Suppression of phase separation in warm condensate mixtures

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AR and D. Angom, arXiv:1502.00473 [cond-mat.quant-gas]

Plan of the talk

Gross-Pitaevskii (GP) equation

Generalized GP equation

Binary BEC

Phase-separation

Correlation function

Conclusions

Gross-Pitaevskii equation (GPE)

 Equation of motion of the condensate wavefunction is given by Gross-Pitaevskii equation(GPE), strictly valid at T = 0K.

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(\mathbf{r}) + gN|\psi|^2 \right] \psi$$

- $\psi \equiv \psi(\mathbf{r}, t)$: condensate wave function • $g = \frac{4\pi\hbar^2 a}{a}$
- a: atomic scattering length > 0 : repulsive
- N: Number of atoms in the condensate

$$V_{\rm trap} = \frac{m}{2} \left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right)$$

- E. P. Gross, Il Nuovo Cimento Series 10 20, (1961),
- L. P. Pitaevskii, Soviet Physics JETP-USSR 13, (1961),
- C. Pethick & H. Smith, Bose-Einstein Condensation in Dilute Gases, (2008)

Finite Temperature models

Stationary Case:

- Hartree-Fock-Bogoliubov-Popov approximation
- Modified Popov approximation

Dynamical Case:

- Stochastic Gross-Pitaevskii equation (SGPE)
- Projected Gross-Pitaevskii equation
- Self-consistent Gross-Pitaevskii-Boltzmann (ZNG formalism)
- Dissipative Gross-Pitaevskii equation

AR, S. Gautam, and D. Angom, *Phys. Rev. A* 89, 013617 (2014),
AR and D. Angom *Phys. Rev. A* 90, 023612 (2014),
S. Gautam, AR, and Subroto Mukerjee, *Phys. Rev. A* 89, 013612 (2014),

Blakie et. al, Adv. Phys. 57, 363 (2008),

- A. J. Allen, Ph.D. Thesis (2010),
- N. P. Proukakis and B. Jackson, J. Phys. B 41, 203002 (2008).

$$\hat{H} = \int \underbrace{d\mathbf{r} \, \hat{\psi}^{\dagger}(\mathbf{r}, t) \left[\hat{h}(\mathbf{r}) - \mu \right] \hat{\psi}(\mathbf{r}, t)}_{\text{single-particle part}} + \frac{1}{2} \iint \underbrace{d\mathbf{r} d\mathbf{r}' \, \hat{\psi}^{\dagger}(\mathbf{r}, t) \hat{\psi}^{\dagger}(\mathbf{r}', t) U(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}', t) \hat{\psi}(\mathbf{r}, t)}_{\text{two-particle interaction term}}$$

where $\hat{h} = K.E + V_{\text{trap}}$ $U(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}'), \left\langle \int d\mathbf{r} \, \hat{\psi}^{\dagger}(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) \right\rangle = N$

U:: Repulsive contact interaction; N:: Total number of atoms

$$\left[\hat{\psi}(\mathbf{r}),\hat{\psi}(\mathbf{r}')\right] = \left[\hat{\psi}^{\dagger}(\mathbf{r}),\hat{\psi}^{\dagger}(\mathbf{r}')\right] = 0; \left[\hat{\psi}(\mathbf{r}),\hat{\psi}^{\dagger}(\mathbf{r}')\right] = \delta(\mathbf{r}-\mathbf{r}')$$

A.Griffin, Phys. Rev. B 53, 9341 (1996)

Hartree-Fock-Bogoliubov(HFB) approximation

The Bose field operator is

$$\hat{\psi}(\mathbf{r},t) = \sum_{i=0} \hat{\alpha}_i(t)\psi_i(\mathbf{r}) = \hat{\alpha}_0(t)\psi_0(\mathbf{r}) + \sum_{i=1} \hat{\alpha}_i(t)\psi_i(\mathbf{r}),$$
$$\hat{\alpha}_i^{\dagger}|n_0n_1,\cdots,n_i,\cdots\rangle = \sqrt{(n_i+1)}|n_0n_1,\cdots,n_i+1,\cdots\rangle,$$
$$\hat{\alpha}_i|n_0n_1,\cdots,n_i,\cdots\rangle = \sqrt{n_i}|n_0n_1,\cdots,n_i-1,\cdots\rangle.$$

BEC occurs when: $n_0 \equiv N_0 \gg 1 \rightarrow N_0, N_0 \pm 1 \approx N_0$ where $N_0 \rightarrow$ Number of **condensate** atoms

