#### Dynamics of Ultracold Quantum Gases in Variable Potentials

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by

Sandeep Gautam



Under the Supervision of

Angom Dilip Kumar Singh, Associate Professor Physical Research Laboratory, Ahmedabad

#### DEPARTMENT OF PHYSICS FACULTY OF SCIENCE MOHANLAL SUKHADIA UNIVERSITY

UDAIPUR

Year of submission: 2011

#### CERTIFICATE

I feel great pleasure in certifying the thesis entitled "**Dynamics of Ultracold Quantum Gases in Variable Potentials**" by Mr. Sandeep Gautam under my guidance. He has completed the following requirements as per Ph.D. regulations of the University

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I am satisfied with the analysis of data, interpretation of results and conclusions drawn.

I recommend the submission of the thesis.

Date: July 8, 2011

Angom Dilip Kumar Singh (Supervisor) Associate Professor Physical Research Laboratory Ahmedabad, India.

Countersigned by Head of the Department

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I Sandeep Gautam, S/O Shri Lekh Raj, resident of E-201, PRL residences, Navrangpura, Ahmedabad - 380 009, hereby declare that the research work incorporated in the present thesis entitled "Dynamics of Ultracold Quantum Gases in Variable Potentials" is my own work and is original. This work (in part or in full) has not been submitted to any university or institute for the award of a Degree or a Diploma. I have properly acknowledged the material collected from secondary sources wherever required. I solely own the responsibility for the originality of the entire content.

Date: July 8, 2011

Sandeep Gautam (Author) Dedicated to,

mummy, daddy,

tinku,

kaala chacha & guddi bua

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## Abstract

Bose and Fermi gases behave quite differently at ultracold temperatures. For Bose gas lowering the temperature below a critical temperature leads to the macroscopic occupation of the single particle ground state, the phenomenon is termed as Bose-Einstein condensation; on the other hand, in Fermi gas, all the single particle states with energy lower than the Fermi energy are filled below a critical temperature. Several studies, both theoretical and experimental, have been done to understand the various properties these quantum degenerate ultracold gases since the first experimental realization of Bose-Einstein condensation [Anderson et al., Science **269**, 198 (1995); C. C. Bradley et al., Phys. Rev. Lett. **75**, 1687 (1995); Davis et al., Phys. Rev. Lett. **75**, 3969 (1995)]. These include studies on binary quantum degenerate mixtures like Bose-Bose, Bose-Fermi and Fermi-Fermi mixtures; various types of dynamical instabilities like modulational, Kelvin-Helmholtz, etc.; collective modes including vortices and many more.

Our studies in the present thesis encompass both the static and dynamical properties of these degenerate systems. We have theoretically examined the Bose-Einstein condensation of an ideal Bose gas in quartic traps instead of conventional harmonic ones. For fermionic alkali atoms, we have examined the use of WKB approximation to calculate the *p*-wave scattering length. We have also employed variable phase method (a numerical method) to calculate *p*-wave scattering length of <sup>6</sup>Li and <sup>40</sup>K for  $a^{3}\Sigma_{u}^{+}$  and  $X^{1}\Sigma_{d}^{+}$  states respectively.

In case of quantum degenerate Bose-Bose mixtures (binary condensates), we have proposed and implemented two semi-analytic methods, valid in two different regimes, to determine the ground state geometry of these condensates in both miscible and immiscible (phase-separated) domains. Extending these studies to quantum degenerate Bose-Fermi mixtures, we have also used mean field approach to study the phenomena of *profile swapping* and *fermion*  pinching in  $^{174}\mathrm{Yb}\text{-}^{173}\mathrm{Yb}$  mixture.

On the dynamics front, we have proposed and theoretically implemented a well controlled experimental scheme to initiate and examine Rayleigh-Taylor instability in phase-separated binary condensate of <sup>85</sup>Rb-<sup>87</sup>Rb. We identify the damping of radial oscillations as a signature of Rayleigh-Taylor instability. And again in <sup>85</sup>Rb-<sup>87</sup>Rb condensate, we have shown that coreless vortex-antivortex pairs or vortex dipoles can be created by moving a Gaussian obstacle potential across the phase-separated condensate.

**Keywords:** Bose-Einstein condensation, binary condensates, phase-separation, Bose-Fermi, Rayleigh-Taylor instability, vortices.

# Chapter 1 Introduction

The statistics of a neutral atom depends upon the total number of fermions in it, which should be even for bosonic and odd for fermionic atoms. As the number of protons is equal to the number of electrons in a neutral atom, bosonic atoms must have even number of neutrons, e.g. <sup>23</sup>Na, <sup>87</sup>Rb and <sup>174</sup>Yb. At normal temperatures and pressures, both bosonic and fermionic gases obey Maxwell-Boltzmann statistics, and there is little to differentiate a bosonic gas from a fermionic one. But as the temperature of the system is lowered, the inherent differences between the bosonic and fermionic systems manifest themselves as significantly different behavior of these systems at ultracold temperatures. In case of bosons, lowering the temperature below a critical temperature  $T_c$  leads to the macroscopic occupation of the single particle ground state [1, 2]; whereas in case of identical fermions, the system enters into a state with a filled Fermi sea. One parameter which characterizes this transition is phase space density, which is defined as the number of particles occupying the volume equal to the cube of thermal de Broglie wavelength  $\lambda_T$  [3]. At  $T_c$ , phase space density becomes of the order 1 and the system can be considered as quantum degenerate. The quantum degenerate bosonic system is also called Bose-Einstein condensate (BEC).

Theoretical and experimental investigations to understand the various aspects of BEC have progressed significantly since the first experimental realization of Bose-Einstein condensation [4, 5, 6] in dilute atomic gases of alkali metals. The species which have been Bose-Einstein condensed include Rubidium [4], Lithium [5], Sodium [6], Hydrogen [7], metastable Helium [8], Potassium [9], Cesium [10], Ytterbium [11], Chromium [12], Strontium [13] and Calcium [14]. BECs in optical lattices have been employed to test several condensed matter phenomena like Josephson currents [15], Bloch oscillations [16], super-

fluid to Mott insulator transition [17], etc. The coherent matter wave nature of BEC, coupled with its non-linear character, has been successfully employed to experimentally observe several well known phenomena in non-linear optics like four-wave mixing [18], superradiant Rayleigh scattering and matter wave amplification [19, 20, 21], parametric amplification of vacuum fluctuations [22], dark solitons [23, 24, 25], bright solitons [26, 27], dark-bright solitons [28, 29], etc. Besides single species BECs, binary quantum degenerate Bose-Bose mixtures, also termed as two species Bose-Einstein condensates (TBECs) or simply binary condensates, have been experimentally realized. The TBEC consisting of two different hyperfine spin sates of <sup>87</sup>Rb was first observed by Myatt et al. [30]. This was followed by another experimental observation by Hall et al. [31], who also used two hyperfine states of  $^{87}$ Rb as the component species of the TBEC. Since then, TBECs of different atomic species (<sup>41</sup>K and <sup>87</sup>Rb) [32] and of different isotopes of the same atomic species [33, 34] have been experimentally realized. These earlier experiments have been followed by plethora of experimental and theoretical studies on different aspects of TBECs. The experiment performed by Hall et al. [31] was revisited in Ref. [35] to study non-equilibrium dynamics and superfluid ring excitations. Vortices, which are crucial to our understanding of superfluidity, have also been experimentally realized in Bose-Einstein condensates (BECs) [36, 37, 38, 39, 40, 41].

#### 1.1 Non-interacting Bose gas

The probability of occupancy of the single particle state  $\nu$  is defined by the Bose distribution function

$$f_{\nu} = \frac{1}{e^{(\epsilon_{\nu} - \mu)/KT} - 1},\tag{1.1}$$

where  $\epsilon_{\nu}$  is the energy of the single particle state  $\nu$  and  $\mu$  is the chemical potential of the system. In classical regime (high temperatures and/or low densities), chemical potential is much less than the ground state energy. As the temperature of the system is lowered the chemical potential increases and at  $T_c$ , it becomes equal to the ground state energy  $\epsilon_0$ . This is the maximum value allowed for the chemical potential as a value greater than  $\epsilon_0$  will make the distribution function negative for some low lying states. From Eq. (1.1) the total number of bosons N and total energy E of the system are

$$N = \sum_{0}^{\infty} f_{\nu},$$
  

$$E = \sum_{0}^{\infty} f_{\nu} \epsilon_{\nu}.$$
(1.2)

For the temperatures high compared to energy difference between adjacent single particle states, i.e.  $KT \gg \Delta \epsilon$ , one can employ semi-classical approximation. In semi-classical approximation, the single particle energy states are assumed to have a continuous distribution. This enables one to replace the summation over the single particle energy states by integration in Eq. (1.2). If  $g(\epsilon)$  is the density of states with energy  $\epsilon$ , the total number of bosons and energy of the system are

$$N = \int_{0}^{\infty} g(\epsilon)f(\epsilon)d\epsilon + N_{0},$$
  

$$E = \int_{0}^{\infty} \epsilon g(\epsilon)f(\epsilon)d\epsilon + E_{0}.$$
(1.3)

Here the contribution of the ground state has been separated from the integral. This is done to avoid assigning a zero statistical weight to the ground state when density of states varies as some positive power of energy [42]. The above equations can be used to calculate  $T_c$  and the various thermodynamic properties like energy, entropy, specific heat, etc.

For an ideal bosonic gas in an anisotropic harmonic-oscillator potential, at T = 0K all the bosons occupy the single particle ground state  $\Phi_0(\mathbf{r})$  of the harmonic-oscillator potential. Below  $T_c$  the de Broglie waves associated with individual atoms overlap, and one can describe the resultant giant matter wave by the condensate wavefunction

$$\Psi(\mathbf{r}) = \sqrt{N}\Phi(\mathbf{r}). \tag{1.4}$$

The ground state wave function of a particle, having mass m, in an anisotropic harmonic-oscillator potential is

$$\Phi(\mathbf{r}) = \frac{1}{\pi^{3/4}} \prod_{i=1}^{3} \frac{e^{-x_i^2/2a_i^2}}{\sqrt{a_{\rm osc}^i}},\tag{1.5}$$

where  $x_i$  and  $a_{\text{osc}}^i$  are coordinate variables and oscillator length along three coordinate axis respectively. Oscillator length along *i*th direction is related to corresponding trap frequency as

$$a_{\rm osc}^i = \sqrt{\frac{\hbar}{m\omega_i}}.$$
 (1.6)

From Eqs. (1.4-1.5), it is evident that number density of the bosons,  $n(\mathbf{r}) =$  $|\Psi(\mathbf{r})|^2$ , has anisotropic Gaussian profile with size of the order of oscillator length along each axis. The number density in the momentum space, which can be calculated by taking the Fourier transform of  $n(\mathbf{r})$ , is also Gaussian but with the *i*th width inversely proportional to  $a_{osc}^i$ . The ratio of widths of density profiles, both in coordinate and momentum space, with the corresponding widths in classical regime, obtained from Maxwell-Boltzmann statistics, is  $\sim \sqrt{\hbar\omega_i/kT} = N^{-1/6}$  at or below  $T_c$ . It means that the condensate density profile is much narrower than the density profile of classical gas (thermal cloud) in both the coordinate and momentum space. In other words, Bose-Einstein condensation takes place both in the coordinate and momentum space [3, 43]. This is not the case for the Bose-Einstein condensation in a box, where condensation occurs in momentum space only [42]. The anisotropic density profile in the momentum space is also responsible for the anisotropic expansion of condensate after trap removal, finally leading to aspect ratio inversion. The anisotropic expansion and aspect ratio inversion are the characteristic signatures of the condensate.

#### 1.2 Weakly interacting Bose gas

At low temperatures, the inter-atomic interaction potential in a dilute bosonic gas is the predominantly due to s-wave binary collisions. One parameter which can completely describe these s-wave binary collisions is s-wave scattering length a. This allows one to formulate the inter-atomic interaction potential between two bosons at positions  $\mathbf{r}$  and  $\mathbf{r}'$  as a contact interaction

$$V_{\rm int} = U_0 \delta(\mathbf{r} - \mathbf{r}'), \qquad (1.7)$$

where  $U_0 = 4\pi\hbar^2 a/m$ . Using this relation, the Hamiltonian for N interacting bosons trapped by an external potential  $V(\mathbf{r})$  is

$$\hat{H} = \int d\mathbf{r} \hat{\Psi}^{\dagger}(\mathbf{r}) \left[ \frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + U_0 \hat{\Psi}^{\dagger}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}), \qquad (1.8)$$

where  $\Psi(\mathbf{r})$  and  $\Psi^{\dagger}(\mathbf{r}')$  are the bosonic field annihilation and creation operators satisfying the following commutation relations

$$\begin{bmatrix} \Psi(\mathbf{r}), \Psi^{\dagger}(\mathbf{r}') \end{bmatrix} = \delta(\mathbf{r} - \mathbf{r}'), \begin{bmatrix} \Psi(\mathbf{r}), \Psi(\mathbf{r}') \end{bmatrix} = \begin{bmatrix} \Psi^{\dagger}(\mathbf{r}), \Psi^{\dagger}(\mathbf{r}') \end{bmatrix} = 0.$$
(1.9)

When the gas is dilute,  $n|a|^3 \ll 1$ , we can use mean field approach to express the annihilation field operator  $\Psi(\mathbf{r})$  as the sum of its expectation value and a fluctuation term, i.e

$$\hat{\Psi}(\mathbf{r}) = \langle \hat{\Psi}(\mathbf{r}) \rangle + \delta \Psi(\mathbf{r}).$$
(1.10)

At T = 0K one can neglect the fluctuation term and replace  $\langle \hat{\Psi}(\mathbf{r}) \rangle$  by a *c*-number  $\Psi(\mathbf{r})$  called order parameter or wavefunction of the condensate to obtain energy,

$$E = \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla \Psi(\mathbf{r})|^2 + V(\mathbf{r}) |\Psi(\mathbf{r})|^2 + U_0 |\Psi(\mathbf{r})|^4 \right], \qquad (1.11)$$

of the condensate. Now, the Lagrangian of the condensate is

$$L = \int d\mathbf{r} \frac{i\hbar}{2} \left( \Psi^{\star}(\mathbf{r}) \frac{\partial \Psi(\mathbf{r})}{\partial t} - \Psi(\mathbf{r}) \frac{\partial \Psi^{\star}(\mathbf{r})}{\partial t} \right) - E.$$
(1.12)

Using the action principle  $\delta \int_{t_1}^{t_2} dt L = 0$ , we obtain the time-dependent Gross-Pitaevskii (GP) equation [44, 45]

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + U_0|\Psi(\mathbf{r},t)|^2\right]\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t},\qquad(1.13)$$

here we have explicitly shown the time dependence of wavefunction. The timeindependent GP equation, which can be obtained by minimizing the energy functional E with respect to  $\Psi^*(\mathbf{r})$  under the constraint that the total number of particles N is conserved, is

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + U_0|\Psi(\mathbf{r})|^2\right]\Psi(\mathbf{r}) = \mu\Psi(\mathbf{r}); \qquad (1.14)$$

here  $\mu$ , a Lagrangian multiplier introduced to impose the constraint of fixed particle number, is called chemical potential of the system. The validity of GP equation requires that the inter-particle spacing should be much larger than the range of interaction (measured by *s*-wave scattering length), i.e.  $n^{-1/3} \gg |a|$ . At low temperatures (ideally at T = 0), the GP equation can be used to study both the static and dynamic properties, characterized by the variations of the order parameter over the distances larger than the mean inter-particle spacing, of the condensates [43].

The presence of non-linear term makes it difficult to solve the GP equation analytically. However, one can obtain the approximate analytic solutions using Thomas-Fermi (TF) approximation or by variational minimization. In TF approximation, one considers that locally the system behaves like uniform Bose gas without any spatial fluctuations in the absolute value of its wavefunction. In other words, kinetic energy of the system can be neglected and the GP equation can be solved trivially. Neglecting kinetic energy is a good approximation for repulsive BECs (a > 0), provided  $Na/a_{osc} \gg 1$  [46]. This condition is easily satisfied for BECs with large number of atoms realized in many experimental set-ups. The kinetic energy contribution is significant over a distance  $\delta = (a_{\rm osc}^4/2R)^{1/3}$  from the surface of the cloud with radius R [46]. In the alternative variational minimization method, one has to minimize the energy functional of the BEC using a suitable *ansatz* with an optimum number of variational parameters. In the current thesis, we only consider repulsive BECs which are quite stable. Attractive BECs, on the other hand, are metastable and collapse above a critical number of atoms.

#### **1.3** Two species Bose-Einstein Condensates

In case of two species Bose-Einstein condensates (TBECs), there is a macroscopic occupation of the two single particle states instead of one. In zerotemperature mean field approximation, the stationary state solution of the TBEC is described by a set of coupled Gross-Pitaevskii equations

$$\left[-\frac{\hbar^2}{2m_i}\nabla^2 + V_i(\mathbf{r}) + \sum_{j=1}^2 U_{ij}|\Psi_j(\mathbf{r})|^2 - \mu_i\right]\Psi_i(\mathbf{r}) = 0, \quad (1.15)$$

where *i* and j = 3 - i are species indices. Here  $U_{ii} = 4\pi\hbar^2 a_{ii}/m_i$ , where  $m_i$  is the mass and  $a_{ii}$  is the *s*-wave scattering length, is the intra-species interaction,

 $U_{ij} = 2\pi \hbar^2 a_{ij}/m_{ij}$ , where  $m_{ij} = m_i m_j/(m_i + m_j)$  is the reduced mass and  $a_{ij}$  is the inter-species scattering length, is the inter-species interaction, and  $\mu_i$  is the chemical potential of the *i*th species. The typical feature of TBECs, which is absent in single component BECs, is the phenomenon of phase separation in coordinate space, i.e. two species tend to occupy different regions of available coordinate space. In TF approximation, the phase separation occurs when all the inter-atomic interactions are repulsive and the inter-species repulsion exceeds the geometric mean of the intra-species repulsive interactions.

### 1.4 Quantum degenerate spin-polarized Fermi gas

In case of spin-polarized Fermi gas, the Pauli's exclusion principle rules out the possibility of *s*-wave scattering. Thus, the lowest partial wave which contributes to interaction (scattering) among the atoms is *p*-wave scattering, which can be safely neglected at low temperatures. It implies that fermions in the ultracold spin-polarized Fermi gas can be considered as non-interacting. The ground state density distribution of inhomogeneous quantum degenerate spin-polarized Fermi gas can be estimated by employing TF approximation [47]. In TF approximation, as mentioned earlier, the Fermi gas is considered homogeneous locally with the local density

$$n(\mathbf{r}) = \frac{k_{\rm F}^3(\mathbf{r})}{6\pi^2},$$
 (1.16)

where  $k_{\rm F}(\mathbf{r})$  is the local Fermi wave number. The chemical potential, energy required to add a fermion to the system, is equal to the sum of local Fermi energy and trapping potential

$$\mu = \epsilon_{\rm F}(\mathbf{r}) + V(\mathbf{r})$$
  
=  $\frac{\hbar^2 k(\mathbf{r})_{\rm F}^2}{2m} + V(\mathbf{r}).$  (1.17)

Form Eq. (1.16) and Eq. (1.17), the density of Fermi gas is

$$n(\mathbf{r}) = \frac{1}{6\pi^2} \left\{ \frac{2m}{\hbar^2} [\mu - V(\mathbf{r})] \right\}^{3/2}, \qquad (1.18)$$

provided  $\mu > V(\mathbf{r})$ . If  $R_i$  (i = 1,2,3) is the spatial extent of the Fermi cloud along *i*th direction, TF approximation is valid provided the Fermi wavelength is much smaller than the dimensions of the cloud, i.e.

$$k_{\rm F}(0)R_i \sim N^{1/3} \gg 1.$$
 (1.19)

Thus for large Fermi clouds one can safely employ TF approximation to calculate  $n(\mathbf{r})$ .

#### 1.5 Excitations of the condensate

Bogoliubov description — The excited states of BEC can be obtained from time-dependent GP equation by searching for solutions of type

$$\Psi(\mathbf{r},t) = e^{-i\mu t/\hbar} \left[ \Psi_{\rm eq}(\mathbf{r}) + u(\mathbf{r})e^{-i\omega t} + v^*(\mathbf{r})e^{i\omega t} \right], \qquad (1.20)$$

where  $\Psi_{eq}(\mathbf{r})$  is the stationary solution of the GP equation, and u and v are complex functions. From Eq. (1.13) and Eq. (1.20), after retaining the terms which are linear in u and v, we get

$$\hbar\omega u(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) - \mu + 2n(\mathbf{r})U_0\right]u(\mathbf{r}) + n(\mathbf{r})U_0v(\mathbf{r}),$$
  
$$-\hbar\omega v(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) - \mu + 2n(\mathbf{r})U_0\right]v(\mathbf{r}) + n(\mathbf{r})U_0u(\mathbf{r}).$$
(1.21)

From these coupled equations, known as Bogoliubov equations, one can obtain the frequency  $\omega$  and hence energy of the excitations. For uniform Bose gas  $(V(\mathbf{r}) = 0)$ , the quasi-particle amplitudes u and v are plane waves and lead to the following energy spectrum

$$(\hbar\omega)^2 = \frac{\hbar^2 q^2}{2m} \left(\frac{\hbar^2 q^2}{2m} + 2U_0 n\right), \qquad (1.22)$$

where q is the wave vector of the plane wave and n is the density of the uniform gas. The excitation energies at long and short wave lengths are

$$\hbar\omega \simeq s\hbar q \quad \text{for } \frac{2\pi}{q} \gg 1,$$

$$\hbar\omega \simeq \frac{\hbar^2 q^2}{2m} + nU_0 \quad \text{for } \frac{2\pi}{q} \ll 1,$$
(1.23)

where  $s = \sqrt{nU_0/m}$  is the sound speed. The transition from linear spectrum at long wavelengths to quadratic one at short wavelengths occurs at  $q \sim \sqrt{2mnU_0}/\hbar = \xi^{-1}$ , where  $\xi$  is the coherence length. It implies that on a length scale shorter than  $\xi$ , the excitations are like those of free particles, while on longer length scales atoms oscillate collectively. For BECs in trapping potentials, numerical solutions of Bogoliubov equations have been calculated in Refs. [48, 49, 50, 51, 52, 53].

Hydrodynamic description — If  $Na/a_{\rm osc} \gg 1$ , excitations of the BEC can be described by the hydrodynamic theory of superfluids in collisionless regime at zero temperature [43]. Using Madelung transformation  $\Psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)}e^{i\phi(\mathbf{r}, t)}$ , Eq. (1.13) can be written as two coupled equations for density and velocity field  $v(\mathbf{r}, t) = \hbar \nabla \phi(\mathbf{r}, t)/m$ 

$$\frac{\partial n}{\partial t} + \nabla .(\mathbf{v}n) = 0,$$

$$m\frac{\partial \mathbf{v}}{\partial t} + \nabla \left(V + U_0 n - \frac{\hbar^2}{2m\sqrt{n}}\nabla^2 \sqrt{n} + \frac{mv^2}{2}\right) = 0,$$
(1.24)

where we have suppressed the explicit spatial and time dependence of the various quantities. In TF approximation, the quantum pressure (term proportional to  $\nabla^2 \sqrt{n}$ ) in Eq. (1.24) can be neglected. Considering  $n = n_{\rm eq} + \delta n$ , where  $n_{\rm eq}$  is the equilibrium density and  $\delta n \propto e^{-i\omega t}$  is the fluctuation about it, one can linearize Eq. (1.24) to get

$$\omega^{2}\delta n = \frac{1}{m} \{\nabla V \cdot \nabla \delta n - [\mu - V(\mathbf{r})] \cdot \nabla^{2} \delta n \}$$
  
=  $-\nabla \cdot [c^{2}(\mathbf{r}) \nabla \delta n],$  (1.25)

where  $mc^2(\mathbf{r}) = \mu - V(\mathbf{r})$  with  $c(\mathbf{r})$  as the local sound speed. This equation can be used to calculate the collective oscillations of the BEC [54]. In presence of trapping potential, oscillations characterized by frequency much larger than trapping frequency (or wavelength much smaller than the size of the system) propagate as usual sound waves. On the other hand, oscillations with frequency of the order of trapping frequency (or wavelengths of the order of system's size) are associated with the motion of the whole system. These collective oscillations correspond to the low-energy solutions of the Bogoliubov equations [43], e.g. vortices, solitons, etc. In case of axisymmetric traps the excitation frequencies of the low lying modes calculated in Ref. [54] are in very good agreement with the experimental results [55, 56] and thus provide an

irrefutable evidence for the validity of GP equation. Hydrodynamic approach breaks down for the oscillations characterized by wavelength of the order of or smaller than  $\xi$ ; whereas for surface oscillations, oscillations characterized by wavelength smaller than  $\delta$  can not be described by hydrodynamic approach.

#### **1.6** Quantized vortices in BEC

As the velocity field of the BEC is proportional to the gradient of its phase, the velocity field is irrotational, i.e.

$$\nabla \times \mathbf{v} = 0, \tag{1.26}$$

provided phase of the order parameter does not have a singularity. The circulation  $\Gamma$  of the velocity field around a closed contour is

$$\Gamma = \oint \mathbf{v}.dl = \frac{\hbar}{m} \oint \nabla \phi.dl = l\frac{h}{m}, \qquad (1.27)$$

where l is an integer. Here we employed the fact that for the single-valuedness of the order parameter, the total phase change around a closed contour should be equal to an integer multiple of  $2\pi$ . Thus the circulation of the velocity field is quantized in units of h/m [57, 58]. Let us assume a purely azimuthal flow of BEC in an axisymmetric trap. The velocity field for such a flow is

$$v_{\phi} = l \frac{\hbar}{mr},\tag{1.28}$$

where r is the distance from the axis of the trap. Because a non-zero value of the order parameter on the trap axis will make the kinetic energy of the system infinite for  $l \neq 0$ , the order parameter must vanish on the trap axis leading to the formation of quantized vortex line. The curl of velocity field, known as vorticity, in the presence of vortex lying along axis (say z-axis) is

$$\nabla \times \mathbf{v} = \hat{z} \frac{lh}{m} \delta^2(r), \qquad (1.29)$$

where  $\delta^2(r)$  is the two dimensional Dirac delta function. Hence vorticity is localized along vortex line as compared to diffused vorticity in case of a rotating rigid body.

#### **1.7** Objectives of the current study

The current study is aimed to study both the static and the dynamic properties of ultracold quantum gases with main focus on binary quantum degenerate mixtures. The objectives of the current study are as follows:

- To study Bose-Einstein condensation of an ideal Bose gas in alternative traps like quartic trapping potentials.
- To calculate *p*-wave scattering length of fermionic alkali atoms.
- To examine the static properties of quantum degenerate Bose-Bose and Bose-Fermi mixtures, especially ground state geometries.
- To examine collective excitations like those leading to Rayleigh-Taylor instability in phase-separated binary condensates.
- To study the creation and evolution of coreless vortex-antivortex pairs in phase-separated binary condensates.

#### **1.8** Outline of the chapters

A brief outline of the chapters in the rest of the thesis is as follows:

In the second chapter, *Physics of ultracold dilute atomic clouds*, we first examine the Bose-Einstein condensation of an ideal Bose gas in quartic trapping potentials in Sec. 2.1. Herein we calculate the critical temperature for Bose-Einstein condensation in quartic traps. Besides this, we also examine the effects of finite particle number and cross terms in trapping potential on the critical temperature. In Sec. 2.2, we examine the use of WKB approximation and variable phase method to calculate p-wave scattering length of fermionic alkali atoms.

In the third chapter, Ground state geometry of quantum degenerate Bose-Bose mixture, we discuss two different methods to determine the ground state geometry of the binary condensate both in miscible and immiscible (phaseseparated) domains. In Sec. 3.1, we provide the details of our semi-analytic scheme based on TF approximation to determine the ground state geometry of TBEC in phase-separated domain. The crucial role played by the interface energy in determining the ground state geometry is underlined in Sec. 3.1.4. In the following Sec. 3.2, we use variational ansatz based semi-analytic method to determine the ground state geometry of very weakly interacting condensate in both miscible and immiscible domains. We extend this method to determine the geometry of TBEC in optical lattices.

In the fourth chapter, *Statics and dynamics of mixtures of quantum fluids*, we first study the ground state geometry of <sup>174</sup>Yb-<sup>173</sup>Yb Bose-Fermi mixture in Sec. 4.1. The choice of this particular Bose-Fermi mixture is based on the experimental feasibility of tuning both the Bose-Bose and Bose-Fermi interactions using optical Feshbach resonances. We use mean field approach to calculate the phase-diagram of this mixture in spherical traps. In Sec. 4.2, we propose a well-controlled experimental scheme to initiate and examine the Rayleigh-Taylor instability in two-species Bose-Einstein condensates. We identify the <sup>85</sup>Rb-<sup>87</sup>Rb mixture as an excellent candidate to observe it experimentally.

In the fifth chapter, *Collective modes in variable potentials*, we study the creation and the dynamics of coreless vortex-antivortex pairs (vortex dipoles) in phase-separated binary condensates. We examine two different mechanisms for vortex dipole generation.

The last chapter of the thesis presents the brief summary of the results and future directions, namely *Future directions*.

# Chapter 2

# Physics of ultracold dilute atomic clouds

In the typical experimental set-ups, used to realize Bose-Einstein condensates (BECs), the ultracold quantum gases are trapped by harmonic potentials. It was shown in Ref. [59] that superfluid to Mott insulator transition, which was experimentally observed earlier in the BEC of <sup>87</sup>Rb atoms trapped in an optical lattice [17], can be more robust with a quartic trapping potential instead of harmonic one. Besides facilitating the quantum phase transition, introducing a quartic confining potential stabilizes fast rotating vortices in BECs [60, 61, 62, 63, 64, 65]. The Bose-Einstein condensation of a non-interacting or ideal Bose gas trapped by one- or two-dimensional power law potentials was earlier studied in Ref. [66]. Later on, Bose-Einstein condensation of an ideal Bose gas trapped by a power law potential of an arbitrary dimensionality was studied in Ref. [67]. The condensation temperature and thermodynamic properties of an ideal Bose gas in an anharmonic trap have been studied in Ref. [68]. In fact, many thermodynamic properties of the BEC like critical temperature, energy, specific heat, entropy, etc., can be calculated to a fairly good approximation by treating the system as non-interacting.

For interacting ultracold bosonic systems, as mentioned in the previous chapter, s-wave scattering length a can be used to define an effective contact interaction potential. Approximating ultracold bosonic system as noninteracting is a good approximation, provided  $Na/a_{osc} \sim 1$ . In the opposite limit  $Na/a_{osc} \gg 1$ , a condition easily realizable in experiments, one can not ignore (weakly) interacting nature of the ultracold bosonic system. Contrary to ultracold bosonic system, a spin polarized Fermi gas, as already stated in the previous chapter, effectively behaves as a non-interacting system at low

temperatures. In this case the most dominant, although small, contribution to the effective potential will be due to the *p*-wave scattering, parameterized in terms of p-wave scattering length  $a_1$ . The calculation of  $a_1$  assumes significance, especially as experiments on fermionic isotopes have made impressive progress since the first experimental observation of degenerate fermions [69]. Superfluidity in a two species fermionic mixture of <sup>6</sup>Li, first predicted theoretically [70], has been observed without any ambiguity [71, 72, 73]. Following which, intense experimental and theoretical investigations continue on the phase diagram of the spin polarized two component <sup>6</sup>Li mixture. Important recent developments are the theoretical calculation of the phase diagram at finite temperature [74] and the experimental investigation of the same at unitarity [75]. Furthermore, the recent achievement of cooling a <sup>6</sup>Li-<sup>40</sup>K fermionic mixture to degeneracy [76] heralds the possibility of observing exotic phases predicted for spin-polarized heteronuclear degenerate fermionic mixtures [77]. Some of the predicted phases are fragile and crucially dependent on the difference in the Fermi energy. For heterogeneous Fermi-Fermi mixtures like <sup>6</sup>Li-<sup>40</sup>K, gapless superfluidity has been studied in Ref. [78]. For such cases, the change in chemical potential induced by p-wave scattering is likely to be an important parameter. The p-wave scattering also plays an important role in determining the stability of trapped Fermi gases against collapse at large densities [79]. The pseudopotentials arising from the p and higher partial waves, discussed in recent works [80, 81], can be used to incorporate the effects of *p*-wave scattering in fermionic isotopes.

In Sec. 2.1, we use semi-classical approximation, introduced in the previous chapter, to calculate the critical temperature for Bose-Einstein condensation in quartic trapping potential. Herein we also calculate the effects of finite particle number and cross-terms in the trapping potential. In Sec. 2.2, we use WKB approximation and variable phase method [82] to calculate the *p*-wave scattering length for fermionic alkali atoms. Based on quantum defect theory, the *p*-wave scattering length can also be determined from the experimental value of the highest bound state energy [83] or by using an analytic expression that relates the *s*- and *p*-wave scattering lengths [84]. The results of quantum defect theory are based on the exact solution of the Schrödinger wave equation for an attractive  $1/r^6$  potential. Since these solutions do not take into account the exact form of the interaction potential, the results of the variable phase method should be much more reliable compared to results based on quantum defect theory. We conclude the chapter with a brief summary of the results.

