Simulating quantum dynamics of boson gases using the positive-P method

Part 3

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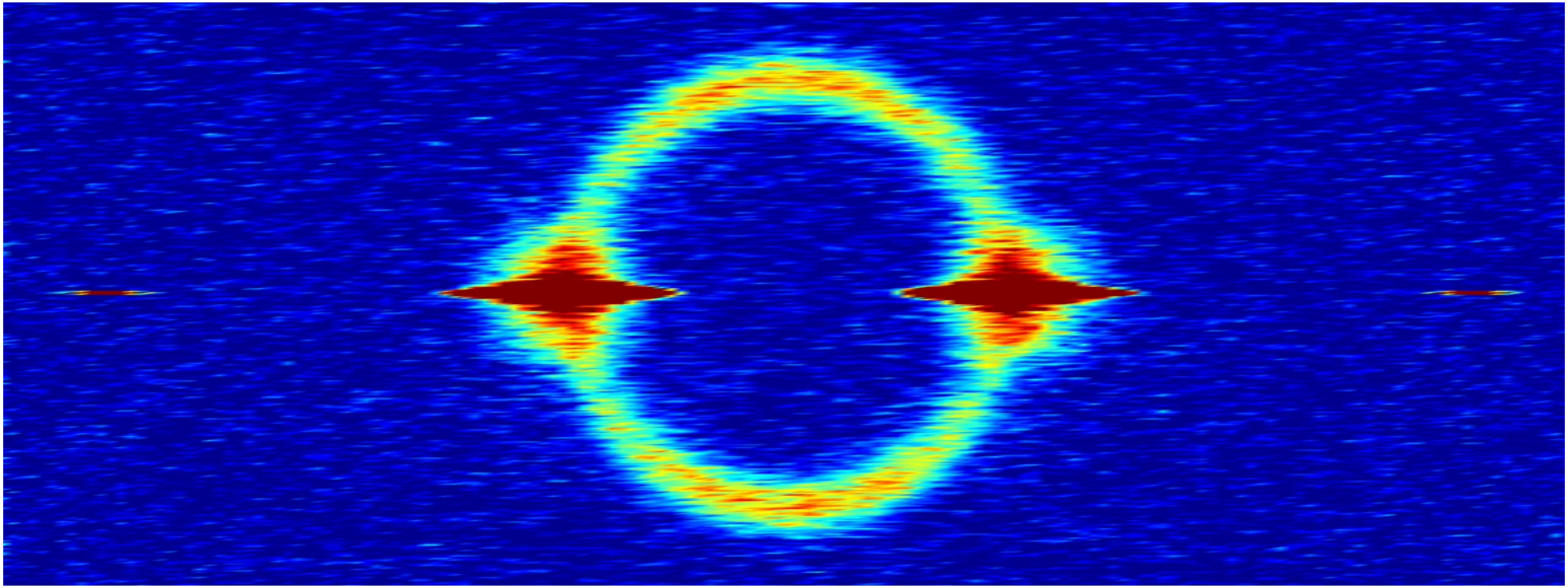
Seminarium - Wydział Fizyki UW



Outline

- Practicalities
  - Algorithm
  - Observables calculation and uncertainties
  - Time-step algorithm
- Sampling issues
- Stochastic instability

  $\longrightarrow$ Limit on the useful simulation time *(Booo!)*
- Bogoliubov quasiparticle description

Equations

1 mode

$$\hat{H} = \hbar\omega \hat{a}^{\dagger}\hat{a} + \hbar\chi \hat{a}^{\dagger}\hat{a}^{\dagger}\hat{a}\hat{a} \qquad n = \alpha\tilde{\alpha}^{*}$$

$$i\hbar\frac{d\alpha}{dt} = \left(\omega + 2\chi n - \sqrt{2\mathrm{i}\chi}\,\zeta(t)\right)\alpha \qquad i\hbar\frac{d\tilde{\alpha}}{dt} = \left(\omega + 2\chi n^{*} - \sqrt{2\mathrm{i}\chi}\,\tilde{\zeta}(t)\right)\tilde{\alpha}$$

