## Finite Temperature Effects in the Condensates of Dilute Atomic Gases

A thesis submitted in partial fulfillment of

the requirements for the degree of

### **Doctor of Philosophy**

by

### Arko Roy

(Roll No. 11330009)

Under the supervision of

### **Prof. Angom Dilip Kumar Singh**

Professor

Theoretical Physics Division

Physical Research Laboratory, Ahmedabad, India.



### DISCIPLINE OF PHYSICS

### INDIAN INSTITUTE OF TECHNOLOGY GANDHINAGAR

2015

# to

# Maa, Baba

for all that you have taught me...

X

K,

#### Declaration

I declare that this written submission represents my ideas in my own words and where others' ideas or words have been included, I have adequately cited and referenced the original sources. I also declare that I have adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/fact/source in my submission. I understand that any violation of the above will be cause for disciplinary action by the Institute and can also evoke penal action from the sources which have thus not been properly cited or from whom proper permission has not been taken when needed.

Signature

Name: Arko Roy

(Roll No: 11330009)

Date:

#### CERTIFICATE

It is certified that the work contained in the thesis titled **"Finite Temperature Effects in the Condensates of Dilute Atomic Gases"** by **Mr. ARKO ROY** (Roll No. 11330009), has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

> Prof. Angom Dilip Kumar Singh (Thesis Supervisor) Professor, Theoretical Physics Division Physical Research Laboratory, Ahmedabad, India.

Date:

Acknowledgments

After piling higher and deeper for the past 5 years, now I find that the thing that's the hardest for me to write is writing the acknowledgments. It also, hands down, takes me longer than any other chapter in this thesis. For me, I think the reason I take these acknowledgments so seriously is because it's when I get to put down on paper how truly grateful I am to be surrounded with such great friends, motivating supervisor, an awesome group, and a family that truly makes my life a joy. That's why it is so tough. I also type a lot slower...

To my supervisor, Prof. Angom Dilip Kumar Singh, I consider myself lucky to have got the opportunity to be your graduate student. I am extremely fortunate and privileged to have got to spend so many years in your company. Thank you for all the formal, and incisive discussions on various topics in physics, computer science, and in particular on the area of my thesis all along; I have learned a lot from you. From introducing me to popular articles on medical science through Siddhartha Mukherjee or Atul Gawande; to graffiti painting of Banksy, magazines like New Yorker, and informative websites like aeon.com, to name a few; thank you. I will remain indebted to you for the trust, faith and confidence you had in me right from the inception of any scientific idea to the final execution of the project. It meant a lot to me. 'What is the status?' was the question that would initiate any conversation kept me motivated and made me enthusiastic to give you a satisfying answer each time. Your truly encouraging words like 'We are heading in the right direction' or 'Don't worry, you will do well' before any review or seminar have always helped me to take things in stride and look forward. I wish I could learn the brilliant acumen you have over academic and non-academic matters. Thank you Dilip for being there, for being extremely patient with me.

It was a pleasure to know Dr. Sandeep Gautam at the beginning of my Ph.D. tenure, who by then was a postdoc in our group. I will remain ever grateful to you for all the time you spent, despite your own research, in giving me the first-hand knowledge on the physics of BEC and related numerical techniques; they were so valuable. The long hours of scientific discussions, providing correct references, sharing codes through mail or chat or phone were highly productive and crucial for me. Now I realize that I had asked you the most naive, simple and trivial questions...P. How fun and tough can debugging a code be, I learned from you; thank you for making me appreciate that. You had been a fantastic and fine trouble-shooter. I could not have expected better than this. Thank you Sandeep, for being extremely helpful and a superb support just at that right point of time.

The first lesson on shock waves, Mach angle, and vortices in classical fluids

from Debolina Dasgupta (currently a Graduate Research Assistant at Department of Aerospace Engineering, Georgia Tech) immensely helped me to understand the various aspects of topological defects in quantum fluids. Thank you so much, they were essential. I take this opportunity to thank Naik (VTech.), Rakesh (UIC), Soumyadeep (Minnesota Univ.) Souvick (UIC), Sayak (Ohio State), Ranjan (IISc), Ankur (Oregon State Univ.), and not to forget Lata (IIT-B) for being so prompt and mailing me the journal articles whenever I had asked for; without your help, I would not have come across several useful and inaccessible papers. A huge part of my research revolved around computers and the men behind the early exposition to the world of Linux were Dr. Siddhartha Chattopadhyay and Dr. Koushik Saha. Thank you Koushik for teaching me how to install OS like Windows/Linux; they were so beneficial. Thank you Siddhartha for divulging the fun of tinkering with the filesystem in Linux. I am deeply indebted to Dr. Shashi Prabhakar for introducing me to the basics of HTML/PHP scripting and helping me out whenever I used to get stuck on a particular step in MATLAB.