#### **2.1** $T_c$ for 3D quartic potential trap

The general form of the quartic oscillator potential is  $\lambda(\mathbf{r}.\mathbf{r})^2$ . It is homogeneous and has cross terms in the Cartesian coordinate representation which couple motions along different axes. Potentials of this form occur in optical lattices, where counter propagating lasers create undulating patterns of standing radiation field. In one dimension, a pair of counter propagating Gaussian laser beams along z-axis of intensity profile  $I_0 \exp(-2r^2/w^2)$  creates an array of periodic intensity minima and maxima. These are located along the z-axis. Depending on the detuning of the laser, the atoms are attracted to the intensity minima or maxima. Usually the wavelength of the laser  $\lambda$  is much smaller than the beam width w. To a very good approximation, the potential across a surface normal to the laser beam

$$V(r) = I_0 \left(\frac{-2r^2}{w^2} + \frac{4r^4}{w^4}\right).$$
 (2.1)

It is possible to retain only the quartic term by tuning the parameters of the laser beams. For simplicity, neglecting the cross terms, in three dimension

$$V(x, y, z) = \lambda (x^4 + y^4 + z^4).$$
(2.2)

The eigen energies of the corresponding Hamiltonian are the sum of eigen values corresponding to each dimension. For the one dimensional quartic oscillator, eigen values can be calculated by minimizing the expectation of the Hamiltonian in the basis states of harmonic oscillator of appropriately chosen frequency[85]. Generalizing the result to three dimensional case, the eigen energy

$$\epsilon(n_1, n_2, n_3) = 1.389 \sum_{i=1}^3 (n_i + \frac{1}{2})^{\frac{4}{3}} \left(\frac{\lambda\hbar^4}{m^2}\right)^{\frac{1}{3}}, \qquad (2.3)$$

where m is the mass of the boson. Since  $1.389(\lambda \hbar^4/m^2)^{1/3}$  has the dimensions of energy, we can represent this factor by  $\hbar \omega$ , then

$$\epsilon(n_1, n_2, n_3) = \sum_{i=1}^3 (n_i + \frac{1}{2})^{\frac{4}{3}} \hbar \omega.$$
(2.4)

We now determine the number of states  $G(\epsilon)$  with energy less than a given value  $\epsilon$ . For energies large compared to  $\hbar\omega$ , we can treat  $n_i$ 's as continuous variables and neglect the ground state energy. To calculate  $G(\epsilon)$ , we introduce a coordinate system in terms of the three variables  $\epsilon_i = n_i^{4/3} \hbar \omega$ . In this coordinate system  $\epsilon = \epsilon_1 + \epsilon_2 + \epsilon_3$  defines a surface of constant energy  $\epsilon$ . Then  $G(\epsilon)$  is proportional to the volume in the first octant bounded by the surface

$$G(\epsilon) = \frac{27}{64(\hbar\omega)^{9/4}} \int_0^{\epsilon} \epsilon_1^{-1/4} d\epsilon_1 \int_0^{\epsilon-\epsilon_1} \epsilon_2^{-1/4} d\epsilon_2 \int_0^{\epsilon-\epsilon_1-\epsilon_2} \epsilon_3^{\epsilon-\epsilon_1-\epsilon_2} d\epsilon_3.$$
(2.5)

We use the relation  $\int_0^u x^{\nu-1}(u-x)^{\mu-1} = u^{\mu+\nu-1}B(\mu,\nu)$ , where  $B(\mu,\nu) = \Gamma(\mu)\Gamma(\nu)/\Gamma(\mu+\nu)$  [86] to evaluate the integral, and then the density of states

$$g(\epsilon) = \frac{dG(\epsilon)}{d\epsilon} = 0.6852 \frac{\epsilon^{5/4}}{(\hbar\omega)^{9/4}}.$$
(2.6)

This expression for density of states is used to calculate  $T_c$ . For bosons, the total number of particles occupying the excited states is

$$N_{\rm exc} = \int_0^\infty \frac{g(\epsilon)}{e^{(\epsilon-\mu)/kT} - 1} d\epsilon.$$
(2.7)

At critical temperature  $\mu \to 0$  in the case of bosons and  $N_{\text{exc}}$  is equal to the total number of bosons N. Evaluating the integral gives  $T_c$  in terms of the number of bosons

$$kT_c = \frac{N^{4/9}\hbar\omega}{\left[0.6852\Gamma(9/4)\zeta(9/4)\right]^{4/9}}.$$
(2.8)

The corresponding expression for three dimensional isotropic harmonic oscillator potential is [3]

$$kT_c = \frac{\hbar\omega_o N^{1/3}}{[\zeta(3)]^{1/3}},\tag{2.9}$$

where  $\omega_o$  is the angular frequency of isotropic harmonic oscillator. From Eq. (2.8) and Eq. (2.9), the ratio of the critical temperatures in the two potentials is

$$\frac{(T_c)_{\text{quartic}}}{(T_c)_{\text{harmonic}}} = \frac{N^{4/9} \zeta(3)^{1/3}}{N^{1/3} \left[0.6852 \Gamma(9/4) \zeta(9/4)\right]^{4/9}}$$
$$= 1.006 N^{1/9}, \qquad (2.10)$$

where we have taken  $\hbar\omega = \hbar\omega_o$  to obtain the ratio. The ratio is proportional to  $N^{1/9}$ , which means that for  $10^7$  atoms,  $T_c$  in the case of 3D quartic potential trap is approximately six times higher than that of the 3D isotropic harmonic trap as is shown in Fig. 2.1.



Figure 2.1: Ratio of the critical temperature  $(T_c)$  to angular frequency  $(\omega_o)$  as a function of the logarithm of number of bosons  $(\log N)$ . Here we have taken  $1.389(\lambda\hbar^4/m^2)^{1/3} = \hbar\omega_o$ ; red and black curves correspond to quartic and quadratic potentials respectively. When  $\log N = 7$ ,  $T_c$  for the 3D quartic potential is approximately six times higher than the 3D isotropic harmonic potential.

#### 2.1.1 Effect of finite particle number

The expression of  $T_c$  in the previous section is with the approximation that the ground state energy is zero, which is a valid approximation when the system has large number of bosons. For finite number of bosons, the zero point energy causes a change in the value of  $T_c$ . For the 3D quartic potential, the ground state energy is [85]

$$\epsilon_{\min} = 2.41 \left(\frac{\lambda \hbar^4}{m^2}\right)^{1/3}.$$
(2.11)

This should be equal to the change in the chemical potential at the critical temperature, that is  $\Delta \mu = \epsilon_{\min}$ . As the total number of bosons is fixed [3]

$$dN = \left(\frac{\partial N}{\partial T}\right)_{\mu} dT + \left(\frac{\partial N}{\partial \mu}\right)_{T} d\mu = 0.$$
 (2.12)
This implies

$$\left(\frac{\partial\mu}{\partial T}\right)_{N} = -\left(\frac{\partial N}{\partial T}\right) \left(\frac{\partial N}{\partial\mu}\right)_{T}^{-1}.$$
(2.13)

Using the expression of N at temperatures slightly above  $T_c$ 

$$N = C_{\alpha} \int_0^\infty \frac{\epsilon^{\alpha - 1}}{e^{(\epsilon - \mu)/kT} - 1} d\epsilon.$$
(2.14)

This relation is obtained by substituting the general expression for the density of states, i.e.  $g(\epsilon) = C_{\alpha} \epsilon^{\alpha-1}$  in Eq. (2.7). Here  $C_{\alpha}$  is a constant whose value depends on the form of the trapping potential. From Eq. (2.13) and Eq. (2.14) we get

$$\left(\frac{\partial\mu}{\partial T}\right)_N = -\alpha \frac{\zeta(\alpha)}{\zeta(\alpha-1)}k.$$
(2.15)

In this expression  $\alpha$  should be greater than 2, otherwise the relation is not valid since  $\zeta(1)$  diverges. Using this expression, the change in the critical temperature due to the finite particle number is

$$\Delta T_c = -\frac{\zeta(\alpha - 1)}{\alpha \zeta(\alpha) k} \Delta \mu.$$
(2.16)

In the case of 3D quartic potential  $\alpha$  is equal to 9/4, then

$$\Delta T_c = \frac{-4\zeta(5/4)}{9\zeta(9/4)k} \Delta \epsilon_{\min} \\ = \frac{-1.071\zeta(5/4)}{\zeta(9/4)k} \left(\frac{\lambda\hbar^4}{m^2}\right)^{1/3}.$$
(2.17)

A relative measure of the effect of zero point energy on the critical temperature is the fractional change of the critical temperature. It is the ratio between  $\Delta T_c$ and  $T_c$ , for the present case

$$\frac{\Delta T_c}{T_c} = \frac{-0.9054\zeta(5/4)}{\zeta(9/4)} \left(\frac{\lambda\hbar^4}{m^2}\right)^{1/3} \frac{\left(\Gamma(9/4)\zeta(9/4)\right)^{4/9}}{\hbar\omega N^{4/9}}.$$
 (2.18)

Noting that  $(\lambda \hbar^4/m^2)^{1/3}$  is equivalent to  $\hbar \omega/1.389$  we get

$$\frac{\Delta T_c}{T_c} = \frac{-0.6891\zeta(1.25)N^{-4/9}}{\zeta(2.25)^{5/9}} \tag{2.19}$$

$$= -2.56N^{-4/9}. (2.20)$$

For the 3D isotropic harmonic potential, the fractional change of the critical temperature is

$$\frac{\Delta T_c}{T_c} = -0.73 N^{-1/3}.$$
(2.21)

If we compare Eq. (2.20) and Eq. (2.21), we find that the percentage decrease in  $T_c$  is larger in the case of 3D quartic potential trap for number of particles  $\leq 80,000$ , but the scenario is reversed for number of particles > 80,000. This is also evident from Fig. 2.2 where cross over point corresponds to the number of particles  $\approx 80,000$ .



Figure 2.2: Fractional change in critical temperature  $(\Delta T_c/T_c)$  as a function of the logarithm of number of bosons (log N). The red and black colored curves correspond to the quartic and quadratic potentials respectively. Below log(N) = 4.9, that is  $N \approx 80,000$ , the 3D quartic potential has larger fractional change. Above this point the 3D isotropic harmonic potential has marginally higher fractional change.

### 2.1.2 Effect of cross terms

3D case: Consider the general form of the quartic potential, as mentioned earlier

$$V(\mathbf{r}) = \lambda(\mathbf{r}.\mathbf{r})^2. \tag{2.22}$$

In optical traps, it is possible to create confining potentials which are approximately close to this form but a truly spherically symmetric one is not realizable. The difficulty is in producing the cross terms of the potential, for example, terms like  $x^2y^2$  in Cartesian coordinate representation. The absence or presence of the cross terms in quadratic and quartic potentials respectively, introduces a key difference between the dynamics in the two potentials. In the absence of the cross terms like xy in quadratic potential, a perturbation to the dynamics of a particle along an axis remains confined along that axis. In contrast, it propagates to other axes in the case of quartic potential. For condensates in traps, an important parameter which reflects the effects of these terms is the critical temperature.

Semiclassically, total number of states available to the system can be obtained by dividing the total phase space volume by  $h^3$ , the volume of a single state, then

$$G(\epsilon) = \frac{1}{h^3} \int d\mathbf{x} \int d\mathbf{p}, \qquad (2.23)$$

$$= \frac{16\pi^2}{h^3} \int_0^{r^*} r^2 dr \int_0^{p^*} p^2 dp. \qquad (2.24)$$

In the above equation  $r^*$  and  $p^*$  are radial coordinate and momentum corresponding to the classical turning point respectively. Transforming the variable of integration from p to  $\epsilon$  [using the relation  $p^2/2m = \epsilon - V(\mathbf{r})$ ] we get

$$G(\epsilon) = \frac{16\pi^2 m}{h^3} \int_0^{r^*} r^2 dr \int_0^{\epsilon^*} \sqrt{2m(\epsilon - V(\boldsymbol{r}))} d\epsilon.$$
 (2.25)

Thus the density of states is

$$g(\epsilon) = \frac{16\pi^2 m}{h^3} \int_0^{r^*} r^2 \sqrt{2m\left(\epsilon - \lambda r^4\right)} dr.$$
(2.26)

Substituting  $r^4 = x$  we can transform the integral into a form which can be evaluated analytically [86]

$$g(\epsilon) = \frac{4\pi^2 m^{3/2} \sqrt{2\lambda}}{h^3} \int_0^{\epsilon/\lambda} \left(\sqrt{\frac{\epsilon}{\lambda} - x}\right) x^{-1/4} dx \qquad (2.27)$$

$$= \frac{4\sqrt{2}\pi^2 m^{3/2} \Gamma(3/2) \Gamma(3/4) \epsilon^{5/4}}{h^3 \lambda^{3/4} \Gamma(9/4)}.$$
 (2.28)

Using this expression for the density of states in Eq. (2.7) we get

$$kT_c = \frac{N^{4/9}}{\left[\Gamma(9/4)\zeta(9/4)\right]^{4/9}} \left[\frac{h^3\lambda^{3/4}\Gamma(9/4)}{\Gamma(3/2)\Gamma(3/4)4\sqrt{2}\pi^2 m^{3/2}}\right]^{4/9}.$$
 (2.29)

Comparing with Eq. (2.8) we can obtain the ratio of  $T_c$  in the two cases, with and without the cross terms, for the 3D isotropic quartic potential. It is found that  $T_c$  with the cross terms is 1.2 times higher. This rise in  $T_c$  can be attributed to the contribution from the cross terms which were neglected while deriving Eq. (2.8). The reason for the difference is, when  $g(\epsilon) = C_{\alpha} \epsilon^{\alpha-1}$  then  $T_c$  varies as  $1/C_{\alpha}^{1/\alpha}$ . Hence, the lower  $T_c$  in 3D quartic potentials without the cross terms is due to the higher value of  $C_{\alpha}$ .

 $2D\ case:$  In the 2D case, neglecting the cross terms, the potential is of the form

$$V(x,y) = \lambda(x^4 + y^4).$$
 (2.30)

Using the same approach as adopted in the 3D case, the total number of states available to the system is

$$G(\epsilon) = \frac{9}{16(\hbar\omega)^{3/2}} \int_0^{\epsilon} \epsilon_1^{-1/4} d\epsilon_1 \int_0^{\epsilon-\epsilon_1} \epsilon_2^{-1/4} d\epsilon_2$$
(2.31)

$$= \frac{3\Gamma(3/4)\Gamma(7/4)}{4(\hbar\omega)^{3/2}\Gamma(5/2)}\epsilon^{3/2}.$$
 (2.32)

Thus the density of states

$$g(\epsilon) = \frac{0.9531\epsilon^{1/2}}{(\hbar\omega)^{3/2}}.$$
(2.33)

Substituting this expression of  $g(\epsilon)$  in Eq. (2.7) we get

$$kT_c = \frac{\hbar\omega N^{2/3}}{\left[\zeta(3/2)\Gamma(3/2)0.9531\right]^{2/3}}.$$
(2.34)

The corresponding expression when cross terms are considered is [66]

$$kT_c = \left[\frac{Nh^2\sqrt{\lambda}}{2\pi^2 m\Gamma(3/2)\zeta(3/2)}\right]^{2/3}.$$
(2.35)

Comparing Eq. (2.34) and Eq. (2.35) we find that  $T_c$  with the cross terms in Eq. (2.35) is approximately 1.12 times higher than  $T_c$  without the cross terms

in Eq. (2.34). Thus the cross terms increase  $T_c$  in 2D as well as 3D case.

### 2.2 Scattering length for fermionic alkali atoms

Hereafter in this chapter, we use atomic units ( $\hbar = m_e = e = 1$ ) for the sake of conciseness. The radial part of the Schrödinger wave equation for two interacting atoms with interaction potential V(R) is

$$\frac{d^2\chi(R)}{dR^2} + \left[k^2 - U(R) - \frac{l(l+1)}{R^2}\right]\chi(R) = 0, \qquad (2.36)$$

where *m* is the reduced mass of the two interacting atoms, U(R) = 2mV(R), *k* is the relative momentum of the two atoms, *l* is the angular momentum quantum number and  $\chi(R)$  is the radial wave-function. This equation is used to calculate the scattering phase shift  $(\eta_l)$  of an atom for each component angular momentum *l* arising from the interaction.

In Eq. (2.36), when  $k \ll 1$ ,  $k^2$  can be neglected in comparison to other terms within the square bracket,

$$\frac{d^2\chi(R)}{dR^2} + \left[-U(R) - \frac{l(l+1)}{R^2}\right]\chi(R) = 0.$$
(2.37)

At large distances from the scattering center, the van der Waal's potential  $U(R) = -2m\alpha/R^6 = -\gamma^2/R^6$  is the dominant inter-atomic interaction. Here  $\alpha$  is the van der Waal's coefficient and  $\gamma = \sqrt{2m\alpha}$ . For low energy collisions  $k \to 0$ , the interaction potential approaches the asymptotic form within the  $kR \ll 1$  region and

$$\frac{d^2\chi(R)}{dR^2} + \left[\frac{\gamma^2}{R^6} - \frac{l(l+1)}{R^2}\right]\chi(R) = 0.$$
(2.38)

The general solution of Eq. (2.38) for a p (l = 1) partial wave is

$$\chi(R) = \sqrt{R} \left[ A J_{3/4} \left( \frac{\gamma}{2R^2} \right) + B J_{-3/4} \left( \frac{\gamma}{2R^2} \right) \right], \qquad (2.39)$$

where  $J_{\pm 3/4}(\ldots)$  are the Bessel functions of first kind. In the limit  $R \to \infty$ , the solution in region kR < 1 after considering only the leading terms of  $J_{3/4}(x)$  and  $J_{-3/4}(x)$  is

$$\chi(R) = A \frac{(\gamma/2)^{3/4}}{2^{3/4} \Gamma(7/4)R} + B \frac{(\gamma/2)^{-3/4} R^2}{2^{-3/4} \Gamma(1/4)},$$
(2.40)

where  $\Gamma(\ldots)$  are the gamma functions.

The *p*-wave phase shift  $\eta_1$  can be expressed in terms of the constants A and B introduced above [87]:

$$\tan \eta_1 = \frac{1}{24} \frac{A}{B} \frac{\gamma^{3/2} \Gamma(1/4)}{\Gamma(7/4)} k^3.$$
 (2.41)

For any arbitrary potential that varies as  $R^{-n}$ , the scattering length  $(a_l)$  and phase shift  $(\eta_l)$  are related by [87]

$$\lim_{k \to 0} k^{2l+1} \cot \eta_l = \frac{-1}{a_l^{2l+1}}.$$
(2.42)

This relation is valid, provided l < (n-3)/2 and is applicable for a p partial wave when n = 6 or higher. From Eqs. (2.41) and (2.42) the scattering volume for the p partial wave is

$$a_1^3 = -\frac{1}{24} \frac{A}{B} \frac{\gamma^{3/2} \Gamma(1/4)}{\Gamma(7/4)}.$$
 (2.43)

We use Eq. (2.43) as a definition for the scattering volume  $a_1^3$  throughout the remaining chapter.

### 2.2.1 Scattering length calculation

The solution of Eq. (2.36) in the asymptotic region, given by Eq. (2.39) and parameterized in terms of A and B, is referred to as the outer solution. To determine A/B, Eq. (2.36) should be solved within the inner part of the interatomic potential: the inner wall and well. This can in principle be accomplished using the WKB method [88, 89]. We can evaluate A/B by matching the outer and inner solutions at a point. The matching point should be in the region where the asymptotic form of the interaction potential begins to dominate and the WKB approximation is applicable.

#### 2.2.1.1 WKB solution

For partial waves other than s, the centrifugal potential is non-zero. Combining the interaction potential and centrifugal term, the effective interaction potential is

$$U_{\rm eff}(R) = U(R) + \frac{l(l+1)}{R^2}.$$
 (2.44)

Then the local momentum of the scattered atom is  $p(R) = \sqrt{-U_{\text{eff}}(R)}$  and the de Broglie wavelength  $\lambda(R) = 2\pi/\sqrt{-U_{\text{eff}}(R)}$ . The WKB approximation is applicable when

$$\left|\frac{d\lambda(R)}{dR}\right| \ll 2\pi \quad \text{or} \quad \frac{m|F|}{p(R)^3} \ll 1.$$
(2.45)

In the above relation  $F = -dU_{\text{eff}}(R)/(2mdR)$  is the net force acting on the atom. At large distances, when the interaction potential approaches the asymptotic form, the above inequality for l = 1 is

$$\left[\frac{3\gamma^2}{R^4} - 2\right] \ll \left[\frac{\gamma^2}{R^4} - 2\right]^{3/2}.$$
 (2.46)

This inequality is in general valid up to large radial distances. As an example Fig. 2.3 shows that for Cs the inequality is satisfied up to  $\approx 30a_o$ . The WKB



Figure 2.3: Terms in the relation  $[3\gamma^2/R^4 - 2] \ll [\gamma^2/R^4 - 2]^{3/2}$ , which defines the validity of the WKB solution, are plotted for cesium. The red and black curves correspond to  $[\gamma^2/R^4 - 2]^{3/2}$  and  $[3\gamma^2/R^4 - 2]$  respectively. Inset shows the ratio of the two terms.

solution at R, which satisfies the inequality and is larger than the classical

turning point  $R_o$ , is given by

$$\chi(R) = \frac{c}{\sqrt{p(R)}} \cos\left(\int_{R_o}^R p(R)dR - \frac{\pi}{4}\right),$$
(2.47)

and the logarithmic derivative is

$$\begin{aligned} \zeta(R) &= \frac{\chi'(R)}{\chi(R)} \\ &= -p(R) \tan\left(\int_{R_o}^R p(R) dR - \frac{\pi}{4}\right) - \frac{1}{2p(R)} \frac{dp(R)}{dR}. \end{aligned} (2.48)$$

An analytic expression of  $\zeta(R)$  for l = 1 is obtained if only the van der Waal's potential is considered:

$$\zeta(R) = -\frac{\sqrt{\gamma^2 - 2R^4}}{R^3} \tan\left[\frac{\sqrt{\gamma^2 - 2R_o^4}}{2R_o^2} - \frac{\sqrt{\gamma^2 - 2R^4}}{2R^2} - \frac{\pi}{4} - \frac{1}{\sqrt{2}}\right] \\ \left(\sin^{-1}\frac{\sqrt{2}R^2}{\gamma} - \sin^{-1}\frac{\sqrt{2}R_o^2}{\gamma}\right) - \left[\frac{2R^4 - 3\gamma^2}{2R(\gamma^2 - 2R^4)}\right].$$
(2.49)

This approximation neglects the well and inner wall part of the interaction potential. It is appropriate for model potentials comprising of the van der Waal's and hard core potentials. Such model potentials, with a tunable position of the repulsive wall, have been used by Crubellier et al. [90] for their analysis related to the photoassociation probability near the threshold. The above expression is reduced to that of the *s*-wave case when l = 0, which is used implicitly in Ref. [88].

From the inequality (2.46), it is evident that when  $\gamma$  is sufficiently large (and this holds true for alkali metal atoms), the WKB solution is valid up to radial distances where the asymptotic form of the potential begins to dominate. Choosing a point  $R^*$  in this region such that the factor 2 in the inequality (2.46) can be neglected, the inequality is modified to

$$R^* \ll (\gamma/3)^{1/2}.\tag{2.50}$$

At this point, as the interaction potential has an asymptotic form, Eq. (2.39) is a solution of Eq. (2.36). The logarithmic derivative of the WKB solution at

the matching point  $R^*$  is

$$\zeta(R^*) = -\sqrt{\frac{\gamma^2}{R^{*6}} - \frac{2}{R^{*2}}} \tan\left(\int_{R_o}^{R^*} p(R)dR - \frac{\pi}{4}\right) + \frac{(3\gamma^2/R^{*5} - 2/R^*)}{2(\gamma^2/R^{*4} - 2)}.$$

Using inequality Eq. (2.50), the above expression simplifies to

$$\zeta(R^*) \simeq -\frac{\gamma}{R^{*3}} \tan\left(\int_{R_o}^{R^*} p(R)dR - \frac{\pi}{4}\right) + \frac{3}{2R^*}.$$
 (2.51)

From here on we shall consider the above expression as the logarithmic derivative of the WKB solution.

### **2.2.1.2** Matching $\chi'(R)/\chi(R)$

We introduce a variable  $x = \gamma/(2R^2)$ . At and around matching point  $R^*$ ,  $x = \gamma/(2R^{*2}) \gg 1$ . We can then use the asymptotic expression of the Bessel function

$$\lim_{x \to \infty} J_n(x) \simeq \sqrt{\frac{2}{\pi x}} \cos\left[x - \left(n + \frac{1}{2}\right)\frac{\pi}{2}\right],$$

and then the solution in Eq. (2.39) is

$$\chi(R) = \frac{2R^{3/2}}{\sqrt{\pi\gamma}} \left[ A \, \cos\left(\frac{\gamma}{2R^2} - \frac{5\pi}{8}\right) + B \, \cos\left(\frac{\gamma}{2R^2} + \frac{\pi}{8}\right) \right]. \tag{2.52}$$

This is the small R limit of the asymptotic solution, whereas the solution in Eq. (2.40), in the limit  $x \to 0$ , is the large R limit of the asymptotic solution. To determine A/B, we match the logarithmic derivatives of the analytical solution in Eq. (2.52) and WKB solution in Eq. (2.47). The logarithmic derivative of the above solution at the matching point  $R^*$  is

$$\frac{\chi(R^*)}{\chi'(R^*)} = \frac{3}{2R^*} + \frac{\gamma}{R^{*3}} \frac{\left[A\sin\left(\frac{\gamma}{2R^{*2}} - \frac{5\pi}{8}\right) + B\sin\left(\frac{\gamma}{2R^{*2}} + \frac{\pi}{8}\right)\right]}{\left[A\cos\left(\frac{\gamma}{2R^{*2}} - \frac{5\pi}{8}\right) + B\cos\left(\frac{\gamma}{2R^{*2}} + \frac{\pi}{8}\right)\right]}.$$
 (2.53)

Equating this logarithmic derivative with the logarithmic derivative of the WKB solution (Eq. (2.51)), A/B is

$$\frac{A}{B} = \frac{\sqrt{2m\alpha}\sin\phi_2 - R^{*2}[R^*\zeta(R^*) - 3/2]\cos\phi_2}{R^{*2}[R^*\zeta(R^*) - 3/2]\cos\phi_1 - \sqrt{2m\alpha}\sin\phi_1} \\
= \frac{1}{\sqrt{2}} \left\{ 1 + \tan\left[\phi_o - \left(3 - 2\sqrt{2}\right)\pi/8\right] \right\},$$
(2.54)

where  $\phi_1 = \gamma/2R^{*2} - 5\pi/8$ ,  $\phi_2 = \gamma/2R^{*2} + \pi/8$ , and  $\phi_o = \int_{R_o}^{R'_o} p(R)dR$ with  $R'_o = \sqrt{\gamma}/2^{1/4}$  is the total phase change between two classical turning points. The final expression for A/B is obtained by splitting the integral in the expression for  $\zeta(R^*)$  at the outer turning point  $R'_o$  [91] and using  $\int_{R^*}^{R_o} p(R)dR \simeq \gamma/(2R^{*2}) - \pi/(2\sqrt{2})$ . Substituting this value of A/B in Eq. (2.43), the value of the *p*-wave scattering volume is

$$a_1^3 = -\frac{1}{24\sqrt{2}} \frac{\gamma^{3/2} \Gamma(1/4)}{\Gamma(7/4)} \Big\{ 1 + \tan\left[\phi_o - \left(3 - 2\sqrt{2}\right)\pi/8\right] \Big\}.$$
 (2.55)

Thus *p*-wave scattering depends upon  $\phi_o$ , which one has to evaluate numerically. We did not pursue the numerical evaluation of  $\phi_o$  because of the availability of more accurate variable phase methods to calculate the *p*-wave scattering length. The above expression can be especially useful for model potentials comprising of van der Waal's and hardcore potentials where  $\phi_o$  can be evaluated analytically.

### 2.2.2 Variable phase method

The variable phase method can used to calculate  $\eta_1$  and hence  $a_1$  from the phase function equation [82]. This method is applicable when the interaction potential satisfies two conditions. The first condition is that the interaction potential should be less singular at the origin than the centrifugal part, that is

$$\lim_{R \to 0} [R^2 U(R)] = 0.$$
(2.56)

This implies that near the origin  $U(R) \to U_0 R^m$  as  $R \to 0$  with m > -2, where  $U_0$  is a constant. The interaction potential satisfies this condition since at shorter radial distances, it approaches the inner wall and is repulsive. The second condition is that the interaction potential should decrease faster than the Coulomb potential or inverse of R. In the variable phase method, the phase shift  $\eta_l$  is a solution of the nonlinear differential equation [82]

$$\eta_l'(R) = -k^{-1} U_{\text{eff}}(R) [\cos \eta_l(R) j_l(kR) - \sin \eta_l(R) n_l(kR)]^2, \qquad (2.57)$$

where  $j_l(kR)$  and  $n_l(kR)$  are the spherical Bessel and Neumann functions respectively. The above equation can be used to evaluate the phase function  $\eta_l(R)$ , which defines the total phase shift up to R; then the phase shift is the limiting value

$$\eta_l = \lim_{R \to \infty} \eta_l(R). \tag{2.58}$$

To calculate  $\eta_l$ , the phase function  $\eta_l(R)$  is evaluated up to a cut-off point at which  $\eta_l(R)$  saturates. The phase shift  $\eta_l$ , as evident from Eq. (2.57), depends on the relative momentum k of the colliding atoms. To remove the  $\text{mod}(\pi)$  ambiguity, the phase shift is normalized such that it approaches zero as  $k \to \infty$ , that is

$$\lim_{k \to \infty} \eta_l = 0. \tag{2.59}$$

In addition to the above condition,  $\eta_l$  is considered to be a regular function of k. Eq. (2.57) is numerically integrated from the point corresponding to the atomic radius of the element to the cut-off point. The solution is the phase shift as defined in Eq. (2.58). An alternative form of variable phase approach has been suggested and implemented by Ouerdane et al. [92, 93]. These authors solve a Riccati equation derived from the variable phase equation in the limit  $k \to 0$ .

### 2.2.3 Results with Variable Phase Method

To evaluate the phase shift and the scattering length, the interaction potential should be known accurately. In this subsection, we present the results of our calculations for fermionic isotopes of cesium, lithium and potassium, for which the interatomic potentials are known accurately and hyperfine interactions are less significant in the long-range part of the potentials. The cesium interaction potential is the one used in the work of Gribakin and Flambaum [88, 89], which is based on Ref. [94, 95]. The lithium interaction potential is based on the work of Zemke and Stwalley [96]. The same authors and their collaborators have also calculated the interaction potential of other alkali metals sodium [97] and potassium [98]. However, these are limited to radial distances where hyperfine interactions are not important.

To calculate the phase shift  $\eta_1$  based on the variable phase method, we integrate Eq. (2.57) numerically, using Runge-Kutta-Fehlberg (RKF) method, from the atomic radius  $R_a$  [99] up to infinity. Ideally, the variable phase equation should be integrated from R = 0 to infinity. But, in atomic collision calculations, the wave function of an incident atom is almost zero inside the atomic radius of the target atom. Hence  $\eta_1(R_a) = 0$  is an appropriate initial condition to integrate Eq. (2.57). It has been discussed in previous works [92, 93] that if the cut-off radius [100] is not sufficiently large, then there are corrections arising from the long-range part of the interaction potential. In order to avoid the corrections, we choose a large cut-off radius so that these corrections, if any, are negligible. One problem that is frequently encountered in choosing a very large cut-off radius is the accumulation of round-off errors. These are relatively severe for small values of k. Hence an appropriate choice of cut-off radius should be made such that round-off errors do not compromise the accuracy of the results. To calculate the scattering length  $a_1$ , the phase shift  $\eta_1$  is evaluated for a range of k close to zero. From the definition in Eq. (2.42),  $-\tan \eta_1/k^3$  converges to  $a_1^3$  for p partial wave as  $k \to 0$ . Alternatively, the slope of  $-\tan \eta_1/k^2$  in the limit  $k \to 0$  is the scattering volume  $a_1^3$ .

Cesium: We consider the scattering of two cesium atoms in the  ${}^{3}\Sigma_{u}$  state. The form of the interaction potential is the one considered in Refs. [88, 94]:

$$V(R) = \frac{1}{2}BR^{\mu}e^{-\eta R} - \left(\frac{C_6}{R^6} + \frac{C_8}{R^8} + \frac{C_{10}}{R^{10}}\right)f_c(R), \qquad (2.60)$$

where the values of the constants are B = 0.0016,  $\mu = 5.53$ ,  $\eta = 1.072$  $C_6 = 7020$ ,  $C_8 = 1.1 \times 10^6$  and  $C_{10} = 1.7 \times 10^8$ . The cut-off function is

$$f_c(R) = \Theta(R - R_c) + \Theta(R_c - R)e^{-(R_c/R - 1)^2},$$
(2.61)

where  $\Theta(x)$  is unit step function. The cut-off parameter  $R_c$  was obtained by comparing Eq. (2.60) to the Cs<sub>2</sub>  ${}^{3}\Sigma_{u}$  potential curve calculated via *ab initio* by Krauss and Stevens [95] from  $R = 7a_{o}$  to  $R = 20a_{o}$ . The best fit to the values of  $V_{\min}$  and  $R_{\min}$  was obtained for  $R_{c} = 23.165a_{0}$ .