Continuous field

$$\hat{\Psi}(x) \sim \frac{\hat{a}}{\sqrt{\Delta v}} \qquad \psi(x) \sim \frac{\alpha}{\sqrt{\Delta v}}$$

$$\hat{H} = \int \left\{ \hat{\Psi}^{\dagger}(x)\left[\mathrm{V}(x) - \frac{\hbar^{٢}}{٢m}\nabla^{٢}\right]\hat{\Psi}(x) + \frac{g}{٢}\hat{\Psi}^{\dagger}(x)\hat{\Psi}^{\dagger}(x)\hat{\Psi}(x)\hat{\Psi}(x) \right\} d^{٣}x$$

$$i\hbar\frac{d\psi(x)}{dt} = \left(V(x) - \frac{\hbar^{٢}}{٢m}\nabla^{٢} + g\,n(x) - \sqrt{i g}\,\xi(x,t) \right)\psi(x)$$

$$n(x) = \psi(x)\tilde{\psi}(x)^{*}$$

$$i\hbar\frac{d\tilde{\psi}(x)}{dt} = \left(V(x) - \frac{\hbar^{٢}}{٢m}\nabla^{٢} + g\,n(x)^{*} - \sqrt{i g}\,\tilde{\xi}(x,t) \right)\tilde{\psi}(x)$$

Algorithm

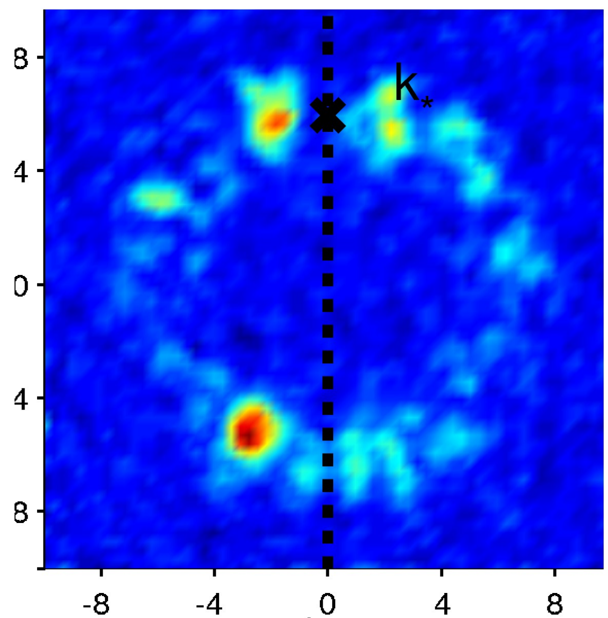
- Zero cumulative sums e.g. $\Sigma^{n(x)} = 0$
- <u>Repeat *S* times:</u>
  - Initialize fields $\psi(x), \tilde{\psi}(x)$ on lattice of *M* points
  - <u>For each small time step dt</u>
    - Generate noise fields $\xi(x), \tilde{\xi}(x)$
    - Advance fields $\psi(x), \tilde{\psi}(x)$ as per evolution equations
    - Add trajectory contribution to cumulative sums e.g. $\Sigma^{n(x)} += \mathrm{Re}[n(x)]$
- Obtain observables (and uncertainties) from cumulative sums at the end e.g. $\bar{n}(x) = \langle \hat{\Psi}^{\dagger}(x) \hat{\Psi}(x) \rangle \approx \frac{\Sigma^{n(x)}}{S}$

Observables as S⟶∞

- For observable $\bar{b} = \langle \hat{B} \rangle$, where $\bar{b} \approx \frac{1}{S} \sum_{j=1}^{S} b_j = \langle b \rangle_S \quad (j = 1, \ldots, S)$
- Uncertainty is given by the Central Limit Theorem

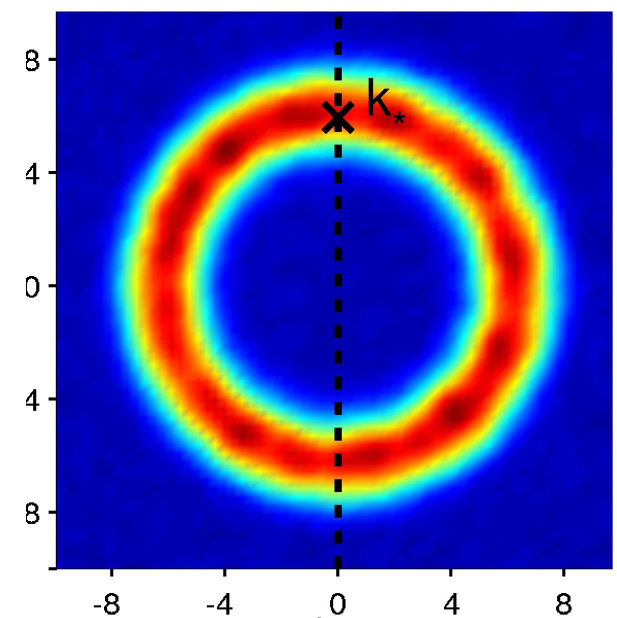
$$\Delta b \approx \sqrt{\frac{\langle b^2 \rangle_S - (\langle b \rangle_S)^2}{S-1}}$$

1 trajectory



k-space Density in the plane ⊥ to collision

≈300 trajectories



Correlations etc.

