Recent Progress on Number-Conserving Formulations in an Ultracold Bose Gas

SA Gardiner (Durham University)
SA Morgan (University College London/Lehman Brothers)

Gardiner, Morgan, PRA 75 043612 (2007)
Introduction/Overview

- Builds on formalism by CW Gardiner [PRA 56 1414 (1997)] and Castin and Dum [PRA 57 3008 (1998)]

- Used by Morgan and coworkers to study finite $T$ BEC excitations

- Also suitable for dynamics leading to condensate depletion [eg Gardiner, Jaksch, Dum, Cirac, Zoller PRA 62 023612 (2000)]

Morgan, Rusch, Hutchinson, Burnett, PRL 91 250403 (2003)

![Graph showing solid circles and open circles with annotations](image)
Low-Temperature Limit

• Consider a dilute gas of interacting bosonic atoms

• If “nearly all” atoms occupy one mode, use Gross-Pitaevskii equation

\[ i\hbar \frac{\partial}{\partial t} \phi(r) = \left[ H_{sp}(r) + \bar{U}|\phi(r)|^2 - \lambda_0 \right] \phi(r) \]

• Quantum field \( \rightarrow \) classical field (justified in various ways)

• What if we wish to account for “other” atoms?

http://cua.mit.edu/ketterle_group/Nice_pics.htm
Can partition system/field operator $\hat{\Psi}(r)$ into condensate and non-condensate components.

Commonly, define condensate $\phi_{SB}(r) = \langle \hat{\Psi}(r) \rangle$ and non-condensate $\delta \hat{\Psi}_{SB}(r) = \hat{\Psi}(r) - \langle \hat{\Psi}(r) \rangle$ (symmetry breaking).
• Symmetry breaking Requires **coherent superposition** of different numbers of particles

• **Number conserving** theories demand a fixed number of particles

• Experimentally, total particle number only known statistically, but shot-to-shot coherences are unlikely
Onsager-Penrose Approach

- Define condensate mode as **eigenfunction** with **largest eigenvalue** of 1-body density matrix \( \rho(r, r') = \langle \hat{\Psi}^+(r') \hat{\Psi}(r) \rangle \)

\[
\int dr' \rho(r, r') \phi(r') = N_c \phi(r)
\]

- Partition field operator

\[
\hat{\Psi}(r) = \hat{a}_c \phi(r) + \delta\hat{\Psi}(r)
\]

- Assumption that non-condensate “small” results in Gross-Pitaevskii equation

\[
i\hbar \frac{\partial}{\partial t} \phi(r) = \left[ H_{sp}(r) + \tilde{U}|\phi(r)|^2 - \lambda_0 \right] \phi(r)
\]
Beyond Gross-Pitaevskii

\[ \int dr' \rho(r, r') \phi(r') = N_c \phi(r) \quad \text{with} \quad \hat{\Psi}(r) = \hat{a}_c \phi(r) + \delta \hat{\Psi}(r) \quad \text{imply} \]

\[ \langle \hat{a}_c^\dagger \delta \hat{\Psi}(r) \rangle = 0 \]

\[ N_c = \langle \hat{N}_c \rangle \equiv \langle \hat{a}_c^\dagger \hat{a}_c \rangle \]

• Candidate **number-conserving fluctuation operators** (analogous to \( \delta \hat{\Psi}_{SB}(r) \))

\[ \hat{\Lambda}_c(r) = \frac{1}{\sqrt{N_c}} \hat{a}_c^\dagger \delta \hat{\Psi}(r) \]

\[ \tilde{\Lambda}(r) = \frac{1}{\sqrt{N_c}} \hat{a}_c^\dagger \delta \hat{\Psi}(r) \]
### Choice of Candidate Operator

\[
\hat{\Lambda}_c(r) = \frac{1}{\sqrt{N_c}} \hat{a}_c^\dagger \delta \hat{\Psi}(r) \\
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\]

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### Choice of Candidate Operator

The candidate operators and their properties are as follows:

\[
\hat{\Lambda}_c(r) = \frac{1}{\sqrt{N_c}} \hat{a}_c \delta \hat{\Psi}(r) \quad \text{and} \quad \tilde{\Lambda}(r) = \frac{1}{\sqrt{N_c}} \hat{a}_c^\dagger \delta \hat{\Psi}(r)
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\[ \hat{\Lambda}_c(r) = \frac{1}{\sqrt{N_c}} \hat{a}^\dagger_c \delta \hat{\Psi}(r) \]

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1st Order: Bogoliubov-de Gennes Equations