HFB approximation: $\hat{\alpha}_0 = \hat{\alpha}_0^{\dagger} = \sqrt{N_0}$, then

$$\hat{\psi}(\mathbf{r},t) = \sqrt{N_0}\psi_0(\mathbf{r})e^{-i\mu t/\hbar} + ilde{\psi}(\mathbf{r},t),$$

such that, $\langle \tilde{\psi}({\bf r},t)
angle = \langle \tilde{\psi}^{\dagger}({\bf r},t)
angle = 0.$

Dalfovo et al, Rev. Mod. Phys. 71, 463 (1999)

Generalized GP equation

Equation of motion of the Bose field operator

$$i\hbar \frac{\partial \hat{\psi}(\mathbf{r},t)}{\partial t} = (\hat{h} - \mu)\hat{\psi}(\mathbf{r},t) + g\hat{\psi}^{\dagger}(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)$$

where, $\hat{\psi}(\mathbf{r}, t) = \phi(\mathbf{r}) + \tilde{\psi}(\mathbf{r}, t)$, and $\phi(\mathbf{r}) = \sqrt{N_0}\psi_0(\mathbf{r})$. $\phi/\tilde{\psi}$ is the condensate/non-condensate part.

$$\tilde{\psi}^{\dagger}(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t) \simeq 2\underbrace{\langle \tilde{\psi}^{\dagger}(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle}_{\tilde{n}}\tilde{\psi}(\mathbf{r},t) + \underbrace{\langle \tilde{\psi}(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle}_{\tilde{m}}\tilde{\psi}^{\dagger}(\mathbf{r},t)$$

 $ilde{n}
ightarrow$ Non-condensate density; $ilde{m}
ightarrow$ Anomalous average

Generalized GPE

Including the thermal component and anomalous term, the generalized GP equation is

$$(\hat{h} - \mu)\phi(\mathbf{r}) + g|\phi(\mathbf{r})|^2\phi(\mathbf{r}) + \underbrace{2g\tilde{n}(\mathbf{r})\phi(\mathbf{r}) + g\tilde{m}(\mathbf{r})\phi^*(\mathbf{r})}_{T-dependent} = 0$$

•
$$\hat{h} = K.E. + V_{\text{trap}}$$

• $\int |\phi(\mathbf{r})|^2 d\mathbf{r} = 1$

A.Griffin, *Phys. Rev. B* **53**, 9341 (1996); Hutchinson *et. al Phys. Rev. Lett.* **78**, 1842 (1997)

Bogoliubov de-Gennes equations

Equation of motion of the thermal component

$$\begin{split} i\hbar\frac{\partial\tilde{\psi}}{\partial t} &= i\hbar\frac{\partial}{\partial t}(\hat{\psi}-\phi), \\ &= (\hat{h}-\mu)\tilde{\psi}+2gn(\mathbf{r})\tilde{\psi}+gm(\mathbf{r})\tilde{\psi}^{\dagger}, \end{split}$$

where,
$$n(\mathbf{r}) = |\phi(\mathbf{r})|^2 + \tilde{n}(\mathbf{r}); \ m(\mathbf{r}) = \phi^2(\mathbf{r}) + \tilde{m}(\mathbf{r});$$

$$\tilde{\psi} = \sum_i \left[u_j \hat{\alpha}_j e^{-iE_j t} - v_j^* \hat{\alpha}_j^\dagger e^{iE_j t} \right];$$

 $u_j, v_j \Rightarrow$ quasiparticle amplitudes Bogoliubov de-Gennes equations:

$$\mathcal{L}u_j - gmv_j = E_ju_j$$

 $\mathcal{L}v_j - gm^*u_j = -E_jv_j$

where $\mathcal{L} = \hat{h} - \mu + 2gn(\mathbf{r})$

Non-condensate density

Density of the thermal component:

$$\langle \tilde{\psi}^{\dagger}(\mathbf{r}) \tilde{\psi}(\mathbf{r}) \rangle = \tilde{n} = \sum_{j} \left\{ \left[|u_{j}|^{2} + |v_{j}|^{2} \right] \langle \hat{\alpha}_{j}^{\dagger} \hat{\alpha}_{j} \rangle + |v_{j}|^{2} \right\}.$$

and multiplying factor

$$\langle \hat{\alpha}_{j}^{\dagger} \hat{\alpha}_{j} \rangle = rac{1}{e^{eta E_{j}} - 1} \equiv N_{0}(E_{j}).$$

is the Bose-Einstein distribution. At T = 0, $\tilde{n} = \sum_{j} |v_j|^2 \rightarrow$ Quantum depletion

The anomalous average:

$$\langle \tilde{\psi}(\mathbf{r}) \tilde{\psi}(\mathbf{r})
angle = ilde{m} = -\sum_{j} u_{j} v_{j}^{*} \left[2 \langle \hat{lpha}_{j}^{\dagger} \hat{lpha}_{j}
angle + 1
ight],$$

AR and D. Angom, *Phys. Rev. A* **90**, 023612 (2014) A.Griffin, *Phys. Rev. B* **53**, 9341 (1996)

Problems in HFB

• HFB theory is not *gapless*. Violates Hugenholtz-Pines theorem.

