Quantum dynamics of correlated atom pairs using the positive-P method

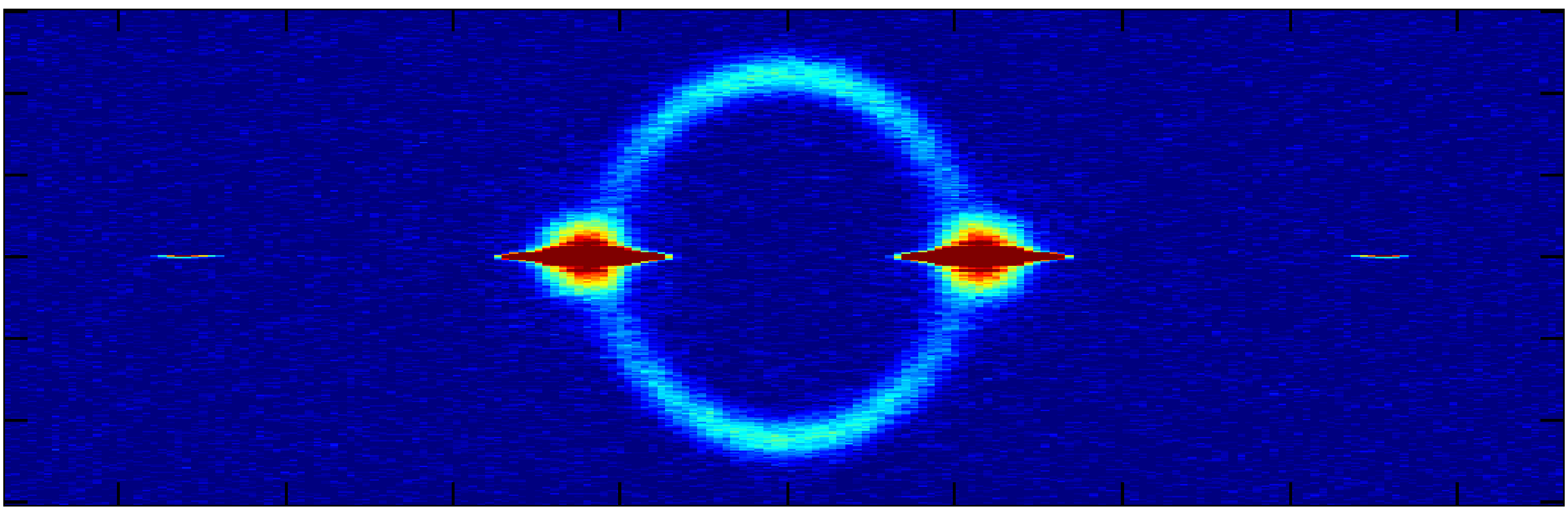
Piotr Deuar

Institute of Physics, Polish Academy of Sciences, Warsaw

Contributions

Chris Westbrook *(Palaiaseau experiment):*
Denis Boiron
Jean-Christophe Jaskula
Valentina Krachmalnicoff
Marie Bonneau
Josselin Ruaudel
Guthrie Partridge
Raphael Lopes

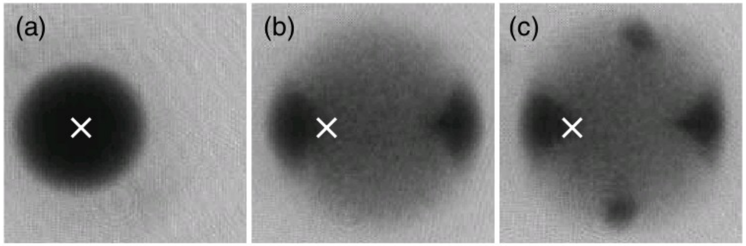
Karen Kheruntsyan (Brisbane)
Peter Drummond (Melbourne)
Marek Trippenbach (Warsaw Uni)
Jan Chwedeńczuk
Paweł Ziń
Tomasz Wasak
Mariusz Gajda (Warsaw IFPAN)
Emilia Witkowska
Kazimierz Rzążewski (Warsaw CFT)



Outline

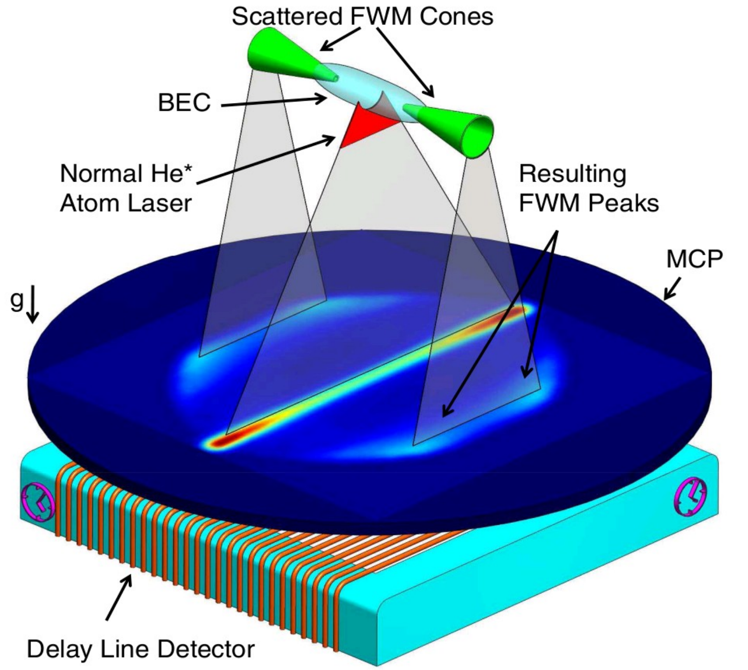
1. Supersonic pair creation
2. Positive-P/Bogoliubov method
3. He* pair scattering at T=0
4. Quasicondensate 0 < T < ~Tc
5. Correlations in the 1D gas at γ ~ 1

Supersonic pair creation

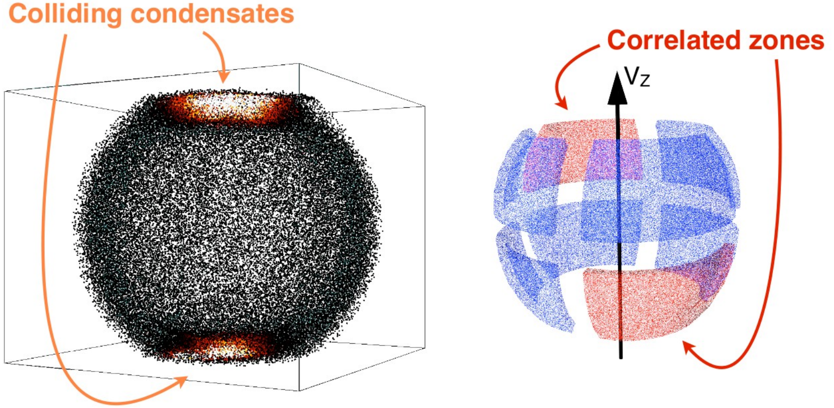


Vogels, Xu, Ketterle, PRL **89,** 020401 (2002)

