New perspectives on classical field simulations of ultracold Bose gases

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• Introduction: a little story

• The quantitative limits of the classical field regime

• A “nonclassical” field with quantum fluctuations
Some things can only be done with c-fields

e.g. Defects in a single realisation from thermal equilibrium


Single realization of evaporative cooling


Full range of quantum gas temperatures
Classical fields approximation in a nutshell

Full quantum field $\rightarrow$ Ensemble of complex-fields

$$\hat{\Psi}(x) = \sum_k \hat{a}_k \psi_k(x) \rightarrow \left\{ \sum_{k \in C} \xi_k \psi_k(x) \right\}$$

Assume highly occupied modes

Replace mode amplitude operators $\hat{a}_k$ with complex number amplitudes $\xi_k$

“Quantum field theory, without discretized particles”

Evolution: nonlinear Schrödinger equation

$$P(\Psi) \sim \exp \left[ -\frac{E(\Psi) - \mu N(\Psi)}{k_B T} \right]$$

$$\hbar \frac{\partial \Psi(x)}{\partial t} = -i \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x) + g |\Psi(x)|^2 \right] \Psi(x)$$

Developed by many authors:

A. Sinatra, M. Brewczyk, M. Gajda, M. Davis, K. Rzazewski, K. Burnett, E. Witkowska, … (no order implied)

Useful Reviews: M. Brewczyk et al, J. Phys B 40, R1 (2007);
Some disappointing caveats

Sensitivity to cutoff

No quantum fluctuations

• The cutoff $k_c$ is a very important parameter. Recommendations differ, though:

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<td>Uniform: $0.30 k_B T$ in 1D</td>
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<td>SGPE calculations of interacting gas</td>
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<td>Match energy in high E modes to $k_B T$ (equipartition) $\sim$ 1 particle in high E modes</td>
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<td>~ 10 particles in mode below cutoff</td>
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AIMS:

• **Quantitatively** determine the conditions under which the physics is that of classical waves.  
  *When can classical field predictions be trusted quantitatively?*

• Untangle the reasons behind the different conflicting prescriptions for the cutoff.

• Give a prescription for the cutoff  
  *Want good predictions of many observables simultaneously.*
Generic case: uniform section of gas

- Local Density approximation (LDA)
  → Grand Canonical ensemble
  (rest of gas acts as a reservoir)

- Thermodynamic limit for these sections of the gas
  (i.e. ignore finite-size effects)

Plan: (1) understand the ideal gas case
(2) benchmark 1D with exact solution


\[
\tau = \frac{T}{T_d}
\]

Dimensionless temperature

\[
\gamma = \frac{mg}{\hbar^2 n}
\]

Interaction strength

\[
f_c = \frac{k_c \Lambda_T}{2\pi}
\]

Dimensionless cutoff
Cutoff optimum for different observables

(ideal gas case)

Pietraszewicz, PD, PRA 92, 063620 (2015)

- $E_{\text{kin}}$ Kinetic energy per particle
- $\text{var}N / N$ Coarse-grained fluctuations
- $l_{pg}$ phase grain volume ($\sim$ coherence length $l_\Phi$)
- Half-width of $g^{(1)}(x)$
- $\rho_0$ condensate fraction

Most extreme behaviour
Global accuracy

Single observable error

\[ \delta_\alpha(\tau, \gamma, f_c) = \frac{\alpha^{(cf)} - \alpha^{(exact)}}{\alpha^{(exact)}} \]

Kinetic energy and coarse-grained fluctuations capture most extreme behaviour.

In the interacting gas need also Total energy for dynamics to be sensible.

\[ \rightarrow \text{use these for an indicator} \]

\[ RMS = \sqrt{\left( \delta_{varN/N} \right)^2 + \max \left[ (\delta_{E_{kin}})^2, (\delta_{E_{total}})^2 \right]} \]

Error in any observable will be < RMS
1D

**Recommendation:**
Accuracy better than 10% for $T < 0.007 \, T_d$

Use $f_c = 0.65$ (Energy cutoff = $1.3 \, k_B T$)

Pietraszewicz, PD, *PRA* 92, 063620 (2015)
Recommendation:
Don't use classical fields,
at the least not near the ideal gas regime