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Gapless finite temperature approximation

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Neglect \tilde{m}.

\downarrow \downarrow

HFB-Popov approximation

Valid in 0 < T \lesssim 0.65 T_c
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N. P. Proukakis and B. Jackson, J. Phys. B 41, 203002 (2008)

Two-component fluid motivations

- Transition from miscible to immiscible phase.
 Example Temperature driven phase-separation in cyclohexane-aniline mixture.
- Dynamical instabilities related to two-component fluid, namely Rayleigh-Taylor instability.
- Are there any similarities and differences in binary mixtures of quantum fluids ?

H. Stanley, Introduction to Phase Transitions and Critical Phenomena, (1971)

Unique feature of binary BEC

Role of interactions

Phase Separation



Papp et. al, *Phys. Rev. Lett.* **101**, 040402 (2008); Inouye et. al, *Nature* **392** 151, (1998); Chin et. al, *Rev. Mod. Phys.* **82**, 1225 (2010).

Unique feature of binary BEC

Dynamical Evolution



AR, S. Gautam, D. Angom, arXiv:1210.0381, (2012),
Takeuchi et. al, *Phys. Rev. B.* 81, 094517 (2010),
Sasaki et al., *Phys. Rev. A* 80, 063611 (2009),
S. Gautam and D. Angom *Phys. Rev. A* 81, 053616 (2010).

Experimental realization of binary BEC

2 different atoms

⁸⁷Rb–⁴¹K

Thalhammer et. al, PRL, 100, (2008)

⁸⁴Sr⁸⁷Rb

Pasquiou et. al, PRA, 88, (2013)

• ²³Na-⁸⁷Rb

Xiong et. al, arXiv:1305.7091, (2013)

McCarron et. al, PRA(R), 84, (2011)

2 different isotopes

• ⁸⁵Rb-⁸⁷Rb Papp et, al. PRL, **101**, (2008)

2 different hyperfine states

• $|F = 1, m_F = +1\rangle$, $|F = 2, m_F = -1\rangle$ of ⁸⁷Rb |F = 2, m = $2\rangle, |F = 2, m = -1\rangle$

Tojo et. al, PRA, 82, (2010)

Coupled Generalized GP equation

From HFB-Popov approximation

$$\begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} + \begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix},$$

$$\hat{h}_1 \phi_1 + U_{11} [n_{1c} + 2\tilde{n}_1] \phi_1 + U_{12} [n_{2c} + \tilde{n}_2] \phi_1 = 0,$$

$$\hat{h}_2 \phi_2 + U_{22} [n_{2c} + 2\tilde{n}_2] \phi_2 + U_{12} [n_{1c} + \tilde{n}_1] \phi_2 = 0.$$

• $n_{kc} = |\phi_k|^2$: Condensate density of k^{th} species • \tilde{n}_k : Non-condensate density of k^{th} species where, $\hat{h}_k = -\frac{\hbar^2 \nabla^2}{2m_k} + V_k(\mathbf{r}) - \mu_k$

BdG Equations

$$\hat{\mathcal{L}}_{1}u_{1j} - U_{11}\phi_{1}^{2}v_{1j} + U_{12}\phi_{1}(\phi_{2}^{*}u_{2j} - \phi_{2}v_{2j}) = \hbar E_{j}u_{1j}, - \hat{\mathcal{L}}_{1}v_{1j} + U_{11}\phi_{1}^{*2}u_{1j} - U_{12}\phi_{1}^{*}(\phi_{2}v_{2j} - \phi_{2}^{*}u_{2j}) = \hbar E_{j}v_{1j}, \hat{\mathcal{L}}_{2}u_{2j} - U_{22}\phi_{2}^{2}v_{2j} + U_{12}\phi_{2}(\phi_{1}^{*}u_{1j} - \phi_{1}v_{1j}) = \hbar E_{j}u_{2j}, - \hat{\mathcal{L}}_{2}v_{2j} + U_{22}\phi_{2}^{*2}u_{2j} - U_{12}\phi_{2}^{*}(\phi_{1}v_{1j} - \phi_{1}^{*}u_{1j}) = \hbar E_{j}v_{2j},$$

where,
$$\hat{\mathcal{L}}_1 = (\hat{h}_1 + 2U_{11}n_1 + U_{12}n_2),$$

 $\hat{\mathcal{L}}_2 = (\hat{h}_2 + 2U_{22}n_2 + U_{12}n_1),$
 $n_1 = n_{1c} + \tilde{n}_1, n_2 = n_{2c} + \tilde{n}_2.$