Using this potential, the phase shift and scattering length are calculated for the <sup>132</sup>Cs and <sup>134</sup>Cs fermionic isotopes. As test calculations, we evaluated *s*-wave phase shifts for the <sup>133</sup>Cs isotope. It should be mentioned that, the value of  $\gamma$  is 41240.1. However, in Ref. [88] the value of  $\gamma$  is defined as 41200. Using the latter, the results of the test calculations were in good agreement with that of Ref. [88].  $\eta_1$  functions calculated from the variable phase method, for varying  $R_c$  for a range of k close to zero are shown in Fig. 2.4. Our calculations show that the value of  $\eta_1$  at higher values of k is more sensitive to  $\gamma$ , the dependence is nonlinear as the equation of phase function is a nonlinear differential equation. Consequently, a small change in  $\gamma$  can result in significant change of  $\eta_1$ . The dependence of  $\eta_1$  on  $\gamma$  is evident from Fig. 2.4, which shows  $\eta_1$  for <sup>132</sup>Cs and <sup>134</sup>Cs. The difference in the interaction potential of the two isotopes is the mass, which manifests as unequal values of  $\gamma$ . The phase function in the neighborhood of k = 0 is also sensitive to the accuracy of the



Figure 2.4: The left and right panel of the figure are the phase shift  $\eta_1(k)$  of  $^{132}$ Cs and  $^{134}$ Cs isotopes respectively. Each panel shows the plots of  $\eta_1(k)$  (measured in radians) for varying cut-off parameter  $R_c$  of the potential. The solid (orange), dotted (black), short-dashed (green), dot-dashed (reddish-brown) and long-dashed (turquoise) curves correspond to  $R_c = 23.115a_o$ ,  $23.140a_o$ ,  $23.165a_o$ ,  $23.190a_o$  and  $23.215a_o$  respectively. The decrease of  $R_c$  enlarges the potential well, increases potential strength and hence leads to the increase in phase shift at constant k. It is analogous to changing the position of the repulsive wall in the model potential considered in Ref. [90].

integration.

In the present calculations, the phase function equation is integrated until  $\eta_1$  converges to the order of  $10^{-6}$ , which is consistent with the choice of tolerance. For Cs, this requires integration up to a radial distance of ~  $500a_o$ . In addition, for the *p*-wave scattering, the centrifugal potential vanishes at a slower rate compared to the van der Waal's potential at large radial distances. This lowers the rate of convergence of the phase shift. A calculation of the *s*-wave phase shift  $\eta_0$  confirms this: it converges to the order of  $10^{-6}$  when the phase equation is integrated to a radial distance of  $\approx 100a_o$ . As discussed in Ref. [88], the *s*-wave scattering cross section for elastic scattering of spinaligned Cs atoms is  $1.5(4) \times 10^{-12}$  cm<sup>2</sup> and is approximately constant from 30 to 250  $\mu$ K. This value is consistent with *s*-wave scattering length of  $\approx \pm 70a_o$ . For  $R_c = 23.165a_o$  and  $R_c = 23.140a_o$ , *s*-wave scattering length values are  $68.0a_o$  and -67.7 respectively and hence close to experimental values. But with  $R_c = 24.140a_o$ , the *s*-wave scattering cross section changes significantly with temperature becoming almost zero at  $64\mu$ K. When  $R_c = 23.165a_o$ , the scattering cross section remains almost constant within the above mentioned temperature range and hence is consistent with experimental results. Thus, we consider  $R_c = 23.165a_o$  as a reasonable choice of cut-off parameter to evaluate the *p*-wave scattering length. For this value of  $R_c$ , the scattering lengths calculated from the slope of  $-\tan(\eta_1)/k^2$  in the limit  $k \to 0$  are  $116a_o$  and  $-93a_o$  for <sup>132</sup>Cs and <sup>134</sup>Cs respectively.

Lithium: For the  $a^{3}\Sigma_{u}^{+}$  state of <sup>6</sup>Li<sub>2</sub>, we use the interaction potential suggested by Zemke and Stwalley [96]. The long-range part of the interaction potential, for <sup>7</sup>Li in particular, is discussed in Ref. [101]. For the  $R \leq 6.388674a_{o}$  and  $R \geq 18.0a_{o}$  regions, the analytic expressions recommended in Refs. [96] and [102] respectively are used. Then, for the  $6.388674a_{o} < R < 18.0a_{o}$  region, the interaction potential is approximated by the cubic spline fitted over the RKR potential values given by Zemke and Stwalley. The resultant interaction potential is shown in Fig. 2.5.

To optimize the calculations, we use the RKF method with a relative tolerance of  $10^{-7}$  from the atomic radius of lithium to the cut-off radius of  $40,000a_o$ . We find that the phase shift stabilizes to 31.42 as  $k \to 0$ , which is shown in Fig. 2.6.

From the calculations, we find that  $-\tan(\eta_1)/k^3$  stabilizes to  $\approx -50000a_o^3$ . The cube root of this is  $a_1$ . Another equivalent way to calculate the scattering volume is to evaluate the slope of  $-\tan(\eta_1)/k^2$  in the  $k \to 0$  limit. We calculate this by least square fitting the data points for  $-\tan(\eta_1)/k^2$  between  $0.0023 \le k \le 0.005$  with an additional point corresponding to the zero phase shift at k = 0. As is evident from Fig. 2.7, a straight line describes the data points very well. The slope of the least-squares fitted line is  $a_1^3 = -46050a_o^3$ , the cube root of which is  $-36a_o$  and can be considered as a reliable value of the *p*-wave scattering length. This value is close to  $-35a_o$  cited by You et al. [103]. Also according to quantum defect theory the *p*-wave scattering volume  $a_1^3$  is related



Figure 2.5: Interatomic potential for  $a\Sigma_u^+$  of <sup>6</sup>Li<sub>2</sub>. The solid (black) and dashed (red) curves are the interatomic potential and the van der Waal's potential respectively. The plot in the inset is the ratio of the van der Waal's potential to the interatomic potential.

to s-wave scattering length  $a_0$  [84]

$$a_{1s}^3 = \frac{[\Gamma(1/4)]^2}{18\pi} \frac{a_{0s} - \overline{a}_{0s}}{2\overline{a}_{0s} - a_{0s}}.$$
(2.62)

Here  $a_{1s}^3 = a_1^3/\beta_6^3$ ,  $a_{0s} = a_0/\beta_6$ ,  $\overline{a}_{0s} = 2\pi/\Gamma(1/4)^2$  and  $\beta_6 = (2m\alpha/\hbar^2)^{1/4}$  is the scaling parameter. Abraham et al. [104] have measured the triplet *s*wave scattering length of <sup>6</sup>Li using two photon photoassociative spectroscopy of the diatomic  $a^3\Sigma_u^+$  state of <sup>6</sup>Li<sub>2</sub>. The value of the *s*-wave scattering length determined by them is  $(-2160 \pm 250)a_o$ . The value of the *p*-wave scattering length  $a_1$  obtained by using this value in Eq. (2.62) is  $\approx -38a_o$ , which is slightly larger than the value obtained by the variable phase method.

Potassium: To calculate the scattering length for  $X^1\Sigma_g^+$  of  $K_2$ , the interaction potential given by Amiot [105] and Zavitsas [106] is used. For  $R \leq 5.42a_o$ and  $R > 28.78a_o$  we use the analytic expressions suggested by Zavitsas [106]. For  $5.42a_o < R \leq 28.78a_o$  we obtain the interaction potential by fitting a cubic spline over the RKR data points given by these authors and taking into account the modification suggested by Zavitsas for v'' = 52 - 81. The variable



Figure 2.6: The *p*-partial wave phase shift  $\eta_1(k)$  (measured in radians) for the  ${}^{3}\Sigma^{+}_{\mu}$  interaction potential of  ${}^{6}\text{Li}_2$ . The phase shift converges to 31.42 as  $k \to 0$ .

phase Eq. (2.57) is integrated from the atomic radius of potassium  $4.59a_o$  to the cut-off radius of  $7000a_o$ . We find that in the case of potassium the accumulation of round-off errors reduces the cut-off radius as compared to lithium. But, as the phase shift  $\eta_1(k)$  stabilizes up to an accuracy of  $\approx 10^{-15}$  even before reaching the radial distance of  $7000a_o$ , we consider it as the cut-off radius. There is no added advantage of increasing the cut-off radius further as it will only lead to an increase of round-off errors without any significant contribution to the phase shift. The value of the scattering length thus obtained is  $-95a_o$ .

### 2.3 Summary of results

We have shown that  $T_c$  in the case of the 3D quartic potential trap is higher than that of the isotropic harmonic potential trap. This is due to the form of the density of states  $g(\epsilon)$ , which varies as  $\epsilon^{5/4}$  and  $\epsilon^2$  in 3D isotropic quartic and quadratic trapping potentials respectively. This implies lower density of states in quartic oscillator potential compared to isotropic harmonic oscillator potential and hence higher  $T_c$ . We have also analyzed the effect of the cross terms in the quartic potential. The cross terms tend to decrease the density of



Figure 2.7: The least square fitted line (solid black curve) on  $a_1^3(k)k$  values in the domain  $0.0023 \le k \le 0.005$  (red crosses). An additional point coinciding with the origin is also considered while drawing the least square fitted curve. The slope of this line is  $\approx -46050$ .

states and raise  $T_c$ . These terms increase  $T_c$  by factor of 1.2 and 1.1 in the 3D and 2D quartic trap potentials respectively, as compared to the case without the cross terms. Experimentally in optical traps, the potentials without the cross terms are more appropriate. We have found that the effect of finite particle number is more pronounced in the 3D quartic potential when the number of particles is  $< 10^5$ . The situation is reversed when the number of particles is  $\gtrsim 10^5$ . The cause of the reversal lies in the form of the fractional change  $\Delta T_c/T_c$  for the two potentials. The ratio of the fractional change between 3D isotropic quartic potential to harmonic potential is  $3.51/N^{1/9}$ . It is  $\approx 1$  for  $N \approx 10^5$ , > 1 for  $N < 10^5$  and < 1 for  $N \gtrsim 10^5$ . Thus, when  $N < 10^5$ the constant factor is dominant in Eq. (2.20) and is responsible for the larger value of  $\Delta T_c/T_c$  in quartic potential. But when  $N \gtrsim 10^5$ ,  $N^{-4/9}$  dominates and  $\Delta T_c/T_c$  of the quartic potential is lower than that of the harmonic potential. We have used WKB approximation to obtain an analytic expression for the p-wave scattering length of alkali metal atoms. We have found that p-wave scattering lengths can be determined from the value of the total phase change between two classical turning points. We have also used the variable phase

method to determine *p*-wave scattering lengths for fermionic isotopes. Based on our calculations using the variable phase method, we have estimated the *p*-wave scattering lengths of <sup>6</sup>Li and <sup>40</sup>K equal to  $-36a_0$  and  $-95a_0$  respectively.

## Chapter 3

## Ground state geometry of quantum degenerate Bose-Bose mixture

Depending upon the properties of the component species and trapping potential parameters, the ground state of two species Bose-Einstein condensate (TBEC) assumes a configuration which minimizes the total energy. This configuration or ground state geometry can either be miscible or immiscible (phase-separated). In the phase-separated regime, the interface energy of the two component species defines the geometry of the ground state. In earlier works, the ground state geometry of TBEC was examined within the TF [107, 108, 109], i.e. without the interface energy. In later works, the contribution from the interface energy was incorporated [110, 111, 112]. From these it is observed that the analytic approximations for interface energy are not sufficient enough to explain the experimental results of strongly segregated ground states [33]. A recent work [113] reported a more accurate determination of the interface energy. It explains the stationary state geometries of the strongly segregated two species Bose-Einstein condensates (TBECs) more precisely. The common salient feature of all these works is the use of TF approximation, which is a good approximation for large number of atoms of each species. In fact if N, a and  $a_{osc}$  are number of atoms of the component species, s-wave scattering length and oscillator length respectively, TF approximation is valid provided  $Na/a_{\rm osc} \gg 1$ . Obviously, this condition is not satisfied for attractive condensates. For small number of atoms as well, say of the order of a few hundreds, and for very weakly interacting condensates  $(Na/a_{\rm osc} \sim 1)$ , the contribution of the kinetic energy to the total energy is significant and can

not be merely treated as a correction to total energy as is done in TF based approaches. For such TBECs, TF approximation is not a good approximation, and hence can not be relied upon to determine their ground state structure.

With the advent of Feshbach resonances [114], it is experimentally possible to tune scattering lengths to reach the very weakly interacting regime or even non-interacting regime [10, 115, 116]. Magnetic Feshbach resonances can tune only one scattering length independently, whereas optical Feshbach resonances [117] open up the possibility of tuning different scattering lengths in a multicomponent system independently. With the experimental observation of optical Feshbach resonances in  $^{172}$ Yb[118] and  $^{174}$ Yb [119], experimental realization of weakly interacting regime in binary condensates appears a distinct possibility.

In this chapter, we give the details of two semi-analytic methods, namely TF approximation and variational minimization, to determine the ground state geometry of the binary condensate. The domains of validity of the two methods,  $Na/a_{\rm osc} \gg 1$  for TF approximation and  $Na/a_{\rm osc} \sim 1$  for variational minimization, makes them supplementary to each other. The chapter is organized as follows: In Sec. 3.1, we describe our semi-analytic scheme based on TF approximation to determine the ground state properties of the TBEC, trapped by axisymmetric trapping potentials, in phase-separated domain. In Sec. 3.2, we employ the variational minimization to study the ground state of the binary condensate both in miscible and phase-separated domains.

# 3.1 Ground state geometry of TBEC - TF approximation

We consider TBEC in axisymmetric trapping potentials

$$V_i(\mathbf{r}) = V_i(r, z) = \frac{m_i \omega^2}{2} (\alpha_i^2 r^2 + \lambda_i^2 z^2), \qquad (3.1)$$

where i = 1, 2 is the species index, and  $\alpha_i$  and  $\lambda_i$  are the anisotropy parameters. In the mean field approximation, the stationary state solution of the TBEC is described by a set of coupled Gross-Pitaevskii (GP) equations (1.15).

When the number of atoms are large, the TF approximation is applicable to obtain the stationary state solutions of Eq. (1.15). In this limit, the kinetic energy is neglected in comparison to interaction energy. We consider the interaction parameter  $U_{12} > \sqrt{U_{11}U_{22}}$  such that the two components are

phase-separated, the two components occupy different regions of the trapping potentials. Neglecting the overlap between the species, stationary state solutions within TF approximation are

$$|\Psi_i(r,z)|^2 = \frac{\mu_i - V_i(r,z)}{U_{ii}},$$
(3.2)

where  $\mu_i$  is fixed by the number of atoms of the corresponding species.

The total energy of the TBEC in the phase-separated regime is

$$E = \int dV \left[ V_1(r,z) |\Psi_1(r,z)|^2 + V_2(r,z) |\Psi_2(r,z)|^2 + \frac{1}{2} U_{11} |\Psi_1(r,z)|^4 + \frac{1}{2} U_{22} |\Psi_2(r,z)|^4 \right].$$
(3.3)

Depending upon the anisotropy parameters, the TBEC can have three distinct spatial distributions in axisymmetric traps. The distinguishing feature of these structures is the geometry of the interface, which can be planar, cylindrical or ellipsoidal. The smooth transition of interface geometry, for the TBEC of <sup>85</sup>Rb-<sup>87</sup>Rb mixture, from planar to ellipsoidal and finally to cylindrical is shown in Fig. 3.1. These features are most prominent when the TBEC is strongly segregated. For the detailed examination of our scheme, we choose <sup>85</sup>Rb-<sup>87</sup>Rb experiments of Papp et al. [33], where two of the geometries planar and ellipsoidal were observed.

### 3.1.1 Planar interface

It has been observed experimentally [33] in cigar shaped traps ( $\lambda_i \ll \alpha_i$ ) that the TBEC assumes a sandwich structure with planar interface between the two species. In this structure the phase separation occurs along the axial direction, and the strongly interacting component sandwiches the weakly interacting one. There are two realizations of this: coincident and shifted trapping potentials.

Coincident trap centers: An idealized choice of  $V_i$  is with coincident centers. If  $z = \pm L_1$  are the locations of the planes separating the two components, and  $L_2$  is the axial extent of the binary condensate, then the problem of determining the structure of the TBEC is equivalent to calculating  $L_1$ . If  $N_i$  and  $R_i$  are the number of atoms and radial size of the *i*th species respectively, then

$$N_i = 2\pi \int_0^{R_i} r dr \int_{-L_i}^{L_i} dz |\Psi_i(r, z)|^2.$$
(3.4)



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Figure 3.1: The false color coded images of  $|\Psi_i(r, z)|$ , for TBEC consisting of <sup>85</sup>Rb (inner component) and <sup>87</sup>Rb (outer component), on r-z plane with vertical and the horizontal directions corresponding to radial and axial coordinate respectively. The wave functions are obtained by numerically solving Eq. (1.15) using  $a_{\text{osc}}$ ,  $a_{ii}$  and  $a_{12}$  taken from Ref. [33], referred to as set a in the text. The images correspond to different values of  $\lambda_i$  but same  $N_i = 50,000$ . (a-e) the values of ( $\lambda_1, \lambda_2$ ) are (0.020, 0.022), (0.50, 0.50) and (0.85,0.85), (1.0, 1.0), (1.5, 1.5) and (50.0, 50.0). As is evident the interface geometry changes continuously from planer to ellipsoidal to cylindrical.

From Eq. (3.2), we get

$$N_{1} = 2\pi \left( \frac{\omega^{2} L_{1}^{5} m_{1} \lambda_{1}^{4}}{20 U_{11} \alpha_{1}^{2}} - \frac{L_{1}^{3} \lambda_{1}^{2} \mu_{1}}{3 U_{11} \alpha_{1}^{2}} + \frac{L_{1} \mu_{1}^{2}}{\omega^{2} m_{1} U_{11} \alpha_{1}^{2}} \right),$$

$$N_{2} = 4\pi \left[ \frac{4\sqrt{2} \mu_{2}^{2} \sqrt{\frac{\mu_{2}}{\omega^{2} \lambda_{2}^{2} m_{2}}}}{15 \omega^{2} m_{2} U_{22} \alpha_{2}^{2}} + \frac{L_{1}}{120 U_{22} \alpha_{2}^{2}} \left( 5 \omega^{2} L_{1}^{4} m_{2} \lambda_{2}^{4} - \frac{8 \omega^{2} m_{2} \left( L_{1}^{2} \lambda_{2}^{2} \right)^{5/2}}{\lambda_{2} L_{1}} + 20 L_{1}^{2} \lambda_{2}^{2} \mu_{2} - \frac{60 \mu_{2}^{2}}{\omega^{2} m_{2}} \right) \right].$$

$$(3.5)$$

Similarly, the total energy in Eq. (3.3) is

$$E = \frac{4\pi}{1680\omega^2 m_2 U_{22}\alpha_2^2} \left( -21\omega^6 L_1^7 m_2^3 \lambda_2^6 + 16\omega^6 L_1^7 m_2^3 \lambda_2^6 + 140\omega^2 L_1^3 m_2 \lambda_2^2 \mu_2^2 - 560L_1 \mu_2^3 + 320\sqrt{2}\mu_2^3 \sqrt{\frac{\mu_2}{\omega^2 \lambda_2^2 m_2}} \right) + 2\pi \left( \frac{\omega^4 L_1^7 m_1^2 \lambda_1^6}{168U_{11}\alpha_1^2} - \frac{L_1^3 \lambda_1^2 \mu_1^2}{6U_{11}\alpha_1^2} + \frac{2L_1 \mu_1^3}{3\omega^2 m_1 U_{11}\alpha_1^2} \right)$$

$$(3.6)$$

Here  $L_1$  is determined through the variational minimization of E with  $L_1$  as the variational parameter and constraints that  $\mu_1$  and  $\mu_2$  satisfy Eq. (3.5) for fixed  $N_i$ . In the constraint equations, we invert the expression of  $N_1$  and obtain  $\mu_1$  as a function of  $L_1$ . However, inverting  $N_2$  to calculate  $\mu_2$  is nontrivial, and hence we implement the minimization numerically.

As mentioned earlier, we consider the TBEC of <sup>85</sup>Rb-<sup>87</sup>Rb with  $N_i =$  50,000. The scattering lengths  $a_{11} = 51a_o$ ,  $a_{22} = 99a_o$  and  $a_{12} = 214a_o$  are from the experimental results of Wieman and collaborators [33]. Likewise, the anisotropy parameters and trap frequency are  $\alpha_i = 1$ ,  $\lambda_1 = 2.9/130$ ,  $\lambda_2 = 2.6/130$  and  $\omega = 130$ Hz respectively. From here on, this choice of parameters is referred as the set a in this chapter. For these parameters, the minima of E occurs at  $32.3a_{\rm osc}$ . Here the unit of length  $a_{\rm osc}$  referred to as the oscillator length is  $\sqrt{\hbar/m_1\omega}$ . To corroborate the results we solve Eq. (1.15) numerically and find the semi-analytic results are in good agreement with the value of  $33.8a_{\rm osc}$  obtained from the numerical solution. For this we employ the split step Crank-Nicholson method [120] implemented for binary condensates. Based on the numerical results, the profile of  $|\Psi|$  for <sup>85</sup>Rb and <sup>87</sup>Rb are shown in Fig. 3.1(a).

Separated trap centers: In the experimental realizations, the gravitational potential of Earth and tilts in the external field configurations tend to separate the minima of the effective potentials. Normally in the cigar shaped traps, the tilt angle is small and separation is effectively along the axial direction. The potentials with separation  $z_0$  are

$$V_1(r,z) = \frac{m_1\omega^2}{2}(\alpha_1^2 r^2 + \lambda_1^2 z^2),$$
  

$$V_2(r,z) = \frac{m_2\omega^2}{2} \left[\alpha_2^2 r^2 + \lambda_2^2 (z-z_0)^2\right].$$
(3.7)

Due to the loss of axial symmetry,  $z = -l_1$  and  $z = L_1$  are the two planes separating the two components. These,  $l_1$  and  $L_1$ , are the parameters to



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Figure 3.2: Surface and contour plot of the variation of E as function of  $l_1$  and  $L_1$ . The minima of E occurs at  $l_1 = 39.5a_{\rm osc}$  and  $L_1 = 26.0a_{\rm osc}$ . These are close to  $l_1 = 40.15a_{\rm osc}$  and  $L_1 = 27.95a_{\rm osc}$  obtained from the numerical solution of coupled GP equations.

minimize E. Like in the previous case with coincident trap centers,  $N_1$ ,  $N_2$ and E can be evaluated, and the expressions are presented in the appendix A. For the parameter set a and  $z_0 = 3.4\mu$ m, the minima of E occurs when  $l_1$  and  $L_1$  are  $39.5a_{\rm osc}$  and  $26.0a_{\rm osc}$  respectively. The overall trend of E as a function of the the variation parameters is shown in Fig. 3.2. It is evident from the figure, for the chosen set of parameters, the energy minima is not strongly localized. In other words, around the energy minima there is variation of E as a function of  $l_1$  and  $L_1$ . Noticeable features of the iso-energy curves, contours in Fig. 3.2, are the ellipse shape and orientation. These indicate the trend of how the change in one parameter  $l_1$  ( $L_1$ ) is balanced with a change in the other parameter  $L_1$  ( $l_1$ ) to maintain constancy of energy. The variations along the iso-energy curves can perhaps occur as temporal variations when the TBEC is excited or ground state is perturbed.

### **3.1.2** Ellipsoidal interface

As the anisotropy parameter  $\lambda$  is increased beyond a critical value  $\lambda_a$ , the interface geometry changes from planer to ellipsoidal where one species envelopes the other. This is the preferred interface geometry for the phase-separated TBEC in axisymmetric traps without interface energy. Consider trapping

potentials with coincident centers. If  $R_i$  and  $L_i$  are equatorial (along radial direction) and polar (along axial direction) radii of the *i*th species respectively, then

$$N_i = 2\pi \int_0^{R_i} r dr \int_{-L_i}^{L_i} dz |\Psi_i(r, z)|^2.$$
(3.8)

From Eq. (3.2) and Eq. (3.3), we get

$$N_{1} = \frac{-2\pi R_{1}\alpha_{1}(3\omega^{2}m_{1}R_{1}^{4}\alpha_{1}^{2} - 10R_{1}^{2}\mu_{1})}{15U_{11}\lambda_{1}},$$

$$N_{2} = \frac{2\pi}{15U_{22}\lambda_{1}^{3}} \left( \omega^{2}m_{2}R_{1}^{5}\alpha_{1}(2\alpha_{2}^{2}\lambda_{1}^{2} + \alpha_{1}^{2}\lambda_{2}^{2}) - 10R_{1}^{3}\alpha_{1}\lambda_{1}^{2}\mu_{2} + \frac{8\sqrt{2}\lambda_{1}^{3}\mu_{2}^{5/2}}{\lambda_{2}\alpha_{2}^{2}\omega^{3}m_{2}^{3/2}} \right),$$

$$E = \frac{\pi}{210\omega^{2}m_{2}U_{11}U_{22}\alpha_{2}^{2}\lambda_{1}^{5}} \left( -15\omega^{6}m_{1}^{2}m_{2}R_{1}^{7}U_{22}\alpha_{1}^{5}\alpha_{2}^{2}\lambda_{1}^{4} + \omega^{6}m_{2}^{3}R_{1}^{7}U_{11} \right)$$

$$\times \alpha_{1}\alpha_{2}^{2}(8\alpha_{2}^{4}\lambda_{1}^{4} + 4\alpha_{1}^{2}\alpha_{2}^{2}\lambda_{1}^{2}\lambda_{2}^{2} + 3\alpha_{1}^{4}\lambda_{2}^{4}) + 160\sqrt{2}U_{11}\lambda_{1}^{5}\mu_{2}^{3}\sqrt{\frac{\mu_{2}}{\omega^{2}m_{2}\lambda_{2}^{2}}}$$

$$+140\omega^{2}m_{2}R_{1}^{3}\alpha_{1}\alpha_{2}^{2}\lambda_{1}^{4}(U_{22}\mu_{1}^{2} - U_{11}\mu_{2}^{2}) \right).$$
(3.9)

In TF approximation, the profile of density  $|\Psi_i(r,z)|^2$  has the same ellipticity

$$e = \begin{cases} \sqrt{\frac{\alpha_1^2 - \lambda_1^2}{\alpha_1^2}} & \text{if } \lambda < 1 \text{ (prolate)}, \\ \\ \sqrt{\frac{\lambda_1^2 - \alpha_1^2}{\lambda_1^2}} & \text{if } \lambda > 1 \text{ (oblate)}, \end{cases}$$
(3.10)

as that of the trapping potential which is a function of  $\lambda$ . This is evident from the expression of density with TF approximation given in Eq. (3.2), where only the trapping potential  $V_i(r, z)$  has spatial dependence. The value of  $R_2$  depends on  $\mu_2$  and reduces the variation parameter to only  $R_1$ . From the ellipticity of the trapping potential, the axial radius of the ellipsoidal interface  $L_i$  is  $\alpha_i R_i/\lambda_i$ . The energy E is then minimized numerically to find the equilibrium geometry of the phase-separated TBEC. To examine the scheme, we consider the <sup>85</sup>Rb-<sup>87</sup>Rb mixture with parameter set a and coincident trapping potentials, but take  $\lambda_i$  as 1.5. Then the equilibrium geometry is ellipsoidal with an equatorial radius  $R_1$  of  $3.72a_{\rm osc}$ . This is in very good agreement with value  $3.75a_{\rm osc}$ obtained from the numerical solution of GP equations. The pseudo color coded images of  $|\Psi_i|$ , numerically computed, with the ellipsoidal interface are shown in Fig. 3.1(b)-3.1(e). It is to be noted that in the images, the interface is prolate when  $\lambda < 1$  and oblate when  $\lambda > 1$ . These correspond to the topologies of the equipotential surfaces of the trapping potential. A highly symmetric case is when  $\lambda$  is unity, the interface geometry is then spherical in shape.

### 3.1.3 Cylindrical interface

On further increase of  $\lambda$  beyond another critical value  $\lambda_b$ , the equilibrium interface geometry is like a cylinder, where the axis of the interface coincides with the polar axis of the trapping potentials. This occurs when  $\lambda_i > \alpha_i$ , i.e. in the oblate condensates. Here the phase separation is along radial direction and is analogous to planar interface in cigar shaped condensates. The reasons for the emergence of the cylindrical geometry as the ground state geometry will become clear in the following subsection where we discuss the role of interface energy. If  $\rho$  is the radius of the interface cylinder, then in TF approximation

$$N_{1} = -\frac{4\pi(\omega^{2}\rho^{2}m_{1}\alpha_{1}^{2} - 2\mu_{1})^{2}\sqrt{-\rho^{2}\alpha_{1}^{2} + 2\mu_{1}/(\omega^{2}m_{1})}{15\omega^{2}m_{1}U_{11}\lambda_{1}\alpha_{1}^{2}} + \frac{16\pi\sqrt{2}\mu_{1}^{5/2}}{15U_{11}\lambda_{1}\alpha_{1}^{2}(m_{1}\omega^{2})^{3/2}},$$

$$N_{2} = \frac{4\pi(\omega^{2}\rho^{2}m_{2}\alpha_{2}^{2} - 2\mu_{2})^{2}\sqrt{-\rho^{2}\alpha_{2}^{2} + 2\mu_{2}/(\omega^{2}m_{2})}}{15\omega^{2}m_{2}U_{22}\lambda_{2}\alpha_{2}^{2}},$$

$$E = \frac{-4\pi}{15U_{11}} \left(\frac{-20\sqrt{2}\mu_{1}^{7/2}}{7\lambda_{1}\alpha_{1}^{2}(m_{1}\omega^{2})^{3/2}} + \frac{(\omega^{2}\rho^{2}m_{1}\alpha_{1}^{2} - 2\mu_{1})^{2}}{7\omega^{2}m_{1}\lambda_{1}\alpha_{1}^{2}} + (\omega^{2}\rho^{2}m_{1}\alpha_{1}^{2} + 2\mu_{1})(\sqrt{-\rho^{2}\alpha_{1}^{2} + \frac{2\mu_{1}}{\omega^{2}m_{1}}}\right) + \frac{\sqrt{-\rho^{2}\alpha_{2}^{2} + 2\mu_{2}/(\omega^{2}m_{2})}}{7U_{22}\lambda_{2}} \left(\frac{4\pi\omega^{4}\rho^{6}m_{2}^{2}\alpha_{2}^{4}}{15} + \frac{4\pi\omega^{2}\rho^{4}m_{2}\alpha_{2}^{2}\mu_{2}}{15} - \frac{64\pi\rho^{2}\mu_{2}^{2}}{15} + \frac{16\pi\mu_{2}^{3}}{3\omega^{2}m_{2}\alpha_{2}^{2}}\right).$$
(3.11)

The above set of equations define the stationary state of TBEC in the oblate shaped condensates. Like in the planar geometry,  $\rho$  is the parameter of variation. To verify the scheme, we consider pan cake shaped ( $\lambda_i \gg \alpha_i$ ) TBEC of <sup>85</sup>Rb-<sup>87</sup>Rb mixture in coincident traps with  $\lambda_i$  as 50.0 and the parameter set a. Then from our scheme, the equilibrium state has cylindrical interface of radius 5.84 $a_{\rm osc}$ . The value from numerical solution of GP equation is 5.80 $a_{\rm osc}$ . The two results are in very good agreement and validate our minimization scheme. The density plots showing the absolute value of wave functions of <sup>85</sup>Rb and <sup>87</sup>Rb, obtained by numerically solving Eq. (1.15), are shown in Fig. 3.1(f). Experimentally, the cylindrical geometry has not been observed in TBECs due to the fact that the  $\lambda_i$  of the trapping potentials were not sufficiently large enough.

### 3.1.4 Role of the interface energy

In the TF calculations discussed so far, as mentioned earlier, the interface energy is neglected. Accordingly, the variational schemes we have adopted incorporate appropriate interface geometries. In other words, the semi-analytic method described in Sec. 3.1.1-Sec. 3.1.3, assumes that one has *a priori* knowledge about the geometry of the interface, i.e. whether it is planar, ellipsoidal or cylindrical. In the absence of such a knowledge, one has to minimize the total energy for each of the three possible interface geometries. However, a such general minimization by considering all the possible interface geometries always favors the ellipsoidal interface as the equilibrium configuration because of its lower energy. For example, though the cylindrical interface for  $\lambda_i = 50.0$ reproduces the numerical results for TBEC of <sup>85</sup>Rb-<sup>87</sup>Rb with parameter *set a*, the minimization with ellipsoidal interface has lower *E*. This is evident from the values of *E*, calculated over a wide range of  $\lambda$  for the three interface geometries, shown in Fig. 3.3.