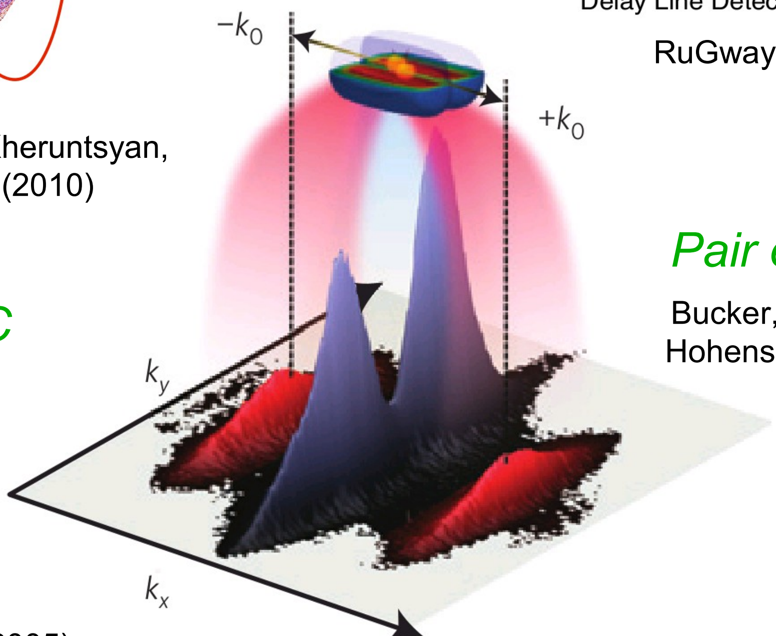
BEC Collisions



RuGway, Hodgman, Dall, Johnsson, Truscott,
PRL **107,** 075301 (2011)



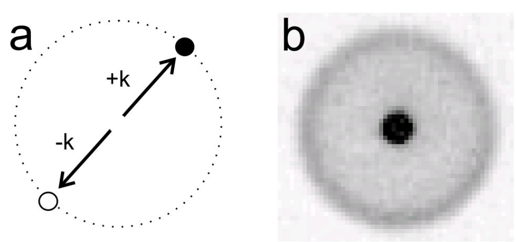
Jaskula, Bonneau, Partridge, Krachmalnicoff, PD, Kheruntsyan,
Aspect, Boiron,Westbrook, PRL **105,** 190402 (2010)



Pair emission from a 1D gas

Bucker, Grond, Manz, Berrada, Betz, Koller,
Hohenster, Schumm, Perrin, Schmiedmayer,
Nature Phys. **7,** 608 (2011)

Dissociation of molecular BEC

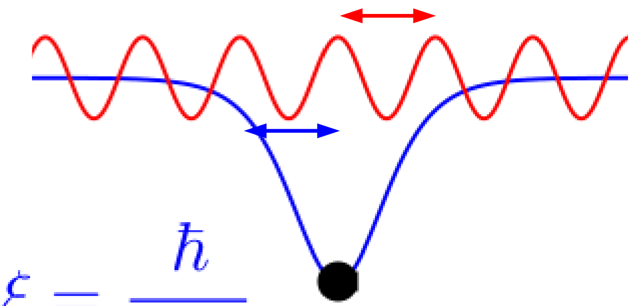


Greiner, Regal, Stewart, Jin, PRL **94,** 110401 (2005)

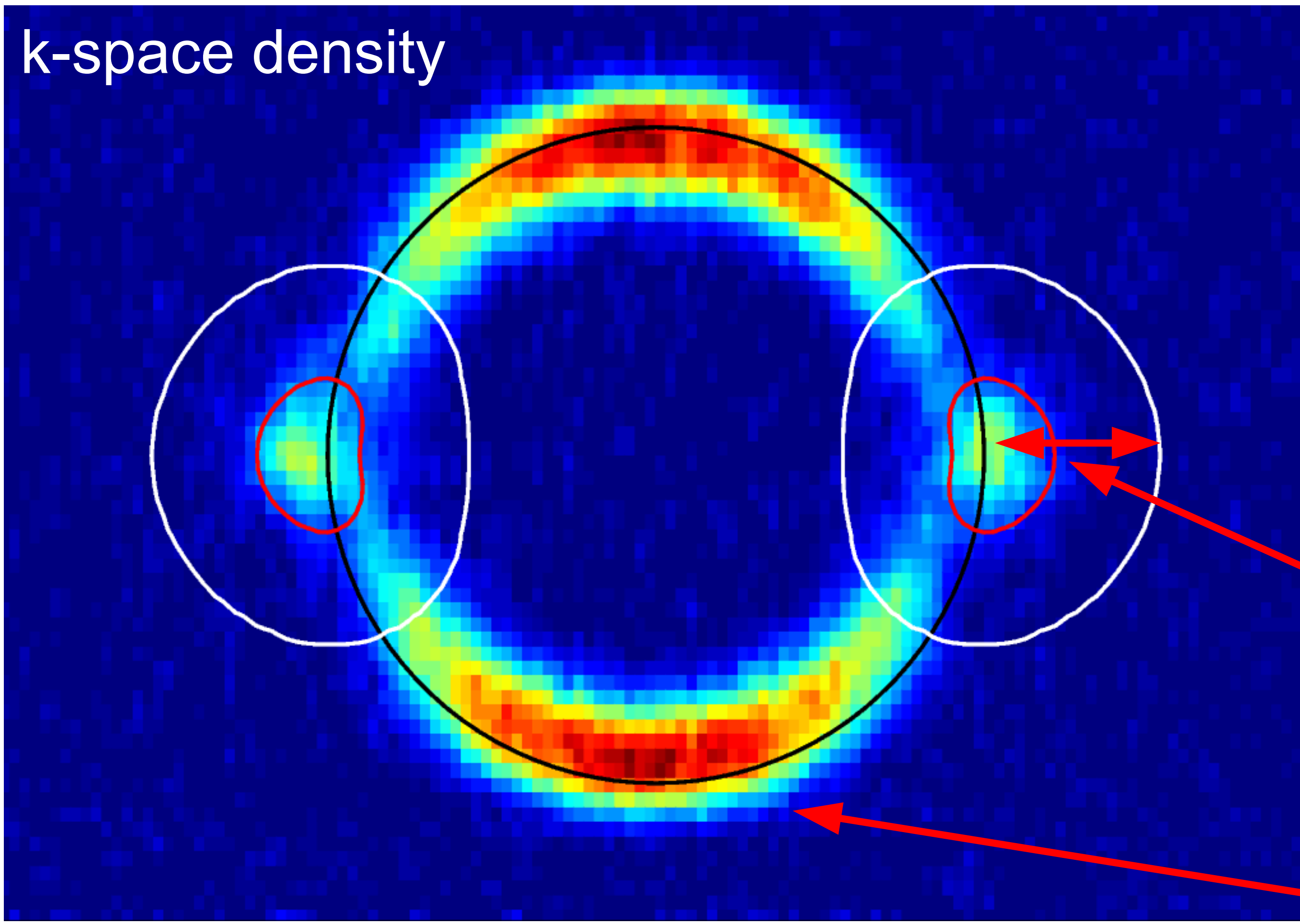
Supersonic scattering

- Above the speed of sound $v_s = \sqrt{\mu/m}$ a condensate no longer behaves as a superfluid

