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

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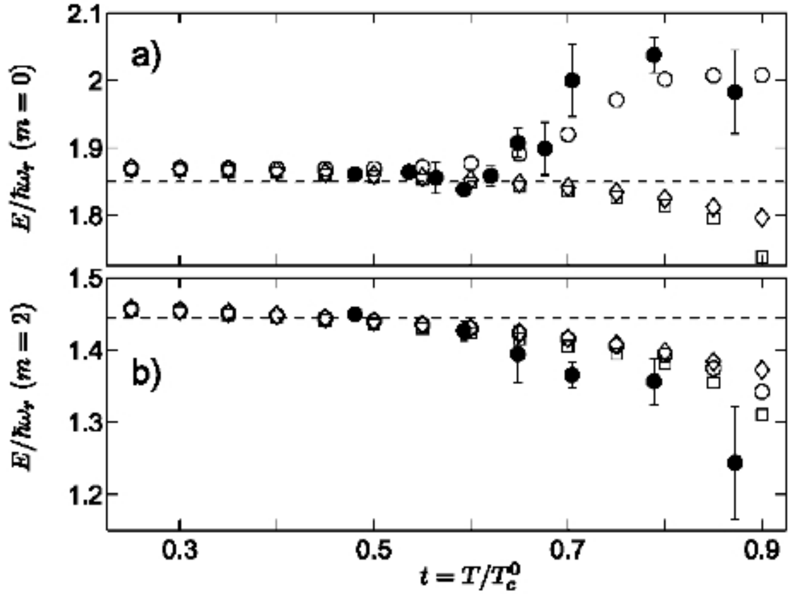
Gardiner, Morgan, PRA **75** 043612 (2007)

Durham University

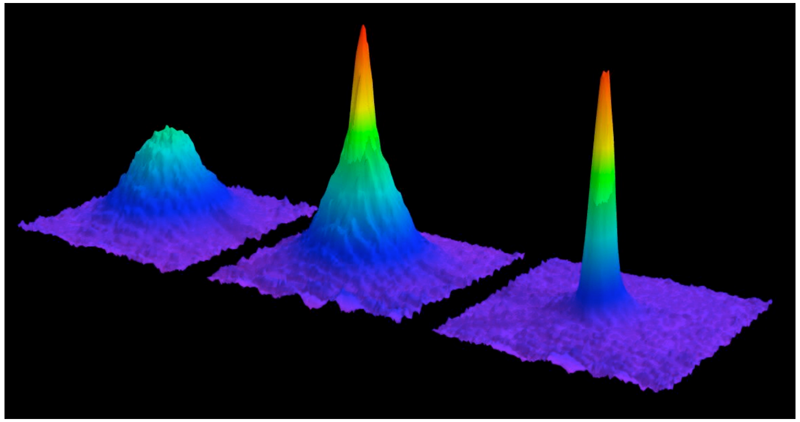
- Builds on formalism by CW Gardiner [PRA **56** 1414 (1997)] and Castin and Dum [PRA **57** 3008 (1998)]
- Used by Morgan and coworkers to study **finite *T*** BEC excitations
- Also suitable for dynamics leading to **condensate depletion** [eg Gardiner, Jaksch, Dum, Cirac, Zoller PRA **62** 023612 (2000)]

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



Solid circles: experiment
Open circles: full theory

http://cua.mit.edu/ketterle_group/Nice_pics.htm



- Consider a dilute gas of interacting bosonic atoms

- If "nearly all" atoms occupy one mode, use **Gross-Pitaevskii** equation

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

- Quantum field ➔ classical field (justified in various ways)

- What if we wish to account for "other" atoms?

Partition

- Can partition system/field operator $\hat{\Psi}(\mathbf{r})$ into **condensate** and **non-condensate** components

- Commonly, define **condensate** $\phi_{SB}(\mathbf{r}) = \langle\hat{\Psi}(\mathbf{r})\rangle$ and **non-condensate** $\delta\hat{\Psi}_{SB}(\mathbf{r}) = \hat{\Psi}(\mathbf{r}) - \langle\hat{\Psi}(\mathbf{r})\rangle$ (symmetry breaking)

Symmetry Breaking vs Number Conservation

- 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

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

$$\int d\mathbf{r}'\rho(\mathbf{r},\mathbf{r}')\phi(\mathbf{r}') = N_c\phi(\mathbf{r})$$