As discussed in Ref. [113], the planer interface observed in experiments [33] emerges as the equilibrium geometry when the interface energy is considered. When  $a_{\rm osc}$  is much larger than the interface thickness, the total excess energy arising from the finite interface tension [113] is

$$\Omega_A = \frac{\sqrt{2m_1}}{4\pi\hbar a_{11}} F(\xi_2/\xi_1, K) \int_A d\mathbf{r} \left[\mu_1 - V(\mathbf{r})\right]^{3/2}.$$
 (3.12)

Here  $\xi_i$ 's are the coherence lengths and K,  $\xi_2/\xi_1$  and  $F(\xi_2/\xi_1, K)$  are defined

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Figure 3.3: The upper (solid) and lower (dashed) set of three plots show the variation of E with and without the interface energy in TBEC of <sup>85</sup>Rb-<sup>87</sup>Rb with parameter set a, where E of planar (brown curve), ellipsoidal (black curve) and cylindrical (orange curve) geometries are examined as function of  $\lambda$ . The inset plots show the region around the cross over points.

as

$$K = \frac{(m_1 + m_2)a_{12}}{2\sqrt{m_1 m_2 a_{11} a_{22}}},$$
  

$$\frac{\xi_2}{\xi_1} = \left(\frac{m_1 a_{11}}{m_2 a_{22}}\right)^{1/4},$$
  

$$F(\xi_2/\xi_1, K) = \frac{\sqrt{2}}{3} \left(1 + \frac{\xi_2}{\xi_1}\right) - \frac{0.514\sqrt{\xi_2/\xi_1}}{K^{1/4}} - \sqrt{\frac{\xi_2}{\xi_1}} \left(\frac{\xi_2}{\xi_1} + \frac{\xi_1}{\xi_2}\right)$$
  

$$\left(\frac{0.055}{K^{3/4}} + \frac{0.067}{K^{5/4}}\right) + \dots,$$

where the integration is over the interface surface area A. The above expression is valid provided  $K \geq 1.5$  and  $\xi_2/\xi_1 \leq 1$ . In our calculations, we consider TBECs in the strongly segregated regime with  $\xi_2/\xi_1 < 1$ , and hence the interface energy in Eq. (3.12) is applicable. Furthermore, the interpene-

tration depth is proportional to  $\sqrt{\xi_2\xi_1}/K^{1/4}$  and approaches zero in the limit  $1/K \to 0$ . In this limit, there is no overlap, and TF solution is an excellent approximation. The equilibrium geometry is then the one which minimizes the total energy: sum of TF energy and  $\Omega_A$ .

A precise determination of  $\Omega_A$  is, therefore, essential to obtain correct geometry of the phase-separated TBEC. In relative comparison, we find the geometry which has the least interface area is also the one with the minimum interface energy. The interface area in planar and cylindrical geometries are

$$A = \begin{cases} 2\pi \frac{2\mu_1 - \lambda_1^2 L_1^2}{\alpha_1^2} & \lambda \ll 1 \text{ (planner)}, \\ 4\pi \rho \frac{\sqrt{2\mu_1 - \alpha_1^2 \rho^2}}{\lambda_1} & \lambda \gg 1 \text{ (cylindrical)}. \end{cases}$$
(3.13)

Similarly, for the prolate and oblate geometries the interface areas are

$$A = \begin{cases} 2\pi R_1^2 + 2\pi R_1^2 \frac{\alpha_1 \sin^{-1} e}{e\lambda_1} & \text{prolate,} \\ 2\pi R_1^2 + \frac{\pi}{e} \left(\frac{\alpha_1 R_1}{\lambda_1}\right)^2 \ln\left(\frac{1+e}{1-e}\right) & \text{oblate.} \end{cases}$$
(3.14)

Here the ellipticities e are as defined earlier in Eq. (3.10). The interface areas in the three geometries for TBEC of <sup>85</sup>Rb-<sup>87</sup>Rb with parameter set a, using our semi-analytic scheme developed in previous section, are shown in Fig. 3.4. The comparative study reveals that planar and ellipsoidal geometries have lower interface area than the cylindrical one for  $\lambda \ll 1$ , whereas the cylindrical and ellipsoidal geometries have lower interface areas for  $\lambda \gg 1$ . In these two domains, the interface area of one geometry is much lower than the other two, and hence interface area can decide the preferred ground state geometry. For  $\lambda$  close to one, the difference in the interface areas of the three geometries is small and surface tension is more crucial than interface area to determine the ground state geometry.

We examine the impact of  $\Omega_A$  in two domains: prolate shaped potentials  $(\lambda_i < 1)$  and oblate shaped potentials  $(\lambda_i > 1)$ . For higher symmetry and simplified analysis we choose  $\lambda_1 = \lambda_2 = \lambda$ .

Prolate trapping potentials: In the  $\lambda < 1$  domain, at low values of  $\lambda$ , the ellipsoidal geometry has higher ground state energy than the planar geometry. As  $\lambda$  is increased, keeping the other parameters fixed, the ground state energies



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Figure 3.4: Plots showing the interface areas as the functions of  $\lambda$ , in the TBEC of <sup>85</sup>Rb-<sup>87</sup>Rb mixture, for three geometries: planar (brown curve), ellipsoidal (black curve) and cylindrical (orange curve). The inset plot shows the interface energy.

of both the geometries increase; however, the planar geometry has higher rate of increase. At  $\lambda_a$ , which is close to one, the energies of the two geometries are equal. Beyond this critical value, the energy of the ellipsoidal geometry is lower and is the ground state geometry. This can be understood from the rate at which the interfaces areas of these two geometries change as  $\lambda$  is increased. With increase in  $\lambda$ , the interface area of planar geometry increases while that of ellipsoidal geometry decreases. Furthermore, the average rate of change in ellipsoidal geometry is higher than that of planar geometry, which is evident from Fig. 3.4. Hence the planar geometry is the ground state geometry due to the much smaller interface area and consequently lower interface energy correction for  $\lambda \ll 1$ . On the other hand, for  $1 > \lambda > \lambda_a$ , ellipsoidal geometry emerges as the ground state geometry due to the lower interface energy correction arising from a smaller interface area.

For the <sup>85</sup>Rb-<sup>87</sup>Rb mixture with the parameter set a, the total energy E, obtained by incorporating  $\Omega_A$  in the semi-analytic scheme developed in previ-

ous subsection, and interface energy  $\Omega_A$  as functions of  $\lambda$  for the two geometries are shown in Fig. 3.3 and Fig. 3.4 (inset plot) respectively. As the value of  $\lambda_a$ depends on the parameters of the system, we examine the variation in  $\lambda_a$  as a function of the ratio  $N_2/N_1$ . For this, we fix  $N_1$  and vary  $N_2$ , then calculate  $\lambda_a$  as a function  $N_2/N_1$ . When  $N_2$  is decreased  $\lambda_a$  increases initially and then decreases. This is shown in Fig. 3.5.



Figure 3.5: Ground state geometry as a function of  $\lambda_c$  ( $\lambda_a$  and  $\lambda_b$  for planarellipsoidal and ellipsoidal-cylindrical transition respectively) and ratio of population  $N_2/N_1$  in the TBEC of <sup>85</sup>Rb-<sup>87</sup>Rb mixture. Inset plots show the variation in energy of two lowest energy structures with  $\lambda$  for oblate trapping potentials with interface energy correction. Black and brown curves correspond to ellipsoidal and cylindrical geometries respectively, whereas orange curve represents E as a function of  $\lambda_b$ . Each pair of curves corresponds to different  $N_2$  but same  $N_1$ . The uppermost pair is for  $N_1 = N_2 = 50,000$ . The next lower pair of curves has  $N_2 = 46,000; 42,000$  and so on.

Oblate trapping potentials: In the  $\lambda > 1$  regime, the ellipsoidal or cylindrical interface geometry is the preferred ground state geometry. The planar interface has higher  $\Omega_A$  and is not favored. For  $\lambda$  close to 1, the ellipsoidal geometry has lower energy, but looses stability as  $\lambda$  is increased. This is due to the higher rate of increase in the  $\Omega_A$  for ellipsoidal geometry as is evident from inset plots in Fig. 3.4. At the critical value  $\lambda_b$  and higher, cylindrical geometry has lower

total energy and takes over as the ground state geometry. To illustrate the spatial configuration of the cylindrical interface geometry, we give the cutaway view of the TBEC in Fig. 3.1.4.



Figure 3.6: The false colour coded cutaway view of  $|\Psi_i(r, z)|$  for the cylindrical interface of the <sup>85</sup>Rb-<sup>87</sup>Rb TBEC. This is the volume rendering of the  $|\Psi_i(r, z)|$  in Fig. 3.1(f).

For the <sup>85</sup>Rb-<sup>87</sup>Rb mixture with the parameter set a, the total energy E and interface energy  $\Omega_A$  as functions of  $\lambda$  for the two geometries are shown in Fig. 3.3 and Fig. 3.4 (inset plot) respectively. For the same parameter set a, the value of  $\lambda_b$ , first decreases and then increases on decreasing  $N_2$ . This is shown in Fig. 3.5.

### 3.2 Ground state geometry of TBEC - Variational ansatz

For simplicity of analysis, we consider identical trap potentials for the component species, i.e.  $\alpha_1 = \alpha_2 = 1$ ,  $\lambda_1 = \lambda_2 = \lambda$ , and  $m_1 = m_2 = m$  in Eq. (3.1). The energy of the TBEC is

$$E = \int_{-\infty}^{\infty} \left[ \sum_{i=1}^{2} \left( \frac{\hbar^{2}}{2m} |\nabla \Psi_{i}|^{2} + V(r, z) \Psi_{i}^{2} + \frac{U_{ii}}{2} |\Psi_{i}|^{4} \right) + U_{12} |\Psi_{1}|^{2} |\Psi_{2}|^{2} \right] d\mathbf{r}.$$
(3.15)

To rewrite the energy in suitable units, define the oscillator length of the trapping potential

$$a_{\rm osc} = \sqrt{\frac{\hbar}{m\omega}},\tag{3.16}$$

and consider  $\hbar\omega$  as the unit of energy. We then divide the Eq. (3.15) by  $\hbar\omega$ and apply the transformations

$$\tilde{r} = \frac{r}{a_{\rm osc}}, \ \tilde{z} = \frac{z}{a_{\rm osc}}, \ \tilde{t} = t\omega \text{ and } \tilde{E} = \frac{E}{\hbar\omega}.$$
 (3.17)

The transformed order parameter

$$\phi_i(\tilde{r}, \tilde{z}) = \sqrt{\frac{a_{\rm osc}^3}{N_i}} \Psi_i(r, z), \qquad (3.18)$$

and energy of the TBEC in scaled units is

$$\tilde{E} = \int d\tilde{\mathbf{r}} \left\{ \sum_{i=1}^{2} N_{i} \left[ \frac{1}{2} |\nabla \phi_{i}|^{2} + V(\tilde{r}, \tilde{z}) |\phi_{i}|^{2} + N_{i} \frac{\tilde{U}_{ii}}{2} |\phi_{i}|^{4} \right] + N_{1} N_{2} \tilde{U}_{12} |\phi_{1}|^{2} |\phi_{2}|^{2} \right\},$$
(3.19)

where  $\tilde{U}_{ii} = 4\pi a_{ii}/a_{\text{osc}}$  and  $\tilde{U}_{12} = 4\pi a_{12}/a_{\text{osc}}$  in the scaled units. For simplicity of notations, from here on we represent the transformed quantities without

tilde in this chapter. We obtain the coupled 2D GP equations,

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial r^2} - \frac{1}{2r}\frac{\partial}{\partial r} + V(r,z) + \sum_{j=1}^2 G_{ij}|\phi_j|^2\right]\phi_i = \mu_i\phi_i, \qquad (3.20)$$

when the energy functional  $\mathcal{E} = E - \sum_{i} \mu_i N_i$  is variationally minimized with  $\phi_i^*$  as parameters of variation, here  $G_{ii} = N_i \tilde{U}_{ii}$  and  $G_{ij} = N_j \tilde{U}_{ij}$ . The equations are then solved numerically. Another approach ideal for semi-analytic treatment is to adopt a predefined form of  $\phi$  with few variational parameters and minimize E. This is outlined for the 2D and 1D in the next subsections.

### 3.2.1 Variational ansatz

As mentioned earlier, the ground state of TBEC can be either be miscible or immiscible (phase-separated) depending on the interaction parameters. An *ansatz* which describes the ground state of the TBEC well, both in the miscible and immiscible domain, when  $a_{ii}, a_{ij} > 0$  and  $a_{22} > a_{11}$  is

$$\Psi_1(r,z) = ae^{-(r^2 + \lambda^2 z^2)/(2b^2)},$$
  

$$\Psi_2(r,z) = \left[f + c(r^2 + \lambda^2 z^2)\right]e^{-(r^2 + \lambda^2 z^2)/(2d^2)},$$
(3.21)

with a, b, f, c and d as the variational parameters. In the phase-separated or immiscible domain, this ansatz is apt for the ellipsoidal interface geometry where the density distribution follows the equipotential surfaces of the trapping potentials. It is applicable, in particular, to weakly interacting TBECs, and this is precisely the underlying assumption for choosing the present ansatz. This ansatz is not suitable for analysis of planar and cylindrical geometries where density distributions do not follow equipotential surfaces. A similar ansatz, perhaps more general, is used in Ref. [121] to examine symbiotic gap and semi gap solitons in TBECs trapped in optical lattice potentials. The parameter c accounts for the flattening of the density profile of the second species as the intra-species non-linearity is increased. Moreover, for symmetric ground state geometries, c is a parameter related to the overlap of two component wave functions. For an ideal case when all the non-linearities are small and equal, c is  $\approx 0$ , and hence the two species of the TBEC completely overlap.

If  $N_1$  and  $N_2$  are the number of particles of the two species, then from

Eq. (3.18) in scaled units

$$\int_{-\infty}^{\infty} d\mathbf{r} |\phi_i(r, z)|^2 = 1.$$
(3.22)

Since the number of atoms of each species is fixed, the normalization conditions are equivalent to two constraint equations and reduce the number of variational parameters by two. After evaluating the integrals, the two constraint equations are

$$b = \frac{(-1)^{2/3} \lambda^{1/3}}{a^{2/3} \sqrt{\pi}},$$
  

$$c = \frac{2\sqrt{3}}{15d^7} \left( \frac{\sqrt{5d^7 \pi^{3/2} \lambda - 2d^{10} f^2 \pi^3}}{\pi^{3/2}} - \sqrt{3}d^5 f \right).$$
 (3.23)

From Eqs. (3.19-3.22), the energy of the first species is

$$E_1 = \frac{a^2 b N_1 \pi^{3/2}}{8\lambda} \left( \sqrt{2}a^2 b^2 G_{11} + 4 + 6b^4 + 2\lambda^2 \right), \qquad (3.24)$$

similarly, for the second species

$$E_{2} = \frac{dN_{2}\pi^{3/2}}{2048\lambda} \left\{ 128 \left[ 4f^{2} \left( 2 + 3d^{4} + \lambda^{2} \right) + 4cd^{2}f(2 + 15d^{4} + \lambda^{2}) + c^{2}d^{4}(22 + 105d^{4} + 11\lambda^{2}) \right] + \sqrt{2}d^{2}G_{22}(945c^{4}d^{8} + 1680c^{3}d^{6}f + 1440c^{2}d^{4}f^{2} + 768cd^{2}f^{3} + 256f^{4}) \right\}, \qquad (3.25)$$

and the energy from the inter-species interaction is

$$E_{12} = \frac{2N_1G_{12}b^2d^3\pi^{3/2}}{2048\lambda(b^2+d^2)^{7/2}} \left[15b^4c^2d^4 + 12b^2cd^2f(b^2+d^2) + 4f^2(b^2+d^2)^2\right].$$
(3.26)

We can then define the energy per boson as

$$\epsilon = \frac{E_1 + E_2 + E_{12}}{N_1 + N_2}.\tag{3.27}$$

This can now be minimized numerically to determine variational parameters and hence the ground state wave functions. The results of minimization with the parameters satisfying  $N_i a_{ij}/a_{osc} \sim 1$  are shown in Fig. 3.7 along with the corresponding numerical results.



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Figure 3.7: The semi-analytic and numerical profiles for a binary condensate with  $N_1 = N_2 = 10,000$ ,  $\lambda = 0.8$ ,  $a_{osc} = 9.566 \times 10^{-7} m$ ,  $a_{11} = 0.5a_0$ ,  $a_{22} = 1.0a_0$ , and  $a_{12} = 0.8a_0$ . Starting from left, the upper panel shows the semi-analytic profiles for the first and the second component, exactly below them in lower panel are wave function profiles obtained by numerically solving Eq. (3.20).

It should be noted that the scenario of all the non-linearities to be equal  $(N_1 = N_2 \text{ and } a_{ii} = a_{ij})$  is not equivalent to single component condensate with  $a_{ii} = a_{ij} = a_s$  as the s-wave scattering length and total number of atoms equal to  $N_1 + N_2$ . This is due to fact that we are still treating the two components as two different species having order parameters  $\phi_1(r, z)$  and  $\phi_2(r, z)$ . It means that experimentally, even if for two different hyperfine states of an isotope above condition is satisfied, the system will be still a binary system having a pair of ground state wave functions  $\phi_1(r, z)$  and  $\phi_2(r, z)$  instead of single ground state wave function for single component BEC. Quantum mechanically, it means that for the system to behave as a single species BEC, the two components needs to be indistinguishable with the same wave function  $\phi(r, z)$ .

### 3.2.2 Quasi-1D condensates

When the radial trapping frequency is much larger than axial trapping frequency ( $\lambda \ll 1$ ), and the TBEC is in the weakly interacting regime  $a_{ii}N_i|\psi(z)|^2 \ll$
1, the order parameter can be factorized into radial and axial parts [122]

$$\phi_i(r,z) = \xi_i(r)\psi_i(z), \qquad (3.28)$$

where  $\xi_i(r)$  is the normalized ground state of radial trapping potential  $V_i^{\text{rad}} = r^2/2$ . From Eq. (3.19), after integrating out the radial order parameter, the energy of the quasi-1D system is

$$E = \int_{-\infty}^{\infty} \left[ \sum_{i=1}^{2} N_i \left( \frac{1}{2} |\nabla_z \psi_i|^2 + V_i^a(z) |\psi_i|^2 + N_i \frac{u_{ii}}{2} |\psi_i|^4 \right) + N_1 N_2 u_{12} |\psi_1|^2 |\psi_2|^2 \right] dz, \qquad (3.29)$$

where  $u_{ii} = 2a_{ii}$ ,  $u_{12} = 2a_{12}$  and  $V_i^a(z) = \lambda^2 z^2/2 + 1$ . We analyze the ground state of the of repulsive TBEC,  $a_{ii}, a_{ij} > 0$ , trapped in quasi-1D traps in both miscible  $a_{12} \leq \sqrt{a_{11}a_{22}}$  and immiscible  $a_{12} > \sqrt{a_{11}a_{22}}$  domains. Without loss of generality we assume  $a_{22} > a_{11}$  and hence, the first species, on account of lower repulsive mean field energy, has larger density at the center when  $N_1 \approx N_2$ . We consider

$$\psi_1(z) = ae^{-(z-\gamma)^2/(2b^2)},$$
  

$$\psi_2(z) = (f+cz^2)e^{-(z+\delta)^2/(2d^2)},$$
(3.30)

as our *ansatz* for the two order parameters with  $a, \gamma, b, f, c, \delta$  and d as variational parameters. Here  $\gamma$  and  $\delta$  represent the location of the order parameter maxima and center of mass motion. This is an apt *ansatz* as it describes the smooth transition between miscible and immiscible phases of the TBEC in a very natural way.

In the miscible domain, the parameter c is a measure of flatness of the  $\psi_2$  profile which arises from the larger intra-species repulsion energy. However, in the immiscible domain, it is the degree of separation between the two species due to the higher inter-species repulsion energy. The order parameters satisfy the normalization conditions

$$\int_{-\infty}^{\infty} dz |\psi_i(z)|^2 = 1, \qquad (3.31)$$

where  $\psi_i(z) = \sqrt{a_{\rm osc}/N_i}\Psi(za_{\rm osc})$ , and hence the number of independent variational parameters is reduced to five. From Eq. (3.29), Eq. (3.30) and Eq. (3.31),

we obtain the expression for energy as a function of five independent parameters. It is a complicated eighth degree polynomial (given in appendix B) and can not be solved analytically. However, one can treat it as a nonlinear optimization problem and use numerical schemes like Nelder-Meade to find a solution [123]. Like in Eq. (3.20), the coupled 1D GP equations

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V_i^a(z) + \sum_{j=1}^2 g_{ij}|\psi_j|^2\right]\psi_i = \mu_i\psi_i, \qquad (3.32)$$

are obtained when  $\mathcal{E} = E - \mu_i N_i$  is variationally extremized with  $\psi_i^{\star}$  as the variational parameters, where  $g_{ii} = N_i u_{ii}$  and  $g_{ij} = N_j u_{ij}$ .

#### **3.2.2.1** Miscible domain with $a_{12} = 0$

As mentioned earlier, the inequality  $a_{12} < \sqrt{a_{11}a_{22}}$  defines the miscible domain. In this parameter range, the two order parameters overlap and in the limiting case of  $a_{12} = 0$ , the two maxima coincide if  $a_{11} = a_{22}$ . Furthermore, in the noninteracting limit  $a_{ij} \rightarrow 0$ , the profiles of the two order parameters are identical for the same number of atoms  $(N_1 = N_2)$ . For the special case of identical intraspecies scattering lengths  $(a_{11} = a_{22})$ , finite inter-species interaction  $(a_{12} \neq 0)$ and identical number of atoms  $(N_1 = N_2)$ , an appropriate *ansatz* is [124]

$$\psi_1(z) = A e^{-(z-B)^2/(2W^2)} e^{i(C+Dz+Ez^2)},$$
  

$$\psi_2(z) = A e^{-(z-B)^2/(2W^2)} e^{i(C-Dz+Ez^2)},$$
(3.33)

originally introduced to describe dynamics of coupled solitons in nonlinear optical fibers [125]. Here the parameters A, B, C, D, E and W are assumed to be time dependent and represent the amplitude, position, phase, wave number, chirp and width of the Gaussian *ansatz* respectively. In our *ansatz* too, a more symmetric choice of the order parameters

$$\psi_i(z) = (f_i + c_i z^2) e^{-(z - \gamma_i)^2 / (2b_i^2)}, \qquad (3.34)$$

can represent the special case mentioned here. The expression of the energy is then much more complicated, and the situation considered being too restrictive, we do not consider this for further analysis and discussion. However, to examine the ground state geometry for a varied range of parameters, interaction strengths and number of atoms, the *ansatz* in Eq. (3.30) is an ideal choice.

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With our ansatz, when  $a_{11} = a_{22} \neq 0$ ,  $a_{12} = 0$  and  $N_1 = N_2$ , the  $cz^2$  dependence in  $\psi_2$  accounts for the self interaction. For this reason, the profile of  $\psi_2$  is broader and more accurate, whereas  $\psi_1$  is a Gaussian and does not reflect the effect of the self interaction in the profile in an equally precise manner as  $\psi_2$ . To examine the density profiles as function of the nonlinearity, arising from the mean field interaction, consider TBEC with  $N_i = 100, 1000$  and 100000. As a specific case take  $a_{11} = a_{22} = 51$ , which corresponds to  $^{85}$ Rb [126], however, to begin with set  $a_{12} = 0$ . The later is experimentally not realizable in  $^{85}$ Rb, but it is a good reference for a comparative study on the role of inter-species interactions. The order parameters for the different  $N_i$  with the chosen parameters are as shown in Fig. 3.8. As mentioned earlier,



Figure 3.8: Order parameters  $\psi_i$  of the two components from the variational calculations with equal intra-species scattering length of  $51a_0$  but no interspecies interaction  $(a_{ij} = 0)$ . Solid (blue) and dashed (orange) curves correspond to the first and second species respectively. The figure on the left hand side is for  $N_1 = N_2 = 1000$ , while that on the right hand side is for  $N_1 = N_2 = 1000$ . The trapping potential parameters are  $\lambda = 0.02$  and  $a_{\rm osc} = 9.566 \times 10^{-7} m$ . For (a)  $N_i a_{ii}/a_{osc} = 2.821$  and for (b)  $N_i a_{ii}/a_{osc} = 282.137$ .

the  $\psi_2$  profiles are flatter and closer to the numerical values. Ideally, the two profiles should be identical as there is no inter-species interaction  $(a_{12} = 0)$ . So the difference between the profiles of the two order parameters is an indication of the error due to the Gaussian *ansatz* of  $\psi_1$ . From the figures, the deviation grows as  $N_i$  is increased, which is expected as the mean field contribution to Eis quadratic in N. In the weakly interacting domain c < 1 and contributions to E from higher order terms of c are negligible. Retaining only the linear

terms, the energy correction arising from the mean field is

$$\Delta E \approx \frac{cf N_2 \sqrt{\pi}}{4} \left[ \frac{2\delta^2 - d^2}{d} + d\lambda^2 (3d^4 + 12d^2\delta^2 + 4\delta^4) + \sqrt{2}df^2 g_{22} (d^2 + 4\delta^2) \right].$$
(3.35)

For identical trapping potentials  $V_1 = V_2$ , the order parameters  $\psi_i$  are centered at the origin (z = 0) and hence  $\delta \approx 0$ . The energy correction then simplifies to

$$\Delta E \approx \frac{cdf N_2 \sqrt{\pi}}{4} (3\lambda^2 d^4 + \sqrt{2}d^2 f^2 g_{22} - 1).$$
(3.36)

The three terms are the leading order corrections from the trapping potential, mean field and kinetic energy respectively. Considering that in quasi 1D case  $\lambda \ll 1$ , the correction arising from c is a competition between the mean field and kinetic energy contributions; at lower values of  $g_{22}$ , the kinetic energy correction dominates and  $\Delta E$  is negative. As mentioned earlier for identical intra-species scattering lengths ( $a_{11} = a_{22}$ ), Eq. (3.33) is more appropriate *ansatz* and for parameters of Fig. 3.8(b), the ground state geometry of the TBEC is shown in Fig. 3.9



Figure 3.9: Order parameters  $\psi_i$  of the two components from the variational calculations using Eq. (3.33) with equal intra-species scattering length of  $51a_0$  but no inter-species interaction  $(a_{ij} = 0)$ . Solid (turquoise) and dotted (black) correspond to the first and second species respectively. The number of atoms and trapping potential parameters are same as those in Fig. 3.8(b).

## **3.2.2.2** Miscible domain with $a_{12} > 0$

Finite inter-species interaction  $(a_{12} \neq 0)$  modifies the density profiles of the two species in a dramatic way. As  $a_{12}$  is increased, the species with the higher repulsion energy, second in the present case, is repelled from the center of trap. This is noticeable in the profiles of TBEC shown in Fig. 3.10. The lower density of the second species around the center of the trap decreases interspecies density product  $|\psi_1|^2|\psi_2|^2$  and minimizes the total energy. However, this must be in proportion with the higher energy from trapping potential due to broader density profile. For identical trapping potentials ( $V_1 = V_2$ ), the profiles of the two species are centered at the origin ( $\gamma = \delta = 0$ ) and symmetric. From Eq. (B.4) in appendix, the inter-species interaction energy is

$$E_{12}^{\text{sym}} = \frac{\sqrt{\pi a^2 b d N_1 g_{12}}}{4(b^2 + d^2)^{9/2}} \bigg[ 4d^8 f^2 + 4b^2 d^6 (4f^2 + cd^2 f) + b^8 (4f^2 + 4cd^2 f + 3c^2 d^4) + 2b^6 d^2 (8f^2 + 3c^2 d^4) + 6cd^2 f) + b^4 d^4 (24f^2 + 3c^2 d^4 + 12cd^2 f) \bigg].$$
(3.37)

Geometrically, with higher  $a_{12}$  the shape of  $\psi_2$  near potential minima undergoes a smooth transition from Gaussian to flat Figs. 3.10(a)-3.10(b) and then to parabola with a local minima at the center of the trap Figs. 3.10(c)-3.10(d). When  $\psi_2$  is flat around the center, to a very good approximation  $\psi'_2(z) = \psi''_2(z) = 0$  for z < 1. With our ansatz  $\psi''_2(0)$  is not zero when  $a_{12} > 0$ , so there are deviations from the actual solutions. Deviations are negligible when  $0 < a_{12} \ll 1$ , however, these grow and become quite prominent when  $\psi_2$  is constant around the center of the trap.

At the center of the trap  $\psi_1$  has the global maximum and  $\psi'_1(0) = 0$ . Close to the center the order parameter

$$\psi_1(z) \approx \psi_1(0) + \frac{z^2}{2} \psi_1''(0),$$
(3.38)

when z < 1. Gaussian ansatz of  $\psi_1$  defined in Eq. (3.30) then gives

$$\psi_1(z) \approx a - \frac{z^2}{2} \frac{a}{b^2}.$$
 (3.39)

For the parameter domain where  $\psi_2$  is constant, close to the center for z < 1,



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Figure 3.10: Ground state wave functions for the two components of the TBEC with  $N_1 = N_2 = 10000$ ,  $g_{11} = 0.553$ ,  $g_{22} = 2g_{11}$ ,  $\lambda = 0.02$  and  $a_{osc} = 9.566 \times 10^{-7}m$ . Starting from left, the values of  $g_{12}$  are  $0.1g_{22}, 0.3g_{22}$  in upper panel, and  $0.5g_{22}$  and  $0.7g_{22}$  in lower panel respectively. The criterion,  $N_j a_{ij}/a_{osc} = g_{ij}/2 \sim 1$ , for the applicability of the variational *ansatz* is satisfied for each case. Turquoise (reddish-brown) and dark-green (orange) curves correspond to first and second component respectively; the solid curves are semi-analytic results, while dashed ones are the numerical solutions of Eq. (3.32).

we can write

$$\psi_2(z) \approx \psi_2(0). \tag{3.40}$$

After substituting these expressions of  $\psi_i$  in Eq. (3.32), the chemical potential of the two species obtained from the zeroth order equations are

$$\mu_1 = \frac{1}{2b^2} + g_{11}a^2 + g_{12}\psi_2(0) + 1,$$
  

$$\mu_2 = g_{22}\psi_2^2(0) + g_{21}a^2 + 1.$$
(3.41)

Since  $\psi'_i(0) = 0$ , the first order terms are zero, and hence second order equation

of  $\psi_1$  is

$$\left[\frac{\lambda^2}{2} + \frac{3g_{11}}{2}\psi_1(0)\psi_1''(0)\right]\psi_1(0) + \frac{g_{12}}{2}\psi_2(0)\psi_1''(0) = \frac{\mu_1}{2}\psi_1''(0).$$
(3.42)

Further simplifications provide the condition

$$g_{11} = \frac{1}{2a^2} \left( \frac{1}{2b^2} + \lambda^2 b^2 + 1 \right)$$
(3.43)

on the intra-species interaction of the first species. Similarly, the second order equation of  $\psi_2$  is

$$\left[\frac{\lambda^2}{2} + g_{21}\psi_1(0)\psi_1''(0)\right]\psi_2(0) = 0.$$
(3.44)

This defines the inter-species interaction as

$$g_{21} = \frac{\lambda^2 b^2}{2a^2},\tag{3.45}$$

to obtain a constant profile of  $\psi_2$  around center of the trap. In other words when this condition holds true, the repulsive inter-species interaction balances the effect of confining potential. And the net outcome is an effective potential around the center which is constant. The  $\psi_2$  profile acquires a local minimum at the center when  $g_{21} > \lambda^2 b^2/(2a^2)$ , our *ansatz* is then the appropriate form of  $\psi_2$ .

#### 3.2.2.3 Immiscible domain: symmetric profile

Phase separation occurs when the TBEC is immiscible. The density profiles of the two species are then spatially separated. Condition for immiscibility is  $a_{12} > \sqrt{a_{11}a_{22}}$  when the TBEC is confined within a square well potential [111]. In which case, the trapping potential is flat and except for the surface effects, limited to within healing length  $\xi = \sqrt{\hbar^2/(2m\mu)}$  from the boundary, there are no trapping potential induced density variations. The TBEC is then homogeneous in the miscible domain and phase-separated in the immiscible domain, where the interface acquires a geometry which minimizes the surface energy. Here the density distributions in the bulk is entirely dependent on the strength of interactions and transition into phase-separated domain is well defined.

With harmonic trapping potentials the densities, to begin with, are not homogeneous in the miscible phase. Even when  $a_{12} < \sqrt{a_{11}a_{22}}$ , miscible do-

main discussed previously, there is a separation between the two maxima of the densities. When  $N_1 \approx N_2$  and  $a_{11} \approx a_{22}$ , the density profiles are symmetric about the center ( $\delta = \gamma = 0$ ) and total energy of the TBEC is

$$E = \frac{\sqrt{\pi}}{4} \left[ \frac{a^2 N_1}{b} + a^2 b^3 \lambda^2 N_1 + \frac{N_2}{4d} (4f^2 - 4cd^2 f + 7c^2 d^4) + \frac{d\lambda^2 N_2}{4} \times (4d^2 f^2 + 12cd^4 f + 15c^2 d^6) + \sqrt{2}a^4 b N_1 g_{11} + \sqrt{2}dN_2 g_{22} \times \left( f^4 + cd^2 f^3 + \frac{9}{8}c^2 d^4 f^2 + \frac{15}{16}c^3 d^6 f + \frac{105}{256}c^4 d^8 \right) \right] + E_{12}^{\text{sym}}, \quad (3.46)$$

where  $E_{12}^{\text{sym}}$  is the inter-species interaction energy defined in Eq. (3.37). For the TBEC in square well described earlier, the criterion for phase separation [111] is the emergence of a dip in the total density  $\rho_1(z) + \rho_2(z) = |\psi_1(z)|^2 + |\psi_2(z)|^2$  at the interface. Such a criterion does not apply for TBEC in harmonic potentials. Instead we define phase separation as the state when the maxima of the densities are well separated. To quantify, define  $z_e$  as the point where the densities of the two species are equal, which implies

$$ae^{-z_{\rm e}^2/(2b^2)} = (f + cz_{\rm e}^2)e^{-z_{\rm e}^2/(2d^2)}.$$
 (3.47)

For large  $a_{12}$ , the order parameter  $\psi_2(z)$  is bimodal. The two maxima are solutions of  $\psi'_2(z) = 0$  and located at

$$z_{\rm m} = \pm \left(\frac{4cd^2 - f}{c}\right)^{1/2}.$$
 (3.48)

The maxima of  $\psi_2$  are well separated from  $\psi_1$  when  $z_{\rm m} > z_{\rm e}$ . We define this as the criterion for phase separation of TBEC in harmonic potentials. This definition of phase separation is an appropriate one in very weakly interacting TBECs  $Na/a_{osc} \approx 1$ , but not so in TF regime  $Na/a_{osc} \gg 1$ , where f = 0 is a better criterion to define phase separation.