$$\lambda_v = \frac{2\pi\hbar}{mv}$$



$$\xi = \frac{\hbar}{mv_s}$$



PD, Ziń, Chwedeńczuk, Trippenbach, EPJD **65,** 19 (2011)

BEC width in K-space is v_s

Scattered atoms Well separated From BEC

Bogoliubov pair creation

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

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

BEC — incoherent part "scattered" atoms

Assume small $\widehat{\delta}(\mathbf{x},t)$

$$\hat{H}_{\text{eff}} = \int d^3\mathbf{x}\, \hat{\delta}^\dagger(\mathbf{x}) H_0(\mathbf{x}) \hat{\delta}(\mathbf{x})$$

K.E. + trap

$$+2g \int d^3\mathbf{x}\, |\phi(\mathbf{x})|^2 \hat{\delta}^\dagger(\mathbf{x}) \hat{\delta}(\mathbf{x})$$

Potential from BEC
For scattered atoms

$$+\frac{g}{2} \int d^3\mathbf{x}\, \phi(\mathbf{x})^2 \hat{\delta}^\dagger(\mathbf{x}) \hat{\delta}^\dagger(\mathbf{x}) + \text{ h.c.}$$

Pair creation

Bogoliubov hurdles

- Looks like a linear problem, so why not just diagonalize $\hat{H}_{\text{eff}}$ and have everything, but.......

1. The numerical lattice might be too large (10^6 – 10^7 points in a 3D calculation)

   (note also the ***"human time"*** bottleneck!)

2. BEC evolves "under" the Bogoliubov field
   $\rightarrow$ would have to re-diagonalize at each time step

3. Assumption of small $\widehat{\delta}(\mathbf{x}, t)$ may fail

- Diagonalization can be avoided by using the positive-P representation

Positive-P representation

Drummond, Gardiner J. Phys. A **13,** 2353 (1980)

Hilbert space dimension

n^M

$$\widehat{\rho} = \int P\left[\psi, \widetilde{\psi}\right] |\psi\rangle \langle\widetilde{\psi}| \, \mathcal{D}^2\psi(\vec{x})\mathcal{D}^2\widetilde{\psi}(\vec{x})$$

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

- The distribution P is positive & real
- Density matrix $\widehat{\rho} \leftrightarrow$ distribution P for the fields $\psi(x), \widetilde{\psi}(x)$
  $\leftrightarrow$ random samples of the fields
- From n^M variables we get samples x M

n = Hilbert space dimension at one point

M = numerical lattice size

Schrodinger → Langevin equations

Evolution of $\widehat{\rho}$ → diffusive evolution of P

(Fokker-Planck equation)

→ random walk of samples of $\psi(x), \widetilde{\psi}(x)$

Observables

$$\langle \hat{O} \rangle = \mathrm{Tr}\left[\hat{\rho}\, \hat{O} \right]$$

Expectation values of observables → moments of P

→ stochastic averages of samples $\psi(x), \widetilde{\psi}(x)$

As samples → ∞ we get better precision

$$\rho_1(\mathbf{x}, \mathbf{x}') = \left\langle \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}(\mathbf{x}') \right\rangle = \mathrm{Re}\langle \widetilde{\psi}(\mathbf{x})^* \psi(\mathbf{x}') \rangle_{st}$$

Bare positive-P equations

PD, Drummond PRL **98,** 120402 (2007)

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

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

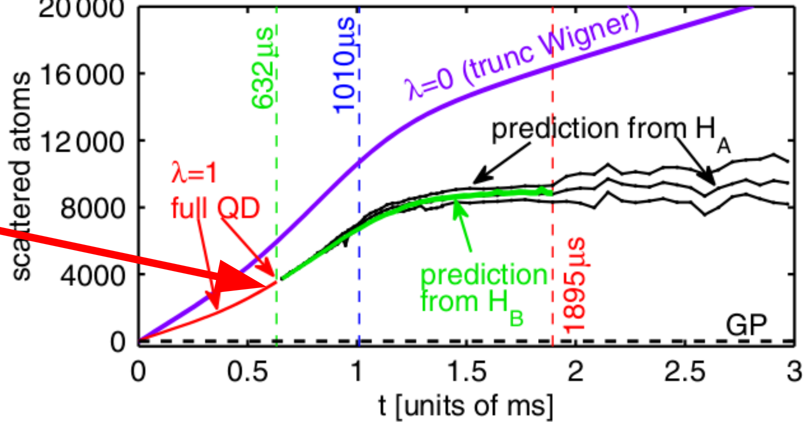
Mean field GP equation

Rest of quantum mechanics

Gaussian real white noise $\xi(x,t),\ \widetilde{\xi}(x,t)$

trouble: noise amplification

PD, PRL **103,** 130402 (2009)



Bogoliubov positive-P equations

PD, Chwedeńczuk, Ziń, Trippenbach, PRA **83,** 063625 (2011)

Krachmalnicoff *et al*, PRL **104,** 150402 (2010)

