

The two kinds of noise when simulating quantum dynamics: thermal and quantum

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Ultracold boson gas

$$\hat{H} = \int d^3\mathbf{x} \left\{ \hat{\Psi}^\dagger(\mathbf{x}) \left[V(\mathbf{x}) - \frac{\hbar^2}{2m} \nabla^2 \right] \hat{\Psi}(\mathbf{x}) + \frac{g}{2} \hat{\Psi}^\dagger(\mathbf{x})^2 \hat{\Psi}(\mathbf{x})^2 \right\}$$

Bose field $\hat{\Psi}(\mathbf{x})$

Phase-space treatments:

$$|\Psi\rangle \longrightarrow \left\{ \psi^{(1)}(\mathbf{x}), \psi^{(2)}(\mathbf{x}), \dots, \psi^{(S)}(\mathbf{x}) \right\}$$

↑
N-body state

↑ ↑ ↑
S samples of 1-body wavefunction, or a related quantity

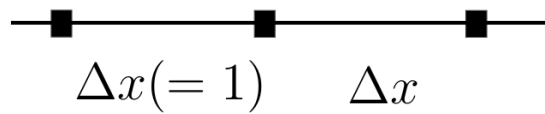
Dynamics:

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle \longrightarrow \frac{d\psi(\mathbf{x})}{dt} = A[\psi(\mathbf{x})] + \underbrace{B[\psi(\mathbf{x})]\xi(\mathbf{x}, t)}_{\text{possibly}}$$

Noise:

$$\langle \xi(\mathbf{x}, t) \xi(\mathbf{x}', t') \rangle = \frac{\delta_{tt'} \delta_{\mathbf{x}, \mathbf{x}'}}{\Delta \mathbf{x} \Delta t} \quad \langle \xi(\mathbf{x}, t) \rangle = 0$$

Quantum & thermal fluctuations: toy model



Box, periodic boundary

3 PARTICLES

$$\hat{H} = -\hat{\Psi}_j^\dagger \frac{\nabla^2}{2} \hat{\Psi}_j + \frac{g}{2\Delta x} \hat{\Psi}_j^{\dagger 2} \hat{\Psi}_j^2$$

g=0 ground state: $|\Psi_G\rangle = |300\rangle$

3 particles in state ϕ_0
0 particles in state ϕ_1
0 particles in state ϕ_2

g=0.3 ground state:

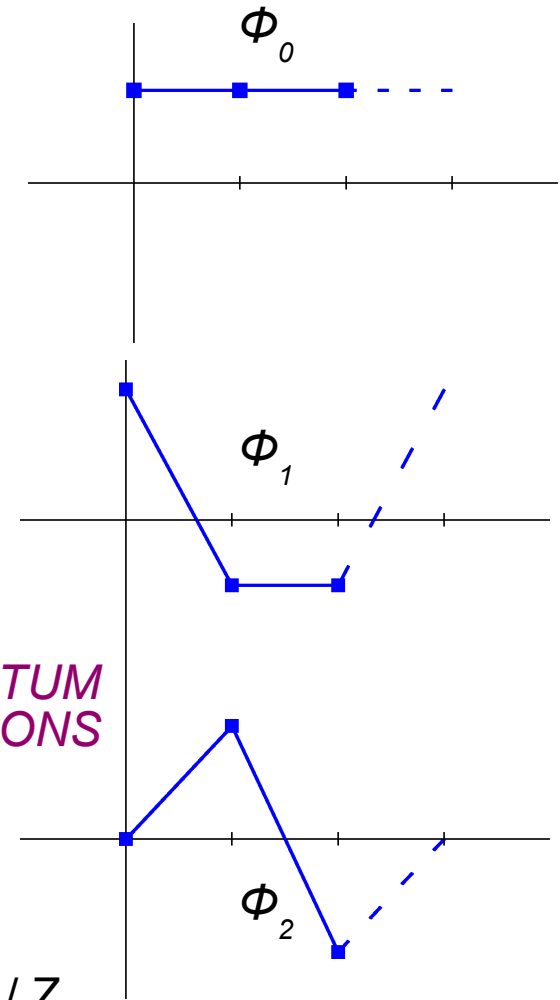
$$|\Psi_G\rangle = 0.997 |300\rangle$$

$$+ 0.052 (|102\rangle - |120\rangle) + 0.005 |012\rangle + 0.003 |030\rangle$$

samples of 1-particle density: 99.630 % ϕ_0

0.185 % ϕ_1 and ϕ_2

$T=0$ QUANTUM FLUCTUATIONS



g=0 T=0.5 thermal state

$$\rho = \{ |300\rangle\langle 300| + e^{-1.5/T} (|\lambda_1\rangle\langle\lambda_1| + |\lambda_2\rangle\langle\lambda_2| + e^{-3/T} (|\lambda_3\rangle\langle\lambda_3| + \dots) + \dots \} / Z$$

samples of 1-particle density: 96.511 % ϕ_0

1.745 % ϕ_1 and ϕ_2

$g=0$ THERMAL FLUCTUATIONS

The usual $T > 0$ methods

Bogoliubov

$$\hat{\Psi}(\mathbf{x}, t) = \phi(\mathbf{x}, t) + \hat{\delta}(\mathbf{x}, t)$$

condensate

the rest
(ASSUMED
SMALL)