#### 3.2.2.4 Imiscible domain: non-symmetric profile

In immiscible domain, if one or both the intra-species non-linearities  $g_{ii}$  are sufficiently small, the stationary state geometry with symmetric  $\psi_i$  can have higher energy than the asymmetric stationary state with the two components lying side by side. There are two reasons for the emergence of asymmetric ground state geometries. First, this geometry has only one interface region, whereas the corresponding symmetric profile has two; as a result the interface



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Figure 3.11: Ground state wave functions for the two components of the TBEC with  $N_1 = N_2 = 10000$ ,  $g_{11} = 0.553$ ,  $g_{22} = 2g_{11}$ ,  $\lambda = 0.02$  and  $a_{osc} = 9.566 \times 10^{-7}m$ . Starting from left, the values of  $g_{12}$  are  $0.9g_{22}$ ,  $1.2g_{22}$  in upper panel, and  $1.4g_{22}$  and  $1.6g_{22}$  in lower panel respectively. The criterion,  $N_j a_{ij}/a_{osc} = g_{ij}/2 \sim 1$ , for the applicability of the variational *ansatz* is satisfied for each case. Turquoise (reddish-brown) and dark-green (orange) curves correspond to first and second component respectively; the solid curves are semi-analytic results, while dashed ones are the numerical solutions of Eq. (3.32).

energy is lower. Second, the smaller kinetic energy as  $\psi'_i(z)$  is prominent at the interface and edges of the condensates.

With our *ansatz*, for the asymmetric profile  $c \sim 0$ , but  $\delta$  and  $\gamma$  are nonzero. The total energy of the TBEC is then

$$E = \frac{\sqrt{\pi}}{4} \left[ \frac{a^2 N_1}{b} + \frac{f^2 N_2}{d} + a^2 b \lambda^2 N_1 (b^2 + 2\gamma^2) + df^2 \lambda^2 N_2 (d^2 + 2\delta^2) \right. \\ \left. + \sqrt{2} a^4 b N_1 g_{11} + \sqrt{2} df^4 N_2 g_{22} + \frac{4a^2 b d e^{-(\gamma + \delta)^2 / (b^2 + d^2)}}{(b^2 + d^2)^{9/2}} \right. \\ \left. \times (d^8 f^2 + 4b^2 d^6 f^2 + b^8 f^2 + 4b^6 d^2 f^2 + 6b^4 d^4 f^2) N_1 g_{12} \right].$$
(3.49)

It must be emphasized that, with our present *ansatz* the asymmetric density

profiles emerges very naturally as a function of  $a_{12}$ . That is not the case with TF based semi-analytic methods which can not account for the existence of asymmetric ground state geometries [127].

Typical ground state geometries of the TBECs obtained by this variational scheme are shown in Fig. 3.11 along with the respective non-linearities and trapping potential parameters mentioned in the caption of each figure. We observe that the present variational scheme also explains the existence of the asymmetric states, as is shown in Fig. 3.11, as the ground state geometry.

## **3.2.3** Gram-Charlier expansion of $|\psi_i|^2$

As mentioned earlier, for the ideal case when all the non-linearities are small and equal, c is  $\approx 0$ . In this limit, both the species have Gaussian distribution. In order to quantify the departure, brought about by interactions among the bosons, of the density distributions from the normalized Gaussian, we resort to an analysis based on Gram-Charlier series A. It is the expansion of a probability density function [128] in terms of the normal distribution. It can be used to analyze the departure from the normal distribution. If F(z) is a nearly normal distribution with cumulants  $\kappa_r$ , then F(z) can be expressed as a series consisting of product of Hermite polynomials  $H_i(z)$  and  $\kappa_r$ . The truncated expression for Gram-Charlier A series up to fourth cumulant is

$$F(\bar{z}) = \frac{e^{-\bar{z}^2/2}}{\sqrt{2\pi\sigma^2}} \left[ 1 + \frac{\kappa_3}{3!\sigma^3} H_3(\bar{z}) + \frac{\kappa_4}{4!\sigma^4} H_4(\bar{z}) \right],$$
  
$$= \frac{e^{-\frac{\bar{z}^2}{2}}}{24\sigma^5\sqrt{2\pi}} \left[ 24\sigma^4 + 4\sigma\bar{z} \left( \bar{z}^2 - 3 \right) \kappa_3 + \left( \bar{z}^4 - 6\bar{z}^2 + 3 \right) \kappa_4 \right], (3.50)$$

where  $\bar{z} = (z - \langle z \rangle)/\sigma$  with  $\langle z \rangle$  and  $\sigma$  as the mean and standard deviation of normal distribution. The departure of a distribution from normal are measured in terms of skewness ( $\gamma_1$ ) and kurtosis ( $\gamma_2$ ). These quantify the asymmetry and peakedness of the distribution function and are defined as

$$\gamma_1 = \frac{\kappa_3}{\kappa_2^{3/2}}, \quad \gamma_2 = \frac{\kappa_4}{\kappa_2^2},$$
 (3.51)

where second cumulant  $\kappa_2$  is equal to the variance  $\sigma^2$ . The  $\langle z \rangle$  and  $\sigma^2$  of the normal distribution are calculated from the numerically calculated  $\psi_i(z)$  using

the definitions

$$\begin{aligned} \langle z \rangle &= \int z |\psi(z)|^2 dz, \\ \sigma^2 &= \int (z - \langle z \rangle)^2 |\psi(z)|^2 dz. \end{aligned}$$

For example, Fig. 3.12 shows the results of Gram-Charlier analysis of density



Figure 3.12: The solid (orange) curve is the approximate  $|\psi_2|^2$  of the TBEC with  $N_1 = N_2 = 10,000$ ,  $a_{\rm osc} = 9.566 \times 10^{-7}$ ,  $g_{11} = 0.553$  and  $g_{22} = 2g_{11}$ , obtained by fitting Gram-Charlier A series over numerically obtained density profile [dashed (dark-green) curve]. In (a)  $g_{12} = 0.6g_{22}$ , while in (b)  $g_{12} = 1.2g_{22}$ . The dash-dotted (reddish-brown) shows the density profile of normal distribution with respect to which  $\gamma_1$  and  $\gamma_2$  of numerical density profile have been calculated. For first figure, the variational parameters f, c,  $\delta$ and d are 0.177, 0.001, 0, 8.675 respectively, while Gram-Charlier values are 0.185, 0, 0, 13.2836 respectively. For second figure, semi-analytic values of f, c,  $\delta$ , and d are 0.267, 0, 8.529, 9.567 respectively, while Gram-Charlier values are 0.270, 0, 7.358, 8.662 respectively.

profile for the second component of the TBEC in miscible and immiscible domains. As is evident from the figure, in the miscible domain, density profile (solid-orange curve) is symmetric and relatively flatter (platykurtic) compared to normal distribution (dot-dashed reddish-brown curve) about origin, and consequently it has zero skewness and negative kurtosis; whereas in second figure, the density distribution has a longer right tail (quantified by positive skewness) and narrow distribution about the mean (leptokurtic) as compared to normal distribution. From Gram-Charlier analysis, we can extract the coefficient of  $z^4$  (excluding exponential part) and compare it with semi-analytic values of  $c^2$ . For both the cases in Fig. 3.12, the two values are same up to second decimal place.

## **3.2.4** TBECs in optical lattices

In this subsection, we analyze the ground state geometry of TBEC in optical lattices with the *ansatz* we have introduced. For this, we consider the optical lattice potential, generated by a pair of orthogonally polarized counter propagating laser beams along axial direction, in presence of the axisymmetric harmonic trapping potential. The period of the lattice potential is half of the laser wavelength. The net external potential experienced by TBEC (in scaled units) is the sum total of the two potentials,

$$V(r,z) = \frac{1}{2}(r^2 + \lambda^2 z^2) + V_0 \cos^2\left(\frac{2\pi z}{\lambda_{\text{las}}}\right),$$
(3.52)

where  $V_0 = sE_r$  is the depth of potential well at each lattice site and  $\lambda_{\text{las}}$  is the wavelength of the laser. Here  $E_r = (2\pi/\lambda_{\text{las}})^2/2$  is the recoil energy of laser light photon and s is the lattice depth scaling parameter. As in the previous section, in weakly interacting regime, the TBEC in cigar shaped traps is like a quasi-1D system and its energy is given by Eq. (3.29). The axial trapping potential is

$$V^{a}(z) = \frac{\lambda^{2} z^{2}}{2} + V_{0} \cos^{2}\left(\frac{2\pi z}{\lambda_{\text{las}}}\right)$$
(3.53)

In tight binding approximation [129]

$$\psi_i(z) = \sqrt{N_i} \sum_n \zeta_i(n) \phi_n(z), \qquad (3.54)$$

where n is index of lattice sites,  $\phi_n(z) = \phi(z - n\lambda_{\text{las}}/2 - \lambda_{\text{las}}/4)$  is the wave function with amplitude  $\zeta(n)$  localized at nth lattice site. Using the tight binding *ansatz*, energy functional of a TBEC in optical lattice is

$$E = \sum_{n} \left\{ \sum_{i=1}^{2} \left[ -2KN_{i}\zeta_{i}(n)\zeta_{i}(n+1) + \epsilon(n)N_{i}|\zeta_{i}(n)|^{2} + \frac{\Lambda_{ii}}{2}N_{i}|\zeta_{i}(n)|^{4} \right] + \Lambda_{12}N_{1}|\zeta_{1}(n)|^{2}|\zeta_{2}(n)|^{2} \right\},$$
(3.55)

where  $\Lambda_{ii}$ ,  $\Lambda_{12}$ , K and  $\epsilon(n)$  are defined as

$$\Lambda_{ii} = 2a_{ii}N_i \int \phi_n^4 dz,$$

$$\Lambda_{12} = 2a_{12}N_2 \int \phi_n^4 dz,$$

$$K = -\int \left[\frac{1}{2}\nabla_z \phi_n \cdot \nabla_z \phi_{n+1} + \phi_n V_i^a(z)\phi_{n+1}\right] dz,$$

$$\epsilon(n) = \int \left[\frac{1}{2}(\nabla_z \phi_n)^2 + V^a(z)\phi_n^2\right] dz.$$
(3.56)

To examine the stationary state of the system we consider  $\zeta_i(n)$  is real while deriving above relation.

### 3.2.4.1 Ground state

In the weakly interacting regime, the localized wave function  $\phi_n$  can be taken as ground state wave function of the lattice site,

$$\phi_n(z) = \frac{1}{\pi^{1/4} \sqrt{\sigma}} e^{-(z - n\lambda_{\text{las}}/2 - \lambda_{\text{las}}/4)/(2\sigma^2)},$$
(3.57)

where  $\sigma = \sqrt{\lambda_{\text{las}}}/(8\pi^2 V_0)^{1/4}$ . Ideally, the energy associated with each individual lattice sites can be minimized to evaluate  $\phi_n(z)$ . Neglecting the energy due to harmonic trapping potential and interaction energy in comparison to potential energy due to optical lattice potential, the energy of the *n*th lattice site is approximately

$$\int \left\{ \frac{1}{2} \left( \frac{d\phi_n}{dz} \right)^2 + V_0 \left( \frac{2\pi}{\lambda_{\text{las}}} \right)^2 \left[ x - \frac{\lambda_{\text{las}}}{4} (2n+1) \right]^2 \right\} dz, \qquad (3.58)$$

where we have used  $V_0 \cos^2(2\pi z/\lambda_{\text{las}}) \approx V_0(2\pi/\lambda_{\text{las}})^2(z - n\lambda_{\text{las}}/2 - \lambda_{\text{las}}/4)^2$  as the potential at the *n*th lattice site. The expressions for  $\epsilon(n)$  and K are

$$\epsilon(n) = \frac{V_0}{2} \left( 1 - e^{-\frac{4\pi^2 \sigma^2}{\lambda_{\text{las}}^2}} \right) + \frac{1}{32\sigma^2} \left[ 8 + 8\lambda^2 \sigma^4 + \lambda^2 \sigma^2 \lambda_{\text{las}}^2 (1+2n)^2 \right],$$
  

$$K = -e^{-\frac{\lambda_{\text{las}}^2}{16\sigma^2}} \left\{ \frac{V_0}{2} \left( 1 + e^{-\frac{4\pi^2 \sigma^2}{\lambda_{\text{las}}^2}} \right) + \frac{1}{32\sigma^4} \left[ 4\sigma^4 \lambda_{\text{las}}^2 \lambda^2 + (1+n)^2 - \lambda_{\text{las}}^2 + 8(\sigma^2 + \lambda^2 \sigma^6) \right] \right\}.$$
(3.59)

Similarly, the energy per boson  $\overline{E} = E/(N_1 + N_2)$  can be calculated, however, as to be expected the expression is complicated and long. Following our *ansatz*, we consider

$$\begin{aligned} \zeta_1(n) &= a e^{-(n-\gamma)^2/(2b^2)}, \\ \zeta_2(n) &= (f+cn^2) e^{-(n+\delta)^2/(2d^2)}, \end{aligned} (3.60)$$

as the envelope profiles with five independent parameters. The length scale associated with the lattice potential, in scaled units, is  $a_{\text{latt}} = \sqrt{\omega/\omega_l}$ , where  $\omega_l$  is the laser frequency of the optical lattice. Considering that the frequency of the harmonic trapping potential  $\omega$  is at the most Khz and  $\omega_l$  is in the optical region  $a_{\text{latt}} \ll 1$ . Hence there are large number of lattice sites within the envelope profile. This implies that  $b \gg \sigma$  and  $d \gg \sigma$ , where  $\sigma$  is the width of the lattice ground state  $\phi_n$ . We can replace summation over lattice sites with integration over the same variable in Eq. (3.55). In fact, due to very weak trapping along axial direction, b and d are of the order of a few  $a_{\text{osc}}$  even for very weak non-linearities. It implies that  $e^{-\pi^2 b^2} \rightarrow 0$  and  $e^{-\pi^2 d^2} \rightarrow 0$ , and in this limit the error incurred in replacing summation by integration approaches zero. From Eq. (3.55), Eq. (3.56) and Eq. (3.60), we calculate the energy per particle which can be minimized to determine the variational parameters. The typical variational results for equal number of atoms of two species are shown in Fig. 3.17.

Symmetric and Non-symmetric Profiles: Similar to TBEC in harmonic trapping potentials, ground sate geometry of binary condensate in optical lattices can be symmetric or asymmetric. In miscible and weakly segregated domain (coherence length of the first component is smaller than the penetration depth of the second component [111]), the ground state geometries are symmetric. For example, a typical symmetric ground state geometry of TBEC in quasi-1D optical lattice is shown in Fig. 3.13.

In strongly segregated domain (coherence length of the first component is greater than the penetration depth of the second component), the ground state geometries can be asymmetric. A typical asymmetric ground state geometry of TBEC in quasi-1D optical lattice is shown in Fig. 3.14.

## 3.2.5 Profile narrowing with lattice depth

The density profiles of the two components in TBEC is more compact with deeper lattice potential. To analyze this, we consider an ideal Bose gas (non-





Figure 3.13: The stationary state solution of the TBEC with  $N_1 = N_2 = 10,000, g_{11} = 0.465, g_{22} = 2g_{11}, g_{12} = g_{21} = 0.8g_{22}, \lambda = 9/92, a_{\rm osc} = 1.137 \times 10^{-6}m, \tilde{\lambda}_{\rm las} = 0.7$  and s = 6.0 as the non-linearity and trapping potential parameters respectively. The criterion,  $N_j a_{ij}/a_{osc} = g_{ij}/2 \sim 1$ , for the applicability of the variational *ansatz* is clearly satisfied. The left and right figures are the profiles obtained by variational minimization and numerically solving quasi-1D GP equation respectively.



Figure 3.14: The stationary state solution of the TBEC with  $N_1 = N_2 = 5,000$ ,  $g_{11} = 0.233$ ,  $g_{22} = 2g_{11}$ ,  $g_{12} = g_{21} = 2g_{22}$ ,  $\lambda = 9/92$ ,  $a_{\rm osc} = 1.137 \times 10^{-6} m$ ,  $\tilde{\lambda}_{\rm las} = 0.7$  and s = 6.0 as the non-linearity and trapping potential parameters respectively. The criterion,  $N_j a_{ij}/a_{osc} = g_{ij}/2 \sim 1$ , for the applicability of the variational *ansatz* is clearly satisfied. The left and right figures are the profiles obtained by variational minimization and numerically solving quasi-1D GP equation respectively.

interacting) trapped in a triple 1D potential well superimposed with a weak

harmonic potential

$$V(x) = \begin{cases} \frac{1}{2}\lambda^2 x^2 + \frac{1}{2}\beta^2 (x+d)^2 & \text{if } -\frac{3d}{2} \leqslant x < -\frac{d}{2}, \\ \frac{1}{2}\lambda^2 x^2 + \frac{1}{2}\beta^2 x^2 & \text{if } -\frac{d}{2} \leqslant x \leqslant \frac{d}{2}, \\ \frac{1}{2}\lambda^2 x^2 + \frac{1}{2}\beta^2 (x-d)^2 & \text{if } \frac{d}{2} < x \leqslant \frac{3d}{2}, \\ \infty & \text{if } |x| > 3d/2, \end{cases}$$
(3.61)

where  $\lambda$  and  $\beta$  are the parameters of harmonic and periodic potentials respectively, and d is the spatial extent of each well. This is most basic model to examine the nearest neighbor effects in a lattice. The central well, in particular, which has two nearest neighbors is a representation of lattice sites in optical lattices. In the experiment set up used by Cataliotti et al. [15], the trap geometry is quasi-1D with  $\omega_z/\omega_r = 9/92$ . For further analysis, the equations are scaled in terms of the transverse oscillator length of the harmonic potential realized in aforementioned experimental set up, which is equivalent to setting  $\lambda = 9/92$ . Accordingly,  $\beta$  and all the coordinates, from here after, are in scaled units. The potential considered is a simplified model and discontinuities are present at the boundary of two neighboring wells. However, the ground state energy is much lower than the barrier height, and it describes the underlying physics very well. In the tight-binding approximation, the total wave function is

$$\psi(x) = \sum_{i=-1}^{1} a_i \phi_i(x), \qquad (3.62)$$

where i = -1, 0 and 1 represent the left, central and right well respectively. Here the normalization is

$$\int_{\infty}^{\infty} |\psi(x)|^2 dx = 1.$$
 (3.63)

We consider  $\beta > \lambda$ , which follows from the tight binding approximation. The width of each of these localized wave functions are calculated by minimizing the localized energies of each well

$$E_{i} = \int N_{i} \left[ \frac{1}{2} |\nabla \phi_{i}|^{2} + V_{i}(x) |\phi_{i}|^{2} \right] dx, \qquad (3.64)$$

where, from the previous definition

$$V_i(x) = \frac{1}{2}x^2 + \frac{1}{2}\beta^2(id+x)^2.$$
(3.65)

The range of each well, as defined earlier, is  $(2i - 1)d/2 \leq x \leq (2i + 1)d/2$ . Neglecting the nearest neighbor overlaps of the wave functions, the integration limits can be considered as  $-\infty$  to  $+\infty$ . The energies are then

$$E_0 = \frac{1}{2}\eta,$$
  
 $E_{\pm 1} = E_0 + \delta E$  (3.66)

where  $\eta = \sqrt{\lambda^2 + \beta^2}$  and

$$\delta E = \frac{\lambda^2 d^2}{2} \tag{3.67}$$

is the energy difference between side and central wells.



Figure 3.15: Variation of v as a function of  $\beta$ .

For the combined system of the three wells, in tight binding approximation, we only consider tunneling between adjacent wells. The lowest eigen energy is the chemical potential of the system, and the eigen vector corresponds to the probability amplitudes for the occupancy of each well. As defined earlier,  $E_{-1}$ ,  $E_0$  and  $E_1$  are the energies localized in left, central and right well respectively.

Define the tunneling matrix element between left and central well as

$$v = \int \left[\frac{1}{2}\nabla\phi_{-1}\cdot\nabla\phi_0 + \phi_{-1}V(x)\phi_0\right]dx,$$
(3.68)

and similarly, for the central and right wells as

$$w = \int \left[\frac{1}{2}\nabla\phi_0 \cdot \nabla\phi_1 + \phi_0 V(x)\phi_1\right] dx.$$
(3.69)

For the symmetric case considered here v = w, and after evaluating the integrals

$$v = \frac{e^{-\frac{17}{4}d^2\eta}}{16\sqrt{\pi\eta}} \left\{ 4d \left[ \beta^2 \left( 1 - 2e^{3d^2\eta} - 2e^{4d^2\eta} \right) - \left( 1 + 2e^{3d^2\eta} \right) \right] - \sqrt{\pi\eta} e^{4d^2\eta} \left[ 2\eta + d^2(5\beta^2 - 3) \right] \operatorname{Erf} \left( d\sqrt{\eta} \right) - \sqrt{\pi\eta} e^{4d^2\eta} \left[ 2\eta - d^2(11\beta^2 + 3) \right] \operatorname{Erf} \left( 2d\sqrt{\eta} \right) \right\}$$
(3.70)

In the above expression  $\text{Erf}(\cdots)$  represents error function. The Hamiltonian matrix of the system is then

$$H = \begin{pmatrix} E_{-1} & v & 0\\ v & E_0 & v\\ 0 & v & E_1 \end{pmatrix}.$$
 (3.71)

The ground state of the system is the lowest energy eigen vector obtained from diagonalizing the Hamiltonian matrix. This is equivalent to solving the secular equation and amounts to calculating the roots of a cubic polynomial, which is possible analytically. The eigen values, in increasing order of magnitude, of the Hamiltonian in Eq. (3.71) are

$$\frac{1}{2}(E_0 + E_1 - E_{12}), \quad E_1, \quad \frac{1}{2}(E_0 + E_1 + E_{12});$$
 (3.72)

where  $E_{12} = \sqrt{\delta E^2 + 8v^2}$ . The eigen vector of the lowest eigen value is

$$a_{\pm 1} = \frac{\sqrt{2v}}{\sqrt{8v^2 + \delta E (\delta E + E_{12})}},$$
  
$$a_0 = -\frac{\sqrt{8v^2 + \delta E (\delta E + E_{12})}}{\sqrt{2}\sqrt{\delta E^2 + 8v^2}},$$

and the ratio of the probability amplitude of occupancy of central to side well is

$$\frac{|a_0|}{|a_{\pm 1}|} = \frac{\delta E(\delta E + E_{12}) + 8v^2}{2v\sqrt{\delta E^2 + 8v^2}}.$$
(3.73)

The energy difference  $\delta E$  is quite small for small values of d. For example based on Ref. [15], consider d = 0.35 and  $\beta = 197.824$ . The associated energy difference and tunneling matrix element are  $\delta E = 0.00049494$  and v = 2.18549respectively. Hence for  $\delta E \ll v$ , using Taylor series expansion Eq. (3.73) simplifies to

$$\frac{|a_0|}{|a_{\pm 1}|} \approx \sqrt{2} + \frac{\delta E}{2v}.\tag{3.74}$$

Since  $\delta E$  is independent of  $\beta$  and v decreases as  $\beta$  is increased (see Fig. 3.15), the above ratio is larger with higher values of  $\beta$ . Using Eq. (3.74), Fig. 3.16 shows the variation of ratio of probability of occupancy of central to side wells with respect to v. This relation is not valid for very large values of  $\beta$  when  $\delta E \ll v$  does not hold true. For trapping potentials without the harmonic



Figure 3.16: The plot shows the  $p_0/p_{\pm 1}$  as a function of v for the values of  $\beta$  ranging from 197.82 to 312.79. In terms of the ratio of barrier height to recoil energy of laser light photon s used in Ref. [15], the aforementioned range of  $\beta$  values is equivalent to s ranging from 6 to 15.

component  $(\lambda = 0)$ , purely lattice potential, the three eigenvalues are identical when the hopping across adjacent wells is zero (v = w = 0). This solution corresponds to all the atoms confined to one of the potential wells. At this stage for further reference, we define the occupancy probability of the *i*th well

as

$$p_i = \left(\int_{-\infty}^{\infty} \phi_i^* \psi dx\right)^2 = |a_i|^2.$$
(3.75)

When v and w are non-zero, then the ground state has nonzero occupancies for all the three wells. The central well has probability of occupancy equal to half ( $p_0 = 0.5$ ), while the wells at the wings have probability equal to one fourth each ( $p_{\pm 1} = 0.25$ ). More importantly, these values are independent of  $\beta$ , i.e. no squeezing of the density profile occurs without the harmonic potential ( $\lambda = 0$ ).

In the presence of a weak harmonic potential, there is an increase in  $p_0$  when  $\beta$  is increased. For  $\beta = 197.82$ , equivalent to s = 6 in Ref. [15], the occupancy probability of the central well is 0.500047, this is marginally larger than the  $\lambda = 0$  case. On the other hand, the wings have occupancy probability of 0.249976, slightly lower probability of occupancy than  $\lambda = 0$  case. The trend continues with further increase of  $\beta$ , and for  $\beta = 1000$  there are almost no atoms in the potential wells at the wings. Thus with increase in value of  $\beta$ , atoms migrate from the wings to central well and lead to the squeezing of the condensate. The squeezing of the condensate profile is evident from the comparative study of plots in Fig. 3.17.



Figure 3.17: The plots show the ground state wave function  $\psi(x)$  (solid curve) and probability density  $|\psi(x)|^2$  (dashed curve) for potential considered in Eq. (3.61). For figure on left side,  $\lambda = 9/92, d = 0.35$  and  $\beta = 197.82$  (s = 6), while for figure on right side,  $\lambda = 9/92, d = 0.35$  and  $\beta = 312.79$  (s = 15)

In three level approximation, a triple well problem can also be analyzed by

considering the following classical Hamiltonian [130]

$$\mathcal{H} = \frac{1}{2}g \left[ n_{-1}^2 + (1 - n_{-1} - n_1)^2 + n_1^2 \right] + n_{-1}\epsilon_{-1} + n_1\epsilon_1 + 2\sqrt{1 - n_{-1} - n_1} \left( v\sqrt{n_{-1}}\cos\theta_{-1} + w\sqrt{n_1}\cos\theta_1 \right), \qquad (3.76)$$

where  $n_j = |a_j|^2$  and  $\theta_j = \arg(a_2) - \arg(a_j)$  are canonical conjugate variables satisfying following equations

$$\frac{dn_j}{dt} = -\frac{\partial \mathcal{H}}{\partial \theta_j} \text{ and } \frac{d\theta_j}{dt} = \frac{\partial \mathcal{H}}{\partial n_j}, \qquad (3.77)$$

and  $\epsilon_{-1}$  and  $\epsilon_1$  are the zero point energies of potential wells at the flanks measured with respect to zero point energy of central well. The stationary states of the system can be calculated by by solving

$$\frac{dn_j}{dt} = \frac{d\theta_j}{dt} = 0 \tag{3.78}$$

In the absence of the harmonic potential,  $\epsilon_{-1}$  and  $\epsilon_1$  are zero and change in tunneling amplitude has no effect on the occupancy of three wells. But the situation is dramatically different with the harmonic potential,  $\epsilon_{-1} = \epsilon_1 \neq 0$ . In this case probability of occupancy of central well increases with decrease in v. This is experimentally realizable by increasing depth of lattice potential. Similarly for four potential wells, the occupancy of the two central wells (whose occupancies are equal) grows as we increase  $\beta$  for non zero  $\lambda$ .

## 3.3 Summary of results

We have studied the ground state properties of TBECs, both in miscible and phase-separated domains, employing two semi-analytic methods. In phaseseparated domain, we show that TF approximation based method, applicable when  $Na/a_{\rm osc} \gg 1$ , is able to explain the emergence of planar and cylindrical geometries as the ground state geometries provided, one takes into account the contribution of interface energy. When  $Na/a_{\rm osc}$  is of the order 1, we employ a suitable variational *ansatz* to determine the ground state geometry of the TBEC both in miscible and phase-separated domains.

## Chapter 4

# Statics and dynamics of mixtures of quantum fluids

The two components of binary quantum degenerate systems can be both bosons, both fermions or one boson and the other fermion. Consequently, the quantum degenerate binary mixtures are of three types: (a) Bose-Bose mixtures, (b) Fermi-Fermi mixtures and (c) Bose-Fermi mixtures. In the previous chapter, we examined, both analytically and numerically, the ground state properties of Bose-Bose mixtures (TBECs). Extending these studies (of previous chapter), we will examine the static properties of Bose-Fermi mixtures in the first part (Sec. 4.1) of the present chapter; in the second part (Sec. 4.2), dynamics of the phase-separated Bose-Bose mixtures will be examined.

## 4.1 Quantum degenerate Bose-Fermi mixtures

The quantum degeneracy in a Bose-Fermi mixture was first experimentally realized for the system consisting of <sup>7</sup>Li and <sup>6</sup>Li [131, 132]. Since then it has been observed in several other Bose-Fermi mixtures, <sup>23</sup>Na-<sup>6</sup>Li [133], <sup>87</sup>Rb-<sup>40</sup>K [134], <sup>87</sup>Rb-<sup>6</sup>Li [135], <sup>4</sup>He-<sup>3</sup>He[136], <sup>174</sup>Yb-<sup>173</sup>Yb[137] and <sup>84</sup>Sr-<sup>87</sup>Sr [138]. These are candidate systems to explore the effects of boson-induced fermionic interactions, of particular interest is the boson mediated fermionic superfluidity. Another property of interest is the dynamical instabilities of the fermionic component arising from the attractive fermionic interactions, which is also boson mediated [139]. Precondition to observe either of these is a precise control of the inter-species interaction through a Feshbach resonance. This has been observed in <sup>87</sup>Rb-<sup>40</sup>K [140, 141] and used to trigger the dynamical collapse of

 $^{40}$ K [139], the same is numerically analyzed in Refs. [142, 143]. A similar set up is suitable to create fermionic ultracold molecules and was theoretically analyzed in a recent work [144]

Density distributions in the phase-separated domain of the Bose-Fermi mixture is also an important property of interest. Like in binary condensates, dynamical instabilities can be initiated in the phase-separated domain through manipulations of interaction strengths. For binary condensates, the recent work on mixtures of two different hyperfine states of <sup>87</sup>Rb [34] is a fine example of controlled experiment on phase separation.

In this regard, Molmer and collaborator [145, 146] examined the zero temperature equilibrium density distributions and predicted widely varying density patterns as a function of inter-species interactions. However, the Bose-Bose and Bose-Fermi interactions considered are extremely strong for experimental realizations. Similar studies have examined the ground state geometry in spherical traps [147, 148]. The conditions for mixing-demixing have been analyzed for homogeneous Bose-Fermi mixture [149] and Bose-Fermi mixtures inside traps [147, 150]. Although, very high interaction strengths are achievable through magnetic Feshbach resonances in alkali atoms, simultaneous tuning of both the boson-boson and boson-fermion interactions is not possible. However, simultaneous tuning is possible with optical Feshbach resonances (OFR) when the resonant frequencies of the boson-boson and boson-fermion interactions are well separated. In an earlier study, the possibility of simultaneous and independent tuning in the <sup>40</sup>K-<sup>6</sup>Li through a magnetic Feshbach resonance and rf-field-induced Feshbach resonance was examined [151]. However, such a possibility does not apply to zero electronic spin (closed-shell) atoms like Yb.

With the realization of quantum degeneracy in the mixture of <sup>174</sup>Yb-<sup>173</sup>Yb where intra-species interactions for <sup>174</sup>Yb can be tuned by OFR [119], we find it pertinent to revisit these studies. With the possibility of tuning interspecies interactions for <sup>174</sup>Yb-<sup>173</sup>Yb mixture, it may be possible to realize the ground state geometries which are hitherto elusive. We, therefore, consider <sup>173</sup>Yb-<sup>174</sup>Yb mixture to study the density profiles for various values of coupling strengths in Sec. 4.1. It must also be mentioned that the isotopes of Yb exhibit a wide range of inter- and intra-species interactions. It has attracted lot of attention as selected isotopic compositions may exhibit dynamical instabilities triggered through the interactions. The <sup>174</sup>Yb-<sup>176</sup>Yb is one such Bose-Bose binary mixture currently investigated for instabilities on account of

the attractive intra-species interaction of  $^{176}$ Yb [152, 153].