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

condensate

Bogoliubov fluctuation field – *MUST BE "small"*

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

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

Mean field

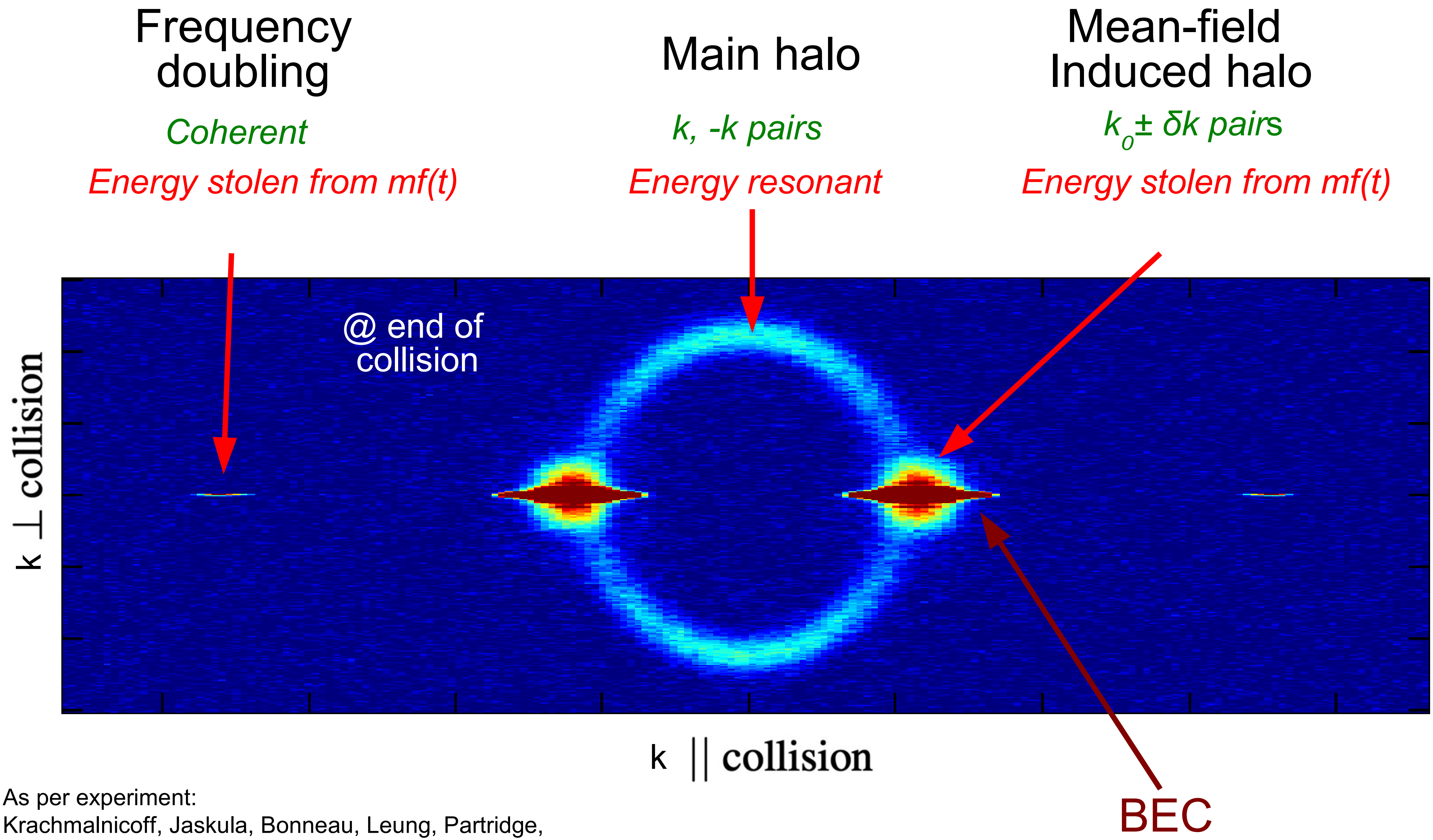
$$i\hbar\frac{d\psi(x)}{dt} = \left\{H_0(x) + 2g|\phi(x)|^2\right\}\psi(x) + g\phi(x)^2\widetilde{\psi}(x)^* + \sqrt{i\hbar g}\,\phi(x)\xi(x,t)$$

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

Now equations are linear ------> no blow-up of noise :)

Can use plane wave basis ---> no diagonalizing of 10^6 X 10^6 matrices :)
---> less human time used! :)

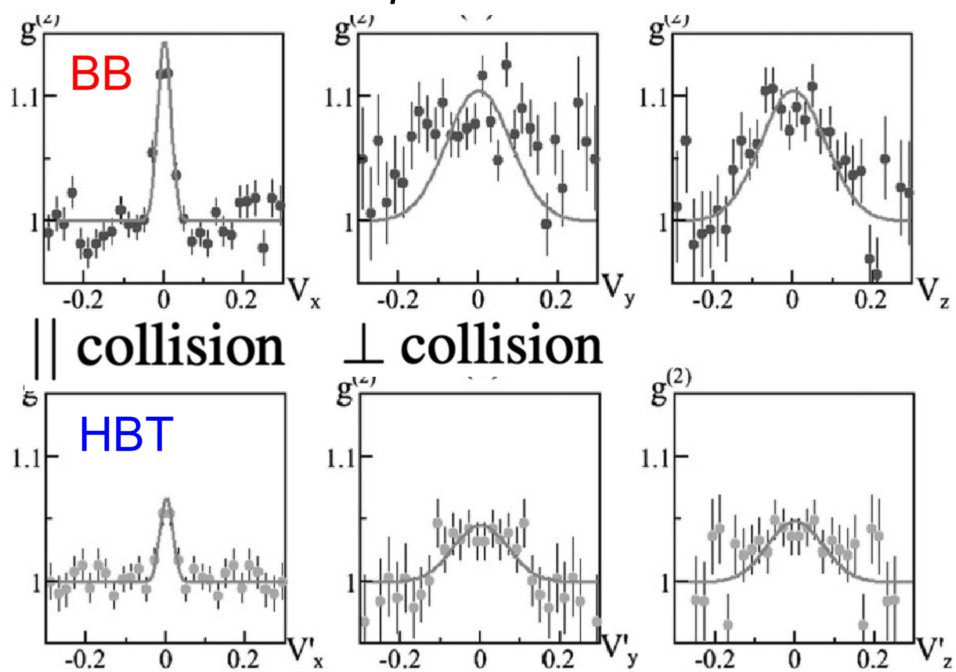
He* BEC collisions (T=0)



As per experiment:
Krachmalnicoff, Jaskula, Bonneau, Leung, Partridge, Boiron, Westbrook, PD, Zin, Trippenbach, Kheruntsyan, PRL **104,** 150402 (2010)