- Both thermal and quantum fluctuations
- Must have dominant condensate
- Only very low temperatures

classical field: PGPE, SGPE, ...

$$\hat{\Psi}(\mathbf{x}) = \sum_j \phi_j(\mathbf{x}) \hat{a}_j \rightarrow \sum_{E_j < E_{\text{cut}}} \phi_j(\mathbf{x}) \alpha_j$$

mode amplitude operator

complex number amplitude
random phase, magnitude

- ONLY thermal fluctuations
- No need for condensate
- Almost all temperatures
- Suffer from cutoff-dependence

truncated Wigner

Like c-fields, but quantum fluctuations are added in vacuum noise initial conditions

- Both thermal and quantum fluctuations
- Any temperature
- Suffer from cutoff-dependence
- Suffer from bogus scattering as $t > 0$
- Impractical if vacuum noise too strong (i.e. modes with occupation $\sim O(1)$ studied)

positive-P

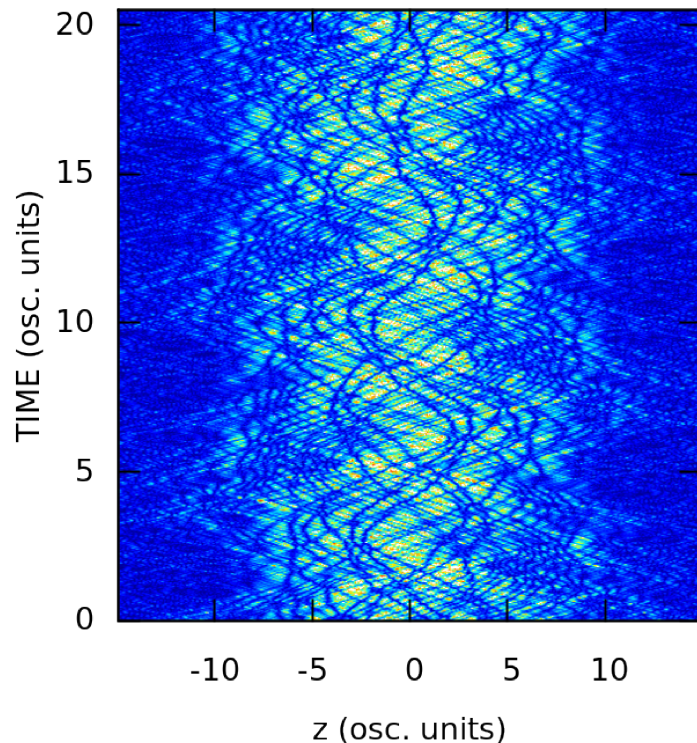
$$\hat{\rho} = \int P[\psi, \tilde{\psi}] |\psi\rangle \langle \tilde{\psi}| \mathcal{D}^2 \psi(\mathbf{x}) \mathcal{D}^2 \tilde{\psi}(\mathbf{x})$$

Probability distribution of bra & ket coherent fields $\psi(\mathbf{x}), \tilde{\psi}(\mathbf{x})$

- Full quantum mechanics
- All fluctuations
- Any temperature
- Restricted to relatively short times by noise

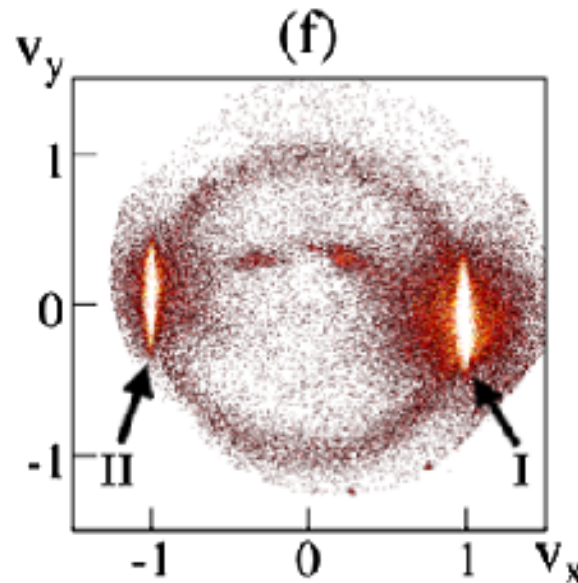
Examples of spontaneous (quantum fluctuation) phenomena at “high” temperature