- **Linearized** equations ($Q(r, r')$ are orthogonal projectors to condensate mode, $\tilde{U} = U_0 N_c$)

\[
i\hbar \frac{d}{dt} \tilde{\Lambda}(r) = \left[ H_{sp}(r) + \tilde{U}|\phi(r)|^2 - \lambda_0 \right] \tilde{\Lambda}(r) + \tilde{U} \int dr' Q(r, r')|\phi(r')|^2 \tilde{\Lambda}(r') + \tilde{U} \int dr' Q(r, r')\phi^2(r')\tilde{\Lambda}^\dagger(r').
\]

- Coupled to **Gross-Pitaevskii equation**

\[
i\hbar \frac{\partial}{\partial t} \phi(r) = \left[ H_{sp}(r) + \tilde{U}|\phi(r)|^2 - \lambda_0 \right] \phi(r)
\]
Fluctuations About a Mean

- Fluctuations assert their existence by having an observable effect, through pair averages (e.g., $T=0$ quantum depletion)

- Non-steady-state evolution of BdG+GPE equations can imply unconstrained growth of non-condensate

- No back-action on condensate
Finite Total Particle Number

- Will need **2nd order** equations of motion, generated by a **3rd order** Hamiltonian
3rd Order Hamiltonian

\[ \hat{H}_3 = N_c \int d\mathbf{r} \phi^*(\mathbf{r}) \left[ \hat{H}_{sp}(\mathbf{r}) + \frac{\tilde{U}}{2} |\phi(\mathbf{r})|^2 \right] \phi(\mathbf{r}) + \sqrt{N_c} \int d\mathbf{r} \left\{ \phi^*(\mathbf{r}) \left[ \hat{H}_{sp}(\mathbf{r}) + \tilde{U} |\phi(\mathbf{r})|^2 \right] \tilde{\Lambda}(\mathbf{r}) + \text{H.c.} \right\} \\
+ \int d\mathbf{r} \tilde{\Lambda}^*(\mathbf{r}) \left[ \hat{H}_{sp}(\mathbf{r}) + 2\tilde{U} |\phi(\mathbf{r})|^2 \right] \tilde{\Lambda}(\mathbf{r}) + \frac{\tilde{U}}{2} \int d\mathbf{r} \left[ \phi^*(\mathbf{r})^2 \tilde{\Lambda}(\mathbf{r})^2 + \text{H.c.} \right] - \frac{\tilde{U}}{2} \int d\mathbf{r} |\phi(\mathbf{r})|^4 \\
+ \int d\mathbf{r} \left[ \langle \tilde{\Lambda}^*(\mathbf{r}) \tilde{\Lambda}(\mathbf{r}) \rangle - \tilde{\Lambda}^*(\mathbf{r}) \tilde{\Lambda}(\mathbf{r}) \right] \int d\mathbf{r} \phi^*(\mathbf{r}) \left[ \hat{H}_{sp}(\mathbf{r}) + \tilde{U} |\phi(\mathbf{r})|^2 \right] \phi(\mathbf{r}) \\
+ \frac{\tilde{U}}{\sqrt{N_c}} \int d\mathbf{r} \left\{ \phi^*(\mathbf{r}) \left[ 2\langle \tilde{\Lambda}^*(\mathbf{r}) \tilde{\Lambda}(\mathbf{r}) \rangle \tilde{\Lambda}(\mathbf{r}) + \tilde{\Lambda}^*(\mathbf{r}) \langle \tilde{\Lambda}(\mathbf{r})^2 \rangle \right] + \text{H.c.} \right\} - \frac{\tilde{U}}{\sqrt{N_c}} \int d\mathbf{r} \left[ \phi^*(\mathbf{r}) |\phi(\mathbf{r})|^2 \tilde{\Lambda}(\mathbf{r}) + \text{H.c.} \right] \\
+ \frac{\tilde{U}}{\sqrt{N_c}} \iint d\mathbf{r} d\mathbf{r}' \left\{ \phi^*(\mathbf{r}) |\phi(\mathbf{r})|^2 \left[ \langle \tilde{\Lambda}^*(\mathbf{r}') \tilde{\Lambda}(\mathbf{r}) \rangle \tilde{\Lambda}(\mathbf{r}') + \tilde{\Lambda}^*(\mathbf{r}') \langle \tilde{\Lambda}(\mathbf{r}) \tilde{\Lambda}(\mathbf{r}) \rangle \right] + \text{H.c.} \right\}. \\
\]

- We have used (Hartree-Fock-like)

\[ \tilde{\Lambda}^*(\mathbf{r}) \tilde{\Lambda}(\mathbf{r}') \tilde{\Lambda}(\mathbf{r}'') \approx \langle \tilde{\Lambda}^*(\mathbf{r}) \tilde{\Lambda}(\mathbf{r}') \rangle \tilde{\Lambda}(\mathbf{r}'') + \langle \tilde{\Lambda}^*(\mathbf{r}) \tilde{\Lambda}(\mathbf{r}'') \rangle \tilde{\Lambda}(\mathbf{r}') + \langle \tilde{\Lambda}(\mathbf{r}') \tilde{\Lambda}(\mathbf{r}'') \rangle \tilde{\Lambda}^*(\mathbf{r}) \]
Hartree-Fock Factorization