$$g^{(1)}(x) = \frac{\left\langle \widehat{\Psi}^{\dagger}(0)\widehat{\Psi}(x)\right\rangle}{\sqrt{\bar{n}(0)\bar{n}(x)}} \approx F = \frac{\langle \tilde{\alpha}^{*}(0)\alpha(x)\rangle_S}{\sqrt{\mathrm{Re}\left\langle \tilde{\alpha}^{*}(0)\alpha(0)\right\rangle_S \mathrm{Re}\left\langle \tilde{\alpha}^{*}(x)\alpha(x)\right\rangle_S}}$$

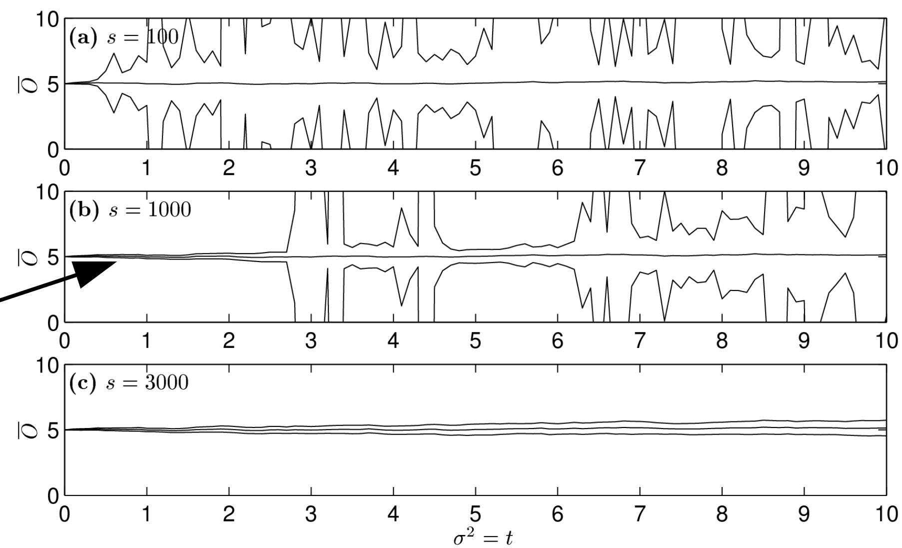
Here the uncertainty $\Delta g^{(1)}(x)$ is more subtle to calculate because the random variables in the averages are not independent

Solution: divide the trajectories into μ subensembles: 1 « μ « S
Calculate separate estimates F_j for each subensemble j, and only then use the Central Limit Theorem

$$\Delta g^{(1)} \approx \sqrt{\frac{\langle F_j^2\rangle_\mu - (\langle F_j\rangle_\mu)^2}{\mu - 1}}$$