## 4.1.1 Zero temperature mean field description

We examine the stationary state properties of a Bose-Fermi (BF) mixture consisting of  $^{174}$ Yb and  $^{173}$ Yb in spherically symmetric trapping potentials

$$V_{\rm B}(\mathbf{r}) = \frac{1}{2} m_{\rm B} \omega^2 r^2, \quad V_{\rm F}(\mathbf{r}) = \frac{1}{2} m_{\rm F} \omega^2 r^2$$
(4.1)

where the subscripts B and F stand for boson and fermion respectively, and  $\omega$  is the radial trapping frequency for the two components. The fermions are spinpolarized (single species) and the fermion-fermion mean field interactions arise from the degeneracy pressure [47], whereas the boson-boson and boson-fermion interactions arise from the *s*-wave scattering between the atoms. Considering these, the mean field energy functional of the Bose-Fermi mixture is [154]

$$E[\Psi_{\rm B}, \Psi_{\rm F}] = \int d\mathbf{r} \left[ N_{\rm B} \left( \frac{\hbar^2 |\nabla \Psi_{\rm B}|^2}{2m_B} + V_{\rm B} |\Psi_{\rm B}|^2 + \frac{1}{2} G_{\rm BB} |\Psi_{\rm B}|^4 \right) + N_{\rm F} \left( \frac{\hbar^2 |\nabla \Psi_{\rm F}|^2}{6m_{\rm F}} + V_{\rm F} |\Psi_{\rm F}|^2 + \frac{3}{5} A |\Psi_{\rm F}|^{10/3} \right) + G_{\rm BF} N_{\rm B} |\Psi_{\rm B}|^2 |\Psi_{\rm F}|^2 \right],$$

$$(4.2)$$

where  $\Psi_{\rm B}(\mathbf{r},t)$  and  $\Psi_{\rm F}(\mathbf{r},t)$  are bosonic and fermionic wave functions satisfying the normalization condition

$$\int d\mathbf{r} |\Psi_{\rm B}(\mathbf{r},t)|^2 = \int d\mathbf{r} |\Psi_{\rm F}(\mathbf{r},t)|^2 = 1.$$
(4.3)

Here  $G_{\rm BB} = 4\pi\hbar^2 a_{\rm BB}N_{\rm B}/m_{\rm B}$ , where  $a_{\rm BB}$  is the bosonic *s*-wave scattering length and  $N_{\rm B}$  is the number of bosons, is the bosonic intra-species interaction,  $G_{\rm BF} = 2\pi\hbar^2 a_{\rm BF}N_{\rm F}/m_R$  and  $G_{\rm FB} = 2\pi\hbar^2 a_{\rm BF}N_{\rm B}/m_R$ , where  $m_R = (m_{\rm B}m_{\rm F})/(m_{\rm B} + m_{\rm F})$  is the reduced mass,  $N_{\rm F}$  is the number of fermions and  $a_{\rm BF}$  is the inter-species scattering length, are the inter-species interactions, and  $A = \hbar^2 (6\pi^2 N_{\rm F})^{2/3}/(2m_{\rm F})$ . The Lagrangian of the system

$$L = \int d\mathbf{r} \frac{i\hbar}{2} \sum_{i=\mathrm{B},\mathrm{F}} \left( \Psi_i^{\star} \frac{\partial \Psi_i}{\partial t} - \Psi_i \frac{\partial \Psi_i^{\star}}{\partial t} \right) - E[\Psi_\mathrm{B}, \Psi_\mathrm{F}]. \tag{4.4}$$

Using the action principle

$$\delta \int_{t_1}^{t_2} L dt = 0, \tag{4.5}$$

we get a set of coupled partial differential equations

$$i\hbar\frac{\partial\Psi_{\rm B}}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2m_{\rm B}} + V_{\rm B}(\mathbf{r}) + G_{\rm BB}|\Psi_{\rm B}|^2 + G_{\rm BF}|\Psi_{\rm F}|^2\right]\Psi_{\rm B},\qquad(4.6a)$$

$$i\hbar\frac{\partial\Psi_{\rm F}}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{6m_{\rm F}} + V_{\rm F}(\mathbf{r}) + A|\Psi_{\rm F}|^{4/3} + G_{\rm FB}|\Psi_{\rm B}|^2\right]\Psi_{\rm F}.$$
 (4.6b)

The above set of equations is valid for Bose-Fermi mixtures consisting of a BEC and a Fermi sea of spin-polarized fermions. For superfluid Bose-Fermi mixtures, consisting of BECs of bosonic component and Cooper pairs between two different hyperfine states of fermions, the modified mean field equation for the fermionic component (BEC of Cooper pairs) has been proposed in Refs. [155, 156].

It is more convenient to rewrite Eq. (4.6) in a dimensionless form by defining dimensionless parameters in terms of the frequency  $\omega$  and the oscillator length  $a_{\rm osc} = \sqrt{\hbar/(m_{\rm B}\omega)}$ . Using  $\tilde{\mathbf{r}} = \mathbf{r}/a_{\rm osc}$ ,  $\tilde{t} = t\omega$  as the scaled dimensionless variables of length and time respectively, Eq. (4.6) can be rewritten as

$$i\frac{\partial\psi_{\rm B}}{\partial\tilde{t}} = \left[-\frac{\nabla_{\tilde{\mathbf{r}}}^2}{2} + V_{\rm B}(\tilde{\mathbf{r}}) + g_{\rm BB} \left|\psi_{\rm B}\right|^2 + g_{\rm BF} \left|\psi_{\rm F}\right|^2\right]\psi_{\rm B},\tag{4.7a}$$

$$i\frac{\partial\psi_{\rm F}}{\partial\tilde{t}} = \left[-\frac{\nabla_{\tilde{\mathbf{r}}}^2}{6m_{\rm ratio}} + m_{\rm ratio}V_{\rm F}(\tilde{\mathbf{r}}) + g_{\rm FF}\left|\psi_{\rm F}\right|^{4/3} + g_{\rm FB}\left|\psi_{\rm B}\right|^2\right]\psi_{\rm F},\qquad(4.7b)$$

where the rescaled wave functions are  $\psi_{\rm B} = a_{\rm osc}^{3/2} \Psi_{\rm B}(\tilde{\mathbf{r}}, \tilde{t})$  and  $\psi_{\rm F} = a_{\rm osc}^{3/2} \Psi_{\rm F}(\tilde{\mathbf{r}}, \tilde{t})$ . Similarly, the interaction strength parameters are

$$g_{\rm BB} = \frac{4\pi a_{\rm BB} N_{\rm B}}{a_{\rm osc}}, \quad g_{\rm BF} = \frac{2\pi a_{\rm BF} N_{\rm F}}{m_R \, a_{\rm osc}},$$
$$g_{\rm FF} = \frac{(6\pi^2 N_{\rm F})^{2/3}}{2m_{\rm ratio}}, \quad g_{\rm FB} = \frac{2\pi a_{\rm BF} N_{\rm B}}{m_R \, a_{\rm osc}},$$

with  $m_{\rm ratio} = m_{\rm F}/m_{\rm B}$ . For the sake of simplicity, we represent the scaled quantities without the tilde ( $\tilde{}$ ) in the rest of the chapter. For spherically symmetric trapping potential, the Eq. (4.6) are reduced to one dimensional

coupled mean field equations

$$i\frac{\partial\psi_{\rm B}}{\partial t} = \left[ -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{r^2}{2} + g_{\rm BB} \left| \frac{\psi_{\rm B}}{r} \right|^2 + g_{\rm BF} \left| \frac{\psi_{\rm F}}{r} \right|^2 \right] \psi_{\rm B}, \qquad (4.8a)$$
$$i\frac{\partial\psi_{\rm F}}{\partial t} = \left[ -\left(\frac{1}{3m_{\rm ratio}}\right) \frac{1}{2}\frac{\partial^2}{\partial r^2} + m_{\rm ratio}\frac{r^2}{2} + g_{\rm FF} \left| \frac{\psi_{\rm F}}{r} \right|^{4/3} + g_{\rm FB} \left| \frac{\psi_{\rm B}}{r} \right|^2 \right] \psi_{\rm F}. \qquad (4.8b)$$

These are the coupled mean field equations which describe the Bose-Fermi mixture in trapping potentials at zero temperature. To obtain the stationary solutions, we solve the equations numerically using Crank-Nicholson scheme [120] with imaginary time propagation.

## 4.1.2 Phase separation

Broadly speaking, for large values of  $G_{\rm BB}$ , the density profiles of the bosonfermion mixture in spherical symmetric traps can have three distinct geometries in phase-separated regime: (a) fermionic core surrounded by bosonic shell, (b) bosonic core surrounded by fermionic shell and (c) shell of bosons between fermionic core and fermionic outer shell [145]. The inter-species interactions begin to play an important role in determining the stationary state structure, when the density profiles of the bosons and fermions are of similar spatial extent. This occurs when the bosonic intra-species interaction is strong. In the TF approximation, the necessary condition for a mixture of equal number of bosons and fermions ( $N_{\rm B} = N_{\rm F} = N$ ) is [145]

$$a_{\rm BB} \approx 1.68 m_{\rm ratio}^{-5/2} a_{\rm osc} N^{-1/6}.$$
 (4.9)

The above condition has been obtained by equating the TF radii of bosons and fermions in the absence of inter-species interaction. The condition ensures the maximum overlap between the two species in the absence of inter-species interactions and hence, accentuates the effect of switching on the inter-species interactions. Hereafter in this chapter, we use  $a_{BB}^*$  to represent the particular value of  $a_{BB}$  at which bosons and fermions have the same spatial extent. For species which are isotopes of the same element the mass difference is small and  $m_{\rm ratio} \approx 1$ . The condition is then reduced to

$$a_{\rm BB}^* \approx 1.68 a_{\rm osc} N^{-1/6}.$$
 (4.10)

Considering  $N \sim 10^6$ , which is the typical value in experimental realizations,  $a_{\rm BB}^* \approx 0.17 a_{\rm osc}$ . As  $a_{\rm osc}$  is in general  $\sim 10^{-6}$  m for harmonic trapping potentials, the required value of  $a_{\rm BB}$  is in the strongly interacting domain. It could be achieved when the interaction is tuned through a Feshbach resonance, magnetic in the case of alkali metal atoms. With the overlapping density profiles, more intricate density patterns are observed when the inter-species interaction is increased, however, tuning  $a_{\rm BF}$  with magnetic Feshbach resonance is ruled out. This complication does not arise when the interactions are tuned with well separated OFRs. In which case, the isotopes of two-valence lanthanide atom Yb is a suitable candidate. It has seven stable isotopes: five bosons (<sup>168</sup>Yb, <sup>170</sup>Yb, <sup>172</sup>Yb, <sup>174</sup>Yb and <sup>176</sup>Yb) and two fermions(<sup>171</sup>Yb, and <sup>173</sup>Yb ); homo-nuclear OFRs of bosonic isotopes ( $^{172}$ Yb and  $^{176}$ Yb ) were recently studied [118]. Among the various possible species pairings <sup>174</sup>Yb-<sup>173</sup>Yb, which has positive intra- and inter-species background scattering lengths [157], is an ideal candidate to study Bose-Fermi mixtures in the strongly interacting domain.

For our studies, we consider a <sup>174</sup>Yb-<sup>173</sup>Yb mixture containing 10<sup>6</sup> atoms of each species and trapped by spherically symmetric trap with trapping frequency  $\omega/(2\pi) = 400$  Hz. The  $a_{\rm BB}$  is chosen to be equal to  $1100a_0$ , which is achievable with the OFR of the  $6s^2 {}^1S_0 \rightarrow 6s6p {}^3P_1$  inter-combination transition. And, the Bose-Fermi inter-species scattering length  $a_{\rm BF}$  can be tuned with OFR of the allowed  $6s^2 {}^1S_0 \rightarrow 6s6p {}^1P_1$  transition. This is a broad line and the disadvantage of using it is high atom loss rate. However, a major advantage of OFR tuned interactions is the fine spatial control it provides. Recently, submicron modulation of scattering length using Feshback resonances was achieved in <sup>174</sup>Yb [119]. Such precise control on the spatial variation of interaction strength is unrealistic with magnetic Feshbach resonances. From here on, where it is not explicitly mentioned, reference to Bose-Fermi mixture in this section implies <sup>174</sup>Yb-<sup>173</sup>Yb isotope mixture . To examine the density profiles of the mixture in the strongly interacting domain, we keep  $a_{BB}$ fixed and vary  $a_{\rm BF}$  so that the system progresses from mixing to full demixing regime via partial demixing regime. It must be emphasized that with TF approximation, from Eq. (4.10) the spatial extent of density profiles with  $a_{BF} = 0$  are same when  $a_{BB}^* = 1191.71a_o$  as is shown in Fig. 4.1(b). However,

we have chosen  $a_{BB} = 1100a_o$ , approximately the value at which the density profiles begin to exhibit the features of interest. The wave-function profiles with  $a_{BB} = 1100a_o$  in the absence of inter-species interactions are shown in Fig. 4.1(a).

## 4.1.3 Mixing to partial demixing regime

Starting from the initial conditions of the mixture, which as mentioned earlier has equal spatial extent of the component species and  $a_{\rm BF} \approx 0$ , the value of  $a_{\rm BF}$  is increased. To analyze the evolution of density profiles, consider the TF profile of the bosons and fermions in scaled units as defined earlier

$$n_{\rm F}(r) = \frac{1}{6\pi^2} \left\{ 2m_{\rm ratio} \left[ E_{\rm F} - V_{\rm F}(r) - u_{\rm FB} n_{\rm B}(r) \right] \right\}^{3/2}, \qquad (4.11a)$$

$$n_{\rm B}(r) = \frac{1}{u_{\rm BB}} \left[ \mu - V_{\rm B}(r) - u_{\rm BF} n_{\rm F}(r) \right], \qquad (4.11b)$$

where  $u_{XY} = g_{XY}/N_Y$  and  $E_F$  is the Fermi energy. From these expressions, the densities at the origin in absence of inter-species interaction are

$$n_{\rm F}(0) = \frac{1}{6\pi^2} \left(2m_{\rm ratio}E_{\rm F}\right)^{3/2},$$
 (4.12a)

$$n_{\rm B}(0) = \frac{\mu}{u_{\rm BB}}.$$
 (4.12b)

In TF approximation, the Fermi energy and chemical potential of the two species are

$$E_{\rm F} = (6N)^{1/3},$$
 (4.13a)

$$\mu = \frac{1}{2} \left( 15 a_{\rm BB} N \right)^{2/5}. \tag{4.13b}$$

Using these in Eq. (4.12), the ratio of the densities at the origin is

$$\frac{n_{\rm F}(0)}{n_{\rm B}(0)} = 0.76a_{\rm BB}^{3/5}(15N)^{1/10}$$

We consider  $a_{\rm BB} \approx 0.17$ , the value at which the profiles of the two species match for  $N = 10^6$ . The population ratio at the origin is then

$$\frac{n_{\rm F}(0)}{n_{\rm B}(0)} \approx 1.35,$$
 (4.14)



Figure 4.1: Wave-function profiles of <sup>174</sup>Yb (dashed green line) and <sup>173</sup>Yb (solid orange line) in a mixture of <sup>174</sup>Yb-<sup>173</sup>Yb with  $N_{\rm B} = N_{\rm F} = 10^6$ ,  $\omega/(2\pi) = 400$ Hz and  $a_{\rm BB} = 1100a_0$  as  $a_{\rm BF}$  is changed from mixing to partial demixing domain. (a) For  $a_{\rm BF} = 0.0$ , (b) for  $a_{\rm BF} = 0.0a_{\rm BB}$  and  $a_{\rm BB} = 1197.11a_0$ , (c) for  $a_{\rm BF} = 0.6a_{\rm BB}$  and (d) for  $a_{\rm BF} = 0.7a_{\rm BB}$ 

that is when  $a_{\rm BF} = 0$  the fermion density is higher than the boson density at the center of the trap. Given this as the initial condition, when the inter-species interaction is switched on, the inter-species mean field energy  $G_{\rm BF}|\Psi_{\rm F}(0)|^2 > G_{\rm FB}|\Psi_{\rm B}(0)|^2$ . Hence, it is energetically favorable to shift the bosons from the center towards the edge of the trap. This is evident in the numerically obtained density profiles shown in Fig. 4.1(a), where the density profile of the bosons is flattened around the origin and has higher density at the edges.

The inter-species interaction energy in mixing regime is

$$E_{\rm int} = \int d\mathbf{r} u_{\rm BF} n_{\rm B} n_{\rm F},$$
  

$$\approx \frac{3 u_{\rm BF} N^2}{4 \pi R_{\rm TF}^3},$$
(4.15)

where we have used  $n_{\rm B} \approx n_{\rm F} \approx N/(4\pi R_{\rm TF}^3/3)$  [150] with  $R_{\rm TF} = \sqrt{2(6N)^{1/3}}$ for the system considered in the present chapter. As  $a_{\rm BF}$  is increased further the system enters the partial demixing regime and the characteristic signature



Figure 4.2: Interspecies interaction energy  $E_{\text{int}}$  between <sup>174</sup>Yb (boson) and <sup>173</sup>Yb (fermion) as a function of  $a_{\text{BF}}$ . The maxima of  $E_{\text{int}}$  occurs at  $a_{\text{BF}} = 0.7a_{\text{BB}}$ .

of which is a maxima in inter-species interaction energy. For our present calculations, the variation of the inter-species interaction energy with  $a_{\rm BF}$  is shown in Fig. 4.2. The condition for attaining partial demixing in spherical traps is [150]

$$a_{\rm BF} \ge \left(c_1 \frac{N_{\rm F}^{1/2}}{N_{\rm B}^{2/5}} + c_2 \frac{N_{\rm B}^{2/5}}{N_{\rm F}^{1/3}}\right) a_{\rm BB},$$
(4.16)

where

$$c_1 = \frac{15^{3/5}}{48^{1/2}} \frac{m_{\rm F}^{3/2}}{2m_R m_{\rm B}^{1/2}} a_{\rm BB}^{3/5}$$
(4.17)

and

$$c_2 = \frac{48^{1/3}}{15^{3/5}} \left(\frac{6}{\pi}\right)^{2/3} \frac{m_{\rm B}}{2m_R} a_{\rm BB}^{2/5}.$$
(4.18)

The above condition for partial demixing is evaluated using TF approximation for the density profiles of both the components. From equation Eq. (4.16), the critical value of  $a_{\rm BF}$  required to reach partial demixing regime for the Bose-Fermi mixture under consideration is  $0.44a_{\rm B}$  and is significantly lower than the value of  $0.7a_{\rm BB}$  obtained from numerical solution of the coupled mean field equations [Eq. (4.8)]. The difference may be attributed to the simplifying assumptions used in deriving the location of the inter-species interaction energy extrema. One of which is choosing the density profiles at  $a_{\rm BF} = 0$  to calculate the inter-species interaction energy. At  $a_{\rm BF} = 0.7a_{\rm BB}$  there is dramatic decrease in the density of the Bosons near the trap center. This is accompanied by corresponding decrease in overlap region between the two components as is shown in Fig. 4.1(d).



Figure 4.3: The wave function profiles of <sup>174</sup>Yb (dashed green line) and <sup>173</sup>Yb (solid orange line) in a mixture of <sup>174</sup>Yb-<sup>173</sup>Yb, with  $N_{\rm B} = N_{\rm F} = 10^6$ ,  $a_{\rm BB} = 1100a_0$  and  $\omega/(2\pi) = 400$ Hz. For (a)  $a_{\rm BF} = 0.75a_{\rm BB}$  and for (b)  $a_{\rm BF} = 1.0a_{\rm BB}$ .

## 4.1.4 Partial demixing to phase separation

A further increase of  $a_{\rm BF}$ , beyond the critical value, enhances the segregation of the two species. This lowers the inter-species overlap and balances the larger interaction energy from higher  $a_{\rm BF}$ . Ultimately, at higher values of  $a_{\rm BF}$ the overlap is almost zero, the system can then be considered fully phaseseparated. The condition to attain phase separation or fully demixed regime is [150]

$$\alpha k_{\rm F} a_{\rm BB} > \left(\frac{a_{\rm BB}}{a_{\rm BF}}\right)^2,\tag{4.19}$$

where

$$k_{\rm F} = (48N_{\rm F})^{1/6}$$
, and  $\alpha = \frac{3^{1/3}}{4(2\pi)^{2/3}} \frac{m_{\rm B}m_{\rm F}}{m_R^2}$ . (4.20)

For <sup>174</sup>Yb-<sup>173</sup>Yb mixture with the previously mentioned parameters, the above criterion translates into  $a_{\rm BF} > 0.9a_{\rm BB}$ . In the phase-separated domain, the

separation occurs around the inner point where densities are equal. To identify the location of this point, consider the  $a_{\rm BF} = 0$  density profiles. If the two profiles intersect at  $r_{\rm i}$ , then from the TF approximation  $r_{\rm i}$  is the solution of the equation

$$\{2m_{\rm ratio} \left[E_{\rm F} - V_{\rm F}(r_{\rm i})\right]\}^3 = \left(\frac{6\pi^2}{u_{\rm BB}}\right)^2 \left[\mu - V_{\rm B}(r_{\rm i})\right]^2.$$
(4.21)

For the system of our interest  $V_{\rm F}$  and  $V_{\rm B}$  are almost identical. Further, when  $a_{\rm BB}$  is chosen [it satisfies Eq. (4.10)] to match the spatial extents of the densities,  $E_{\rm F} \approx \mu$ . Following which, to a very good approximation  $[E_{\rm F} - V_{\rm F}(r_{\rm i})] \approx [\mu - V_{\rm B}(r_{\rm i})]$ . The solution of Eq. (4.21) is then

$$r_{\rm i} = \left[2E_{\rm F} - \frac{1}{4m_{\rm ratio}^3} \left(\frac{6\pi^2}{u_{\rm BB}}\right)^2\right]^{1/2}.$$
 (4.22)

The importance of  $r_i$  is for the following:  $n_F(r) > n_B(r)$  for  $r < r_i$ , and  $n_F(r) < n_B(r)$  for  $r > r_i$ . For the <sup>174</sup>Yb-<sup>173</sup>Yb mixture, based on the above relation  $r_i = 13.09a_{osc}$  for  $N_B = N_F = 10^6$  and  $a_{BB} = 0.17a_{osc}$ , while the numerical value is  $r_i = 12.42a_{osc}$ . Energetically, when  $a_{BF}$  is switched on it is favorable to accommodate the bosons and fermions at the outer and inner regions about  $r_i$  respectively. As  $a_{BF}$  is increased, the position of  $r_i$  tends to migrate outward but not dramatically.

With further increase in  $a_{\rm BF}$ , the bosons are expelled towards the edge of trapping potential while fermions are squeezed towards the trap center (see Fig. 4.3). With TF approximation, the effective potential experienced by <sup>173</sup>Yb in the overlap region is

$$V_{\text{eff}} = \left( m_{\text{ratio}} - \frac{g_{\text{BF}}}{g_{\text{BB}}} \right) \frac{r^2}{2}$$
$$\approx \left( 1 - \frac{g_{\text{BF}}}{g_{\text{BB}}} \right) \frac{r^2}{2}, \qquad (4.23)$$

where we have considered  $m_{\rm ratio} \approx 1$  for <sup>174</sup>Yb-<sup>173</sup>Yb mixture. Obviously, the effective potential experienced by fermions vanishes at  $a_{\rm BF} = a_{\rm BB}$ , and this explains the constant wave function profile of <sup>173</sup>Yb in the overlap region as is shown in Fig. 4.3(b). Unlike two component BECs, the density of the fermions in the region occupied by bosons is not zero when the criterion for full demixing is satisfied.



Figure 4.4: The wave function profiles of <sup>174</sup>Yb (dashed green line) and <sup>173</sup>Yb (solid orange line) in a mixture of <sup>174</sup>Yb-<sup>173</sup>Yb, with  $N_{\rm B} = N_{\rm F} = 10^6$ ,  $a_{\rm BB} = 1100a_0$  and  $\omega/(2\pi) = 400$ Hz, as  $a_{\rm BF}$  is steadily increased from an initial value of  $a_{\rm BF} = a_{\rm BB}$ . For (a)  $a_{\rm BF} = 1.05a_{\rm BB}$ , for (b)  $a_{\rm BF} = 1.1a_{\rm BB}$ , for (c)  $a_{\rm BF} = 1.15a_{\rm BB}$ , and for (d)  $a_{\rm BF} = 1.25a_{\rm BB}$ .

## 4.1.5 Fermion pinching

For the values of  $a_{BB}$  marginally below  $a_{BB}^*$ , besides  $r_i$  there is another point  $r_o$  where the densities are identical as is evident from Fig. 4.1(a). The location of  $r_o$  is rather sensitive to kinetic energy corrections of the bosons [158]

$$E_{\rm kin} = 2.5 \frac{N_{\rm B}}{R_{\rm TF}^2} \ln\left(\frac{R_{\rm TF}}{1.3}\right).$$
 (4.24)

Without the kinetic energy correction, that is with TF approximation,  $r_{\rm o}$  exists up to higher values of  $a_{\rm BF}$ . However, the kinetic energy correction softens the profile at the edges and  $r_{\rm o}$  vanishes as  $a_{\rm BB}$  approach  $a_{\rm BB}^*$  [see Fig. 4.1(b)]. In the phase-separated domain when  $r_{\rm o}$  is close to the edge, the fermion density is depleted at  $r_{\rm i} < r < r_{\rm o}$  for higher  $a_{\rm BF}$ , and there is fermion density enhancement at  $r < r_{\rm i}$  and  $r > r_{\rm o}$ . For the bosons it is opposite: there is density enhancement at  $r_{\rm i} < r < r_{\rm o}$ , and depletion at  $r < r_{\rm i}$  and  $r > r_{\rm o}$ .

As  $a_{\rm BF}$  is increased to values larger than  $a_{\rm BB}$ , the effective potential within

the overlap region  $(r_{\rm i} < r < r_{\rm o})$  is approximately

$$V_{\rm eff} \approx \mu \frac{g_{\rm BF}}{g_{\rm BB}} - \eta \frac{r^2}{2},\tag{4.25}$$

where  $\eta = |m_{\text{ratio}} - g_{\text{BF}}/g_{\text{BB}}|$ , and like in the previous case, we can take  $m_{\text{ratio}} \approx 1$ . The form of  $V_{\text{eff}}$  is repulsive with a maxima at  $r_i$  and decreases towards  $r_o$ . The net effect is that the fermion density profile is pinched at the region where r is marginally larger than  $r_i$ . Onset of pinching is clearly discernible in Fig. 4.4(a), and it is more pronounced in Fig. 4.4(b). At higher values of  $a_{\text{BF}}$  the pinching is complete and an island of fermions appears at the edge. Figures 4.4(c) and 4.4(d) show the formation of the fermionic island due to pinching in the <sup>173</sup>Yb-<sup>174</sup>Yb mixture.

## 4.1.6 **Profile swapping**

A remarkable feature in the evolution of density profiles as a function of  $a_{\rm BF}$  is the observation of profile swapping for certain range of parameters, in which the fermions are initially at the core and bosons form a shell. However, at higher values of  $a_{\rm BF}$  the bosons occupy the core and fermions forms a shell around it. As an example to illustrate profile swapping, consider  $N_B = N_F =$  $10^5$ , from Eq. (4.10) the spatial extents are equal at  $a_{\rm BB} = 0.24 a_{\rm osc}$ . However, retain the value  $a_{BB} = 1100a_o$  as in the case of  $10^6$  atoms in each species. In this case, the spatial extent of the bosons is less than the fermions, however, there are two points at which the densities of the bosons and fermions are the same. When  $a_{\rm BF}$  is set to a non-zero value, at lower values the changes in the equilibrium density profiles exhibit a pattern similar to fermion *pinching*. Like in fermion *pinching* as  $a_{\rm BF}$  is ramped up, there is a depletion of fermions from the overlap region as shown in Fig. 4.5(a-d). However, at some value of  $a_{\rm BF}$  a dramatic departure occurs. The fermions from the core are expelled to the edges and bosons settle at the core (Fig. 4.6). At intermediate values of  $a_{\rm BF}$ , the bosons form a shell sandwiched between fermions at the core and an outer shell. This is evident from the density profiles shown in Fig. 4.5(d). As is evident from the figures, the migration of the fermions to the flanks occurs at a relatively minute change in  $a_{\rm BF}$ , from  $1.15a_{\rm BB}$  to  $1.16a_{\rm BB}$ .

To analyze the profile swapping based on total energy considerations, take the density profiles just prior to the expulsion of fermions from the core. The



Figure 4.5: The wave function profiles of <sup>174</sup>Yb (dashed green line) and <sup>173</sup>Yb (solid orange line) in a mixture of <sup>174</sup>Yb-<sup>173</sup>Yb, with  $N_{\rm B} = N_{\rm F} = 10^5$ ,  $a_{\rm BB} = 1100a_0$  and  $\omega/(2\pi) = 400$ Hz, as  $a_{\rm BF}$  is steadily increased from an initial value of  $a_{\rm BF} = a_{\rm BB}$ . For (a)  $a_{\rm BF} = 1.0a_{\rm BB}$ , for (b)  $a_{\rm BF} = 1.05a_{\rm BB}$ , for (c)  $a_{\rm BF} = 1.1a_{\rm BB}$ , and for (d)  $a_{\rm BF} = 1.15a_{\rm BB}$ .

inter-species interaction energy is

$$E_{\rm int} \approx \int_{r_{\rm i}-\delta}^{r_{\rm i}+\delta} d\mathbf{r} u_{\rm BF} n_{\rm B} n_{\rm F} + \int_{r_{\rm i}+\delta}^{\infty} d\mathbf{r} u_{\rm BF} n_{\rm B} n_{\rm F}.$$
 (4.26)

Here,  $r_i$  like defined earlier is the inner point where the two densities are equal. The first term is the inter-species interaction energy arising from the inner boundary of the overlap region, and  $\delta$  is the interpenetration depth considered symmetric for simplicity. The second term is the interaction energy from the remaining overlap region. Although the upper limit of integration is taken as  $\infty$ , in reality it extends up to the point where  $n_B$  is nonzero. To simplify the analysis, we assume that the fermions from the core, after the position swapping, are pushed beyond the overlap domain. The interaction energy when swapping occurs is

$$E_{\rm int} \approx \int_0^{r_{\rm i}+\delta} d\mathbf{r} u_{\rm BF} n_{\rm B} n_{\rm F} + \int_{r_{\rm i}+\delta}^\infty d\mathbf{r} u_{\rm BF} n_{\rm B} n_{\rm F}, \qquad (4.27)$$



Figure 4.6: The wave function profiles of <sup>174</sup>Yb (dashed green line) and <sup>173</sup>Yb (solid orange line) in a mixture of <sup>174</sup>Yb-<sup>173</sup>Yb, with  $N_{\rm B} = N_{\rm F} = 10^5$ ,  $a_{\rm BB} = 1100a_0$  and  $\omega/(2\pi) = 400$ Hz, as  $a_{\rm BF}$  is steadily increased from its initial value of  $a_{\rm BF} = 1.16a_{\rm BB}$ . For (a)  $a_{\rm BF} = 1.16a_{\rm BB}$ , for (b)  $a_{\rm BF} = 1.17a_{\rm BB}$ , for (c)  $a_{\rm BF} = 1.18a_{\rm BB}$  and for (d)  $a_{\rm BF} = 1.2a_{\rm BB}$ .

where in the first term, the lower limit accounts for the nonzero fermion density around the core. The occurrence of profile swapping implies that

$$\int_{r_{\rm i}-\delta}^{r_{\rm i}+\delta} d\mathbf{r} u_{\rm BF} n_{\rm B} n_{\rm F} > \int_{0}^{r_{\rm i}+\delta} d\mathbf{r} u_{\rm BF} n_{\rm B} n_{\rm F}, \qquad (4.28)$$

at some value of  $a_{\rm BF}$ . In other words, like in binary mixtures of condensates, at some point the geometry of the overlap region determines the nature of the density profiles. To illustrate the various geometries discussed as a function of  $a_{\rm BB}$  and  $a_{BF}$ , the phase diagram of <sup>174</sup>Yb-<sup>173</sup>Yb mixture with with  $N_{\rm B} = N_{\rm F} =$  $10^6$  and  $\omega/(2\pi) = 400$ Hz is shown in Fig. 4.7. From the figure it is evident that the fermion pinching and profile swapping occur across a strip of parameter space. It lies between the domains of bosonic core and fermionic core. Among the different possible geometries, profile swapping initiated by tuning interspecies scattering length, appears to be a promising tool to study Rayleigh-Taylor type of instability [159, 160] in Bose-Fermi mixtures. For degenerate Bose-Fermi mixtures, the idea is to start with a ground state geometry with


Figure 4.7: The phase diagram of <sup>174</sup>Yb-<sup>173</sup>Yb mixture with  $N_{\rm B} = N_{\rm F} = 10^6$ and  $\omega/(2\pi) = 400$ Hz. Dashed (green) and dash-dotted (orange) curves are the semi-analytic conditions for mixing to partial demixing and demixing to phase separation (or full demixing) transitions, while solid (blue) is the numerically obtained criterion for mixing to partial demixing transition. In phaseseparated regime, for  $a_{\rm BB} \lesssim 750$  bosonic core is surrounded by fermionic shell, for  $750 \lesssim a_{\rm BB} \lesssim 1100$  there is fermion pinching along with profile swapping at  $a_{\rm BB} \approx 750$ . For  $750 \lesssim a_{\rm BB} \lesssim 1100$ , bosonic shell is surrounded by fermionic core and shell. For  $a_{\rm BB} \gtrsim 1100$ , fermionic core is surrounded by bosonic shell.

fermions forming the core, and then increase  $a_{\rm BF}$  so that the new ground state has the fermionic core swapped by bosonic one. In the next section, we explore similar idea to initiate and study Rayleigh-Taylor instability in phase-separated binary condensates.