I remain grateful to the Director, Dean, Academic Committee for the academic & non-academic support and help I got all throughout. Thank you for providing all the necessary facilities and a homely atmosphere, I will surely cherish my stay at PRL forever. I am thankful to Dr. Bhushit G. Vaishnav for his continual support. A warm thanks to all the faculty members, course-work instructors, research scholars, PDFs of Theoretical Physics Division, and specially the members of DSC for attending my seminars, and giving encouraging remarks on the thesis work. I thank Prof. R. P. Singh, Prof. K. P. Subramanian, Prof. Subroto Mukerjee, and the anonymous external examiners for their constructive feedbacks, suggestions and encouraging comments while reviewing the thesis; they were much-needed and indispensable.

All throughout these brilliant 5 years, I used to share the office space with Avdhesh and Girish Kumar. Thank you for tolerating me despite my gossipy nature, and listen to my ramblings. Let me take this moment to thank Mr. Razaahmed Maniar, Secretary of Theory Office for the numerous help in official matters related to the Division. I will always remember the enormous help I got from Mr. Senthil Babu, Mr. Pradeep Sharma of PRL, and Dr. Nithin V. George, Mr. Piyush Vankar of IIT Gandhinagar (IIT-GN) in all academic & administrative matters. I am deeply indebted to the PRL and IIT-GN Library staff for all the facilities and help they provided. Thank you Dr. T. S. Kumbar of IIT-GN for mailing many interesting articles and allowing me to access the journals subscribed by IIT-GN. I am highly obliged to the American Physical Society, NIST Virtual Library, and Macmillan Publishers Ltd.(on behalf of Nature Publishing Group) for permitting me to reprint some of their published figures in this thesis. A big thanks to Mr. Samuel Johnson and Mr. Jigar Raval for a smooth and seamless computing experience on PRL HPC, and recently on Vikram-100. Without your help, life would not have been that easy. I thank the other members of the Computer Center, PRL for their endless advice, support and cooperation.

I must thank Abhishek and Koushik for giving me the first hands-on training on cooking. I had an amazing time. Priyanka and Sneha, thank you for baking the most exquisite cakes, for the absolutely yummy and mouth-watering food I have ever had. 'A Bird's Rhapsody' would have remained implausible, but because of you...I am pleased with Tanushree for the awesome dinner treats at her place. Thank you; I enjoyed a lot. I also thank the canteen staff for the tireless effort put in serving food  $16 \times 7$ . I continue to be a foodie because of you all. This thesis would not have been possible without the innumerable late-night parties, hangouts and the amusing time spent together with Tanmoy Chattopadhyay, Monojit, Naveen, Chandan Hati - thank you for the camaraderie. Without you, life would have been so wretched. I am thrilled with all the fun and exciting things we have been able to do together. Ujal, Gaurava, Lalit; dude, you are just excellent! Your strange quirks are really entertaining; thanks Chandan Gupta and Ribhu for all the photography outings and the criticisms thereafter. I am fortunate to be among so many sensible and responsible guys, specially Deepak, Diptiranjan, Bivin, Jabir, Prahlad and Kuldeep Pandey for taking care of the hostel activities and make it a better one. I am grateful to have had the company of Dr. Susanta Kumar Bisoi, Dr. Sunil Chandra, Dr. Amrendra Pandey, Diganta Kumar for the many initiatives we had taken together and for the several chitchat sessions. A huge shout to thank all my batchmates and junior & senior colleagues for making my stay at PRL cozy and making the hostel a happening place. I sincerely thank and acknowledge the group members Kuldeep Suthar, Rukmani, Soumik and the intense journal-club sessions with Nabyendu, Sudip, Manpreet, Pankaj, Pradeep for the stimulating discussions on various topics in condensed-matter physics.

For all that I have learned, everything that I have gained, whatever I have achieved - I owe my deepest thanks and express my gratitude to my parents, grandparent for their constant love, support and encouragement. Without you I could not have been so happy.