Non-Condensate density:

$$\tilde{n}_k = \sum_j \left\{ \left[|u_{kj}|^2 + |v_{kj}|^2 \right] N_0(E_j) + |v_{kj}|^2 \right\}$$

AR, S. Gautam, D. Angom, Phys. Rev. A. 89, 013617 (2014)

Phase-separation in binary BEC T = 0

Density profiles

from miscible to immiscible(phase-separated) $^{133}Cs - ^{87}Rb$ mixture in quasi-1D trap $\omega_{z(Rb)} = 2\pi \times 3.89Hz, \omega_{z(Cs)} = 2\pi \times 4.55Hz,$ $\omega_{\perp(Cs)} = 8.835\omega_{z(Cs)}; \omega_{\perp(Rb)} = 8.277\omega_{z(Rb)}$ $\omega_{\perp} \gg \omega_{z}, \ \hbar\omega_{\perp} \gg \mu$ $a_{CsCs} = 280a_0, a_{RbRb} = 100a_0$

Measure of phase separation

$$\Lambda = \frac{\left[\int n_1(z)n_2(z)dz\right]^2}{\left[\int n_1^2(z)dz\right]\left[\int n_2^2(z)dz\right]}.$$

$$\label{eq:lambda} \begin{split} \Lambda &= 1 \to \text{Miscible and signifies complete overlap of the two species,} \\ \Lambda &= 0 \to \text{the binary condensate is completely phase-separated.} \end{split}$$

Phase-separation in binary BEC T = 0through a_{12} $\Lambda = 1$ $\Lambda = 0.95$ $\Lambda = 0.08$



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Suppression of phase-separation $T_{T=0} \neq 0, a_{12} = 300a_{0}a_{12}$



(a)-(c)The solid blue (green) lines represent $n_{\rm Cs}(n_{\rm Rb})$. The dashed red(brown) lines represent $\tilde{n}_{\rm Cs}(\tilde{n}_{\rm Rb})$ at T = 0, 10, 25 nK respectively.

Λ increases.

Suppression of phase-separation $T_{T=0} \neq 0, a_{12} = 300a_{0}$



(d)-(f) The solid dark cyan (maroon) lines represent $n_{cCs}(n_{cRb})$. The dashed crimson(black) lines $n_{cCs}(n_{cRb})$ at T = 0 with the same number of condensate atoms at T = 0, 10, 25nK respectively. Effect of \tilde{n} on miscibility-immiscibility transition

Suppression of phase-separation origin

$$T = 0 \qquad \qquad T = 10$$



The fourth excited mode has maximum contribution to the thermal cloud.



(a)-(c) The solid blue (green) lines represent 85 Rb(87 Rb). The dashed red(brown) lines represent $\tilde{n}_1(\tilde{n}_2)$.

Λ increases.

Correlation function measure of coherence

The normalized first order correlation function is given by

$$egin{aligned} g_k^{(1)}(z,z') &=& rac{\langle \hat{\Psi}_k^\dagger(z) \hat{\Psi}_k(z')
angle}{\sqrt{\langle \hat{\Psi}_k^\dagger(z) \hat{\Psi}_k(z)
angle \langle \hat{\Psi}_k^\dagger(z') \hat{\Psi}_k(z')
angle}} \ &=& rac{n_{ck}(z,z') + ilde{n}_k(z,z')}{\sqrt{n_k(z)n_k(z')}}, \end{aligned}$$

where,

$$n_{ck}(z, z') = \phi_k^*(z)\phi_k(z')$$

$$\tilde{n}_k(z, z') = \sum_j \{ [u_{kj}^*(z)u_{kj}(z') + v_{kj}^*(z)v_{kj}(z')]N_0(E_j) + v_{kj}^*(z)v_{kj}(z') \}.$$

Correlation function measure of coherence



At T = 0, $g_{Cs/Rb}^{(1)}(0, z) = 1$ for $a_{12} = 300a_0$. When $T \neq 0$, the $g_{Cs/Rb}^{(1)}(0, z)$ is maximum at z = 0 and decays to zero with increasing z. The rate of decay of the $g_{Cs/Rb}^{(1)}(0, z)$ increases with temperature.