Spontaneous solitons in trapped gas



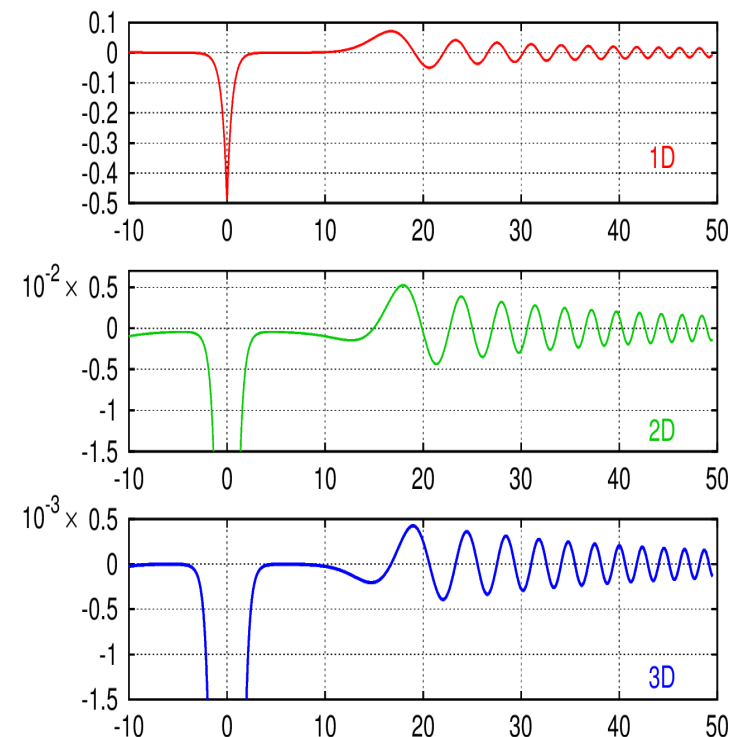
Karpiuk, PD, Bienias, Witkowska, Pawłowski, Gajda, Rzążewski, Brewczyk, PRL **109**, 205302 (2012)

Pair scattering out of colliding quasicondensates



Perrin, Chang, Krachmalnicoff, Schellekens, Boiron, Aspect, Westbrook, PRL **99**, 150405 (2007)

Pair creation in-situ after a quantum quench



PD, Stobińska, arXiv:1310.1301; Carusotto, Balbinot, Fabbri, Recati, EPJD **56**, 391 (2010)

Q: How to get thermal and spontaneous fluctuations together when:

- Temperature is too high for a condensate (Bogoliubov excluded)
- Thermal state required (positive-P excluded)
- Low occupied modes needed (truncated Wigner excluded)

T=0 STAB method – BEC collision

$$\widehat{\Psi}(\mathbf{x}, t) = \phi(\mathbf{x}, t) + \widehat{\delta}(\mathbf{x}, t)$$

(Stochastic Time-Adaptive Bogoliubov)