$$O = \frac{1}{v + 0.2} \quad \text{where} \quad dv = dW(t)$$

S = μ s



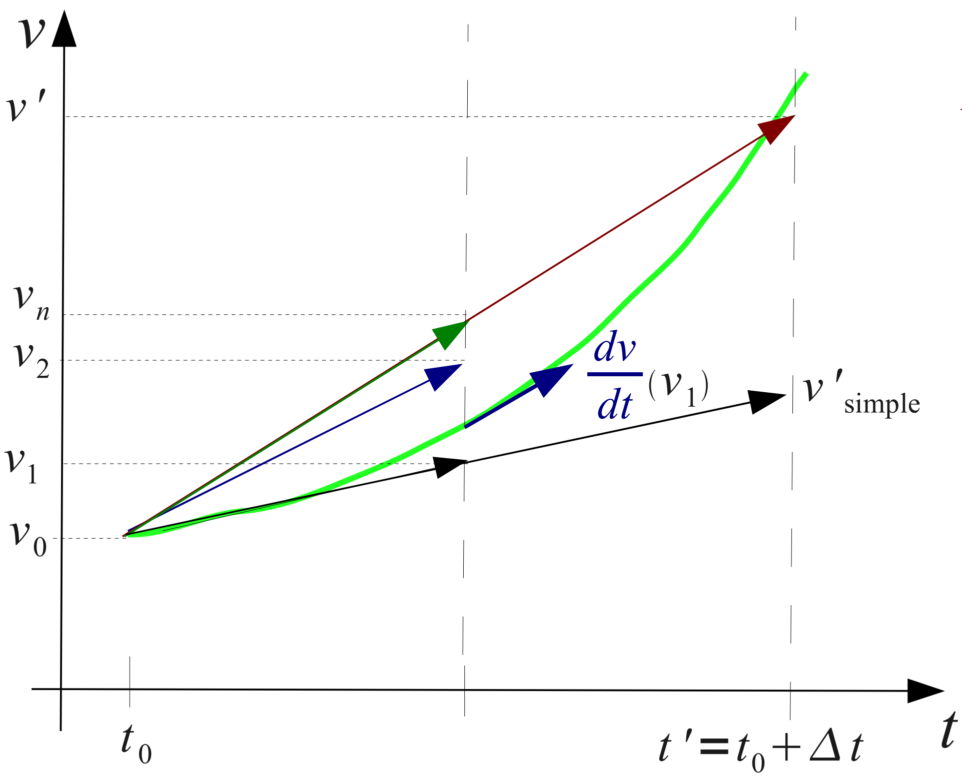
Integration

$$\frac{dv}{dt} = A(v) + B(v)\xi(t)$$

- <u>Simple method</u>

  $$v' = v_0 + [A(v_0) + B(v_0)\xi]\Delta t$$

  not very good: unstable



- <u>Mid-step estimation method</u>

$$\begin{aligned} v_1 &= v_0 + [a(v_0) + B(v_0)\xi](\Delta t/2) \\ v_2 &= v_0 + [a(v_1) + B(v_1)\xi](\Delta t/2) \\ &\dots \\ v_n &= v_0 + [a(v_{n-1}) + B(v_{n-1})\xi](\Delta t/2) \\ v' &= v_0 + [a(v_n) + B(v_n)\xi]\Delta t \end{aligned}$$

stable, but need

$$a(v) = A(v) - \frac{B(v)}{2} dB(v) dv$$

to offset artificial noise correlations due to $\langle \xi^2 \rangle = \frac{1}{\Delta t}$

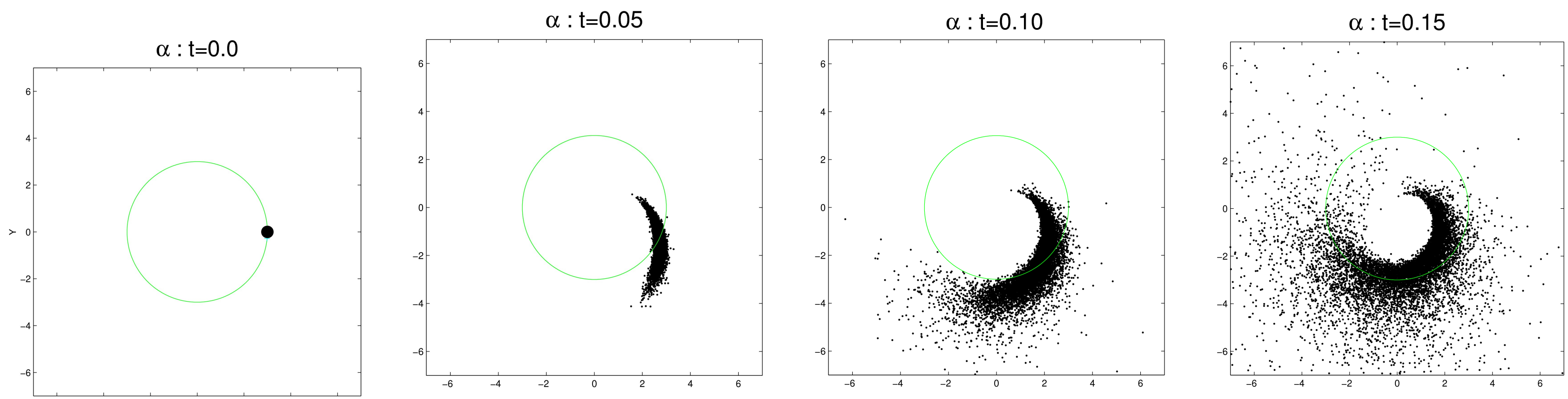
Sampling issues

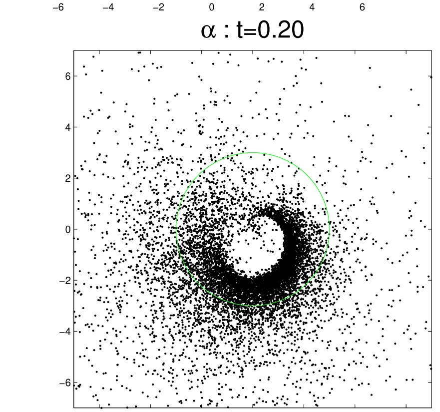
- Consider the 1 mode equations: <u>multiplicative noise</u>