Arko

### Abstract

The stationary state solutions and dynamics of Bose-Einstein condensates (BECs) at T = 0 are well described by the Gross-Pitaevskii (GP) equation. BECs of dilute atomic gases have been experimentally achieved at ultracold temperatures of the orders of  $10^{-9}$  K. To include the effects of finite temperature on these condensates one needs to generalize the GP equation. We report here the development of the Hartree-Fock-Bogoliubov theory with the Popov (HFB-Popov) approximation for trapped twocomponent BECs (TBECs). It is a gapless theory and satisfies the Hugenholtz-Pines theorem. The method is particularly well suited to examine the evolution of the lowlying energy excitation spectra at T = 0 and  $T \neq 0$ . Apart from the two Goldstone modes corresponding to each of the species in quasi-1D TBEC, we show that the third Goldstone mode, which emerges at phase-separation due to softening of the Kohn mode, persists to higher interspecies interaction for density profiles where one component is surrounded on both sides by the other component. These are termed as *sandwich* type density profiles. This is not the case with symmetry-broken density profiles where one species is entirely to the left and the other is entirely to the right which we refer to as *side-by-side* density profiles. However, the third Goldstone mode which appears at phase-separation gets hardened when the confining potentials have separated trap centers. This hardening increases with the increase in the separation of the trap centers in which the TBECs have been confined. Furthermore, we demonstrate the existence of mode bifurcation near the critical temperature. We also examine the role of thermal fluctuations in quasi-1D TBECs of dilute atomic gases. In particular, we use this theory to probe the impact of non-condensate atoms to the phenomenon of phase-separation in TBECs. We demonstrate that, in comparison to T = 0, there is a suppression in the phase-separation of the binary condensates at  $T \neq 0$ . This arises from the interaction of the condensate atoms with the thermal cloud. We also show that, when  $T \neq 0$  it is possible to distinguish the phase-separated case from miscible from the trends in the correlation function. However, this is not the case at T = 0. In a BEC, a soliton enhances the quantum depletion which is sufficient enough to induce dynamical instability of the system. For phase-separated TBECs with a dark soliton in one of the components, two additional Goldstone modes emerge in the excitation spectrum. We demonstrate that when the anomalous mode collides with a higher energy mode it renders the solitonic state oscillatory unstable. We also report soliton induced change in the topology of the density profiles of the TBEC at phase-separation. For quasi-2D BECs, at T = 0, we show that with the transformation of a harmonically to toroidally trapped BECs, the energy of the Kohn modes gets damped. This is examined for the case when the radial angular frequencies of the trap are equal. The other instance, when the condensate is asymmetric, the degeneracy of the modes gets lifted. The variation in the anisotropy parameter is accompanied by the damping of the modes, the quasiparticle modes form distinct family of curves; each member being different from the other by the principal quantum number n. When  $T \neq 0$ , with the production of a toroidally trapped BEC, the maxima of the thermal density tends to coincide with the maxima of the condensate density profiles. This is different from the case of a harmonically trapped BEC in which due to the presence of repulsive interaction between the atoms, the thermal density gets depleted where the condensate atoms are the highest.

eskPOKSU

# Contents

Ac	know	ledgme	ents	1
Ał	ostrac	:t		5
Co	ontent	ts		7
Li	st of l	Figures		11
1	Intro	oductior	ı	15
	1.1	Bose-I	Einstein Condensation	18
		1.1.1	Off-Diagonal Long-Range Order (ODLRO)	20
		1.1.2	Two-component Bose-Einstein condensates	21
	1.2	Liquid	He and BEC	25
	1.3	Spin-p	olarized Hydrogen	26
	1.4	Finite	Temperature Models	26
	1.5	Object	ives of the Present Study	32
	1.6	Overvi	iew of the Chapters	33
2	Finit	te Temp	perature Theory	35
	2.1	Single	-component BEC	36
		2.1.1	Gross-Pitaevskii equation	36
		2.1.2	Many-body Hamiltonian	37
		2.1.3	Bogoliubov approximation	38
		2.1.4	Hartree-Fock-Bogoliubov approximation	39
		2.1.5	Hartree-Fock-Bogoliubov-Popov approximation	44
		2.1.6	Local-Density approximation	45