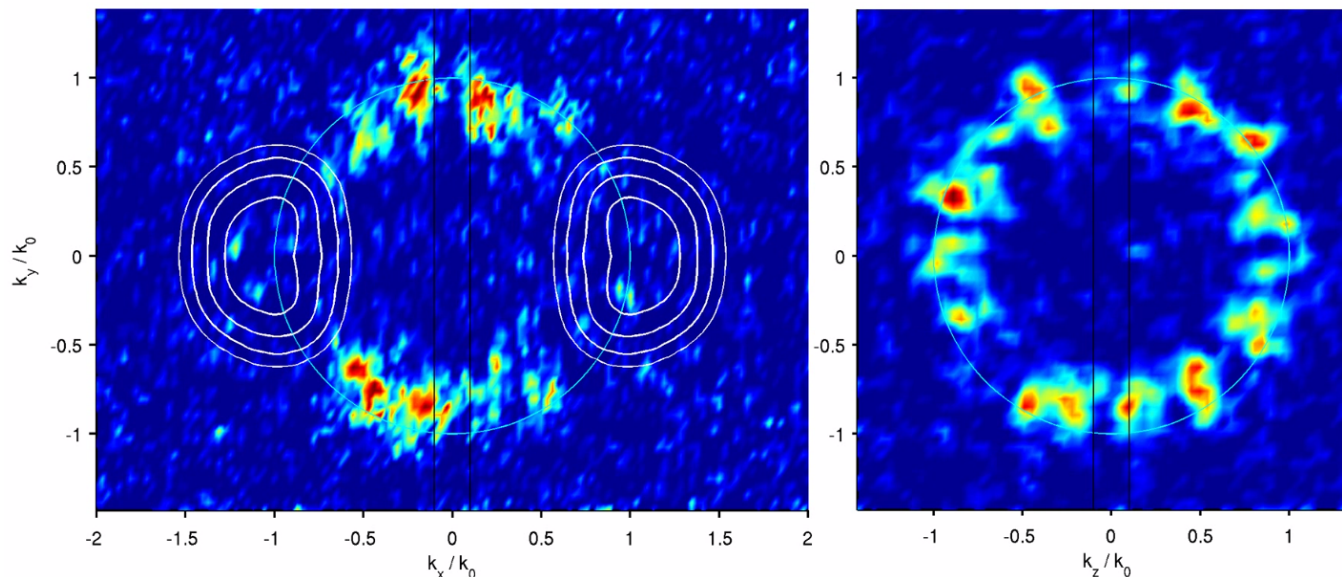
Treat condensate using GP equation

Treat $\widehat{\delta}(\mathbf{x}, t)$ using positive-P representation

$$i\hbar \frac{d\phi(x)}{dt} = [H_0(x) + g|\phi(x)|^2] \phi(x)$$

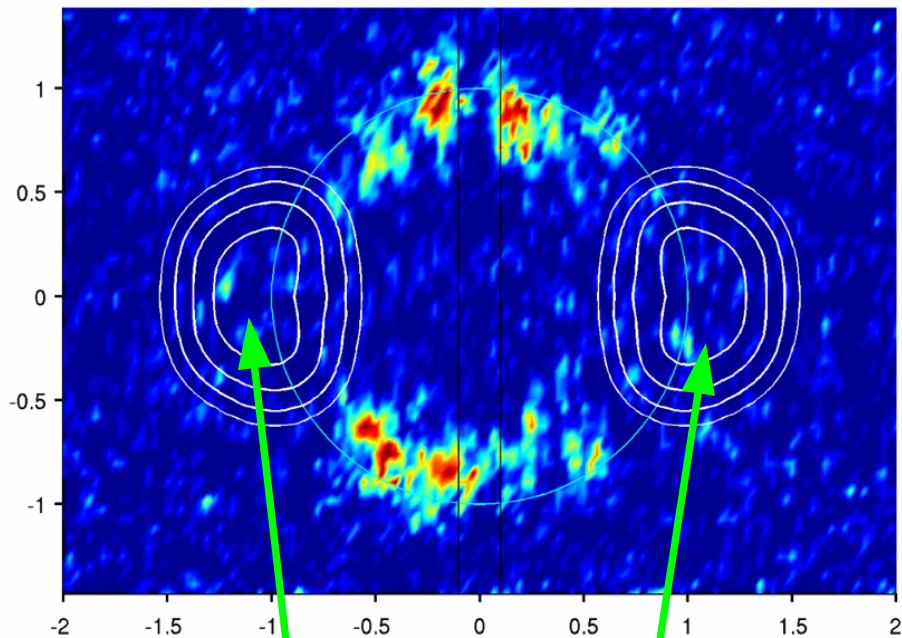
$$i\hbar \frac{d\psi(x)}{dt} = \{H_0(x) + 2g|\phi(x)|^2\} \psi(x) + g\phi(x)^2 \widetilde{\psi}(x)^* + \sqrt{i\hbar g} \phi(x) \xi(x, t)$$

$$i\hbar \frac{d\widetilde{\psi}(x)}{dt} = \{H_0(x) + 2g|\phi(x)|^2\} \widetilde{\psi}(x) + g\phi(x)^2 \psi(x)^* + \sqrt{i\hbar g} \phi(x) \widetilde{\xi}(x, t)$$

