Fragmentation and Merging Dynamics of Bose-Einstein Condensates with oscillating fields

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"In fact, it is often stated that of all the theories proposed in this century, the silliest is quantum theory. Some say that the only thing that quantum theory has going for it, in fact, is that it is unquestionably correct."

Michio Kaku

Hyperspace: A Scientific Odyssey Through Parallel Universes, Time Warps, and The Tenth Dimension (1994), 262

Certificate of Examination

This is to certify that the dissertation titled **Fragmentation and Merging Dynamics of Bose-Einstein Condensates with oscillating fields"** submitted by **Mr. Abhijeet Roy (Reg. No. MS12018)** for the partial fulfilment of BS-MS dual degree programme of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

Dr. Rajeev Kapri | Dr. K.R. Shamasundar | Dr. P. Balanarayan (Supervisor)

Dated: April 21, 2017

Declaration

The work presented in this dissertation has been carried out by me with Dr. P. Balanarayan at the Indian Institute of Science Education and Research Mohali. This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Abhijeet Roy
(Candidate)
Dated: April 21, 2017

In my capacity as the supervisor of the candidates project work, I certify that the above statements by the candidate are true to the best of my knowledge.

Dr. P. Balanarayan
(Supervisor)

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Abbreviations

BEC	**B**ose **E**instein **C**ondensate
ODLRO	**O**ff-**D**iagonal **L**ong **R**ange **O**rder
KH	**K**ramers-**H**enneberger
DVR	**D**iscrete **V**ariable **R**epresentation
GPE	**G**ross-**P**itaevskii **E**quation
TDGPE	**T**ime **D**ependent **G**ross-**P**itaevskii **E**quation
TDSE	**T**ime **D**ependent **S**chrödinger **E**quation
EUR	**E**ntropic **U**ncertainty **R**elations
BBM	**B**ialynicki-**B**irula **M**ycielski
MCTDHB	**M**ulti-**C**onfiguration **T**ime **D**ependent **H**artree for **B**osons

Dedicated to my family and friends

For their endless love, support and encouragement

Abstract

Bose-Einstein condensate is a very robust state of a bosonic system below a certain critical temperature. Bosons have a much higher tendency to get accommodated in a single non-degenerate state than the distinguishable particles. Therefore, it is very difficult to create stable fragmented condensates. But, there have been successful attempts to fragment or cut a single condensate experimentally by employing optical tweezers and knives. Fragmentation of a condensate naturally occurs when there are inherent degeneracies in a system. In this work, fragmentation of condensates is studied theoretically in the case of a symmetric double well trap. Fragmentation is shown to occur when a single well is made to oscillate very fast and with sufficiently large amplitude in the so-called Kramers-Henneberger framework. The dual-space information entropy for the condensate density is calculated for different oscillation parameters to understand the evolution of the state from a single condensate to a fragmented condensate. Besides, merging of fragmented condensates is also studied in the Kramers-Henneberger framework.

Chapter 1

Introduction

1.1 Brief History

In 1924, the Indian Physicist Satyendra Nath Bose derived the Planck's radiation law without any reference to classical physics. But this paper was rejected by the then scientific community. Therefore, he sent it to the then famous Albert Einstein. He immediately sensed the importance of the work and arranged for its publication [1]. He also extended Bose's ideas to matter. In 1925, Einstein predicted that cooling matter made up of particles with integer spin, now known as bosons, to very low temperatures would cause them to condense into a single quantum state resulting in a new form of matter —the Bose-Einstein condensate. In 1995, the first ever Bose-Einstein condensate was prepared in the lab [2][3][4] leading to a resurgence of interest in this field. Cornell, Wieman and Ketterle shared the 2001 Nobel Prize for their achievement of preparing the first BECs and studying their properties. From then on, Bose-Einstein condensation has emerged as an area of research of fundamental importance. BEC's have become critical systems for the study of many kinds of purely quantum mechanical properties.

1.2 Bose-Einstein condensation

Bose-Einstein condensation is a very peculiar phenomenon that occurs at a low temperature in bosonic systems. But the interesting thing about BEC transition is that it does not take place due to interactions but is purely a consequence of Bose-Einstein statistics. To quote Einstein verbatim, 'it is condensation without interaction' [5]. But interactions determine the properties of the condensate.

The phenomenon of Bose-Einstein condensation has at its roots the fact that bosons are indistinguishable and the bosonic many-body wavefunction is symmetric in nature [5].

$$\Psi(\epsilon_1, \epsilon_2) = \frac{1}{\sqrt{2}} \left[\phi(\epsilon_1, \epsilon_2) + \phi(\epsilon_2, \epsilon_1)\right] \tag{1.1}$$

where $\Psi(\epsilon_1, \epsilon_2)$ and $\phi(\epsilon_1, \epsilon_2)$ are the many-body wavefunctions and ϵ_1, ϵ_2 are the degrees of freedom of the system.