### 4.2 Rayleigh-Taylor instability in binary condensates

Rayleigh-Taylor instability (RTI) sets in when a lighter fluid supports a heavier one in the gravitational field or when a lighter fluid pushes a heavier one. It leads to turbulent mixing of the two fluids as the perturbations at the interface grow exponentially. It is present across a wide spectrum of phenomena in nature. The turbulent mixing in astrophysics, inertial confinement fusion and geophysics originate from RTI. In superfluids RTI sets up crystallization waves at the superfluid-solid interface. This has been observed in <sup>4</sup>He [161]. Despite the ubiquitous nature and importance, controlled experiments with RTI are difficult and rare. However, we show that the TBECs or binary condensates in a trap are ideal systems for a controlled study of RTI in superfluids. In a recent work [162], the magnetic-field-gradient-induced RTI at the interface of the TBEC consisting of two hyperfine states of <sup>87</sup>Rb was analyzed. Another instability related to RTI, which has attracted growing interest, is the Kelvin Helmholtz instability (KHI). The prerequisites of KHI are phase separation and relative tangential velocities at the interface. Quantum KHI has been observed in experiments with <sup>3</sup>He [163] and recently studied theoretically for TBEC [164]. The other dynamical phenomena studied in TBECs include modulational instability [165, 166, 167, 168], pattern formation at the interface [169], countersuperflow instability [170, 171] and Richtmyer-Meshkov instability [172], etc. Among these, the countersuperflow instability was recently realized experimentally [173].

In this section, we will examine a different mechanism to set up RTI in TBECs and study its impact on the collective excitations. To initiate RTI we consider a TBEC, confined in a harmonic trapping potential, where all the interatomic interactions are repulsive. We choose the ground state in the immiscible domain as the initial state, i.e. phase-separated configuration where the species with the stronger intra-species repulsive interaction surrounds the other [174, 175]. Here the trapping potential is an analogue of the gravitational potential, and we may consider the species with the stronger intra-species repulsive interaction as the lighter fluid. We then increase the intra-species repulsive interaction of the inner species by increasing the scattering length through a Feshbach resonance. A critical state is reached when the repulsive interactions of the inner and outer species are equal. The system is unstable to any further increase as the intra-species repulsive interaction of the inner species is higher. This is the quantum analogue of RTI in fluid dynamics. As a case study, we choose the TBEC of <sup>85</sup>Rb-<sup>87</sup>Rb mixture. In this system, the <sup>85</sup>Rb intra-species interaction is tunable through a Feshbach resonance [176] and was recently used to study the miscibility [33] of the TBEC. More recently, the dynamical pattern formation during the growth of this system was theoretically investigated [168]. The other feature is that the inter-species  $^{85}$ Rb- $^{87}$ Rb interaction is also tunable and well studied [177]. Considering the parameters of the experimental realization, we choose the axisymmetric (cigar shaped) trap geometry.

#### 4.2.1 Phase-separated cigar shaped TBECs

To study RTI, we consider the phase-separated state  $(U_{12} > \sqrt{U_{11}U_{22}})$  in the axis symmetric trapping potentials with coincident centers, i.e. Eq. (3.1)

$$V_i(r,z) = \frac{m_i \omega^2}{2} (\alpha_i^2 r^2 + \lambda_i^2 z^2),$$

where  $\omega$  is the smaller of the two radial trapping frequencies, and  $\alpha_i$  and  $\lambda_i$ are the scaling factors of the radial and axial trapping frequencies respectively. We consider  $\alpha_i > \lambda_i$  to generate cigar shaped potentials, and  $U_{ij}$ 's are all positive. As elaborated in the previous chapter, when  $\alpha_i \gg \lambda_i$ , the interface of the phase-separated state is planar and species having larger scattering length sandwiches the other one [174]. This is clearly visible in the first column of Fig. 4.10, which shows the typical ground state density profile of the cigar shaped TBEC.

As mentioned earlier, we consider the parameters of the recent experiment [33] with <sup>85</sup>Rb and <sup>87</sup>Rb as the first and second species respectively, in the case study. In the experiment the radial trapping frequencies are identical  $(\alpha_i = 1)$ , and the scale factors or the anisotropy parameters of the axial trapping frequencies  $\lambda_1$  and  $\lambda_2$  are 0.022 and 0.020 respectively. The scattering lengths are  $a_{11} = 51a_0$ ,  $a_{22} = 99a_0$  and  $a_{12} = a_{21} = 214a_0$ , and we take  $N_i = 50,000$ . If  $z = \pm L_1$  are the equations of two interface planes located symmetrically about origin, one can calculate  $L_1$  using the method described in the previous chapter (see Sec. 3.1.1). For aforementioned set of parameter values, the plot in Fig. 4.8 shows the variation of E as a function of  $L_1$ . The value of  $L_1$  where minimum of E occurs is  $32.3a_{osc}$ . Here the unit of length  $a_{\rm osc} = \sqrt{\hbar/m_1 \omega}$  with the radial trapping frequency  $\omega = 130$  Hz. This is in agreement with the numerical result  $33.8a_{\rm osc}$  calculated using split-step Crank-Nicholson method with imaginary time propagation [120]. We refer to this state as *phase I*, where  ${}^{85}$ Rb and  ${}^{87}$ Rb are at the center and flanks respectively.

#### 4.2.2 Binary condensate evolution

In the fluid dynamics parlance, the gradient of the trapping potentials are the equivalents of gravity and the dynamics of the condensates is modelled as potential flows. The dynamical evolution of the interface is then described through a combination of the continuity equation, Euler's equation and Bernoulli's



Figure 4.8: The variation in energy E with  $L_1$  in phase-separated regime. The upward arrow indicates the position of minimum E at  $L_1 = 32.3a_{\text{osc}}$ . The inset shows the same plot along with the variation of  $\mu_1$  and  $\mu_2$  with respect to  $L_1$ , the magenta (light gray) and gray curves correspond to  $\mu_1$  and  $\mu_2$  respectively.

theorem with suitable boundary conditions [159, 160]. For a phase-separated TBEC with a planar interface along the xy-plane, from linear stability analysis a small perturbation at the interface have independent modes of the form  $A(s)e^{i(k_xx+k_yy)+st}$ . Here  $k_x$  and  $k_y$  are wave numbers along x and y coordinates, s is the temporal decay constant and A(s) is the amplitude of the mode. After solving the linearized equations [159, 160], we get

$$s = \pm \left[ \frac{\sqrt{k_x^2 + k_y^2} m \omega^2 \lambda^2 L_1(n_2 - n_1)}{n_1 + n_2} \right]^{1/2}.$$
 (4.29)

The densities of the condensates  $n_1$  and  $n_2$  are at a point  $(r, L_1)$  on the interface. Recollect that the  $n_1$  and  $n_2$  refer to the densities of the species at the center and flanks respectively. To simplify the analysis, we consider  $m_1 = m_2 = m$  and  $\lambda_1 = \lambda_2 = \lambda$  while deriving the above relation.

The decay constant s is imaginary and the interface is stable when  $n_1 > n_2$ but it oscillates when perturbed. However, when  $n_1 < n_2$  the value of s is real and any perturbation, however small, grows exponentially. This is the prerequisite for RTI in binary condensates. From the TF approximation, this condition is equivalent to  $a_{11} > a_{22}(\mu_1 - V)/(\mu_2 - V)$ . Here V is the trapping potential of the two species at the interface. In normal fluids with RTI, the lighter fluid rises to the top as bubbles and heavier fluid sinks as finger like extensions till the entire bulk of the lighter fluid is on top of the denser one. On the other hand, binary condensates in a similar situation evolve in a very different way.

To examine the dynamical evolution of the binary condensate with RTI, we choose phase I ( $a_{11} < a_{22}$ ) as the initial state. In this phase, the <sup>87</sup>Rb BEC at the flanks is considered as resting over the <sup>85</sup>Rb BEC at the center. To set up RTI, we increase  $a_{11}$  till  $a_{11} > a_{22}(\mu_1 - V)/(\mu_2 - V)$  through the  $^{85}\mathrm{Rb}-^{85}\mathrm{Rb}$  magnetic Feshbach resonance [176]. However, we maintain  $U_{12}>$  $\sqrt{U_{11}U_{22}}$  so that the TBEC remains in the immiscible domain. This is an unstable state, and we refer to this as the *phase Ia*. The stationary state of the TBEC corresponding to the new parameters is phase-separated and similar in structure to the initial state but with the species interchanged. Let us call the stationary state corresponding to the new parameters as phase II. The binary condensate should dynamically evolve from *phase Ia* to *phase II*. However, unlike in normal fluids with RTI, there are no bulk flows of either <sup>85</sup>Rb or <sup>87</sup>Rb atoms across the interface. Instead the condensates expands with interference effects and modulations. At the same time, there is tunnelling as well. These occur due to the coherence in the quantum liquids. To examine the evolution, we solve the pair of time-dependent GP equations

$$i\hbar \frac{\partial \Psi_i(r,z)}{\partial t} = \left[\frac{-\hbar^2}{2m_i}\nabla^2 + V_i(r,z) + \sum_{j=1}^2 U_{ij}|\Psi_j|^2\right]\Psi_i(r,z),$$
 (4.30)

which describe the dynamical evolution of the TBEC. During evolution the density profiles is approximated as

$$n_i(r, z) = n_i^{\rm eq}(r, z) + \delta n_i(r, z).$$
(4.31)

Here  $n_i^{\text{eq}}(r, z)$  and  $\delta n_i(r, z)$  are the equilibrium density and density fluctuations arising from the increase in  $a_{11}$  respectively. From the hydrodynamic approximations,  $\delta n_i(r, z)$  or the collective modes follow the equations

$$m_i \frac{\partial^2}{\partial t^2} \delta n_i = \boldsymbol{\nabla} n_i \cdot \boldsymbol{\nabla} \sum_{j=1}^2 U_{ij} \delta n_j + n_i \nabla^2 \sum_{j=1}^2 U_{ij} \delta n_i.$$
(4.32)

Consider  $\delta n_i(r, z, t) = b_i(t)r^l \exp(\pm il\phi)$  as the form of the solution. Here  $b_i(t)$  subsumes the time dependent part of the solution arising from the temporal

variation of the amplitude and l is an integer. Then as  $\nabla^2 \delta n_i = 0$ , only the first term on the right hand side remains in the equation. The profile of the interface acquires complex pattern as it evolves under the influence of RTI. This increases the area of the interface and couples the two species more strongly through the inter species interaction. Furthermore, as the inner species expands and penetrates in the outer species, the density decreases and hence the mean field energy. This damps the radial oscillations of the inner component. In the miscible phase, the evolution equation simplifies to

$$\ddot{b}_{i} = -\frac{l\omega^{2}}{U_{ii}} \left( U_{ii}b_{i} + U_{ij}b_{j} \right).$$
(4.33)

We can also get a similar set of coupled equations for the other form of the collective modes  $\delta n_i(r, z, t) = b_i(t)zr^{l-1}\exp(\pm i(l-1)\phi)$ . In this case, the prefactor is  $(l-1+\lambda_i^2)$  instead of l in the expression for  $\ddot{b}_i$ . In either of the cases, the equations are similar to two coupled oscillators. For the phase-separated state, the form of the TF solutions are significantly different from the miscible one. We resort to numerical schemes to solve the coupled-GP equations with RTI. An analytical description is difficult as the interface geometry evolves to a highly complex structure.

#### 4.2.3 Numerical results

TBEC evolution with RTI — To examine the evolution of TBEC with RTI, as mentioned earlier, we choose the *phase I* as the initial state. We then change  $a_{11}$  to  $80a_0$ ,  $102a_0$ ,  $200a_0$ ,  $306a_0$ ,  $408a_0$  and  $780a_0$ ; the last value is in the miscible parameter region. The dynamical variables which are the coarse grained representative of the evolution are  $r_{\rm rms}$  and  $z_{\rm rms}$ , the *rms* radial and axial sizes respectively.

When  $a_{11}$  is increased to  $80a_0$ , the <sup>85</sup>Rb condensate oscillates radially to accommodate excess repulsion energy. This is the only available degree of freedom as tight confinement, arising from <sup>87</sup>Rb at the flanks, along z-axis restricts axial oscillations. In TF approximation, the effective potential  $V_{\text{eff}} =$  $V + (\mu_2 - V)U_{12}/U_{22}$ . The angular frequency of the oscillation is  $\approx 0.32\omega$ . This is close to one of the eigen modes of the Bogoliubov equations. The temporal variation of  $r_{\text{rms}}$  is shown as the plots in the inset in Fig. 4.9. These show that the oscillations of the <sup>87</sup>Rb are sympathetically initiated and arise from the coupling between the two condensate species. The oscillations are more prominent with smaller number of atoms.



Figure 4.9: The temporal variation of  $r_{\rm rms}$  for <sup>85</sup>Rb and <sup>87</sup>Rb when  $a_{11}$  is changed from  $51a_0$  to  $408a_0$ . In the main plot, the upper and lower black curves correspond to evolution of the <sup>85</sup>Rb and <sup>87</sup>Rb respectively. The magenta (light gray) and red (gray) correspond to evolution with loss terms. The plot in the inset shows the variation in  $r_{\rm rms}$  of <sup>85</sup>Rb (gray) and <sup>87</sup>Rb (black) without loss terms.

There is a change in the nature of oscillations when the new value of  $a_{11}$ is such that  $a_{11} > a_{22}(\mu_1 - V)/(\mu_2 - V)$ . The corresponding stationary state has <sup>87</sup>Rb and <sup>85</sup>Rb at the core and flanks respectively. The  $r_{\rm rms}$  oscillation frequency is the same as in  $a_{11} < a_{22}$  case, but there is a temporal decay of the amplitude till it equilibrates. This is due to the expansion of <sup>85</sup>Rb along the z-axis and is an unambiguous signature of RTI. The expansion is clearly discernible in the density profile of the condensates shown in Fig. 4.10. The main plot in Fig. 4.9 shows temporal variation of  $r_{\rm rms}$  for  $a_{11} = 408a_0$ close to the miscible domain. There is a strong correlation between the decay rate and nature of oscillations. For  $a_{11}$  marginally larger than  $a_{22}$ , the <sup>85</sup>Rb condensate tunnels through the <sup>87</sup>Rb condensate, whereas at larger values the <sup>85</sup>Rb expands and spreads into the <sup>87</sup>Rb.

A dramatic change in the nature of the coupled oscillations occurs when  $U_{12} < \sqrt{U_{11}U_{22}}$ , that is when the TBEC is in the miscible domain. The <sup>85</sup>Rb expands through the <sup>87</sup>Rb cloud, and the two species undergo radial oscillations which have a beat pattern. Figure 4.11 shows the  $r_{\rm rms}$  when  $a_{11}$  is increased to 780 $a_0$ . Besides the radial oscillations, as to be expected when  $a_{11} > a_{22}(\mu_1 - V)/(\mu_2 - V)$ , the axial size  $z_{\rm rms}$  increases steadily. This accommodates the



Figure 4.10: Evolution of the TBEC with RTI. The first and second row are density profiles of <sup>85</sup>Rb and <sup>87</sup>Rb BECs respectively after increasing  $a_{11}$  to  $408a_0$ . Starting from left, the density profiles are at 0, 24.5, 49.0 and 73.5 ms after the increase of  $a_{11}$ .

excess repulsion energy along the axial direction. Along with the oscillations, there are density fluctuations reminiscent of modulational instability. It is to be mentioned that in earlier works [165, 167] modulational instability in the miscibility domain was analyzed in depth.

Evolution with loss terms — We also study the effect of loss terms, arising from the inelastic collisions, on the evolution of the condensate. There are two types of the inelastic collisions that lead to the loss of atoms from the trap: dipolar relaxation where the two atoms change their spin states after binary collision and three body recombination where three atoms collide, resulting in the formation of a diatomic molecule. To model the effect of loss of atoms from the trap, we add the phenomenological loss term

$$\frac{-i\hbar}{2} \left[ \sum_{j=1}^{2} K_{2(ij)} |\Psi_j(r,z)|^2 + K_{3i} |\Psi_i(r,z)|^4 \right], \qquad (4.34)$$

to right hand side of Eq. (4.30). Here  $K_{2(ii)}$  and  $K_{2(ij)}$  with  $j \neq i$  are the two body dipolar loss rate coefficients for collisions between same and different species, and  $K_{3i}$  are the three body recombination loss rate coefficients.

In the experiment by Papp et al. [33], it is possible to vary  $a_{11}$  from  $51a_0$ to  $900a_0$  by tuning the magnetic field in the range of 164.6-158.6 G [126]. In this range of the magnetic field,  $K_{2(22)}$  and  $K_{2(12)} = K_{2(21)}$  are approximately constant [178]. Based on a previous work [178], the inelastic two body loss rate coefficients of the <sup>85</sup>Rb-<sup>87</sup>Rb TBEC at the magnetic field of 161G are  $K_{2(11)} \simeq 10^{-14} \text{cm}^3 \text{s}^{-1}$ ,  $K_{2(22)} \simeq 4.5 \times 10^{-17} \text{cm}^3 \text{s}^{-1}$  and  $K_{2(12)} = K_{2(21)} \simeq$ 



Figure 4.11: The variation in  $r_{\rm rms}$  for <sup>85</sup>Rb and <sup>87</sup>Rb with time when  $a_{11}$  is increased from  $51a_0$  to  $780a_0$ . In the main plot, the upper and lower black curves correspond to evolution of <sup>85</sup>Rb and <sup>87</sup>Rb respectively. The magenta (light gray) and red (gray) curves correspond to the evolution with the loss terms.

 $1.6 \times 10^{-16} \text{cm}^3 \text{s}^{-1}$ . For  $K_{2(11)}$ , the maximum value occurs when  $a_{11}$  is  $51a_0$  and decreases at the most by an order of magnitude for higher values of  $a_{11}$ .

For the inelastic three body loss rate coefficients, value of  $K_{31}$  is minimum when  $a_{11}$  is  $51a_0$  [176] and changes by more than two order of magnitude for higher values of  $a_{11}$ , but  $K_{32}$  remains constant. From previous works, rate coefficients for <sup>85</sup>Rb and <sup>87</sup>Rb are  $1.7 \times 10^{-27}$ cm<sup>6</sup>s<sup>-1</sup> (near resonance) and  $3.8 \times 10^{-29}$ cm<sup>6</sup>s<sup>-1</sup> [179] respectively. Between the two loss mechanisms, within the magnetic field range of 158-162G the two body losses of <sup>85</sup>Rb dominate over three body losses [176]. Taking these factors into account, we consider the above mentioned loss rates as the appropriate values when  $a_{11}$  is increased to  $408a_0$  and  $780a_0$  in our numerical simulations. For the case of  $a_{11}$  increased to  $80a_0$ , we consider  $K_{2(11)} \simeq 2.5 \times 10^{-14}$ cm<sup>3</sup>s<sup>-1</sup> and  $K_{31} = 3.8 \times 10^{-31}$ cm<sup>6</sup>s<sup>-1</sup> while the other loss rate coefficients remain unchanged. We find that when RTI sets in, the nature of oscillations of  $r_{\rm rms}$  do not change significantly with the inclusion of loss term. The maximum change is  $\approx 4\%$  and this is evident from Fig. 4.9 and Fig. 4.11. This implies that the decay of  $r_{\rm rms}$  oscillation amplitude can be mainly ascribed to RTI and not to the loss of atoms from the trap.

#### 4.3 Summary of results

We have analyzed the equilibrium density profiles of the <sup>174</sup>Yb-<sup>173</sup>Yb Bose-Fermi mixture for a range of interaction strengths. In this Bose-Fermi mixture, it is possible to tune both the Bose-Bose and Bose-Fermi interactions across a range of values. Density profiles of the two species display pinching and position swapping when the boson-boson scattering length is close to  $a_{BB}^*$ , the value at which the spatial extent of the bosons is same as the fermions. Pinching occurs when the  $a_{BB}$  is marginally below  $a_{BB}^*$ ; at these values as  $a_{BF}$ is increased, fermions at the edges are pinched to form a thin shell, whereas at even lower values of  $a_{BB}$ , as  $a_{BF}$  is increased the fermions are expelled to the edge and density profiles are swapped. At intermediate values of  $a_{\rm BF}$  the profiles undergo through a series of configurations, and these are significantly different from the ones in Bose-Bose mixtures. We have also examined the onset of Rayleigh-Taylor instability in TBEC and identified the observable signature in the dynamics. Starting from  $a_{11} < a_{22}$ , RTI sets in when the TBEC is tuned to  $a_{11} > a_{22}(\mu_1 - V)/(\mu_2 - V)$  in the TF approximation. The damping of  $r_{\rm rms}$  oscillations of the species at the core marks the onset of RTI.

## Chapter 5

## Collective modes in variable potentials

Vortices are among the most fundamental topological defect structures in fluid flows. These occur in a variety of fluids at different length scales and in different settings. In BECs, vortices carry integral angular momenta and serve as evidence of superfluidity. Formation and dynamics of solitary and multiple vortices in single species condensates is well studied. An important development in vortex dynamics is the realization of vortex dipoles, a pair of vortex and anti-vortex, due to superfluid flow past an obstacle [180]. Furthermore, the recent development to observe vortex dipoles in real time [181] opens up the possibility to examine its dynamics. The vortex dipoles can also be considered as the embedded section of a vortex ring, which were first observed in BEC as the decay product of dark solitons [25]. Another phenomenon in superfluids, where vortex dipoles are crucial is transition to quantum turbulence. The initial requirement is the formation of multiple vortex dipoles, followed by reconnections to form a vortex tangle, which then leads to quantum turbulence [182]. In multi-component condensates, coreless vortices [183] and Skyrmions [184] have been experimentally observed in spinor condensates. Coreless vortices in multi-component spinless condensates are, however, yet to be experimentally realized.

In this chapter, we theoretically study the vortex dipole formation when a Gaussian obstacle moves across a phase-separated binary condensate. As a specific case, we consider the binary condensate consisting of <sup>85</sup>Rb and <sup>87</sup>Rb. In this one of the scattering lengths can be tuned by using magnetic Feshbach resonances [33]. This allows us to choose values of scattering lengths suitable for the generation of coreless vortex dipoles. Theoretically, the flow of the miscible binary and spinor condensates across a Gaussian obstacle potential has been investigated [185, 186, 187]. A related work is the seeding of vortex rings when a condensate bubble moves through the bulk of another condensate in binary condensates. This has been examined in a recent work [188]. The chapter is organized as follows: in Sec. 5.1, we derive the time dependent mean field equations for quasi two dimensional binary condensates, in Sec. 5.2, we theoretically describe the effects of obstacle potential on the density profile of the condensate in TF approximation; in the same section we discuss the obstacle assisted transport of one species across the other. It is followed by the Sec. 5.3 where we elucidate two different mechanisms leading to the coreless vortex dipole generation, and finally in the last section, we summarize the main results of the chapter.

#### 5.1 Binary condensates and vortex dipoles

Dynamics of weakly interacting binary condensate at zero temperature is well described by a set of coupled GP equations

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V_i(\mathbf{r},t) + \sum_{j=1}^2 U_{ij}|\Psi_j(\mathbf{r},t)|^2 - i\hbar\frac{\partial}{\partial t}\right]\Psi_i(\mathbf{r},t) = 0 \qquad (5.1)$$

in mean field approximation, where i = 1, 2 is the species index and rest of the symbols have the same meanings as used in earlier chapters. In the present chapter, we consider binary condensate consisting of <sup>85</sup>Rb and <sup>87</sup>Rb for which  $m_1 \approx m_2$ .

Furthermore, we also consider identical trapping potentials, which are axially symmetric, for both the species. The total potential is then

$$V(\mathbf{r},t) = \frac{m\omega^2}{2}(x^2 + \alpha^2 y^2 + \lambda^2 z^2) + V_{\rm obs}(x,y,t),$$

where  $V_{\text{obs}}(x, y, t) = V_0(t) \exp\{-2([x - x_0(t)]^2 + y^2)/w_0^2\}$  is the blue detuned Gaussian obstacle potential and  $\lambda$  is the anisotropy parameter. Like in previous two chapters, we define the oscillator length of the trapping potential  $a_{\text{osc}} = \sqrt{\hbar/(m\omega)}$ , and consider  $\hbar\omega$  as the unit of energy. We can then rewrite the equations in dimensionless form with transformations  $\tilde{\mathbf{r}} = \mathbf{r}/a_{\text{osc}}$ ,  $\tilde{t} = t\omega$  and  $\phi_i(\tilde{\mathbf{r}}, \tilde{t}) = \sqrt{a_{\text{osc}}^3/N_i}\Psi_i(\mathbf{r}, t)$ . From here on, we will represent the scaled quantities without tilde unless stated otherwise. In pancake-shaped traps ( $\lambda \gg 1$ ),  $\phi(\mathbf{r},t) = \psi(x,y,t)\zeta(z)\exp(-i\lambda t/2)$  [120], where  $\zeta = (\lambda/(2\pi))^{1/4}\exp(-\lambda z^2/4)$  is the ground state wave function in axial direction. The Eq. (5.1) can then be reduced to the two dimensional form

$$\begin{bmatrix} -\frac{1}{2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{x^2 + \alpha^2 y^2}{2} + V_{\text{obs}}(x, y, t) + \sum_{j=1}^2 u_{ij} |\psi_j(\mathbf{r}, t)|^2 \\ -i \frac{\partial}{\partial t} \end{bmatrix} \psi_i(\mathbf{r}, t) = 0, \quad (5.2)$$

where  $u_{ii} = 2a_{ii}N_i\sqrt{2\pi\lambda}/a_{\rm osc}$  and  $u_{ij} = 2a_{ij}N_j\sqrt{2\pi\lambda}/a_{\rm osc}$ . We consider  $u_{12} > \sqrt{u_{11}u_{22}}$  so that the ground state of the binary condensate is phaseseparated. As explained in the third chapter, geometry of the density distribution is such that the species with the lower repulsion energy forms a core and the other species forms a shell around it. For convenience, we identify the former and later as the first and second species respectively. With this labelling, interaction energies  $u_{11} < u_{22}$  and for equal populations, this implies  $a_{11} < a_{22}$ .

To be specific, we consider <sup>85</sup>Rb-<sup>87</sup>Rb binary condensate with  $a_{11} = 460a_0$ ,  $a_{22} = 99a_0$ , and  $a_{12} = 214a_0$  as the scattering length values and  $2N_1 = N_2 = 10^6$  as the number of atoms. Here  $a_{11}$  is tunable with magnetic Feshback resonance [126]. With these set of parameters, the stationary state of <sup>85</sup>Rb-<sup>87</sup>Rb binary condensate is just phase-separated. The trapping potential and obstacle laser potential parameters are same as those considered in Ref. [180], i.e.  $\omega/(2\pi) = 8$ Hz,  $\alpha = 1$ ,  $\lambda = 11.25$ ,  $V_0(0) = 93.0\hbar\omega$  and  $w_0 = 10\mu$ m. Hereafter in this chapter, we term this set of scattering lengths, number of atoms and trapping potential parameters as *set a*.

In hydrodynamics, the velocity field of a vortex dipole is the vector sum of two component fields. One of the fields arises due to the inhomogeneous density of the condensate and leads to the precession of an off center vortex around the trap center [189, 190]. In addition to this, each vortex has a velocity field which varies inversely with the distance from its center, which is experienced by the other vortex of vortex dipole. In our study, we move the obstacle along x-axis and generate vortex dipoles located symmetrically about x-axis. These vortex dipoles consist of pairs of singly charged vortices and antivortices. The energy associated with these vortex dipoles is of the order of trapping frequency, and hence these correspond to the collective modes of the BEC. If (x, y) and (x, -y) are the locations of the positively and negatively charged vortices of the vortex dipole respectively, then the velocity field of the positively charged vortex is

$$\mathbf{v}(x,y) = \omega_{\rm pr}\hat{k} \times \mathbf{r} + \frac{1}{2y}\hat{i},$$

where  $\omega_{pr}$  is the rotational frequency of a vortex with charge +1 in the condensate. A similar equation describes the velocity field of the negatively charged vortex.



Figure 5.1: Stationary state  $|\psi|$  of binary condenstate with obstacle potential at (a)  $-6.0a_{\text{osc}}$ , (b)  $-5.9a_{\text{osc}}$  and (c)  $-5.0a_{\text{osc}}$ .

#### 5.2 Obstacle modified condensate density

To analyze the density perturbations in presence of the obstacle beam, let  $R_{\rm in}$  be the radius of the inner species or the interface boundary. And, let  $R_{\rm out}$  be the radial extent of the outer species. In the absence of the obstacle beam, the chemical potential of first species is  $\mu_1 = R_{\rm in}^2/4 + u_{11}/(\pi R_{\rm in}^2)$ . Here, the second term is correction arising from the presence of the second species. The chemical potential of the second species is  $R_{\rm out}^2/2$ . Both of these are in scaled units. The theoretical approach to calculate  $R_{\rm in}$  and  $R_{\rm out}$ , based on TF approximation, has been outlined in appendix C. The obstacle beam initially (t = 0) located at  $(-R_{\rm out}, 0)$  traverses towards the center with velocity  $v_{\rm obs}$  and its intensity is ramped down at the rate  $\eta = -\partial V_0(t)/t$ . The location of

the beam at a later time is

$$x_0(t) = -R_{\rm out} + v_{\rm ob}t,$$
 (5.3)

and the intensity of the beam is

$$V_0(t) = V_0(0) - \eta t, \tag{5.4}$$

where  $V_0(0)$  is the initial intensity of the obstacle beam. At the starting point, the total potential  $V(R_{out}, 0, 0) > R_{out}^2/2$  and the density of the outer species  $|\psi_2|^2$  is zero around the center of the obstacle beam. However, as it traverses the condensates with decreasing intensity, at some later time t',  $V(x_0(t'), 0, 0) < R_{out}^2/2$ . Density  $|\psi_2|^2$  is then finite within the obstacle. For compact notations, hereafter we drop the explicit notation of time dependence while writing  $x_0(t)$  and  $V_0(t)$ .

#### 5.2.1 Density modification at interface

As the obstacle beam approaches the interface, the intensity is weak to expel out the outer species. However, when the beam enters the inner species with any finite intensity  $V(R_{\rm in}, 0, t) > \mu_1$ , it is sufficient to make  $|\psi_1|^2$  zero around the beam. The interface is modified and equipotential curve of the interface is

$$\frac{x^2 + y^2}{2} + V_0 \exp\left[-2\frac{(x - x_0)^2 + y^2}{w^2}\right] = \frac{R_{\rm in}^2}{2}.$$
(5.5)

Around the center of the obstacle beam  $\sqrt{(x-x_0)^2 + y^2} < w/\sqrt{2}$ , and the obstacle potential is

$$V_{\rm obs} \approx V_0 - \frac{2V_0}{w^2} \left[ (x - x_0)^2 + y^2 \right].$$
 (5.6)

Hence from Eq. (5.5) the equipotential curve in the neighborhood of the obstacle beam is

$$\left(x + \frac{C}{2A}\right)^2 + y^2 = \tilde{R}_{\rm in}^2,\tag{5.7}$$

where

$$A = \frac{1}{2} - \frac{2V_0}{w^2},$$
  

$$C = \frac{4V_0x_0}{w^2},$$
  

$$\tilde{R}_{in}^2 = \frac{1}{A} \left( \frac{R_{in}^2}{2} + \frac{C^2}{4A} + C\frac{x_0}{2} - V_0 \right)$$

Equipotential curve in the vicinity of the obstacle is thus modified into a circle with center at (-C/2A, 0) and radius  $\tilde{R}_{in}$ . In our numerical calculations, the Gaussian obstacle potential is quite narrow and  $w^2/(4V_0) \ll 1$ . Retaining only the leading order terms in  $w^2/4V_0$ , the center is approximately located at  $(x_0 + w^2 x_0/(4V_0), 0)$  and radius is

$$\tilde{R}_{\rm in} \approx \sqrt{\frac{w^2}{2V_0} \left(1 + \frac{w^2}{4V_0}\right) \left(V_0 + \frac{x_0^2}{2} - \frac{R_{\rm in}^2}{2}\right)}.$$
(5.8)

Sufficiently away from the obstacle,  $\sqrt{(x-x_0)^2 + y^2} > w/\sqrt{2}$  and the obstacle potential is negligible. The equipotential curve then remains unchanged,  $R_{\rm in}^2 = x^2 + y^2$ . Thus an approximate piecewise expression of the equipotential curve is

$$\left(x + \frac{C}{2A}\right)^2 + y^2 = \tilde{R}_{in}^2, \text{ if } |R_{in} - x_0| < \frac{w}{\sqrt{2}},$$
$$x^2 + y^2 = R_{in}^2, \text{ if } \sqrt{(x - x_0)^2 + y^2} > \frac{w}{\sqrt{2}}.$$
(5.9)

This expression defines the interface geometry in the TF approximation and has discontinuity at  $\sqrt{(x-x_0)^2 + y^2} = w/\sqrt{2}$ . Surface effects, however, smoothen the density profile around this point. The obstacle beam is repulsive and expels the condensate around it such that bulk density is regained over a distance of one healing length.