- Partition field operator

$$\hat{\Psi}(\mathbf{r}) = \hat{a}_c\phi(\mathbf{r}) + \delta\hat{\Psi}(\mathbf{r})$$

- Assumption that non-condensate "small" results in Gross-Pitaevskii equation

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

- $\int d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}')\phi(\mathbf{r}') = N_c \phi(\mathbf{r})$ with $\hat{\Psi}(\mathbf{r}) = \hat{a}_c \phi(\mathbf{r}) + \delta\hat{\Psi}(\mathbf{r})$ imply

$$\langle \hat{a}_c^\dagger \delta\hat{\Psi}(\mathbf{r}) \rangle = 0 \qquad N_c = \langle \hat{N}_c \rangle \equiv \langle \hat{a}_c^\dagger \hat{a}_c \rangle$$

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

$$\hat{\Lambda}_c(\mathbf{r}) = \frac{1}{\sqrt{\hat{N}_c}} \hat{a}_c^\dagger \delta\hat{\Psi}(\mathbf{r}) \qquad \tilde{\Lambda}(\mathbf{r}) = \frac{1}{\sqrt{N_c}} \hat{a}_c^\dagger \delta\hat{\Psi}(\mathbf{r})$$

Choice of Candidate Operator

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$$\hat{\Lambda}_c(\mathbf{r}) = \frac{1}{\sqrt{\hat{N}_c}}\hat{a}_c^\dagger \delta\hat{\Psi}(\mathbf{r}) \qquad \tilde{\Lambda}(\mathbf{r}) = \frac{1}{\sqrt{N_c}}\hat{a}_c^\dagger \delta\hat{\Psi}(\mathbf{r})$$

Candidate operator	Number conserving?	Bosonic commutation relations?	Expectation value =0?
$\delta\hat{\Psi}_{\mathrm{SB}}(\mathbf{r})$	✖	✔	✔
$\hat{\Lambda}_c(\mathbf{r})$	✔		
$\tilde{\Lambda}(\mathbf{r})$	✔		

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$\tilde{\Lambda}(\mathbf{r})$	✔		

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$\hat{\Lambda}_c(\mathbf{r})$	✔	✔	✖
$\tilde{\Lambda}(\mathbf{r})$	✔		

Choice of Candidate Operator

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$$\hat{\Lambda}_c(\mathbf{r}) = \frac{1}{\sqrt{\hat{N}_c}}\hat{a}_c^{\dagger}\delta\hat{\Psi}(\mathbf{r}) \qquad \tilde{\Lambda}(\mathbf{r}) = \frac{1}{\sqrt{N_c}}\hat{a}_c^{\dagger}\delta\hat{\Psi}(\mathbf{r})$$

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$\delta\hat{\Psi}_{\rm SB}(\mathbf{r})$	✖	✔	✔
$\hat{\Lambda}_c(\mathbf{r})$	✔	✔	✖
$\tilde{\Lambda}(\mathbf{r})$	✔		✔

Choice of Candidate Operator

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$$\hat{\Lambda}_c(\mathbf{r}) = \frac{1}{\sqrt{\hat{N}_c}}\hat{a}_c^\dagger \delta\hat{\Psi}(\mathbf{r}) \qquad \tilde{\Lambda}(\mathbf{r}) = \frac{1}{\sqrt{N_c}}\hat{a}_c^\dagger \delta\hat{\Psi}(\mathbf{r})$$

Candidate operator	Number conserving?	Bosonic commutation relations?	Expectation value =0?
$\delta\hat{\Psi}_{\mathrm{SB}}(\mathbf{r})$	✖	✔	✔
$\hat{\Lambda}_c(\mathbf{r})$	✔	✔	✖
$\tilde{\Lambda}(\mathbf{r})$	✔	✖	✔

Choice of Candidate Operator

$$\hat{\Lambda}_c(\mathbf{r}) = \frac{1}{\sqrt{\hat{N}_c}}\hat{a}_c^\dagger \delta\hat{\Psi}(\mathbf{r}) \qquad \tilde{\Lambda}(\mathbf{r}) = \frac{1}{\sqrt{N_c}}\hat{a}_c^\dagger \delta\hat{\Psi}(\mathbf{r})$$

Candidate operator	Number conserving?	Bosonic commutation relations?	Expectation value =0?
$\delta\hat{\Psi}_{\mathrm{SB}}(\mathbf{r})$	✖	✔	✔
$\hat{\Lambda}_c(\mathbf{r})$	✔	✔	✖
$\tilde{\Lambda}(\mathbf{r})$	✔	✖	✔