	2.2	Two-co	omponent BEC	47
		2.2.1	HFB approximation for the TBEC	49
3	Evo	ution of	f Goldstone mode in binary BECs	57
	3.1	Mode e	evolution of trapped TBEC at $T = 0$	60
		3.1.1	Third Goldstone mode	62
		3.1.2	Avoided crossings and quasidegeneracy	66
		3.1.3	Mode hardening in displaced trap centers	68
	3.2	Mode e	evolution in TBEC with dark soliton at $T = 0$	70
		3.2.1	The Dark Soliton	72
		3.2.2	Fluctuation induced instability in single-species BEC	73
		3.2.3	Interaction induced instability in TBEC with soliton	77
		3.2.4	Mode collisions	79
		3.2.5	Third and fourth Goldstone modes	81
		3.2.6	Different mass ratios	82
	3.3	Summa	ary of the Chapter	85
4	Finit	e temp	erature effects in condensate mixtures	87
	4.1	Overla	p measure and correlation function	88
	4.2	Mode e	evolution of trapped TBEC at $T \neq 0$	90
	4.3	Suppre	ssion of phase segregation	93
	4.4	Segreg	ation independent of temperature	99
	4.5	Therma	al suppression in <sup>85</sup> Rb- <sup>87</sup> Rb BEC	101
	4.6	Summa	ary of the Chapter	102
5	Fluc	tuations	s in quasi-2D condensates	105
	5.1	Quasi-2	2D BEC : Theory	106
	5.2	Mode e	evolution at $T = 0$	110
		5.2.1	Variation in $U_0$	111
		5.2.2	Variation in $\alpha$	117
	5.3	$T \neq 0$	results	121
	5.4	Summa	ary of the Chapter	123

6	Scope for Future Work	125
A	Numerical Details	127
Bik	bliography	129
Lis	t of Publications	145
Pu	blications attached with thesis	147

Studio Frida

# **List of Figures**

1.1	Experimental images of the velocity distribution of trapped <sup>87</sup> Rb atoms	17
1.2	Experimental images of condensates of <sup>87</sup> Rb atoms in a ring-shaped magnetic	
	trap	19
1.3	Experimental images of sandwich type density profiles in a TBEC	22
1.4	Absorption images of <sup>85</sup> Rb - <sup>87</sup> Rb TBEC showing the miscible and immisci-	
	ble phases.	24
1.5	Equilibrium condensate and thermal density profiles	27
2.1	Feynman diagrams of scattering processes in a single-species BEC	40
2.2	Feynman diagrams of scattering processes due to the intraspecies interactions	
	$U_{11}$ and $U_{22}$ in a TBEC	51
2.3	Feynman diagrams of scattering processes arising due to the interspecies in-	
	teractions $U_{12}$ in a TBEC	52
3.1	False color coded experimental images of <sup>87</sup> Rb- <sup>133</sup> Cs TBEC taken by the	
	method of absorption imaging.	59
3.2	Transition to phase-separation and structure of the density profiles in TBEC.	60
3.3	The evolution of the modes as a function of the interspecies scattering length	
	$a_{\rm CsRb}$ in Cs-Rb TBEC.	63
3.4	Evolution of quasiparticle amplitude corresponding to the Rb Kohn mode as	
	$a_{\rm CsRb}$ is increased from 0 to $400a_0$ .	65
3.5	Low-lying modes of ${}^{85}$ Rb- ${}^{87}$ Rb as a function of $a_{85}$ Rb ${}^{87}$ Rb	66
3.6	The quasiparticle amplitudes of the 5th and 6th modes at quasidegeneracy.	67
3.7	The evolution of the low-lying quasiparticle eigenfrequencies in the Rb-Na	
	TBEC	68

