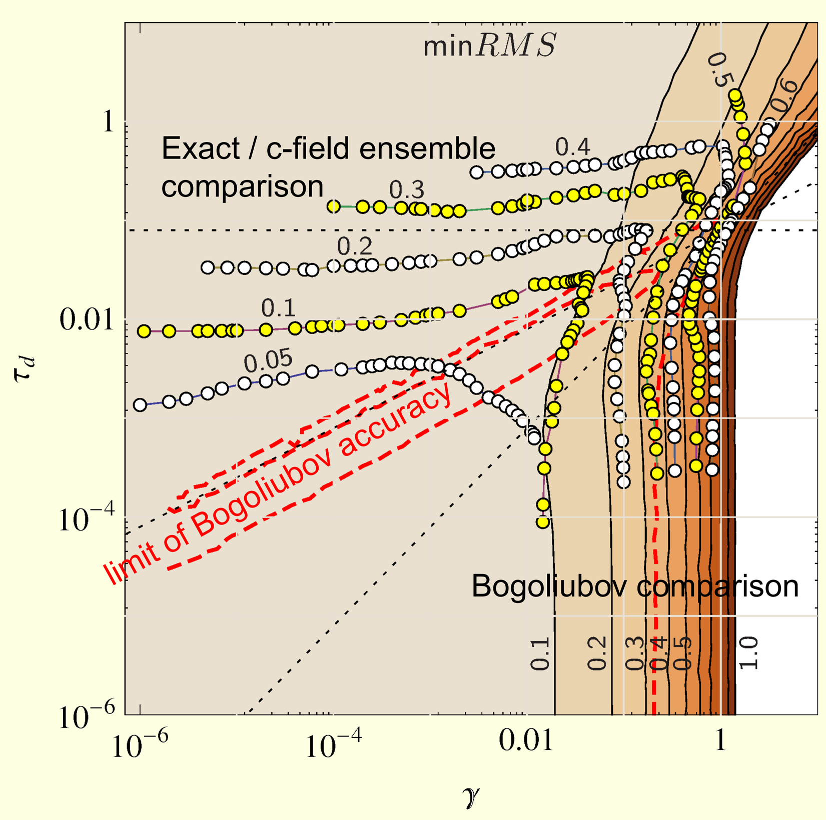


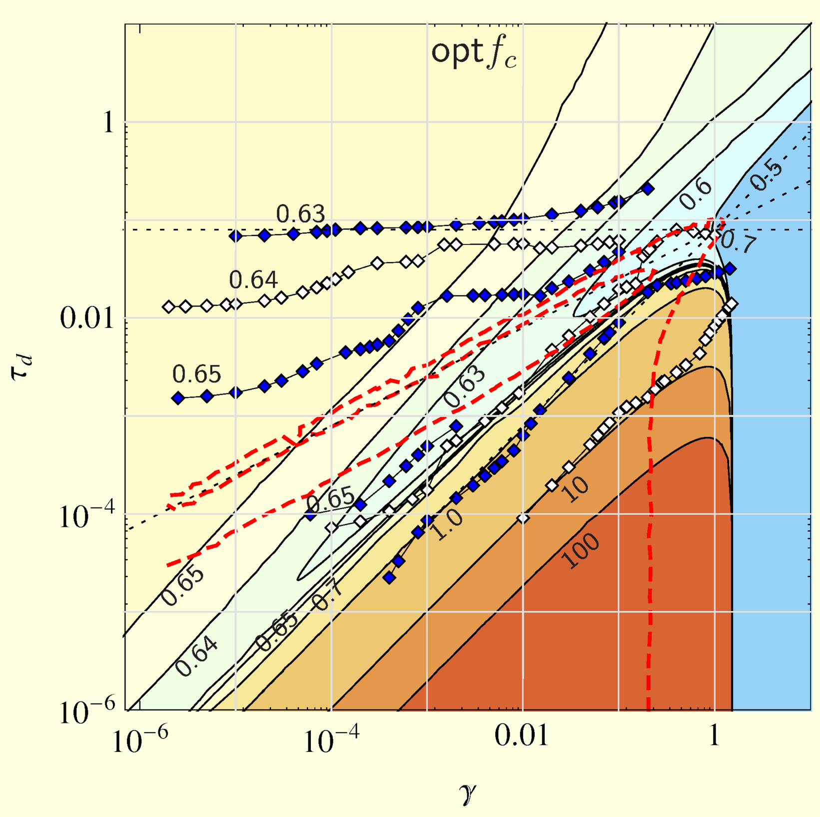
Raw data

- Exact results were obtained using the Yang-Yang solution.
  Yang, Yang, J Math. Phys. **10**, 1115 (1969)
  Plus a new algorithm to extract density fluctuations.
  Pietraszewicz, Deuar, arXiv: 1708:00031
- C-field ensembles were obtained using:
  - Metropolis algorithm
    Witkowska, Gajda, Rzążewski, Opt. Commun. **283**, 671 (2010)
  - Thermalization of SGPE equations
    Gardiner, Davis, J. Phys. B **36**, 4731 (2003)
- When k_BT <~ μ, extendend Bogoliubov was used:
  Mora, Castin, Phys. Rev. A **67**, 053615 (2003)
  - quantum results using
  - c-field results using complex amplitudes for quasiparticle modes