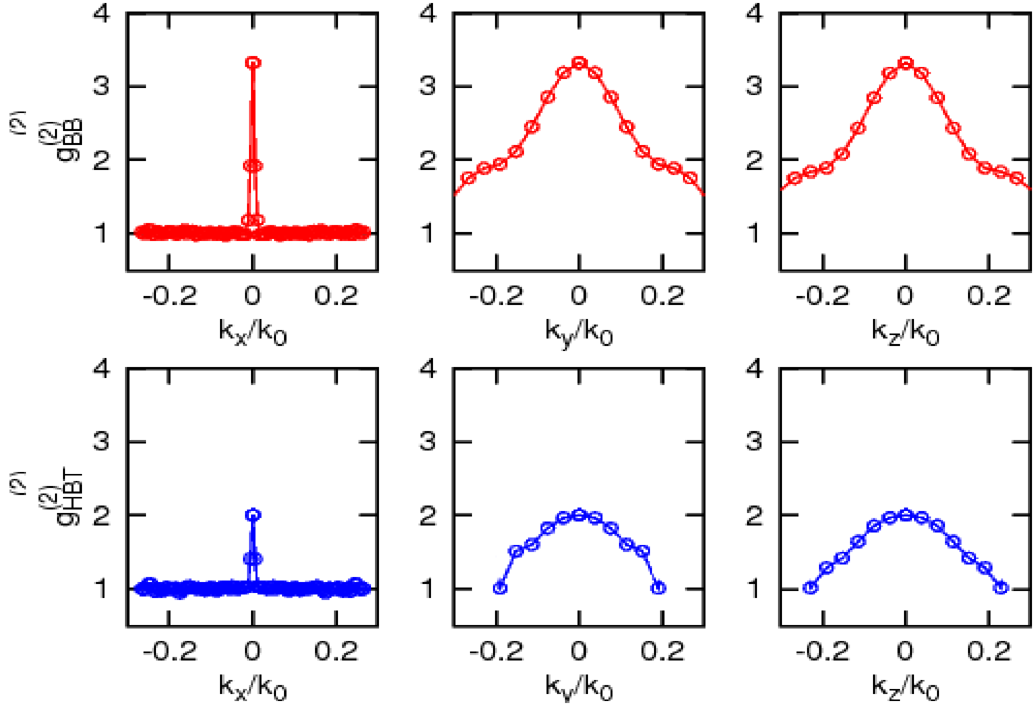
Halo correlations

experiment



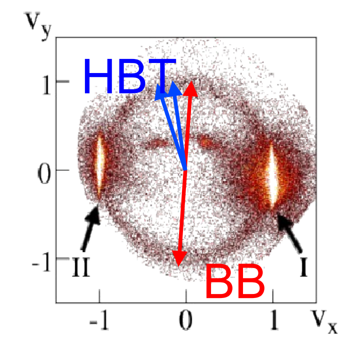
Perrin, Chang, Krachmalnicoff, Schellekens, Boiron, Aspect, Westbrook, PRL **99**, 150405 (2007)

simulation



Pair correlations along collision

experiment			numerics		
BB width	BB width / HBT width	BB height / HBT height	BB width	BB width / HBT width	BB height / HBT height
$0.017\ k_0$	1.1	2.1	$0.004\ k_0$	1	2.2



Krachmalnicoff, Jaskula, Bonneau, Leung, Partridge, Boiron, Westbrook, PD, Zin, Trippenbach, Kheruntsyan, PRL **104,** 150402 (2010)

Cauchy-Schwartz inequality violation

Kheruntsyan, Jaskula, PD, Bonneau, Partridge, Ruaudel, Boiron, Lopes, Westbrook, arXiv:1204.0058

Cross-correlation ≤ Auto correlation

e.g. currents

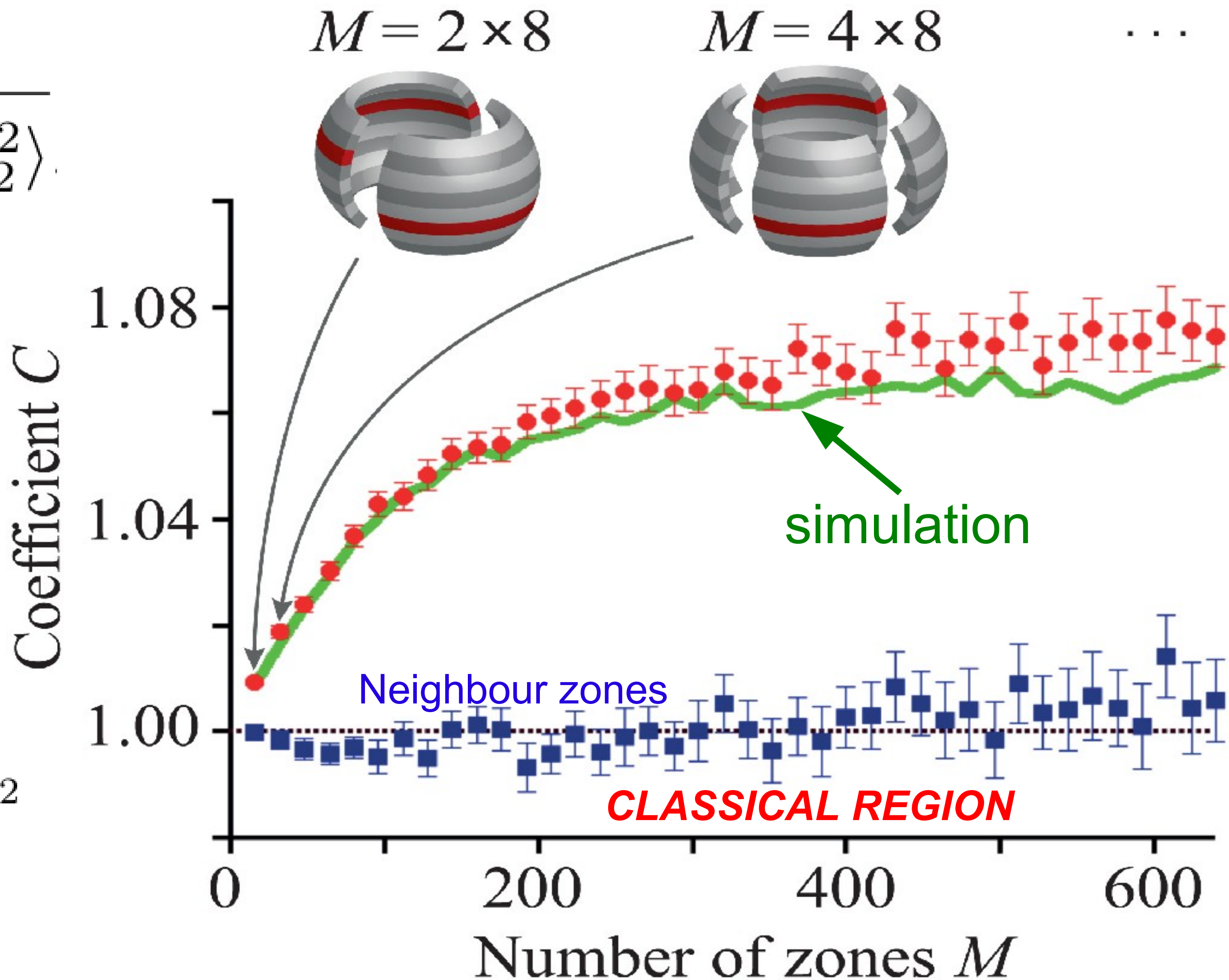
$$|\langle I_1 I_2\rangle| \leq \sqrt{\langle I_1^2\rangle\langle I_2^2\rangle}$$

local correlations

$$G_{12}^{(2)} \leq [G_{11}^{(2)} G_{22}^{(2)}]^{1/2}$$

Bin averaged correlations

$$C = \overline{\mathcal{G}}_{12}^{(2)} / [\overline{\mathcal{G}}_{11}^{(2)} \overline{\mathcal{G}}_{22}^{(2)}]^{1/2}$$