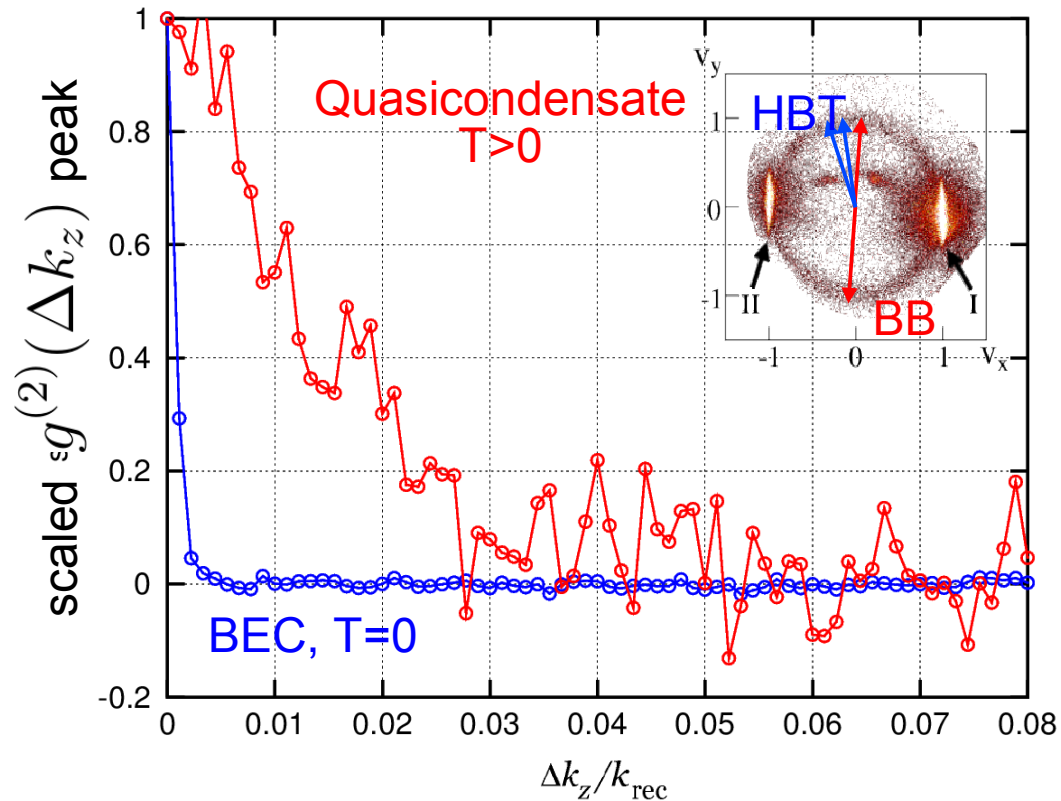


PD, Wasak, Zin,
Chwedenczuk,
Trippenbach, PRA **88**,
013617 (2013)

T>0 Adaptation



Use c-field ensemble for $\phi(\mathbf{x}, t)$



Westbrook group experiment,
e.g. Kheruntsyan, Jaskula, PD, Bonneau, Partridge, Raudel, Lopes, Boiron, Westbrook, PRL **108**, 260401 (2012)

method	coherence length l_ϕ	Pair correlation $g^{(2)}(k, -k)$ width
EXPERIMENT	$\sim 45\mu\text{m}$	$0.017 k_{\text{rec}}$
$T = 0$ STAB	∞	$0.0004 k_{\text{rec}}$
$T > 0$ adaptation	$45\mu\text{m}$	$0.013 k_{\text{rec}}$

Caveat:
Scattered field is only accurate
When well separated from source

In situ situations - SGPE

$$i\hbar \frac{d\psi(\mathbf{x})}{dt} = (1 - i\gamma) \left\{ V(\mathbf{x}) - \frac{\hbar^2 \nabla^2}{2m} - \mu + g|\psi(\mathbf{x})|^2 \right\} \psi(\mathbf{x}) + \sqrt{\gamma T} \eta(\mathbf{x}, t)$$

Gross-Pitaevskii equation (GPE)
Complex white noise

reservoir coupling
 (weak $\gamma \ll 1$)

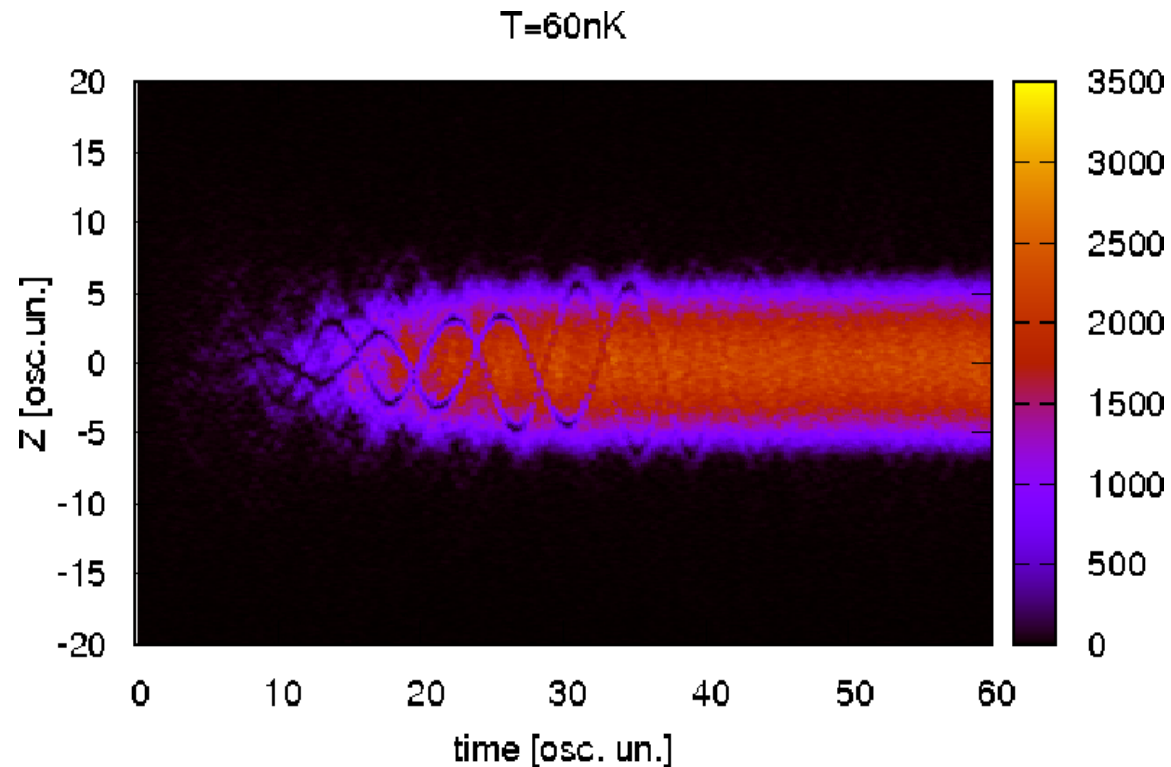
General assumptions:

Low energy modes (high occupation):

C-field

High energy modes (low occupation):

Thermal reservoir



Observation

Observation: the positive- P equations (full quantum mechanics) for a Bose field coupled to a naïve Markovian thermal reservoir

$$i\hbar \frac{d\psi(\mathbf{x})}{dt} = \left\{ V(\mathbf{x}) - \frac{\hbar^2 \nabla^2}{2m} + g\tilde{\psi}^* \psi - i\bar{\gamma} + \sqrt{i\hbar g} \xi(\mathbf{x}, t) \right\} \psi + \sqrt{\bar{\gamma} T} \eta(\mathbf{x}, t)$$

$$i\hbar \frac{d\tilde{\psi}(\mathbf{x})}{dt} = \left\{ V(\mathbf{x}) - \frac{\hbar^2 \nabla^2}{2m} + g\psi^* \tilde{\psi} - i\bar{\gamma} + \sqrt{i\hbar g} \tilde{\xi}(\mathbf{x}, t) \right\} \tilde{\psi} + \sqrt{\bar{\gamma} T} \eta(\mathbf{x}, t)$$

Real white noises
(quantum fluctuations)

Complex white noise
(thermal fluctuations)

Are quite similar to the SGPE equation (with a less naïve reservoir):

$$i\hbar \frac{d\psi(\mathbf{x})}{dt} = (1 - i\gamma) \left\{ V(\mathbf{x}) - \frac{\hbar^2 \nabla^2}{2m} - \mu + g|\psi|^2 \right\} \psi + \sqrt{\gamma T} \eta(\mathbf{x}, t)$$

Hybrid: thermal Initial conditions, full evolution

This suggests a hybrid equation that would include:

- both thermal and quantum fluctuations:
- equilibrated thermal cloud from SGPE
- quantum fluctuations, atom pair production, etc. from positive- P
- probably the positive- P instability?

$$i\hbar \frac{d\psi(\mathbf{x})}{dt} = (1 - i\gamma) \left\{ V(\mathbf{x}) - \frac{\hbar^2 \nabla^2}{2m} - \mu + g\tilde{\psi}^* \psi + \sqrt{i\hbar g} \xi(\mathbf{x}, t) \right\} \psi + \sqrt{\gamma T} \eta(\mathbf{x}, t)$$

$$i\hbar \frac{d\tilde{\psi}(\mathbf{x})}{dt} = (1 - i\gamma) \left\{ V(\mathbf{x}) - \frac{\hbar^2 \nabla^2}{2m} - \mu + g\psi^* \tilde{\psi} + \sqrt{i\hbar g} \tilde{\xi}(\mathbf{x}, t) \right\} \tilde{\psi} + \sqrt{\gamma T} \eta(\mathbf{x}, t)$$

Quantum fluctuations
Thermal fluctuations

Observables are calculated as by replacing: $\hat{\Psi}(\mathbf{x}) \rightarrow \psi(\mathbf{x}), \quad \hat{\Psi}^\dagger(\mathbf{x}) \rightarrow \tilde{\psi}(\mathbf{x})^*$
 In normally ordered moments.

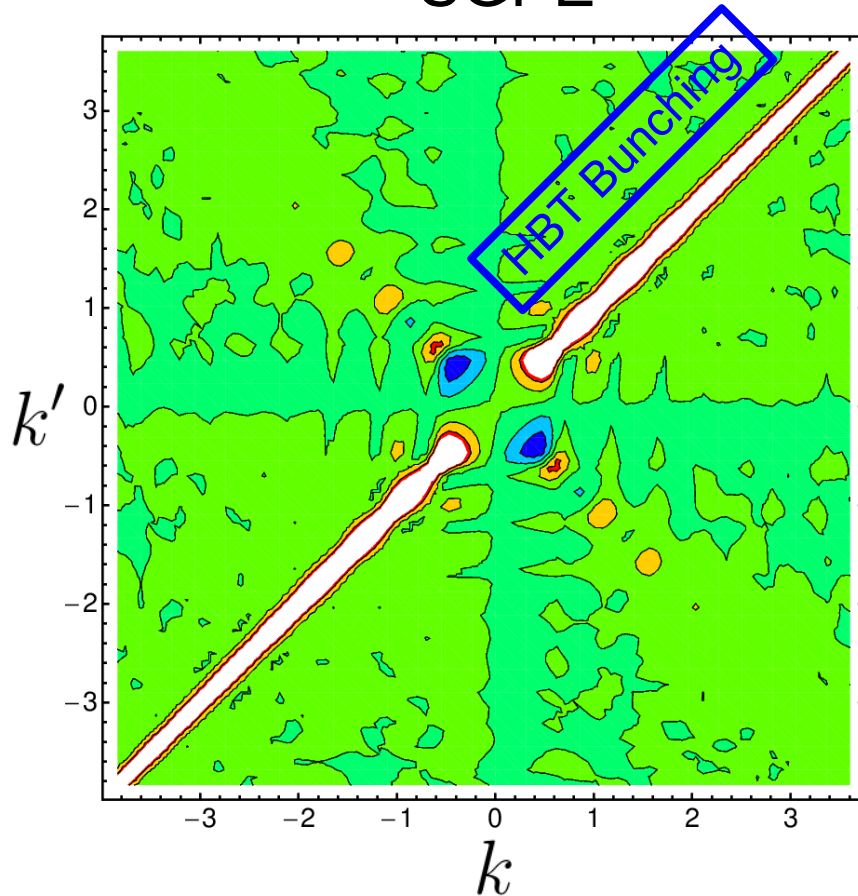
e.g. $\rho_1(\mathbf{x}, \mathbf{x}') = \langle \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}(\mathbf{x}') \rangle = \text{Re} \langle \tilde{\psi}(\mathbf{x})^* \psi(\mathbf{x}') \rangle_{\text{samples}}$