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

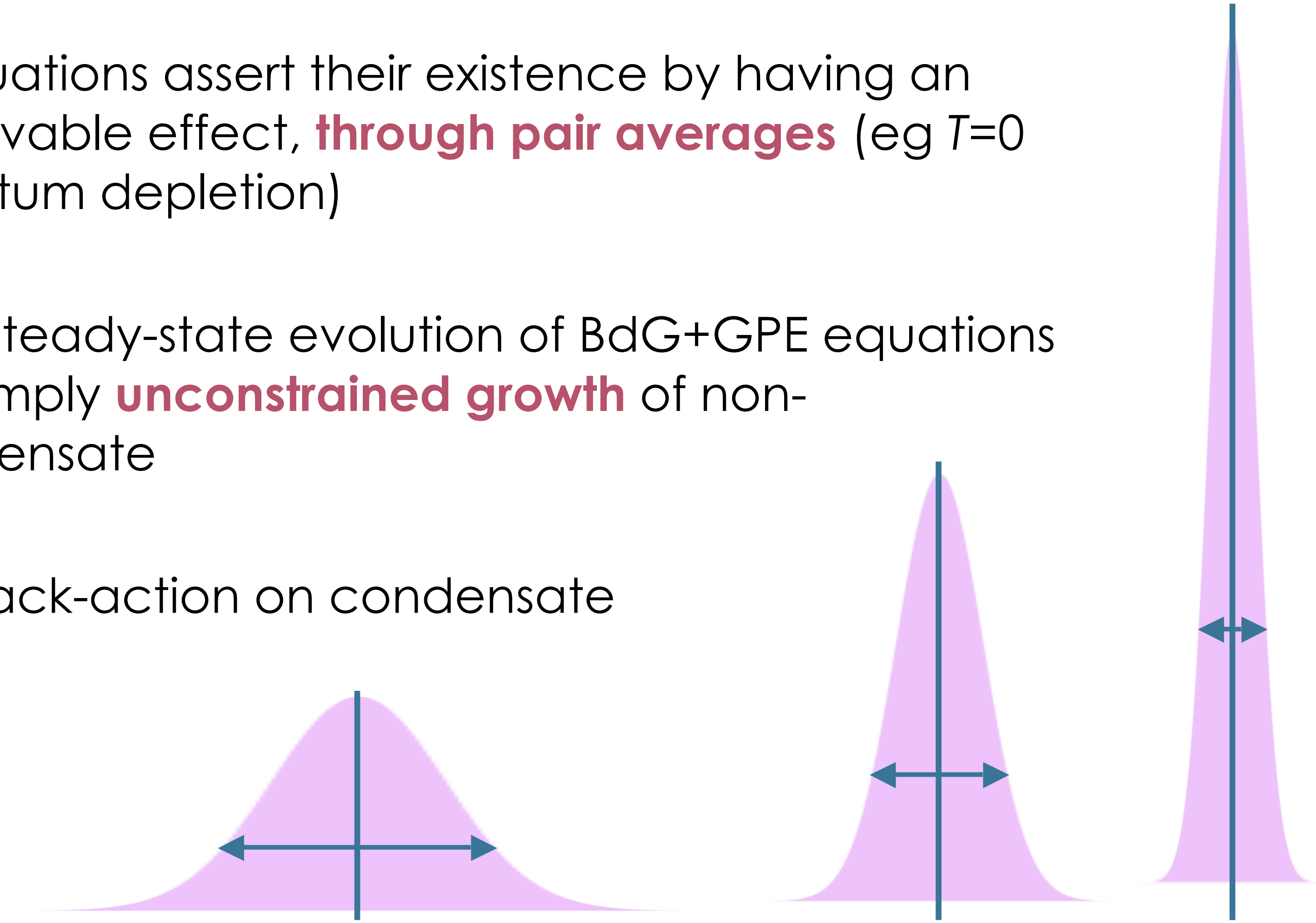
$$i\hbar\frac{d}{dt}\tilde{\Lambda}(\mathbf{r}) = \left[H_{\mathrm{sp}}(\mathbf{r}) + \tilde{U}|\phi(\mathbf{r})|^2 - \lambda_0\right]\tilde{\Lambda}(\mathbf{r}) + \tilde{U}\int d\mathbf{r}'\,Q(\mathbf{r},\mathbf{r}')|\phi(\mathbf{r}')|^2\tilde{\Lambda}(\mathbf{r}') + \tilde{U}\int d\mathbf{r}'\,Q(\mathbf{r},\mathbf{r}')\phi^2(\mathbf{r}')\tilde{\Lambda}^\dagger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