Classical field model for T>0

e.g. free space : plane wave basis

Full quantum field

c-fields

$$\Psi(\mathbf{r}) = \sum_{\mathbf{k}} a_{\mathbf{k}} \frac{1}{\sqrt{V}} e^{i\mathbf{k}\mathbf{r}} \longrightarrow \Phi(\mathbf{r}) = \sum_{|\mathbf{k}|\leqslant \mathbf{K}_{max}} \alpha_{\mathbf{k}} \frac{1}{\sqrt{V}} e^{i\mathbf{k}\mathbf{r}}$$

Replace mode amplitude operators $a_{\mathbf{k}}$
with complex number amplitudes $\alpha_{\mathbf{k}}$

Thermal initial state:

- $|\alpha_{\mathbf{k}}|^2$ Distributed according to Bose-Einstein distribution
- Phase of $\alpha_{\mathbf{k}}$ is random
- Use many realizations to get thermal ensemble

Useful papers:

Brewczyk, Gajda, Rzazewski, J. Phys B **40,** R1 (2007)
Blakie, Bradley, Davis, Ballagh, Gardiner, Adv. Phys. **57**, 363 (2008)
Proukakis, Jackson, J. Phys A **41,** 203002 (2008)
Brewczyk, Borowski, Gajda, Rzazewski, J Phys B **37**, 2725 (2004)

Validity of classical field

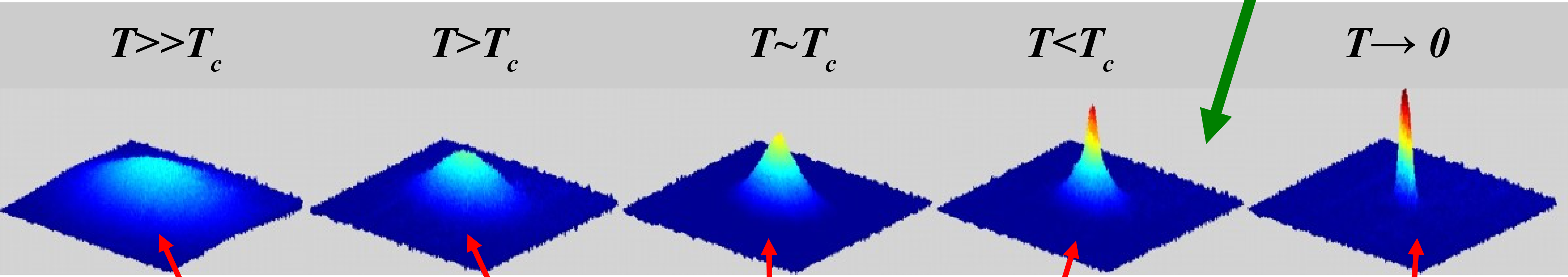
$$\left[\hat{\Psi}(x), \hat{\Psi}^\dagger(x')\right] = \delta(x - x') \quad \longrightarrow \quad [\psi^*(x), \psi(x')] = 0$$

→ it will be fine, ...

.... as long as there are always many atoms involved

in whatever it is we are studying

Quasicondensate



http://www-matterwave.physics.ox.ac.uk/node/1

Mode occupation getting small

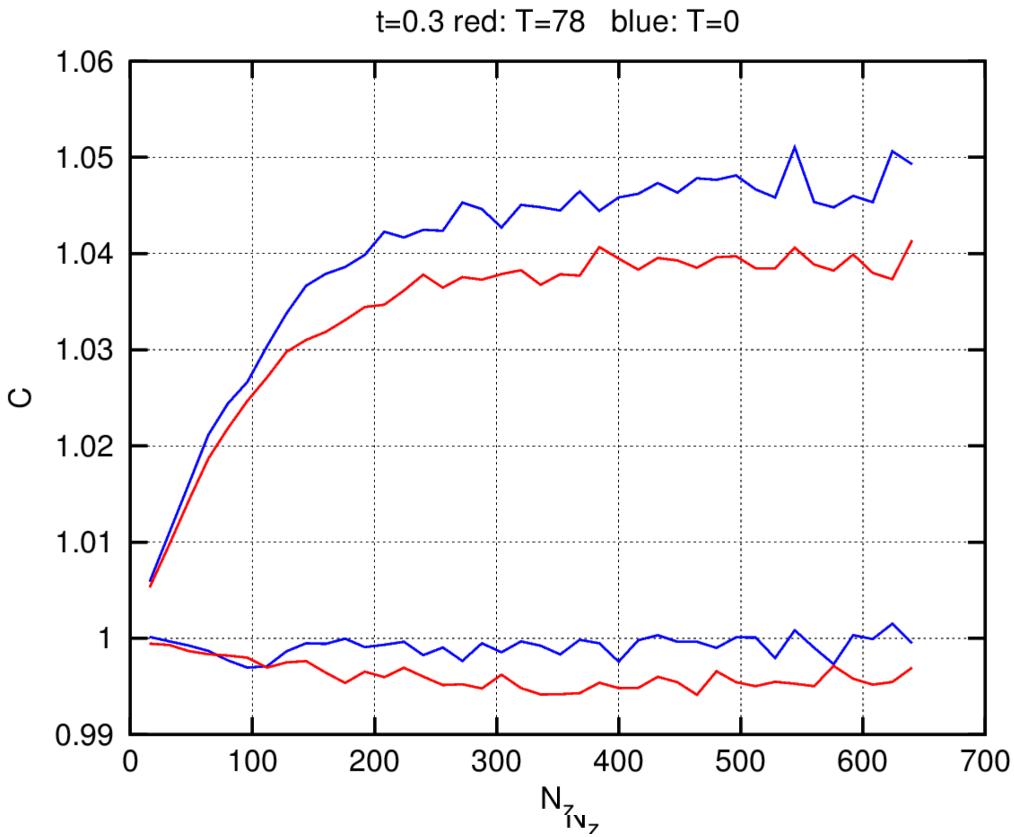
OK for Classical-field method:
All relevant modes highly occupied