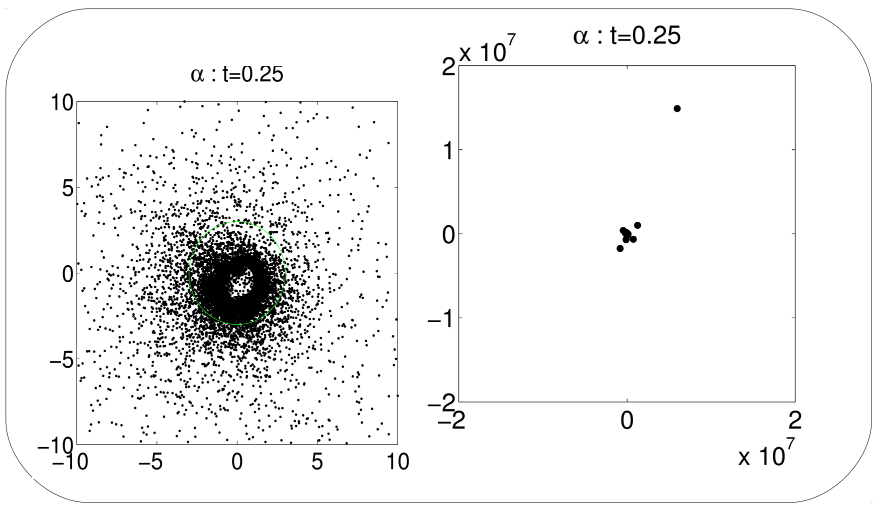
$$\frac{d\alpha}{dt} \approx \ldots + \text{const} \times \alpha \zeta(t)$$

hence $\alpha(t) \approx \alpha(0) e^{Z(t)}$ where $\langle Z(t)^2 \rangle = \text{const} \times t = \sigma^2$

This develops very long tails once σ ≥ O(1)







Noise amplification instability

Logarithmic variables: $n_L = \log \alpha \tilde{\alpha}, \quad m_L = \log \alpha / \tilde{\alpha}$

$$i\hbar \frac{dn_L}{dt} = 2\mathrm{i}\sqrt{i\chi}\, d\eta(t) \qquad i\hbar \frac{dm_L}{dt} = 2(\omega - \chi) + 4\chi e^{n_L} + 2\mathrm{i}\sqrt{i\chi}\, d\eta(t)^*$$

$$\langle \eta(t) \rangle = 0, \quad \langle \eta(t)^2 \rangle = 0, \quad \langle \eta(t) \eta(t')^* \rangle = \delta(t - t')$$

- Noise in n_L causes e^{n_L} to acquire imaginary part
- This imaginary part is random
- It leads to exponential growth or decay in $m = e^{m_L}$ and in α or $\tilde{\alpha}$
- Some trajectories randomly get growth, some decay
- Variance of e^{m_L} and so of α or $\tilde{\alpha}$ grows very rapidly
- When var$[m_L]$ reaches O(10) signal-to-noise becomes unusable

Useful simulation times

1 mode

$$t_{\text{sim}} \sim \frac{O(1)}{\chi N^{2/3}}$$

field

$$t_{\text{sim}} \sim \left(\frac{\hbar}{g}\right) \frac{(\Delta v)^{(1/3)}}{n_{\max}^{2/3}}$$

Simple criterion

$$t_{\text{sim}} \sim \left|\frac{\hbar}{g}\right| \frac{(\Delta v)^{(1/3)}}{n_{\max}^{2/3}}$$

Smallest relevant length : Healing length:

$$\xi = \frac{\hbar}{\sqrt{2 m n g}}$$

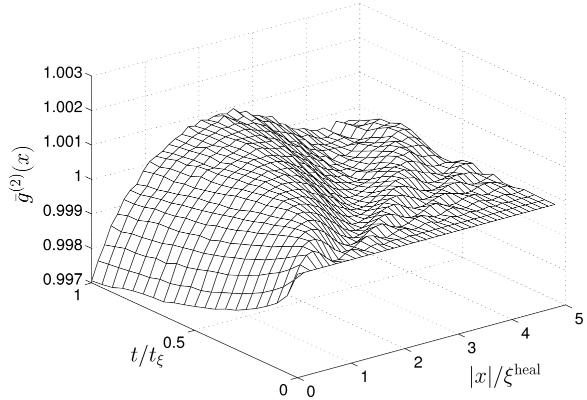
Related smallest relevant „healing time”

$$t_{\text{heal}} = \frac{m \xi^2}{\hbar} = \frac{\hbar}{2 n g}$$

In terms of this time,

$$\frac{t_{\text{sim}}}{t_{\text{heal}}} \sim (\Delta x\, n)^{1/3} \leq (\xi n)^{1/3}$$

Therefore, some relevant dynamics can be seen
iff there are O(1) or more particles per healing length (volume)



Bogoliubov treatment

To deal with short simulation time one can use the Bogoliubov quasiparticle approximation

- $\widehat{H}(\widehat{\Psi}) \rightarrow \widehat{H}(\Phi + \widehat{\Psi}_B)$
- Kill all terms of $O(\widehat{\Psi}_B)^3$

  (this assumes that the quasiparticles in $\widehat{\Psi}_B(x)$ do not interact)
- Treat the quasiparticle field $\widehat{\Psi}_B(x)$ using the positive-P representation in the same way that the full field $\widehat{\Psi}(x)$ was treated before.
- Allows
  - Bogoliubov description of 10^7 modes (difficult to diagonalise)
  - Description of dilute systems (when truncated Wigner is incorrect)
- Problems: when quantum depletion is large.