- Coupled to **Gross-Pitaevskii equation**

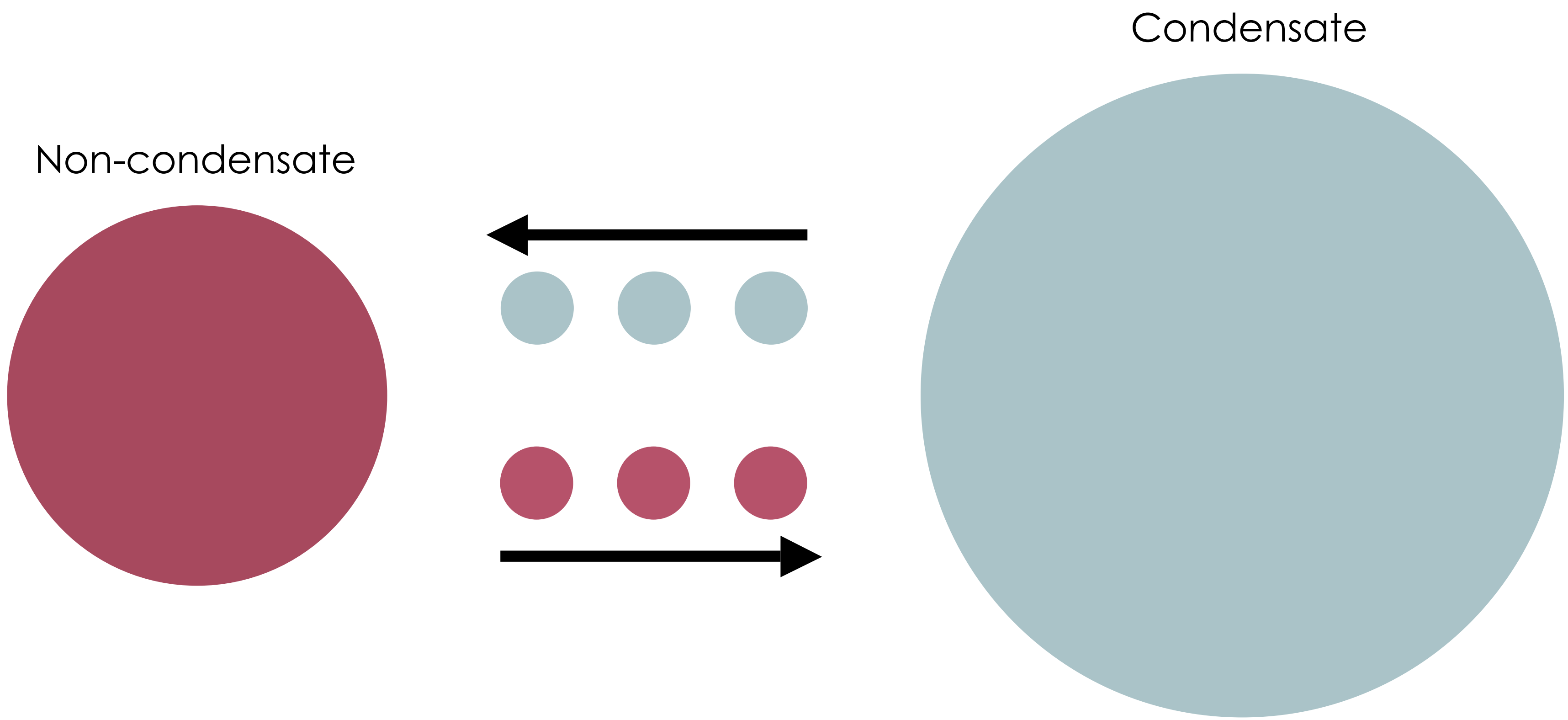
$$i\hbar\frac{\partial}{\partial t}\phi(\mathbf{r}) = \left[H_{\mathrm{sp}}(\mathbf{r}) + \tilde{U}|\phi(\mathbf{r})|^2 - \lambda_0\right]\phi(\mathbf{r})$$