Occupation in excited modes getting small

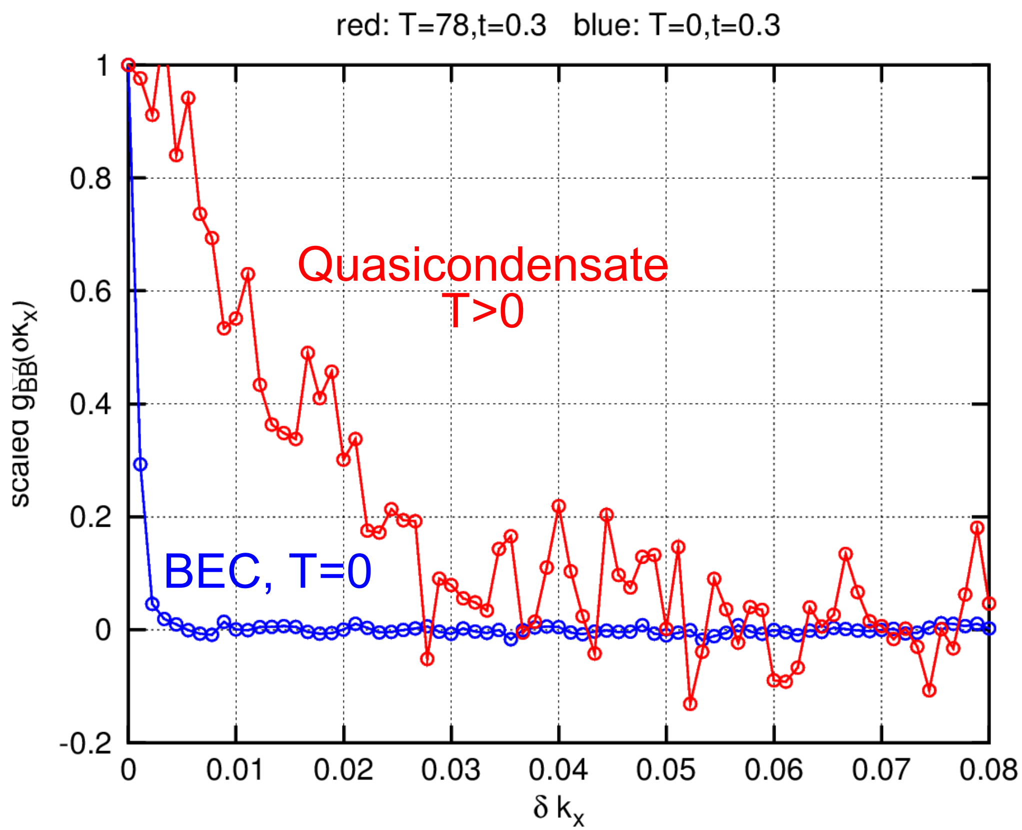
Quasicondensate effects on correlations

Initial classical field described by model of
Phase-fluctuating 3D condensates in elongated traps
Petrov, Shlyapnikov, Walraven, PRL **87**, 050404 (2001)

CS-violation not affected much



k,-k correlations strongly affected



1D Bose gas – exact results : crossover regime

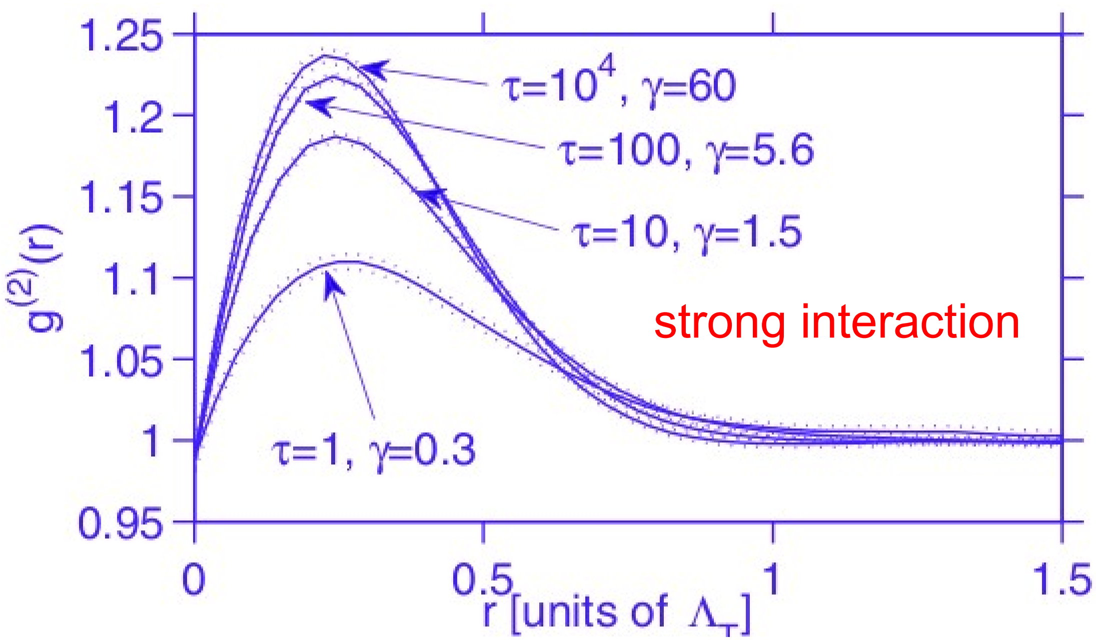
PD, Sykes, Gangardt, Davis, Drummond, Kheruntsyan, PRA 79, 043619

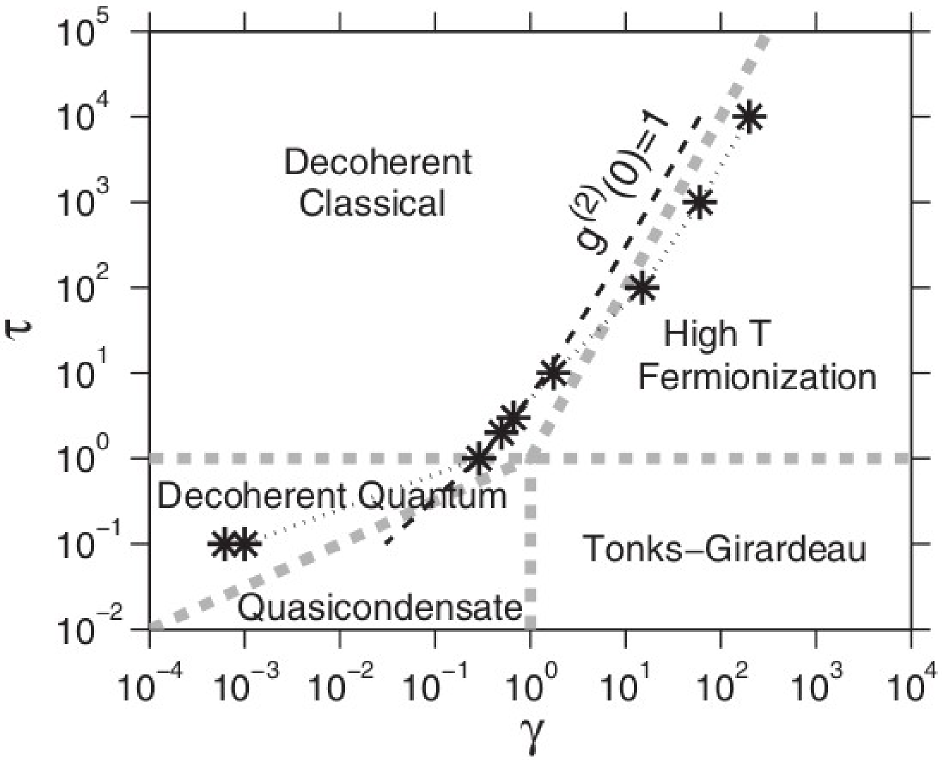
- Here a direct positive-P calculation can be made in *imaginary time* to obtain correlations in the thermal ensemble.