Pietraszewicz, PD, PRA 92, 063620 (2015)
Recommendation:
Accuracy better than 10% for $T < 0.49 \ T_c$
Use $f_c = 0.78$ ( Energy cutoff $= 1.9 \ k_BT$)

Pietraszewicz, PD, PRA 92, 063620 (2015)
Interacting gas: accuracy

\[ \min[RMS] \]

- Generated by Metropolis sampling

- Generated by SGPE

- Sampled from Bogoliubov spectrum
  - As per Mora, Castin, PRA 67, 053615 (2003)

- Interaction strength: \( \gamma \)
- Temperature: \( T = T_d \)
- RMS = 0.1
- "soliton" gas
- "thermal" quasicondensate
- "quantum" quasicondensate \( \mu \ll T \)
Interacting gas: best cutoff

\[ \varepsilon_c = \pi k_B T f_C^2. \]

Pietraszewicz, PD, arXiv:1607.xxxxx
PART 2: Quantum fluctuations

• The issue:
  * Semiclassical field theories do not include quantum fluctuations.
    • antibunching
    • shot-noise
    • zero point phase fluctuations
    • Usually are not sensitive to N, only $gN$

• Stopgap measure: truncated Wigner
  * GPE evolution, but $\frac{1}{2}$ virtual particle per mode to emulate quantum fluctuations.
  * Good for short times :)
  * Bad for long times/stationary state :(  
    • Thermalizes to classical field ensemble, regardless of initial state.
    • Virtual particles convert to heat.
    • Temperature of this ensemble set by cfield energy + vacuum energy + cutoff
Stochastic GPE – alternative classical field model

low energy c-field region
 coupled modes
 ensemble of fields $\phi(x)$

high energy
 thermal region
 indep. modes
 $F_j(T, \mu)$

$P_C I - P_C$
Naturally generates a Grand canonical ensemble at long times

\[
\frac{d\phi(x)}{dt} = \mathcal{P}_C \left\{ -\frac{i + \gamma(x)}{\hbar} \mathcal{P}_C \left[ (H_{sp} - \mu + g|\phi(x)|^2) \phi(x) \right] + \sqrt{\frac{2\gamma(x)k_B T}{\hbar}} \eta(x, t) \right\}.
\]

\[
\langle \eta(x, t)^* \eta(x', t') \rangle = \delta(t - t') \delta^d(x - x')
\]

- Still no quantum fluctuations.

- However...
  it turns out that the several derivations always begin with the full quantum Wigner representation.

- Then why no quantum fluctuations?
  ... because they were always removed by hand by everyone to make the equation easier to handle.

- SO,
  what happens when we leave them be?

Wigner SGPE with quantum fluctuations

\[ \frac{d\phi(x)}{dt} = \mathcal{P}_C \left\{ -\frac{i}{\hbar} \mathcal{P}_C \left[ (H_{sp} - \mu + g \left[ |\phi(x)|^2 - P_C(x, x) \right] ) \phi(x) \right] \right\} \]

\[ - \frac{\mathcal{P}_C[\gamma(x)]}{\hbar} \mathcal{P}_C \left[ (H_{ke} + D_{x}^{\text{reg}}(x) - 2k_B T) \phi(x) \right] \]

\[ + \sqrt{\mathcal{P}_C[\gamma(x)]} \left[ \sqrt{D_{x}^{\text{reg}}(x)} \eta(x, t) + \frac{1}{(2\pi)^{d/2}} \int d^d k e^{i k \cdot x} \frac{\hbar |k|}{\sqrt{2m}} \tilde{\eta}(k, t) \right] \}

\[ D_{x}^{\text{reg}}(x) = \max \left[ 2k_B T - \mu + V(x) + g \left[ |\phi(z)|^2 - P_C(x, x) \right] \right], \quad k_B T \]

Energy dependent diffusion

In x-space

Coupling to High energy tails

in k-space

Small correction

White noises

\[ \langle \eta(x, t)^{*} \eta(x', t') \rangle = \delta(t - t') \delta^d(x - x') \]

\[ \langle \tilde{\eta}(k, t)^{*} \tilde{\eta}(k', t') \rangle = \delta(t - t') \delta^d(k - k') \]