Fluctuations About a Mean

- Fluctuations assert their existence by having an observable effect, **through pair averages** (eg *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

$$\begin{aligned}\hat{H}_3 =& N_c \int d\mathbf{r}\phi^*(\mathbf{r})\left[H_{\mathrm{sp}}(\mathbf{r}) + \frac{\tilde{U}}{2}|\phi(\mathbf{r})|^2\right]\phi(\mathbf{r}) + \sqrt{N_c}\int d\mathbf{r}\left\{\phi^*(\mathbf{r})\left[H_{\mathrm{sp}}(\mathbf{r}) + \tilde{U}|\phi(\mathbf{r})|^2\right]\tilde{\Lambda}(\mathbf{r}) + \mathrm{H.c.}\right\}\\
&+ \int d\mathbf{r}\tilde{\Lambda}^\dagger(\mathbf{r})\left[H_{\mathrm{sp}}(\mathbf{r}) + 2\tilde{U}|\phi(\mathbf{r})|^2\right]\tilde{\Lambda}(\mathbf{r}) + \frac{\tilde{U}}{2}\int d\mathbf{r}\left[\phi^*(\mathbf{r})^2\tilde{\Lambda}(\mathbf{r})^2 + \mathrm{H.c.}\right] - \frac{\tilde{U}}{2}\int d\mathbf{r}|\phi(\mathbf{r})|^4\\
&+ \int d\mathbf{r}'\left[\langle\tilde{\Lambda}^\dagger(\mathbf{r}')\tilde{\Lambda}(\mathbf{r}')\rangle - \tilde{\Lambda}^\dagger(\mathbf{r}')\tilde{\Lambda}(\mathbf{r}')\right]\int d\mathbf{r}\phi^*(\mathbf{r})\left[H_{\mathrm{sp}}(\mathbf{r}) + \tilde{U}|\phi(\mathbf{r})|^2\right]\phi(\mathbf{r})\\
&+ \frac{\tilde{U}}{\sqrt{N_c}}\int d\mathbf{r}\left\{\phi^*(\mathbf{r})\left[2\langle\tilde{\Lambda}^\dagger(\mathbf{r})\tilde{\Lambda}(\mathbf{r})\rangle\tilde{\Lambda}(\mathbf{r}) + \tilde{\Lambda}^\dagger(\mathbf{r})\langle\tilde{\Lambda}(\mathbf{r})^2\rangle\right] + \mathrm{H.c.}\right\} - \frac{\tilde{U}}{\sqrt{N_c}}\int d\mathbf{r}\left[\phi^*(\mathbf{r})|\phi(\mathbf{r})|^2\tilde{\Lambda}(\mathbf{r}) + \mathrm{H.c.}\right]\\
&+ \frac{\tilde{U}}{\sqrt{N_c}}\iint d\mathbf{r}d\mathbf{r}'\left\{\phi^*(\mathbf{r})|\phi(\mathbf{r})|^2\left[\langle\tilde{\Lambda}^\dagger(\mathbf{r}')\tilde{\Lambda}(\mathbf{r})\rangle\tilde{\Lambda}(\mathbf{r}') + \tilde{\Lambda}^\dagger(\mathbf{r}')\langle\tilde{\Lambda}(\mathbf{r}')\tilde{\Lambda}(\mathbf{r})\rangle\right] + \mathrm{H.c.}\right\}.\end{aligned}$$

- We have used (Hartree-Fock-like)

$$\tilde{\Lambda}^\dagger(\mathbf{r})\tilde{\Lambda}(\mathbf{r}')\tilde{\Lambda}(\mathbf{r}'') \approx \langle\tilde{\Lambda}^\dagger(\mathbf{r})\tilde{\Lambda}(\mathbf{r}')\rangle\tilde{\Lambda}(\mathbf{r}'') + \langle\tilde{\Lambda}^\dagger(\mathbf{r})\tilde{\Lambda}(\mathbf{r}'')\rangle\tilde{\Lambda}(\mathbf{r}') + \langle\tilde{\Lambda}(\mathbf{r}')\tilde{\Lambda}(\mathbf{r}'')\rangle\tilde{\Lambda}^\dagger(\mathbf{r})$$