$$\gamma = \frac{mg}{\hbar^2 n}$$

$$\tau = T/T_d, \; T_d = \hbar^2 n^2 / (2m)$$

degeneracy temperature





Correlation waves after a quantum quench

PD, P. Drummond, J. Phys A **39,** 1163 (2006)

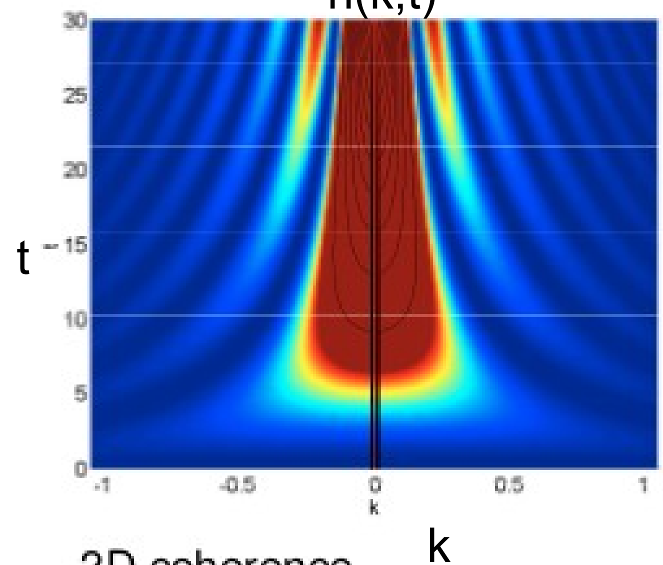
t = 0

uniform
undepleted
condensate

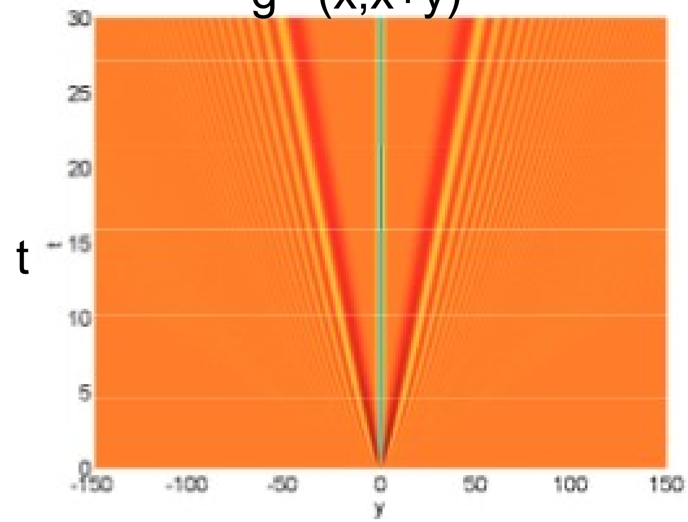
t > 0

Contact
interaction
turned on
g>0

1D k-space density
$n(k,t)$

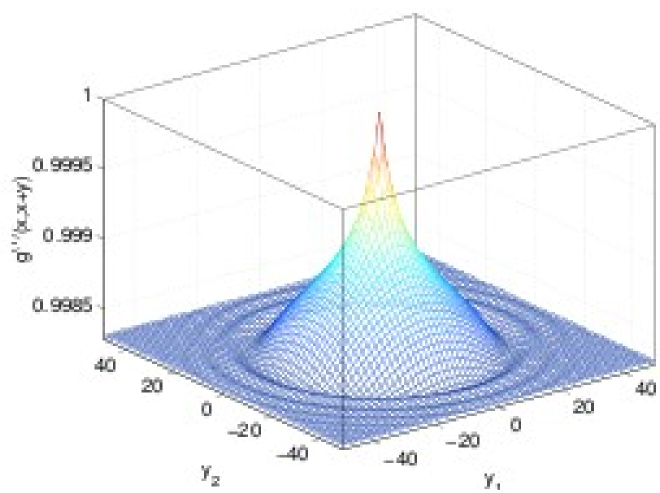


1D density-density correlations
$g^{(2)}(x,x+y)$

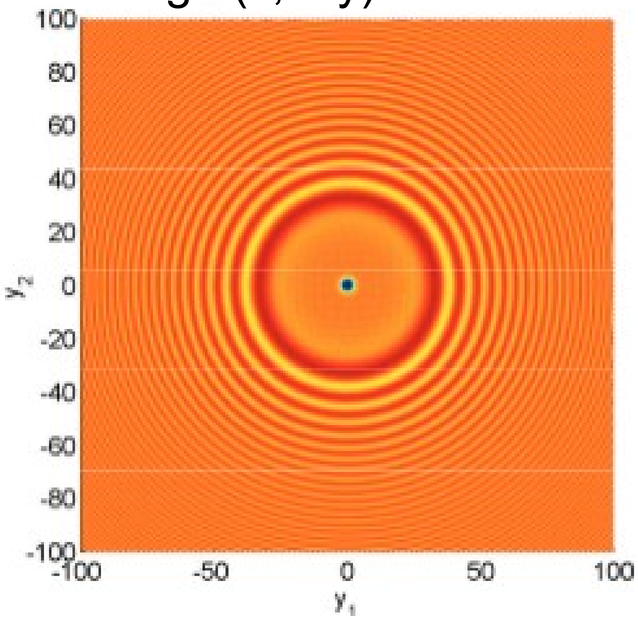


2D coherence

$g^{(1)}(x,x+y)$ t=20



2D density-density correlations
$g^{(2)}(x,x+y)$ t = 20



Conclusions / Outlook

- "Straightforward" simulation of supersonic quantum dynamics

  With positive-P treatment of Bogoliubov field

- Bogoliubov dynamics made tractable for large systems

  By use of plane wave modes + stochastic noise

- Treat classical field realizations as condensates for T>0

  Quasicondensate (and near Tc?)

- Exact treatment of 1D gas in crossover regime:

  Thermal, and quantum quench

- To be developed: Number-conserving Bogoliubov

  Would allow treatment of sub-sonic pair scattering