- Morgan [J Phys B 33 3847 (2000)] found HFB factorizations of cubic products omitted terms as large as terms of quartic origin which were retained

- However ...
  - We have neglected quartic terms altogether
  - Cubic terms eliminated in the steady state
Generalized Gross-Pitaevskii Equation

- Use Hamiltonian to generate EOM for $\tilde{\Lambda}(\mathbf{r})$

$$i\hbar \frac{\partial}{\partial t} \phi(\mathbf{r}) = \left\{ H_{sp}(\mathbf{r}) + \tilde{U} \left[ \left( 1 - \frac{1}{N_c} \right) |\phi(\mathbf{r})|^2 + 2 \frac{\langle \tilde{\Lambda}^\dagger(\mathbf{r})\tilde{\Lambda}(\mathbf{r}) \rangle}{N_c} \right] - \lambda_2 \right\} \phi(\mathbf{r}) + \tilde{U} \phi^*(\mathbf{r}) \frac{\langle \tilde{\Lambda}(\mathbf{r})^2 \rangle}{N_c}$$

$$- \tilde{U} \int d\mathbf{r}' |\phi(\mathbf{r}')|^2 \left[ \frac{\langle \tilde{\Lambda}^\dagger(\mathbf{r}')\tilde{\Lambda}(\mathbf{r}) \rangle}{N_c} \phi(\mathbf{r}') + \phi^*(\mathbf{r}') \frac{\langle \tilde{\Lambda}(\mathbf{r}')\tilde{\Lambda}(\mathbf{r}) \rangle}{N_c} \right]$$

- $\lambda_2$ is a (possibly complex) scalar
• Substituting the generalized Gross-Pitaevskii equation back into the EOM for \( \tilde{\Lambda}(\mathbf{r}) \) yields

\[

i\hbar \frac{d}{dt} \tilde{\Lambda}(\mathbf{r}) = \left[ H_{sp}(\mathbf{r}) + \tilde{U}|\phi(\mathbf{r})|^2 - \lambda_0 \right] \tilde{\Lambda}(\mathbf{r}) + \tilde{U} \int d\mathbf{r}' Q(\mathbf{r}, \mathbf{r}') |\phi(\mathbf{r}')|^2 \tilde{\Lambda}(\mathbf{r}') \\
+ \tilde{U} \int d\mathbf{r}' Q(\mathbf{r}, \mathbf{r}') \phi^2(\mathbf{r}') \tilde{\Lambda}^\dagger(\mathbf{r}').
\]

• **No change** from 1st order BdG equations
Orthogonality and Nonlocality

- **Linear** Schrodinger equation preserves orthogonality

- **Not so** with nonlinear field equations

- Must “know” about orthogonal component everywhere in space, hence **nonlocal terms**
If we let $N_c \to \infty$, then the generalized GPE

\[
i\hbar \frac{\partial}{\partial t} \phi(\mathbf{r}) = \left\{ H_{\text{sp}}(\mathbf{r}) + \bar{U} \left[ \left( 1 - \frac{1}{N_c} \right) |\phi(\mathbf{r})|^2 + 2 \frac{\langle \tilde{\Lambda}^+(\mathbf{r})\tilde{\Lambda}(\mathbf{r}) \rangle}{N_c} \right] - \lambda_2 \right\} \phi(\mathbf{r}) + \bar{U} \phi^*(\mathbf{r}) \frac{\langle \tilde{\Lambda}(\mathbf{r})^2 \rangle}{N_c}
\]

\[
- \bar{U} \int d\mathbf{r}' |\phi(\mathbf{r}')|^2 \left[ \frac{\langle \tilde{\Lambda}^+(\mathbf{r}')\tilde{\Lambda}(\mathbf{r}) \rangle}{N_c} \phi(\mathbf{r}') + \phi^*(\mathbf{r}') \frac{\langle \tilde{\Lambda}(\mathbf{r}')\tilde{\Lambda}(\mathbf{r}) \rangle}{N_c} \right]
\]

reduces to the standard GPE

\[
i\hbar \frac{\partial}{\partial t} \phi(\mathbf{r}) = \left[ H_{\text{sp}}(\mathbf{r}) + \bar{U} |\phi(\mathbf{r})|^2 - \lambda_0 \right] \phi(\mathbf{r})
\]

while the BdG equations remain unchanged.
Infinite Particle Limit

Non-condensate

Condensate
Conclusions

• Offers a **consistent** number-conserving treatment for coupled condensate and non-condensate dynamics

• 2nd order: minimal **non-trivial** treatment

**Acknowledgements: UK EPSRC, Royal Society**