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 $\tilde{\Lambda}(\mathbf{r})$
- Using $\left\langle i\hbar \frac{d}{dt} \tilde{\Lambda}(\mathbf{r}) \right\rangle = 0$ produces

$$i\hbar \frac{\partial}{\partial t}\phi(\mathbf{r}) = \left\{ H_{\text{sp}}(\mathbf{r}) + \tilde{U}\left[\left(1 - \frac{1}{N_c}\right)|\phi(\mathbf{r})|^2 + 2\frac{\langle \tilde{\Lambda}^\dagger(\mathbf{r})\tilde{\Lambda}(\mathbf{r})\rangle}{N_c} \right] - \lambda_2 \right\} \phi(\mathbf{r}) + \tilde{U}\phi^*(\mathbf{r})\frac{\langle \tilde{\Lambda}(\mathbf{r})^2\rangle}{N_c}$$
$$- \tilde{U}\int d\mathbf{r}'|\phi(\mathbf{r}')|^2 \left[\frac{\langle \tilde{\Lambda}^\dagger(\mathbf{r}')\tilde{\Lambda}(\mathbf{r})\rangle}{N_c}\phi(\mathbf{r}') + \phi^*(\mathbf{r}')\frac{\langle \tilde{\Lambda}(\mathbf{r}')\tilde{\Lambda}(\mathbf{r})\rangle}{N_c} \right]$$

- λ_2 is a (possibly **complex**) scalar

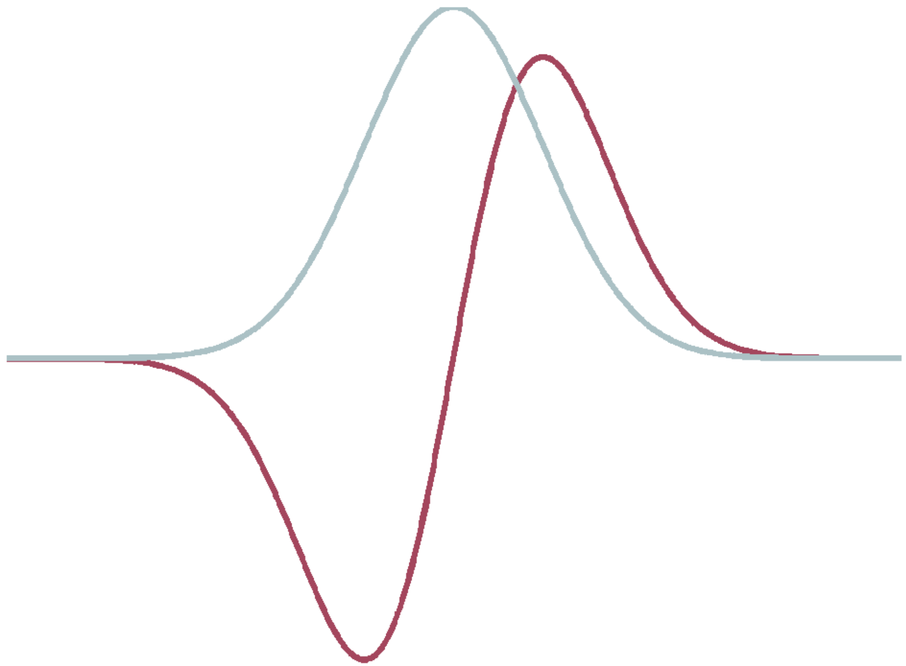
- Substituting the generalized Gross-Pitaevskii equation back into the EOM for $\tilde{\Lambda}(\mathbf{r})$ yields