Minimal diffusion at low energy

Skip 15 pages, … and voila!
Observables

Need to be done properly in Wigner representation:

\[ \langle \hat{\Psi}^\dagger(x)\hat{\Psi}(x') \rangle = \langle \phi(x)^*\phi(y) \rangle_{\text{ensemble}} - \frac{1}{2} P_C(y, x). \]

\[ \langle \hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x')\hat{\Psi}(x)\hat{\Psi}(x') \rangle \]

\[ = \left\langle \left[ |\phi(x)|^2 - \frac{P_C(x, x)}{2} \right] \left[ |\phi(y)|^2 - \frac{P_C(y, y)}{2} \right] \right. \]

\[ \left. - \text{Re} \left[ \phi(x)^*\phi(y) P_C(x, y) \right] + \frac{1}{4} |P_C(x, y)|^2 \right\rangle_{\text{ensemble}} \]

Allows e.g. for antibunching
Sensitivity to absolute particle number

Classical fields:

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

GPE / SGPE is unchanged under the transformation:

But quantum fluctuations rise with

$$\gamma_{LL} = g/n \sim \lambda^2$$

Small absolute particle numbers can be obtained

$$\langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x') \rangle = \langle \phi(x)^* \phi(y) \rangle_{\text{ensemble}} - \frac{1}{2} P_C(y, x).$$
Antibunching appears

\[ g \rightarrow g \lambda \]

\[ \psi(x) \rightarrow \frac{\psi(x)}{\sqrt{\lambda}} \]

\[ T \rightarrow \frac{T}{\lambda} \]

Increasing \( \gamma_{LL} = \frac{g}{n} \)

\( \gamma_{LL} = \frac{g}{n} \sim \lambda^2 \)

Classical field (SGPE)

WSGPE

PD, Pietraszewicz, Proukakis, Swisłocki, arXiv:1608.xxxxx
Phase fluctuations with quantum contribution

As interaction rises, keeping constant chemical potential $\mu$ and $T/T_d$, ....

Small $\gamma_{LL} = g/n$

Larger $\gamma_{LL} = g/n \sim 0.001$

Largest $\gamma_{LL} = g/n \sim 0.01$

The expected drop in phase correlation length

Phase coherence length

Thermal fluctuations:

$$\ln\left[\frac{g_1(r)}{\rho}\right] = \frac{r}{l_c} + o(1/r^n)$$

Quantum+thermal fluctuations:

$$\ln\left[\frac{g_1(r)}{\rho}\right] = \frac{r}{l_c} + K + o(1/r^n)$$

$\gamma_{LL} = g/n$

PD, Pietrasziewicz, Proukakis, Swisłocki, arXiv:1608.xxxxx

Thermal fluctuations:

$$g_1(r)/\rho = \frac{r}{l_c} + o(1/r^n)$$

Quantum+thermal fluctuations:

$$g_1(r)/\rho = \frac{r}{l_c} + K + o(1/r^n)$$
Strong soliton regime $\frac{\tau}{\sqrt{\gamma_{LL}}} \approx 1.0$, $\mu = 22.4$

SGPE $\gamma_{LL} \rightarrow 0$, $N \rightarrow \infty$, e.g. $N \approx 20\,000$
Strong soliton regime $\frac{\tau}{\sqrt{\gamma_{LL}}} \approx 1.0, \mu = 22.4$

WSGPE $\gamma_{LL} \approx 0.001, N \approx 2000$
Strong soliton regime $\frac{\tau}{\sqrt{\gamma_{LL}}} \approx 1.0$, $\mu = 22.4$

WSGPE $\gamma_{LL} \approx 0.01$, $N \approx 500$
Wrap-up

- We have determined the range of conditions for which a consistent and accurate classical field description exists. It is most necessary to take into account at least: density, density fluctuations, and kinetic energy.

- A “nonclassical” field theory has been derived which allows for treatment of quantum and thermal fluctuations together. Can see quantum depletion, antibunching, ...

- This “Wigner SGPE” has similar numerical properties to the standard SGPE and is not much more numerically intensive.

Thank you!