Preliminary results: atom pairs in situ

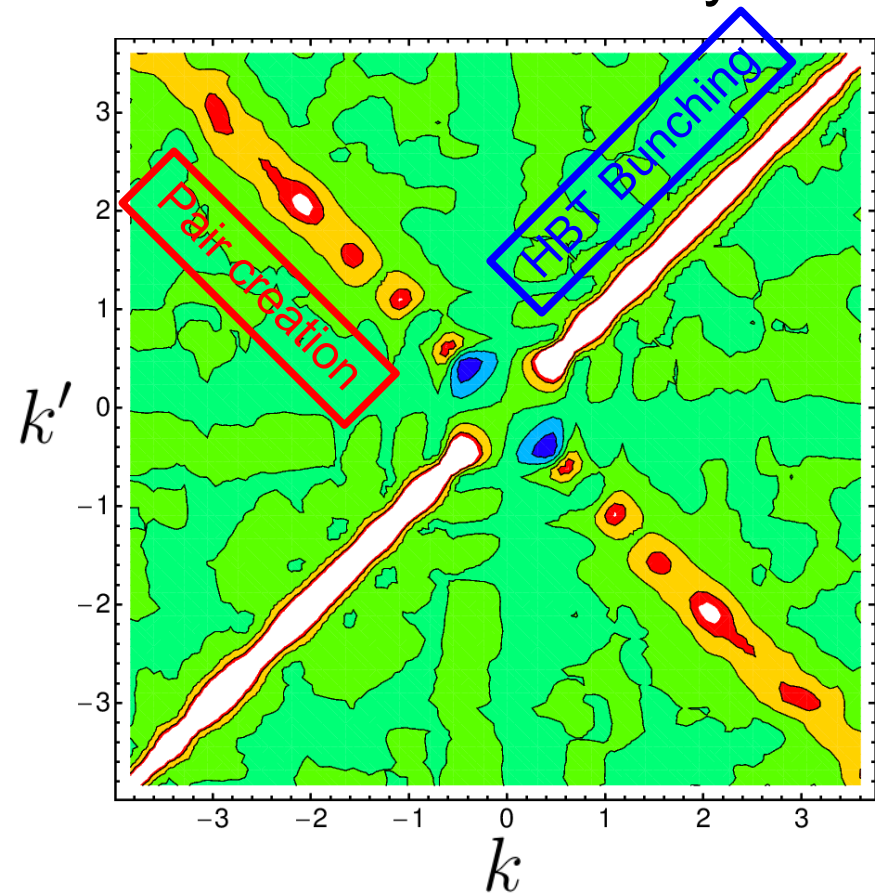
$N=1000$ $\mu = 22.41 \hbar\omega$ $k_B T = 140 \hbar\omega$ $T_\phi \approx 900 \hbar\omega$ $T_c \approx 1900 \hbar\omega$