#### 5.2.2 Fully immersed obstacle beam

A critical requirement to form coreless vortices is complete immersion of the obstacle beam within the inner species. Based on the previous discussions, as the beam approaches the origin, the last point of contact between the beam and interface at  $R_{\rm in}$  lies along x-axis. To determine the condition when complete

immersion occurs, consider the total potential along x-axis

$$V(x,0,t) \approx \frac{x^2}{2} + V_0(t) \left[ 1 - 2\frac{(x-x_0(t))^2}{w^2} + 4\frac{(x-x_0(t))^4}{w^4} \right], \quad (5.10)$$

where the Gaussian beam potential is considered up to the second order term. The expression is appropriate in the neighborhood of the beam and has one local minima and maxima each. There is also a global minima, however, it is not the correct solution as it lies in the domain where  $x > \frac{w}{\sqrt{2}}$ , and hence Eq. 5.10 is no longer valid. Correct global minima is the one located at x = 0 and associated with the harmonic potential. The obstacle is considered well immersed when the local minima is located at the interfacial radius  $R_{\rm in}$ . The local minima is a root of the polynomial

$$x^3 + a_2 x^2 + a_1 x + a_0 = 0, (5.11)$$

obtained from the condition dV/dx = 0. Here,

$$a_{2} = -3x_{0},$$
  

$$a_{1} = -\frac{w^{2}}{2} + 3x_{0}^{2} + \frac{w^{4}}{8V_{0}},$$
  

$$a_{0} = \frac{1}{2}x_{0} \left(w^{2} - 2x_{0}^{2}\right).$$

For the trapping potential parameters considered in the present work, all the three roots are real. The root corresponding to local minima is

$$x_{\min}(t) = -\frac{(s_+ + s_-)}{2} - \frac{a_2}{3} + i\frac{\sqrt{3}}{2}(s_+ - s_-), \qquad (5.12)$$

where

$$s_{\pm} = \left[ -\frac{a_2^3}{27} + \frac{1}{6} \left( -3a_0 + a_1 a_2 \right) \pm \sqrt{\left(\frac{a_1}{3} - \frac{a_2^2}{9}\right)^3 + \left(-\frac{a_2^3}{27} + \frac{1}{6} \left( -3a_0 + a_1 a_2 \right) \right)^2} \right]^{1/3},$$

and  $x_{\min}$  is a function of time as the obstacle potential is time dependent. However, for compact notations like in  $V_0$  and  $x_0$ , hereafter we drop the explicit notation of time dependence while writing  $x_{\min}(t)$ . Value of  $x_{\min}$  is real when it satisfies certain conditions [191], and these are met for the experimentally realizable parameters. The obstacle is then completely immersed when  $x_{\min} = R_{\text{in}}$ , and let  $t_{\text{im}}$  denote the time at which this condition is satisfied. Once the obstacle beam is well inside the inner species, within the beam density of inner species  $(n_1)$  is zero but density of outer species  $(n_2)$  is nonzero. This leads to the formation of second interface layer, which embeds a bubble of the  $n_2$  within  $n_1$ . Recollect, the first interface layer is located at  $R_{\text{in}}$  and it is where  $n_2$  encloses  $n_1$ . The second interface, unlike the one at  $R_{\text{in}}$ , is a deformed-ellipse, and we label it as  $\Gamma$ . It touches x-axis at two points and  $x_{\min}$ is the one farther from the origin. From TF-approximation, the density of  $n_2$ within  $\Gamma$  is

$$n_{2\Gamma}(x, y, t_{\rm im}) = \frac{\mu_2 - V(x, y, t_{\rm im})}{u_{22}}, \qquad (5.13)$$

where the subscript  $\Gamma$  is to indicate the density is within  $\Gamma$ . At  $t_{\rm im} n_{2\Gamma}$  is in equilibrium with the bulk of  $n_2$ , and let the number of atoms within  $\Gamma$  be  $N_{2\Gamma}$ , which can be calculated from  $n_{2\Gamma}$ .

Except for deviations arising from mean field energy, the second interface  $\Gamma$  closely follows an equipotential surface. From the condition of pressure balance at two interfaces

$$\mu_{1} - \sqrt{\frac{u_{11}}{u_{22}}} \mu_{2} = \frac{R_{\text{in}}^{2}}{2} \left(1 - \sqrt{\frac{u_{11}}{u_{22}}}\right),$$
  
$$\mu_{1} - \sqrt{\frac{u_{11}}{u_{22}}} \mu_{2} = V(x_{\min}, 0, t) \left(1 - \sqrt{\frac{u_{11}}{u_{22}}}\right).$$
(5.14)

The first equation is valid all along the interface at  $R_{in}$ . However, the second is derived at  $(x_{\min}, 0)$ , but to a good approximation the condition is valid along  $\Gamma$  as it is close to an equipotential surface. The density of the first species at  $(x_{\min}, 0)$  is

$$n_1(x_{\min}) = \frac{1}{\sqrt{u_{11}u_{22}}} \left[ \frac{R_{\text{out}}^2 - 2V(x_{\min}, 0, t)}{2} \right].$$
 (5.15)

Similarly density of second species at at  $(x_{\min}, 0)$  is

$$n_2(x_{\min}) = \frac{1}{u_{22}} \left[ \frac{R_{\text{out}}^2 - 2V(x_{\min}, 0, t)}{2} \right].$$
 (5.16)

Inside  $\Gamma$ , where the obstacle potential is dominant,  $n_1$  decays exponentially.

Along the x-axis

$$n_1(\delta x_-, 0) = n_1(x_{\min}, 0) \exp\left(-\frac{2}{\Lambda_1}\delta x_-\right), \qquad (5.17)$$

where  $\delta x_{-}$  is the distance of the point measured from  $\Gamma$ . Similarly the density of the second species just outside  $\Gamma$  is

$$n_2(\delta x_+, 0) = n_2(x_{\min}, 0) \exp\left(-\frac{2}{\Lambda_2}\delta x_+\right), \qquad (5.18)$$

where  $\delta x_+$  is distance from  $\Gamma$  but away from the obstacle beam, and  $\Lambda_2$  is the penetration depth of the second species. In these expressions the penetration depth is

$$\Lambda_i = \xi_i \left[ \frac{\sqrt{a_{11}a_{22}}}{a_{12} - \sqrt{a_{11}a_{22}}} \right]^{1/2}.$$
(5.19)

Based on the densities at the interface region, we can incorporate the interspecies interaction and calculate the effective potential of each species.

#### 5.2.3 Obstacle assisted bubble

At a time  $\Delta t$  after the obstacle is immersed in  $n_1$ , the location and amplitude of the obstacle potential are

$$x_0(t_{\rm im} + \Delta t) = -R_{\rm out} + v_{\rm ob} \times (t_{\rm im} + \Delta t), \qquad (5.20)$$

$$V_0(t_{\rm im} + \Delta t) = V_0(0) - \eta \times (t_{\rm im} + \Delta t).$$
 (5.21)

Equilibrium TF  $n_2$  within the obstacle potential at this instant is

$$n_{2\Gamma}(x, y, t_{\rm im} + \Delta t) = \frac{\mu_2 - V(x, y, t_{\rm im} + \Delta t)}{u_{22}}.$$
 (5.22)

This, however, is higher than the density distribution at  $t_{\rm im}$ , that is  $n_{2\Gamma}(x, y, t_{\rm im} + \Delta t) > n_{2\Gamma}(x, y, t_{\rm im})$  as the potential V is lower. This is on account of two factors: first, the amplitude of the obstacle potential decreases with time; and second, the harmonic oscillator potential is lower at  $x_0(t_{\rm im} + \Delta t)$ . The number of atoms, however, does not change from the value at  $t_{\rm im}$  unless there is a strong Josephson current. Density  $n_{2\Gamma}$  is thus below the equilibrium value once the obstacle beam is well within  $n_1$ . This creates a stable bubble of  $n_2$  assisted or trapped within the beam and is transported across  $n_1$ .

Departure of  $n_2$  from the equilibrium is not the only density evolution within the beam. There is a progressive change of  $n_{1\Gamma}$  as the beam moves deeper into  $n_1$ . At time  $t_{\rm im}$ , when the obstacle is completely immersed in  $n_1$ the effective potential, experienced by  $n_1$ ,  $V(x, y, t_{\rm im}) + n_{2\Gamma}u_{12}$  is larger than  $\mu_1$ ; so  $n_1$  is zero within the beam. However, if the rate of ramping  $\eta$  is such that at a later time  $V(x, y, t_{\rm im} + \Delta t) + n_{2\Gamma}u_{12} < \mu_1$ , while the beam is still within  $n_1$ , there is a finite  $n_1$  within the beam.

$$n_{1\Gamma} = \frac{\mu_1 - V(x, y, t_{\rm im} + \Delta t) - u_{12}n_{2\Gamma}}{u_{11}}$$
(5.23)

As the growth of  $n_{1\Gamma}$  is in its nascent stage, Eq. (5.22) is still applicable. Since  $a_{12} > \sqrt{a_{11}a_{22}}$  for the condensate, in TF approximation both  $n_{1\Gamma}$  and  $n_{2\Gamma}$  can not be simultaneously non-zero. At the same time,  $n_{2\Gamma}$  is forbidden to migrate to the bulk  $n_2$  due to the  $n_1$  generated potential barrier in the region between interfaces  $\Gamma$  and  $R_{\rm in}$ . To accommodate both  $n_1$  and  $n_2$  within the beam, the shape of interface  $\Gamma$  is transformed to increase  $n_{2\Gamma}$ . So that  $n_2$  is zero in certain regions within the beam where the condition,  $V(x, y, t_{\rm im} + \Delta t) + n_{2\Gamma}u_{12} < \mu_1$  is satisfied. This mechanism is responsible for obstacle assisted transport of  $n_2$  across  $n_1$ .

#### 5.3 Formation of coreless vortex dipoles

To examine the formation of coreless vortex dipoles in finer detail, we resort to numerical solution of Eq. (5.2) with a modified version of the split-step Crank-Nicholson code reported in Ref. [120]. We consider obstacle potential is initially located in the outer component and is moved across the interface, towards the origin.

#### 5.3.1 Obstacle generated coreless vortex dipoles

For this case, we consider <sup>85</sup>Rb-<sup>87</sup>Rb binary condensate with parameters set a, however, with maximum value of obstacle laser potential  $V_0(0) = 125.0$ . The obstacle potential is initially located at  $x = -15a_{osc}$ . The obstacle moves with the speed of  $180\mu$ m/s, progressively decreases in strength with rate constant  $\eta = 10.1$  (in scaled units) and vanishes at  $x = 8a_{osc}$ . The obstacle potential creates a normal vortex dipole as it traverses  $n_2$ . As the obstacle penetrates the interface, it carries the vortex dipole generated in the outer component in



Figure 5.2:  $|\psi_i|$  and phase of binary condensates after the creation of coreless vortex dipole. (a) Coreless vortex dipole is fully formed but yet to dissociate from the obstacle, (b) center of obstacle beam is at origin and coreless vortex dipole is separated, (c) additional coreless vortex dipoles are generated when the obstacle reaches the interface, (d) phase of the binary condensate corresponding to (b), and (e) density of the condensates parallel to x-axis and passing through the center of the coreless vortex. Blue arrow marks the center of the coreless vortex dipole.

its region of influence. Further motion of the obstacle in  $n_1$  creates coreless vortices.

The key factor which influences the generation of coreless vortex dipoles is the deformation at the aft region of the obstacle confined  $n_2$ . The deformation accompanied by large mixing is initiated when the interface is about to break up. This is evident even in the stationary state density distribution shown in Fig. 5.1(b). At break up, the interface repulsion and potential gradient are highest along the x-axis and lead to the formation of a dimple. Curvature is large around the deformed interface, and flow of  $n_1$  past it generates vortex dipoles. However, as the vortex dipoles are generated within the penetration zone, the build up of  $n_1$  around the vortex core drives  $n_2$  from the penetration zone to the core of the vortex. For the parameters considered, first coreless vortex dipole is formed soon after the interface break up and is shown in Fig. 5.2(a) at t = 0.21s. The vortex dipole is almost detached when the obstacle reaches origin as is shown in Fig. 5.2(b). From the phase, Fig. 5.2(d), it is evident that the phase singularity is associated with  $\psi_1$  and  $\psi_2$  is non-zero at the core. This is seen in the plot of density along a line parallel to x-axis and passing through the vortex core in Fig. 5.2(e); the blue arrow in the figure marks the location of the vortex core. Another important density modification is, although the obstacle potential is repulsive,  $n_2$  has a maxima at the center. This is due to the repulsion energy from  $n_1$ . More coreless vortex dipoles are created when the obstacle crosses the center of harmonic potential as is shown in Fig. 5.2(c).

The other initial configuration is to place the obstacle potential within  $n_1$ . If  $V_{\text{obs}}$  is such  $\mu_1 < V(\mathbf{r}, t_0) < \mu_2$ , then within the obstacle potential  $n_2$  is nonzero. Initial density distribution is like in Fig. 5.1(c). Due to inertia,  $n_2$  lags behind the beam when the obstacle suddenly starts to move. When the obstacle has shifted from its initial position  $x_0$  to  $x_0 + \delta x_0$ , the points of intersection of the inner interfaces, located at  $x_0$  and  $x_0 + \delta x_0$  and assumed to be circular with a radius  $R_{\Gamma}$ , are

$$(x_c, y_c) = \left(\frac{1}{2}(2x_0 + \delta \mathbf{x}), \pm \frac{1}{2}\sqrt{4R_{\Gamma}^2 - \delta \mathbf{x}^2}\right).$$
(5.24)

Due to inertia  $n_2$  still occupies the region  $\delta\Gamma$  defined as

$$(x - x_0)^2 + y^2 < R_{\Gamma}^2 < (x - x_0 - \delta x)^2 + y^2$$

The potential experienced by  $n_2$  along the left interface of  $\delta\Gamma$  decreases as one moves from x-axis. This leads to redistribution of  $n_2$  in  $\delta\Gamma$  region and creation of a pressure difference  $\delta P = (n_1^2 u_{11} - n_2^2 u_{22})/2 \ge 0$  at the left bounding arc of  $\delta\Gamma$ . Along this arc,  $\delta P$  decreases from  $(x_0 - R_{\Gamma}, 0)$  to  $(x_c, y_c)$  and tends to flatten it. Another equally important dynamical process is the redistribution of  $n_1$  as  $V_{\text{eff}} = V(x, y) + n_2(x, y)u_{12}$  increases along the left interface from xaxis to  $(x_c, y_c)$ . Due to this,  $n_1$  starts to penetrate the interface from the point where  $V_{\text{eff}} \le \mu_1$ . Thus the repulsive interaction at the interface and gradient of harmonic potential combine to form a dimple on the interface. The dimple formation initiates the formation of (coreless) ghost vortices in the obstacle region [192], which detach to form coreless vortex dipole.

#### 5.3.2 Interface generated coreless vortices

This mechanism to generate the coreless vortices is observable only in the phase-separated binary condensates. We consider <sup>85</sup>Rb-<sup>87</sup>Rb with  $a_{11} = 80a_0$ ,  $N_1 = N_2 = 10^6$  and the rest of the parameters same as those defined in parameters set a. The obstacle is initially located at  $x = -12.5a_{osc}$  as is shown in Fig. 5.3(a). In our simulations, it moves with a speed of  $140 \mu m/s$ , continuously decreases in strength and finally vanishes at  $x = 5a_{osc}$ . The motion of the obstacle across the outer species initially generates a normal vortex dipole as is shown in Fig. 5.3(b). Since  $a_{12} \geq \sqrt{a_1 a_2}$  in the present case, the vortex dipole is is unable to penetrate the bulk of the inner species and is captured by the interface as is shown in Fig. 5.3(c) at  $t \approx 0.16$ s. As a result of this capture, the interface starts executing complex surface oscillations which in turn lead to the formation of protrusions and crevices on the interface [see Fig. 5.4(a)]. The protrusions on the interface, which penetrate the outer species, can move with the speed greater than the local sound speed for the outer species. When it happens, it can lead to the generation of coreless vortex dipoles in the outer species [see Fig. 5.4(b)]. It means that the protrusions, which are filled by the inner species, actually can the play the role of obstacle for the outer species. From the phase, Fig. 5.4(d), it is evident that the phase singularity is associated with  $\psi_2$  and  $\psi_1$  is non-zero at the core. This is also manifested in the plot of density along a line parallel to x-axis and passing through the vortex core as is shown Fig. 5.4(e). As  $a_{12} \gtrsim \sqrt{a_1 a_2}$ , detachment of the crevices on the interface, which are filled with outer species, is not energetically favorable. Hence this mechanism leads to the generation of coreless vortices in the outer species as is illustrated in Fig. 5.4(a-c).

#### 5.3.3 Summary of results

We have shown that the motion of the Gaussian obstacle across a phaseseparated binary condensate can lead to the generation of coreless vortex dipoles. We have identified two different mechanisms responsible for coreless vortex dipole generation. Depending upon the scattering length values of the component species, coreless vortices are generated in either inner or outer



Figure 5.3: (a)-(c) The absolute value of wavefunctions  $|\psi_i|$  for the binary condensate at different times, here (a) shows the binary condensate at t = 0s, (b) shows the binary condensate with a normal vortex dipole at t = 0.12s and (c) shows the capture of the normal vortex dipole by the interface at t = 16s. (d) and (e), both corresponding to figure (b), are the phase and density of the condensate parallel to x-axis and passing through the location of the vortex. The arrow in (c) indicates the location of the vortex at t = 0.12s.

species. Besides generating vortex dipoles, obstacle can also be used to create an obstacle assisted bubble of one species inside the bulk distribution of other.



Figure 5.4: The decay of surface oscillations of the interface into coreless vortices. (a)-(c) The absolute value of wavefunctions  $|\psi_i|$  for the binary condensate at different times, here (a) shows the fully formed protrusion at t = 0.39s, (b) shows the binary condensate after the detachment of the protrusion at t = 0.40s and (c) shows the coreless vortex dipole at t = 0.88s. (d) and (e), both corresponding to figure (c), are the phase and density of the condensate parallel to x-axis and passing through the location of the vortex. The arrow in (c) indicates the location of the coreless vortex at t = 0.88s.

## Chapter 6

### **Future directions**

We have shown that the critical temperature for Bose-Einstein condensation of an ideal gas in 3D quartic potential trap is higher than the critical temperature in isotropic harmonic potential trap. We have found that cross terms in the trapping potential increase critical temperature both in 2D and 3D geometries. In case of spin polarized fermionic alkali atoms, we have calculated the *p*-wave scattering length of <sup>6</sup>Li and <sup>40</sup>K for the  $a^{3}\Sigma_{u}^{+}$  and  $X^{1}\Sigma_{g}^{+}$  states respectively, using the variable phase method.

We have analyzed the static properties, with a special emphasis on the ground state geometry, of quantum degenerate Bose-Bose and Bose-Fermi mixtures. In case of Bose-Bose mixtures, we have described two semi-analytic methods with different domains of validity to determine the ground state geometry. In case of Bose-Fermi mixtures, we have considered <sup>174</sup>Yb-<sup>173</sup>Yb mixture to underline the phenomena of *fermion pinching* and *profile swapping*.

We have studied the initiation and the evolution of Rayleigh-Taylor instability in phase-separated binary condensates. We have identified <sup>85</sup>Rb-<sup>87</sup>Rb binary condensate as an apt candidate to explore it experimentally. In the phase-separated binary condensate, we have theoretically investigated the generation of coreless vortices, which are the collective excitations of the system, using a moving Gaussian obstacle. We have identified two different mechanisms leading to the coreless vortex dipole generation. One of these mechanisms where interfacial oscillations decay to create coreless vortices is peculiar to phase-separated binary condensates. In future, we shall study this particular mechanism in its finer detail. Another important question is the dynamical stability of these coreless vortices, which we plan to unravel in our future studies. Extending these studies to 3D geometries to examine vortex reconnections is also on our future agenda. It is well understood that solitons are dynamically unstable in 2D geometries due to the onset of *snake instability*. In future, one of our objective is to study *snake instability* of dark-bright solitons in phase-separated binary condensates.

## Appendix A

## Separated trap centers

In case of planar interface between the two species trapped in potentials with separated minima, the expressions for  $N_1$ ,  $N_2$  and E are:

$$N_1 = \frac{\pi}{60U_{11}\alpha_1^2} \left( 3\omega^2 (l_1^5 + L_1^5)m_1\lambda_1^4 - 20(l_1^3 + L_1^3)\lambda_1^2\mu_1 \frac{60(l_1 + L_1)\mu_1^2}{\omega^2 m_1} \right),$$

$$N_{2} = \frac{1}{3\lambda_{2}U_{22}}\pi \left[ \frac{8\sqrt{2}\mu_{2} \left(\frac{\mu_{2}}{\omega^{2}m_{2}}\right)^{3/2}}{5\alpha_{2}^{2}} + \frac{1}{20\omega^{2}m_{2}\alpha_{2}^{2}} \left(5\omega^{4}l_{1}^{5}m_{2}^{2}\lambda_{2}^{5} - \omega^{4}l_{1}^{4}m_{2}^{2}\lambda_{2}^{4}\right) \\ \times \left(15z_{0}\lambda_{2} + 8l_{1}\lambda_{2}\right) - 10z_{0}\omega^{2}l_{1}^{2}m_{2}\lambda_{2}^{3} \left(z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} - 6\mu_{2}\right) + 20z_{0}\lambda_{2} \\ \times \left(z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} - 3\mu_{2}\right)\mu_{2} + 60\lambda_{2}l_{1} \left(z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} - \mu_{2}\right)\mu_{2} + 10\omega^{2}l_{1}^{3}m_{2}\lambda_{2}^{3} \\ \times \left(-3z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} + 2\mu_{2}\right)\right)\right] - \frac{1}{3\lambda_{2}U_{22}}\pi \left[ -\frac{8\sqrt{2}\mu_{2} \left(\frac{\mu_{2}}{\omega^{2}m_{2}}\right)^{3/2}}{5\alpha_{2}^{2}} \\ + \frac{1}{20\omega^{2}m_{2}\alpha_{2}^{2}} \left(-5\omega^{4}L_{1}^{5}m_{2}^{2}\lambda_{2}^{5} + \omega^{4}L_{1}^{4}m_{2}^{2}\lambda_{2}^{4} \left(-15z_{0}\lambda_{2} + 8L_{1}\lambda_{2}\right) \\ - 10z_{0}\omega^{2}L_{1}^{2}m_{2}\lambda_{2}^{3} \left(z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} - 6\mu_{2}\right) + 20z_{0}\lambda_{2} \left(z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} - 3\mu_{2}\right)\mu_{2} \\ - 60\lambda_{2}L_{1} \left(z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} - \mu_{2}\right)\mu_{2} + 10\omega^{2}L_{1}^{3}m_{2}\lambda_{2}^{3} \left(3z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} - 2\mu_{2}\right)\right)\right],$$

$$E = \frac{1}{60U_{22}} \pi \left[ \frac{160\sqrt{2}\mu_{2}^{2}\sqrt{\frac{\omega^{2}\lambda_{2}^{2}m_{2}}{7\omega^{2}m_{2}\alpha_{2}^{2}}}{7\omega^{2}m_{2}\alpha_{2}^{2}} - \frac{1}{14\omega^{2}m_{2}\alpha_{2}^{2}} \left(21\omega^{6}l_{1}^{7}m_{2}^{3}\lambda_{2}^{6} + \omega^{6}l_{1}^{6}m_{2}^{3}\lambda_{2}^{6}\right) \\ \times \left(35z_{0} - 16l_{1}\right) + 7\omega^{4}l_{1}^{5}m_{2}^{2}\lambda_{2}^{4} \left(15z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} - 16\mu_{2}\right) + 7\omega^{4}l_{1}^{4}m_{2}^{2}\lambda_{2}^{4} \\ \times \left(25z_{0}^{3}\omega^{2}m_{2}\lambda_{2}^{2} + 16l_{1}\mu_{2}\right) + 7z_{0}\omega^{2}l_{1}^{2}m_{2}\lambda_{2}^{2} \left(3z_{0}^{4}\omega^{4}m_{2}^{2}\lambda_{2}^{4} - 40z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} \right) \\ \times \mu_{2} - 60\mu_{2}^{2} \right) - 14z_{0}\mu_{2} \left(3z_{0}^{4}\omega^{4}m_{2}^{2}\lambda_{2}^{4} + 10z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2}\mu_{2} - 40\mu_{2}^{2}\right) + 70l_{1} \\ \times \mu_{2} \left(-3z_{0}^{4}\omega^{4}m_{2}^{2}\lambda_{2}^{4} - 6z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2}\mu_{2} + 8\mu_{2}^{2}\right) + 35l_{1}^{3} \left(3z_{0}^{4}\omega^{6}m_{2}^{3}\lambda_{2}^{6} \right) \\ -4\omega^{2}m_{2}\lambda_{2}^{2}\mu_{2}^{2}\right)\right)\right] \\ + \frac{1}{60U_{22}}\pi \left[\frac{160\sqrt{2}\mu_{2}^{3}\sqrt{\frac{\mu^{2}}{\omega^{2}\lambda_{2}^{2}m_{2}}}{7\omega^{2}m_{2}\alpha_{2}^{2}} + \frac{1}{14\omega^{2}m_{2}\alpha_{2}^{2}} \left(-21\omega^{6}L_{1}^{7}m_{2}^{3}\lambda_{2}^{6} + \omega^{6}L_{1}^{6}m_{2}^{3}\lambda_{2}^{6} \right) \\ \times \left(35z_{0} + 16L_{1}\right) - 7\omega^{4}L_{1}^{5}m_{2}^{2}\lambda_{2}^{4} \left(15z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} - 16\mu_{2}\right) + 7\omega^{4}L_{1}^{4}m_{2}^{2}\lambda_{2}^{4} \\ \times \left(25z_{0}^{3}\omega^{2}m_{2}\lambda_{2}^{2} - 16L_{1}\mu_{2}\right) + 7z_{0}\omega^{2}L_{1}^{2}m_{2}\lambda_{2}^{2} \left(3z_{0}^{4}\omega^{4}m_{2}^{2}\lambda_{2}^{4} - 40z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2} \right) \\ \times \mu_{2} - 60\mu_{2}^{2}\right) - 14z_{0}\mu_{2} \left(3z_{0}^{4}\omega^{4}m_{2}^{2}\lambda_{2}^{4} + 10z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2}\mu_{2} - 40\mu_{2}^{2}\right) + 70L_{1} \\ \times \mu_{2} \left(3z_{0}^{4}\omega^{4}m_{2}^{2}\lambda_{2}^{4} + 6z_{0}^{2}\omega^{2}m_{2}\lambda_{2}^{2}\mu_{2} - 8\mu_{2}^{2}\right) - 35L_{1}^{3} \left(3z_{0}^{4}\omega^{6}m_{2}^{3}\lambda_{2}^{6} \right) \\ -4\omega^{2}m_{2}\lambda_{2}^{2}\mu_{2}^{2}\right)\right)\right]$$

These equations reduce to those for coincident centers on substituting  $l_1 = L_1$ and  $z_0 = 0$ .

## Appendix B Quasi-1D condensates

The energy of the TBEC in quasi-1D trap using ansatz Eq. (3.30) is

$$E = E_1 + E_2 + E_{12}, \tag{B.1}$$

where  $E_1$  and  $E_2$  are the energy contributions from the first and second component respectively, while  $E_{12}$  is inter-species interaction energy. The expressions for  $E_1$ ,  $E_2$  and  $E_{12}$  are:

$$E_{1} = \frac{\sqrt{\pi}N_{1}}{4} \left[ \frac{a^{2}}{b} + a^{2}b\lambda^{2}(b^{2} + \gamma^{2}) + \sqrt{2}a^{4}bg_{11} \right],$$
(B.2)  

$$E_{2} = \frac{\sqrt{\pi}N_{2}}{1024} \left\{ \frac{64}{d} \left[ 4f^{2} - 4cf(d^{2} - 2\delta^{2}) + c^{2}(7d^{4} + 20d^{2}\delta^{2} + 4\delta^{4}) \right] + 64d \left[ 4f^{2}(d^{2} + 2\delta^{2}) + 4cf(3d^{4} + 12d^{2}\delta^{2} + 4\delta^{4}) + c^{2} + (15d^{6} + 90d^{4}\delta^{2} + 60d^{2}\delta^{4} + 8\delta^{6}) \right] \lambda^{2} + \sqrt{2}d \left[ 256f^{4} + 256cf^{3} + (d^{2} + 4\delta^{2}) + 96c^{2}f^{2}(3d^{4} + 24d^{2}\delta^{2} + 16\delta^{4}) + 16c^{3}f + (15d^{6} + 180d^{4}\delta^{2} + 240d^{2}\delta^{4} + 64\delta^{6}) + c^{4}(105d^{8} + 1680d^{6}\delta^{2} + 3360d^{4}\delta^{4} + 1792d^{2}\delta^{6} + 256\delta^{8}) \right] g_{22} \right\},$$
(B.3)

$$E_{12} = \frac{\sqrt{\pi a^2 b d N_1 g_{12} e^{-\frac{(\gamma+\delta)^2}{b^2+d^2}}}}{4(b^2+d^2)^{9/2}} \left\{ 4d^8(f+c\gamma^2)^2 + 4b^2d^6 \left[ 4f^2 + cf(d^2+4\gamma^2-4\gamma\delta) + c^2\gamma^2(3d^2-4\gamma\delta) \right] + b^8 \left[ 4f^2 + 4cf(d^2+2\delta^2) + c^2(3d^4+12d^2\delta^2+4\delta^4) \right] + 2b^6d^2 \left[ 8f^2 + c^2(3d^4-8\gamma\delta^3-12d^2\delta\gamma+6d^2\delta^2) + 2cf(3d^2-4\delta\gamma+4\delta^2) \right] + b^4d^4 \left[ 24f^2 + 3c^2(d^4+4d^2\gamma^2-8d^2\gamma\delta+8\gamma^2\delta^2) + 4cf(3d^2+2\gamma^2-8\gamma\delta+2\delta^2) \right] \right\}.$$
(B.4)

The dependent parameter c is

$$c = \frac{2}{3d^5 + 12d^3\delta^2 + 4d\delta^4} \left[ -d^3f - 2df\delta^2 + \frac{1}{\sqrt{\pi}} \left( 3d^5\sqrt{\pi} - 2d^6f^2\pi + 12d^3\sqrt{\pi}\delta^2 - 8d^4f^2\pi\delta^2 + 4d\sqrt{\pi}\delta^4 \right)^{1/2} \right].$$
 (B.5)

## Appendix C

# Theoretical approach to calculate $R_{in}$

For simplicity of analysis, we assume that the obstacle is located at origin. Since the wavefunctions are normalized to unity, we have

$$1 = 2\pi \int_{\tilde{R}_{in}}^{R_{in}} \frac{\mu_1 - r^2/2}{u_{11}} r dr,$$
  

$$1 = 2\pi \left[ \int_0^{\tilde{R}_{in}} \frac{1}{u_{22}} \left( \mu_2 - Ar^2 - V_0 \right) r dr + \int_{R_{in}}^{\sqrt{2\mu_2}} \frac{\mu_2 - r^2/2}{u_{22}} r dr \right].$$
(C.1)

On integration, aforementioned equations yield

$$1 = \frac{\pi \left(\tilde{R}_{in}^2 - R_{in}^2\right) \left(\tilde{R}_{in}^2 + R_{in}^2 - 4\mu_1\right)}{4u_{11}},$$
  

$$1 = \frac{\pi \left(-2A\tilde{R}_{in}^4 + (R_{in}^2 - 2\mu_2)^2 - 4\tilde{R}_{in}^2 (V_0 - \mu_2)\right)}{4u_{22}},$$
 (C.2)

which can be solved to obtain  $\mu_i$ 's

$$\mu_{1} = \frac{\pi \tilde{R}_{\rm in}^{4} - \pi R_{\rm in}^{4} - 4u_{11}}{4\pi \left(\tilde{R}_{\rm in}^{2} - R_{\rm in}^{2}\right)},$$
  
$$\mu_{2} = \frac{\sqrt{(\pi + 2A\pi)\tilde{R}_{\rm in}^{4} + 4u_{22} - 2\pi \tilde{R}_{\rm in}^{2} \left(R_{\rm in}^{2} - 2V_{0}\right)}}{2\sqrt{\pi}} + \frac{R_{\rm in}^{2} - \tilde{R}_{\rm in}^{2}}{2} \quad (C.3)$$

Eq. (C.3) defines  $\mu_i$ 's in terms of  $R_{\rm in}$  and along with first equation of Eq. (5.14) defines the unique value of  $R_{\rm in}$  for given non-linearity parameters. For the



Figure C.1: Solid black curve shows the variation of  $\delta P = P_1 - P_2$  as a function of  $R_{\rm in}$ . The pressure becomes zero at  $R_{\rm in} = 8.5 a_{\rm osc}$ .

parameters set a, the value of  $R_{\rm in}$  thus obtained is  $8.5a_{\rm osc}$  as is shown in Fig. C.1. The values of  $\mu_1$ ,  $\mu_2$ ,  $\tilde{R}_{\rm in}$  and  $R_{\rm out}$  are 121.2, 165.7, 1.4 and 18.2 respectively, in scaled units.

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