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

- **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

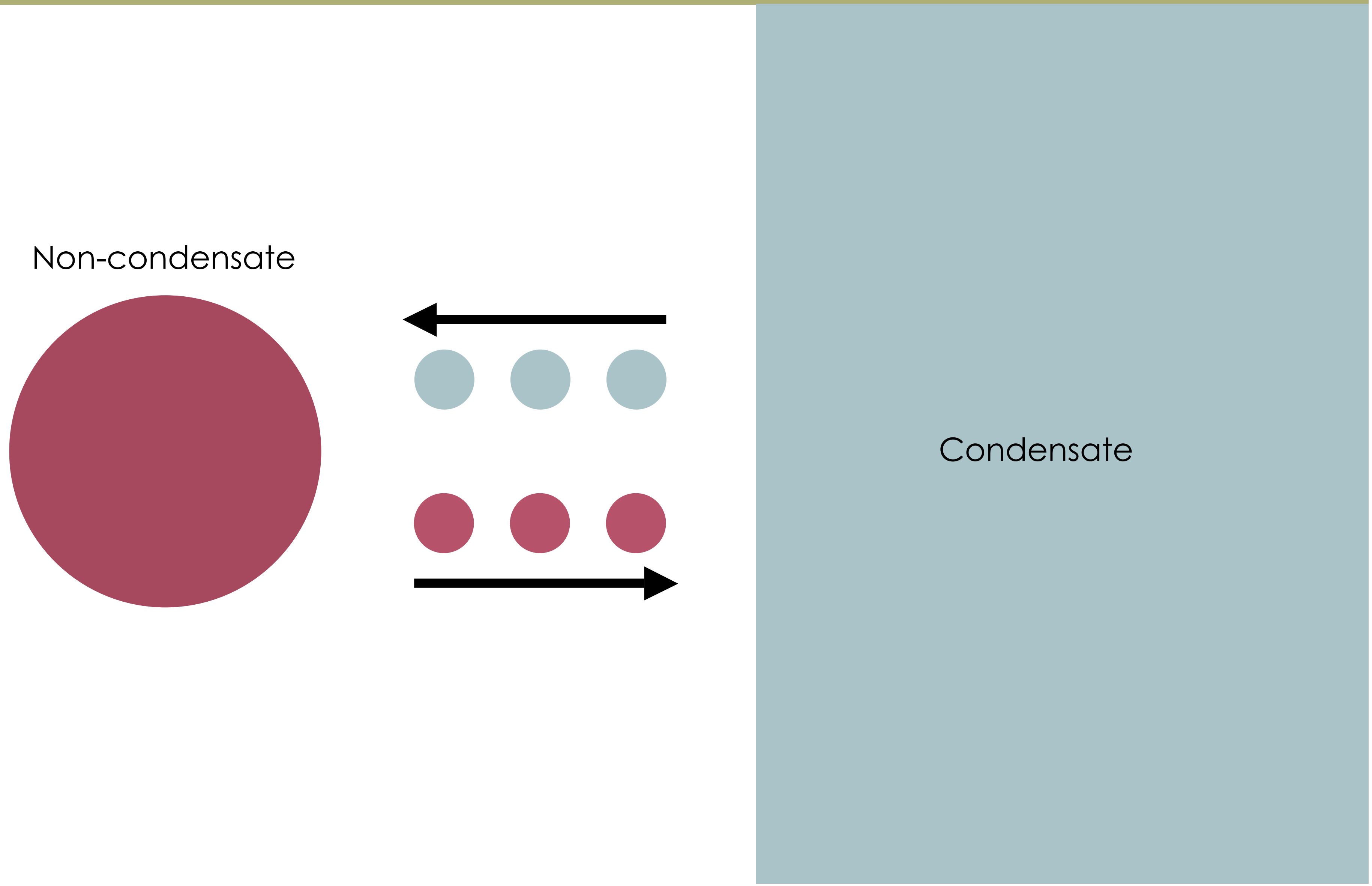
$$i\hbar \frac{\partial}{\partial t}\phi(\mathbf{r}) = \left\{ H_{\mathrm{sp}}(\mathbf{r}) + \tilde{U}\left[\left(1 - \frac{1}{N_c}\right)|\phi(\mathbf{r})|^2 + 2\frac{\langle \tilde{\Lambda}^\dagger(\mathbf{r})\tilde{\Lambda}(\mathbf{r})\rangle}{N_c} \right] - \lambda_2 \right\}\phi(\mathbf{r}) + \tilde{U}\phi^*(\mathbf{r})\frac{\langle \tilde{\Lambda}(\mathbf{r})^2\rangle}{N_c}$$
$$- \tilde{U}\int d\mathbf{r}'|\phi(\mathbf{r}')|^2 \left[\frac{\langle \tilde{\Lambda}^\dagger(\mathbf{r}')\tilde{\Lambda}(\mathbf{r})\rangle}{N_c}\phi(\mathbf{r}') + \phi^*(\mathbf{r}')\frac{\langle \tilde{\Lambda}(\mathbf{r}')\tilde{\Lambda}(\mathbf{r})\rangle}{N_c} \right]$$

reduces to the **standard** GPE

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

while the BdG equations remain **unchanged**

Infinite Particle Limit



Conclusions

- Offers a **consistent** number-conserving treatment for coupled condensate and non-condensate dynamics
- 2nd order: minimal **non-trivial** treatment

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