Momentum correlations $g^{(2)}(k, k')$

SGPE



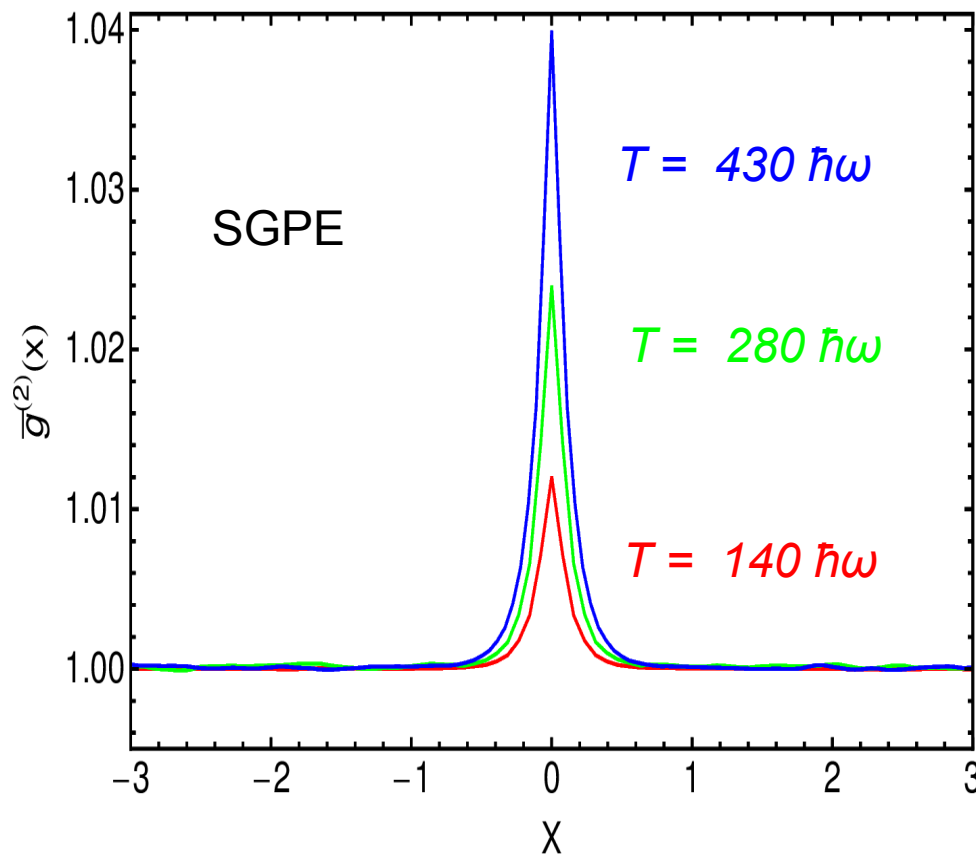
Quantum-thermal hybrid



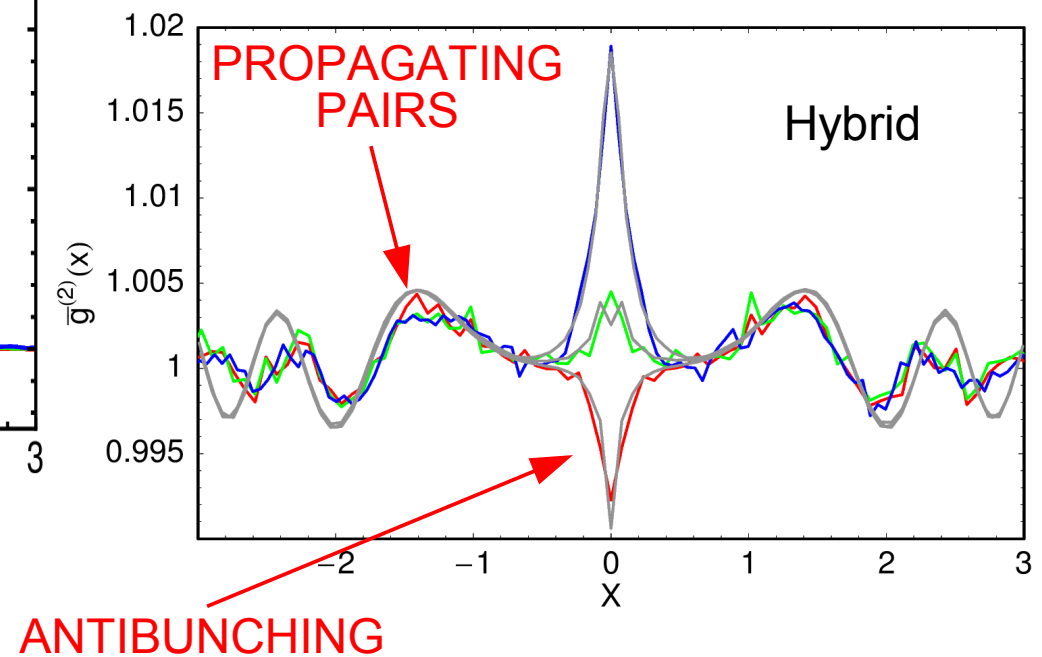
Preliminary results: atom pairs in situ

Spatial density correlations $g^{(2)}(0, x)$

$N=1000$ $\mu = 22.41 \hbar\omega$ $T = 140 \hbar\omega - 430 \hbar\omega$ $T_\phi \approx 900 \hbar\omega$ $T_c \approx 1900 \hbar\omega$



Effects of the "quench" caused by turning on quantum fluctuations at $t=0$



Scaling of spontaneous effects

Spatial density correlations $g^{(2)}(0, x)$

$$\mu = 22.41 \hbar\omega \quad T = 140 \hbar\omega$$

→ $Ng = \text{constant}$