Bogoliubov Hamiltonian

Condensate obeys GP equation

$$\Phi(x,t) = \Phi_L(x,t) + \Phi_R(x,t)$$

Quasiparticles

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

Single-particle Hamiltonian

$$+ 2g |\Phi(t)|^2 \hat{\Psi}_B^\dagger \hat{\Psi}_B$$

collective potential

$$+ 2g\, \Phi_L(t) \Phi_R(t) \hat{\Psi}_B^\dagger \hat{\Psi}_B^\dagger + \text{h.c.}$$

Pair production

$$+ g \left[\Phi_L(t)^2 + \Phi_R(t)^2 \right] \hat{\Psi}_B^\dagger \hat{\Psi}_B^\dagger + \text{h.c.} \Big\}$$

Off-resonant terms

Positive-P equations

Condensate (split into L and R parts for later convenience)

$$i\hbar\frac{d\Phi_R}{dt}=\left[V(x)-\frac{\hbar^2}{2m}\nabla^2+g\left(\left|\Phi_R{}^2\right|+2\left|\Phi_L{}^2\right|+\Phi_L^*\Phi_R\right)\right]\Phi_R$$

$$i\hbar\frac{d\Phi_L}{dt}=\left[V(x)-\frac{\hbar^2}{2m}\nabla^2+g\left(\left|\Phi_L{}^2\right|+2\left|\Phi_R{}^2\right|+\Phi_R^*\Phi_L\right)\right]\Phi_L$$