3.8	The evolution of the low-lying quasiparticle eigenfunctions as a function of	
	$z_0$ in the Rb-Na TBEC.	69
3.9	Image showing experimental arrangements to imprint a dark soliton in a BEC.	71
3.10	Quasiparticle amplitudes corresponding to the first two excited modes of a	
	single-species BEC with a dark soliton.	74
3.11	The temporal evolution in the profile of the non-condensate atom density $\tilde{n}$ at	
	$T = 0. \ldots $	75
3.12	Variation in the total number of non-condensate atoms $\tilde{N}$ at $T = 0$ as a	
	function of the scattering length $a_{11}$	76
3.13	Transition to phase-separation and structure of the density profiles in TBEC	
	with soliton.	77
3.14	The evolution of the modes as a function of the interspecies scattering length	
	$a_{\rm CsRb}$ in the Cs-Rb TBEC with soliton	79
3.15	Variation in the nature of mode evolution near mode crossing and collision.	80
3.16	Evolution of quasiparticle amplitudes corresponding to the Rb Kohn mode as	
	$a_{\text{CsRb}}$ is increased from 0 to $400a_0$ .	81
3.17	Evolution of the quasiparticle amplitudes corresponding to the fourth excited	
	mode as $a_{CsRb}$ is increased from 0 to $420a_0$	83
3.18	The evolution of the low-lying modes of the TBEC with soliton for different	
	mass ratios as a function of the interspecies scattering length $a_{12}$	85
4.1	Self-energy diagrams for TBEC in the HFB-Popov approximation	89
4.2	Frequencies $(\omega_j)$ of the low-lying modes at $T/T_c \neq 0$	91
4.3	Density profile of $n_c$ and $\tilde{n}$ at 25nK	92
4.4	The suppression of phase-separation in ${}^{87}\text{Rb}$ - ${}^{133}\text{Cs}$ TBEC at $a_{12} = 295a_0$ .	94
4.5	The first order spatial correlation function, $g^{(1)}_{\mathrm{Cs/Rb}}(0,z)$ with $z \geqslant 0$ with	
	varying $T$	95
4.6	The first order spatial correlation function, $g^{(1)}_{\mathrm{Cs/Rb}}(0,z)$ with $z \geqslant 0$ with	
	varying $a_{12}$ .	96
4.7	The equilibrium density profiles and first order spatial correlation function	
	$g^{(1)}(0,z)$ with $z \ge 0$ of Cs and Rb BEC respectively at $T = 10$ nK	98

4.8	Quasiparticle amplitudes corresponding to the fourth excited mode in <sup>85</sup> Rb-
	<sup>87</sup> Rb TBEC at $T = 0, 10$ nK
4.9	Density profiles showing complete phase-separation at $T = 0$ and $T = 10$ nK. 100
4.10	The suppression of phase-separation in ${}^{85}$ Rb- ${}^{87}$ Rb TBEC at $a_{11} = 120a_0$ . 101
5.1	Density profiles showing transformation of a harmonically trapped to a toroidal
	<b>BEC.</b>
5.2	Evolution of Kohn mode function as $U_0$ is increased from 0 to $20\hbar\omega_x$ for $\alpha = 1.107$
5.3	The evolution of the mode energies as a function of $U_0$ for $\alpha = 1$ at $T = 0$ . 109
5.4	Evolution of $l = 0$ mode function as $U_0$ is increased from 0 to $15\hbar\omega_x$ for $\alpha = 1.110$
5.5	Evolution of quasiparticle amplitude corresponding to the hexapole mode as
	$U_0$ is increased from 0 to $15\hbar\omega_x$ for $\alpha = 1. \dots $
5.6	The plots show the variation in the profile of $u_{\rm Na}$ , and $v_{\rm Na}$ along x-axis at
	y = 0 corresponding to the $l = 0$ mode
5.7	The evolution of the quasiparticle modes as a function of $\alpha$ for $U_0 = 0$ at $T = 0.113$
5.8	Evolution of Bogoliubov quasiparticle amplitudes for the family of curves
	connected by solid red dots ( ) as shown in Fig. 5.7
5.9	Evolution of Bogoliubov quasiparticle amplitudes for the family of curves
	connected by solid purple triangles ( $\blacktriangle$ ) as shown in Fig. 5.7
5.10	Evolution of the quasiparticle amplitudes corresponding to the eigenvalues
	traced by the red arrows in Fig. 5.7
5.11	Evolution of the quasiparticle amplitudes corresponding to the eigenvalues
	traced by the green arrows in Fig. 5.7
5.12	Evolution of the Bogoliubov quasiparticle amplitude corresponding to the
	Kohn mode which remains steady as $\alpha$ is varied when $U_0 = 0. \ldots 118$
5.13	Evolution of the Bogoliubov quasiparticle amplitude corresponding to the
	Kohn mode which goes soft as $\alpha$ is varied when $U_0 = 0. \ldots 119$
5.14	Density profiles showing transformation of a rotationally symmetric to an
	ellipsoidal BEC for $U_0 = 5120$
5.15	The evolution of the quasiparticle modes as a function of $\alpha$ for $U_0 = 5$ at $T = 0.121$
5.16	The $y = 0$ cut showing the variation in condensate and (b) thermal density
	profiles along x at $T = 10$ nK for varying $U_0$

5.17 Condensate and non-condensate density profiles at T = 10 nK for varying  $U_0$ . 123

desk for the subject of the second