The $g_k^{(1)}(0,z)$ of the individual species cross each other at a certain z_0 . Two species have equal $g_{\rm Cs/Rb}^{(1)}(0,z_0)$. With increase in a_{12} , z_0 increases, and $g_{\rm Cs/Rb}^{(1)}(0,z_0)$ decreases. Difference in the decay rates of $g_{\rm Cs/Rb}^{(1)}(0,z_0)$; it is much faster in Cs.





The solid red(black) line represents $g_{Cs}^{^{z}(1)}(0, z)$ in Cs BEC(Cs-Rb TBEC). The solid red(black) line represents $g_{Rb}^{(1)}(0, z)$ in Rb BEC(Cs-Rb TBEC).



Phase-separation in ⁸⁷Rb-¹³³Cs TBEC for $a_{12} = 650a_0$. The solid blue (green) lines represent $n_{cCs}(n_{cRb})$ at T = 0. The solid maroon (yellowish brown) lines represent $n_{cCs}(n_{cRb})$, and the dashed crimson (black) lines represent $\tilde{n}_{cCs}(\tilde{n}_{cRb})$ at T = 25nK.

Conclusions

- To examine the properties of TBECs in the neighbourhood of phase separation, it is essential to incorporate the thermal component.
- There is a delay or suppression of phase-separation due to the thermal component generic to any binary BEC mixture.
- Different from the classical binary fluids which undergo miscible-immiscible transition with temperature as control parameter.
- Each species has two sub-components, the condensate and non-condensate atoms. The condensate components are coherent, but the non-condensate components are incoherent and like the normal gas.

Conclusions

- Spatial density variations of all the components due to the nature of the confining potential.
- The transition to the phase separated domain at finite temperatures is associated with a distinct change in the profile of the correlation function.
- In the strongly phase separated domain, temperature does not alter the density profiles.

Conclusions

- Spatial density variations of all the components due to the nature of the confining potential.
- The transition to the phase separated domain at finite temperatures is associated with a distinct change in the profile of the correlation function.
- In the strongly phase separated domain, temperature does not alter the density profiles.

...and finally

THANK YOU the group

Prof. Dilip Angom

Dr. Brajesh K. Mani

Dr. S. Chattopadhyay

Dr. Sandeep Gautam

Mr. Kuldeep Suthar

THANK YOU the group

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Gross-Pitaevskii (GP) equation Generalized GP equation Binary BEC Phase-separation Correlation function Conclusions

Backup Slides

Phase-separation in binary BEC T = 0

$\begin{array}{l} \textbf{Density profiles} \\ \text{from miscible to immiscible(phase-separated)} \\ {}^{133}\text{Cs} - {}^{87}\text{ Rb mixture in quasi-1D trap} \\ \omega_{z(\text{Rb})} = 2\pi \times 3.89\text{Hz}, \\ \omega_{z(\text{Cs})} = 2\pi \times 4.55\text{Hz}, \\ \omega_{\perp}(\text{Cs}) = 50.0\omega_{z(\text{Cs})}; \\ \omega_{\perp}(\omega_{\perp}) = 50.0\omega_{z(\text{Rb})} \\ \omega_{\perp} \gg \omega_{z}, \\ \hbar\omega_{\perp} \gg \mu \\ a_{\text{CsCs}} = 280a_{0}, \\ a_{\text{RbRb}} = 100a_{0} \end{array}$

Suppression of phase-separation $T_{T=0} \neq 0, a_{12} = 295a_{0}$



(a)-(c)The solid blue (green) lines represent $n_{\rm Cs}(n_{\rm Rb})$. The dashed red(brown) lines represent $\tilde{n}_{\rm Cs}(\tilde{n}_{\rm Rb})$ at T = 0, 5, 10 nK respectively.

Λ increases.

Suppression of phase-separation $T_{T=0} \neq 0, a_{12} = 295a_{0}$



(d)-(f) The solid dark cyan (maroon) lines represent $n_{cCs}(n_{cRb})$. The dashed crimson(black) lines $n_{cCs}(n_{cRb})$ at T = 0 with the same number of condensate atoms at T = 0, 5, 10 nK respectively. Effect of \tilde{n} on miscibility-immiscibility transition

Suppression of phase-separation $T \neq 0, a_{11} = 120a_0$ T = 0 T = 5 T = 10T = 0 T = 5 T = 10



dashed red(brown) lines represent $\tilde{n}_1(\tilde{n}_2)$.

Λ increases.

Correlation function measure of coherence



At T = 0, $g_{Cs/Rb}^{(1)}(0, z) = 1$.

When $T \neq 0$, the $g_{Cs/Rb}^{(1)}(0,z)$ is maximum at z = 0 and decays to zero with z.

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