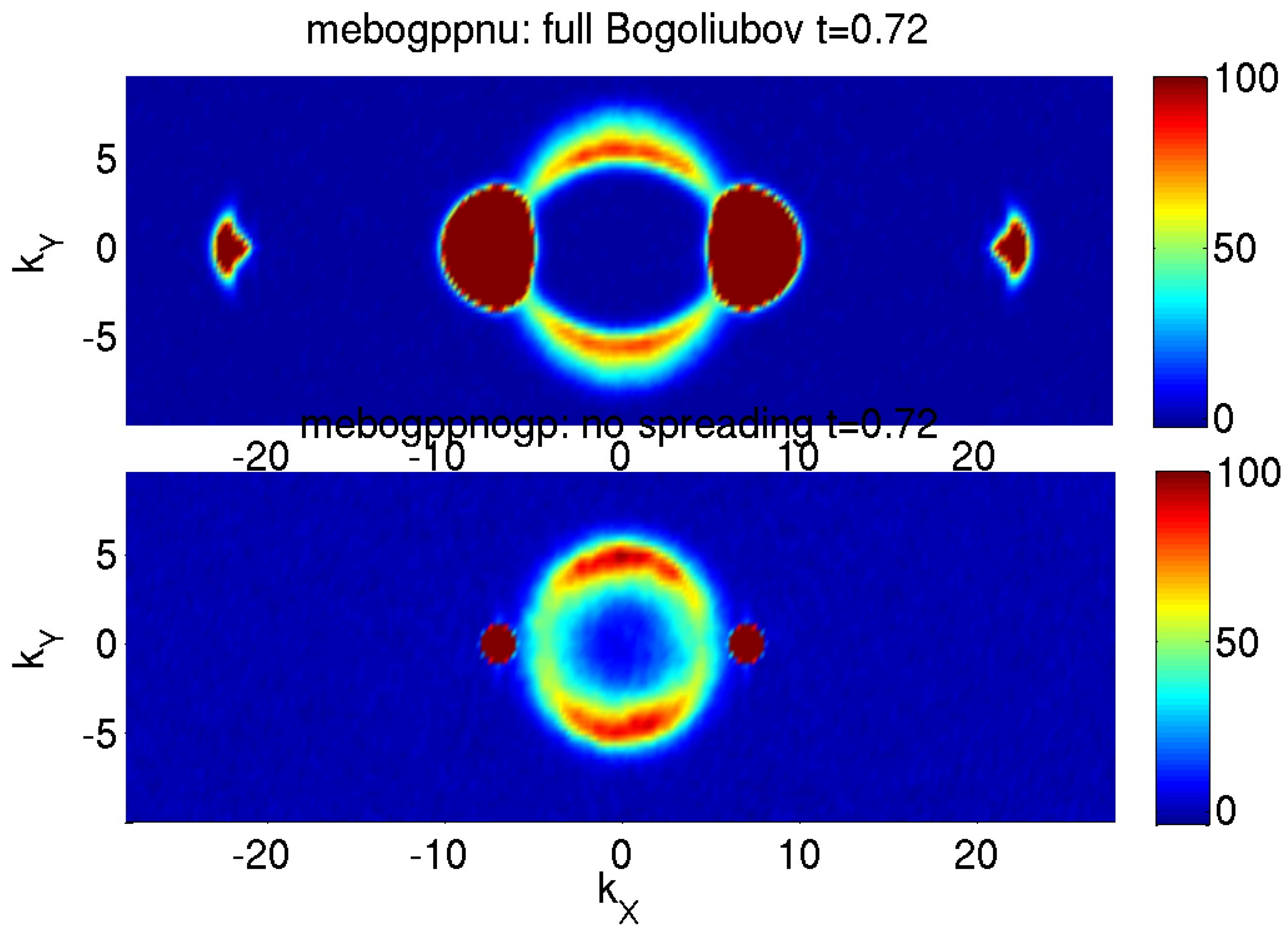
Quasiparticles

$$i\hbar\frac{d\psi}{dt}=\left[V(x)-\frac{\hbar^2}{2m}\nabla^2+2\mathrm{g}\left|\Phi^2\right|\right]\psi+g\Phi^2\tilde{\psi}^*-\sqrt{ig}\,\psi\,\xi(x,t)$$

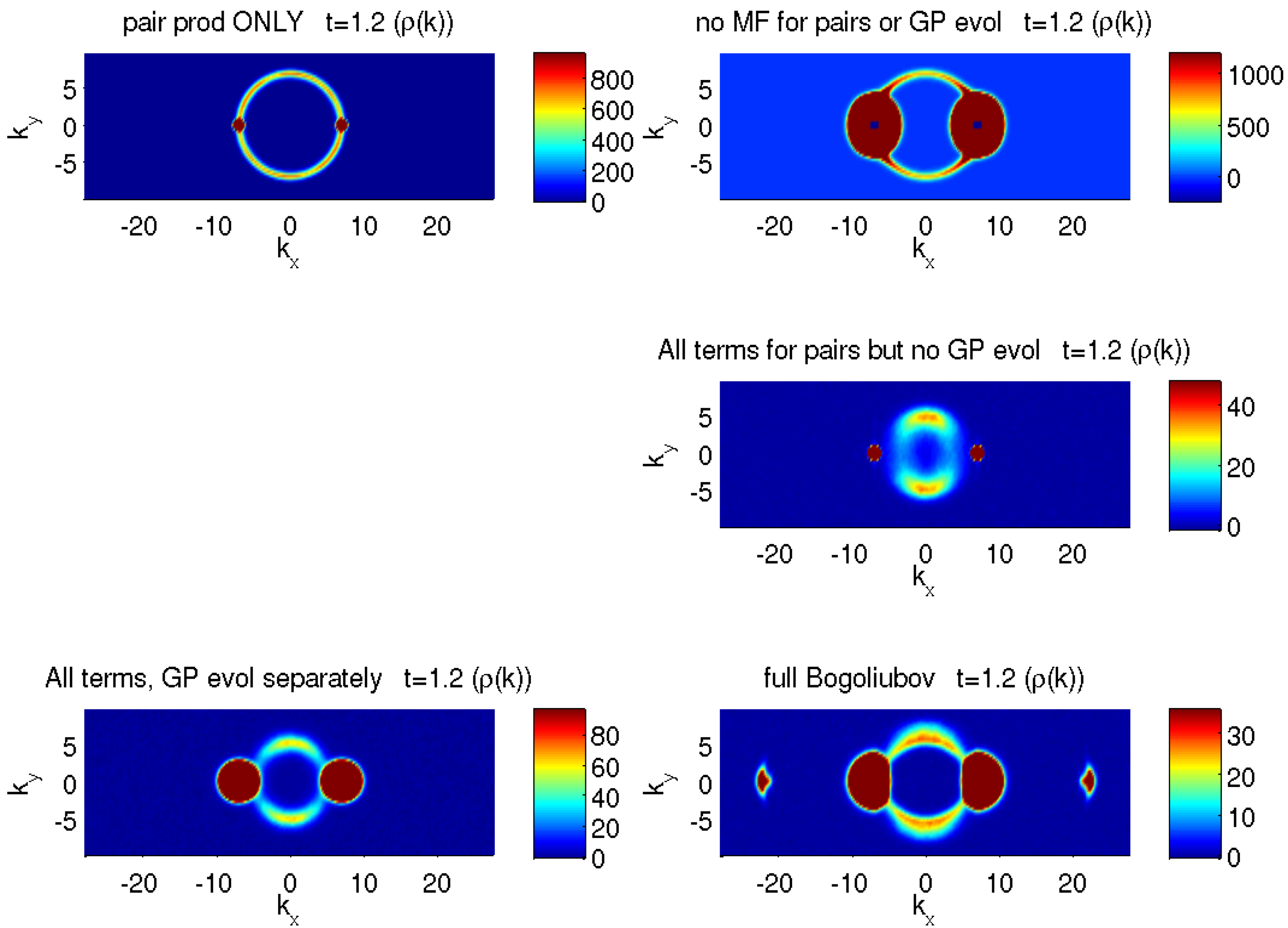
$$i\hbar\frac{d\tilde{\psi}}{dt}=\left[V(x)-\frac{\hbar^2}{2m}\nabla^2+2\mathrm{g}\left|\Phi^2\right|\right]\tilde{\psi}+g\Phi^2\psi^*-\sqrt{ig}\,\tilde{\psi}\,\tilde{\xi}(x,t)$$