c-field ensembles generated





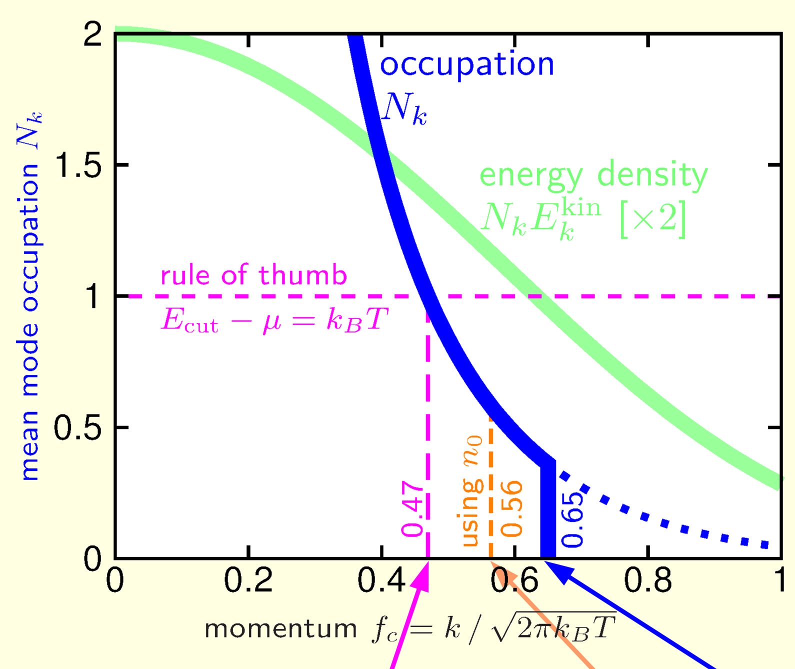


Cutoff mode occupation

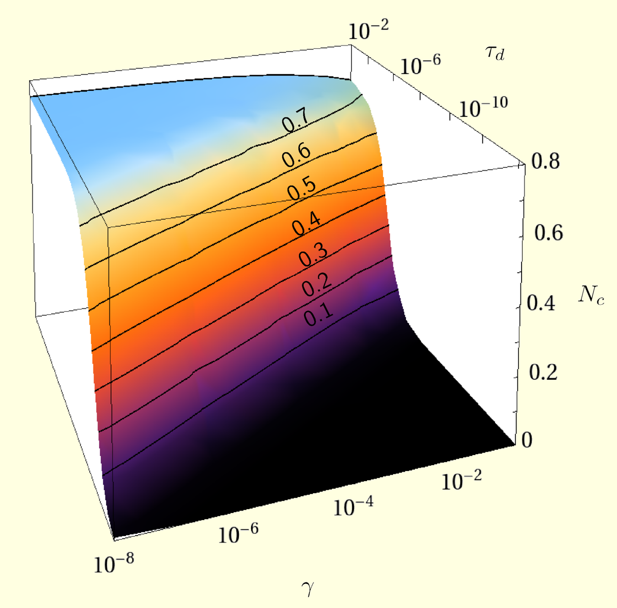
$$E_{\rm cut} = f_c^2\,\pi\,k_BT$$

$$N_{\rm cut} = \frac{1}{e^{E_{\rm cut}/k_BT} - 1} = \frac{1}{e^{\pi f_c^2} - 1}$$

In c-fields: $\approx \dfrac{k_BT}{E_{\rm cut}} = \dfrac{1}{\pi f_c^2}$



Best cutoff is significantly higher than usually used



Blakie et al. Adv. Phys. **57**, 363 (2008)

Global optimum optf_c

Witkowska, Gajda, Rzążewski, Phys. Rev. A **79**, 033631 (2009)

Closing comments

- A higher than expected cutoff is indicated. Reasons:
  - High energy modes are needed to correctly reproduce kinetic energy
  - Other observables depend on low energy modes → not adversely affected.
- 2D/3D: can be similarly studied by comparing to:
  - Extended Bogoliubov for quasicondensates Mora, Castin, Phys. Rev. A **67**, 053615 (2003)
  - Hartree Fock for the high-T limits Henkel, Sauer, Proukakis, arXiv:1701.03133

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