Linear - no noise instability!

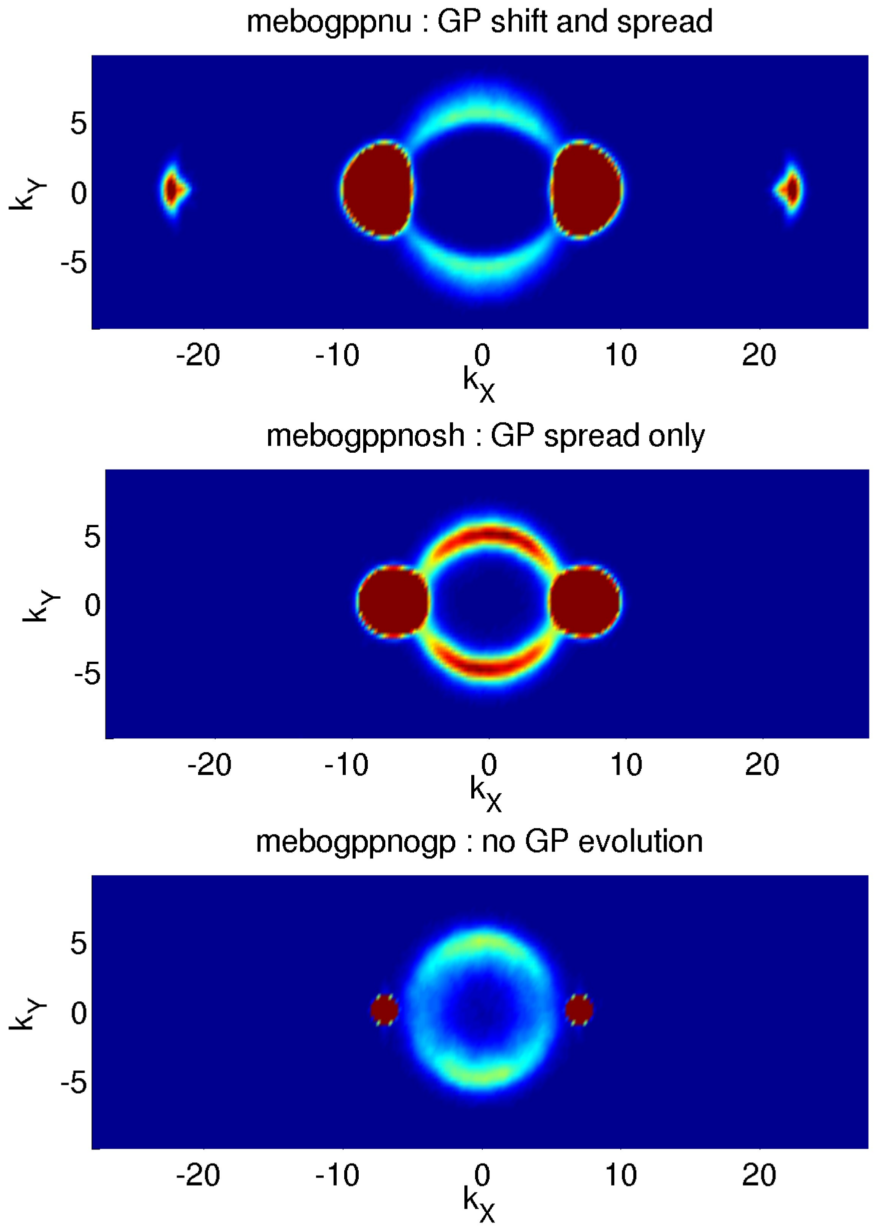
Dissection of the system (1)



Dissection of the system (2)



Dissection of the system (3)



Thankyou!