$$\Rightarrow |\Psi(\epsilon_1, \epsilon_2)|^2 = \frac{1}{2} \left[|\phi(\epsilon_1, \epsilon_2)|^2 + |\phi(\epsilon_2, \epsilon_1)|^2 + 2Re(\phi^*(\epsilon_1, \epsilon_2)\phi(\epsilon_2, \epsilon_1))\right] \tag{1.2}$$

$$\Rightarrow |\Psi(\epsilon, \epsilon)|^2 = 2|\phi(\epsilon, \epsilon)|^2 \tag{1.3}$$

For an N-body system,

$$|\Psi(\epsilon, \epsilon, ...\epsilon)|^2 = N! \, |\Psi(\epsilon, \epsilon, ...\epsilon)|^2 \tag{1.4}$$

This equation says that the probability for finding N bosons in the same state is very large as compared to that for distinguishable particles. Therefore, the bosons have a great tendency to condense into a single state when the single particle wavefunctions overlap [5], i.e, the de-Broglie wavelengths of the particles is lesser than or of the order of the inter-particle distance.

Bose-Einstein statistics is described by the distribution function

$$N_i = \bar{n}_i = \frac{1}{\exp\left[\beta(\epsilon_i - \mu)\right] - 1} \tag{1.5}$$

where N_i is the ensemble average of the occupation number in the ith state, n_i is the actual occupation number in the ith state for a particular microstate in the

ensemble and μ is the chemical potential of the system.

This shows that when $\mu \to \epsilon_0$, N_0 becomes very large, i.e., it becomes macroscopically occupied. So, the statistics itself leads to Bose Einstein condensation even in the absence of any interaction. The total number of particles can be written as

$$N = N_0 + N_T, \quad N_T = \sum_{i \neq 0} \bar{n}_i(T, \mu) \tag{1.6}$$

N_0 is the number of particles in the condensed state and N_T is the number of particles out of the condensate at temperature T and chemical potential μ and is proportional to the density of states and increases with the size of the system.

N_T is smooth with μ and reaches a maximum value of N_c at $\mu = \epsilon_0$. The temperature at which $N_c = N$ is called the critical temperature. Below this temperature, N_0 must rise abruptly leading to Bose-Einstein condensation.

1.3 Motivation and Plan of the Thesis

The theoretical starting point of studying BEC is the Gross-Pitaevskii equation which assumes a mean-field approximation. It is justified in cases where the condensates are dilute given by the condition $na^3 \ll 1$ which means that the range of interaction is far lesser than the average inter-particle distance [6][9]. For non-dilute condensates, beyond mean-field approach is required. But the GPE is quite accurate for dilute condensates close to absolute zero.

The condensates are described by an order parameter $\Psi = \rho e^{i\phi}$ where ρ represents the condensate density and ϕ describes the phase of the condensate. ϕ acts like a potential for velocity field [9]. This phase is not an observable by itself. The number-phase uncertainty relation $\Delta N \Delta\phi \approx 1$ does not allow the complete determination of both the parameters of the condensate but interference patterns emerge when two condensates are brought together as the two condensates get entangled in the detection process [8]. This makes the coherence in the condensate an important property to study.

An important theorem, irrespective of the equation by which the BECs are described, states that 'Given no internal symmetry present in the system, the ground

state of a condensate can be taken to be real, nodeless and non-degenerate.' [5] This theorem has great consequences. It means that the ground state is very robust and it is very difficult to fragment a condensate since the fragmented state has to compete with the single condensate for the ground state whenever there is degeneracy in the system [11]. This thesis tries to look at the question of fragmentation of condensates through a different framework.

The coherence in fragmented condensates cannot be understood by just computing the single-particle reduced density matrix [11]. Second-order correlation functions are necessary to characterise the coherence in the condensate [15]. It may be desirable to know the coherence properties of the condensates for quantum interference experiments, but it can be difficult to compute second-order correlation functions directly. Therefore, we try to study the coherence of the condensates in different states [11] by computing the information entropy [14] of the system. This is because information entropy is known to be a good measure of uncertainty when the probability distribution has sharp peaks with gaps in between, and this kind of distribution seems a good candidate for a fragmented state. Therefore, we seek to compute the dual-space information entropy of the condensate system when it evolves from one kind of state to another.

Kramers-Henneberger framework is a useful way to study the above evolution of condensate state. This framework has been used earlier to study fragmentation of condensates [10]. In this work also, this approach is used to study fragmentation of condensates as a function of an oscillation parameter of the single well trap which leads to a change in the trap potential [10]. The objective of this thesis is to try and understand how the dual-space information entropy of the condensate behave as the ground state of the system changes and to look for states which can have its dual-space entropy sum minimised within the mean-field approximation or equivalently, in the GP framework.

The work also tries to understand the dynamics of condensate merging when two independent condensates are brought together [27], thereby also explaining the mechanism of fragmentation when the opposite is done.

Chapter 2

Theoretical Framework

2.1 Bose-Einstein condensates and Density Matrix

An alternative and more general definition of BEC, other than all the bosons occupying a single state, is given in terms of the single particle reduced density matrix which is given, in the language of second quantisation, by [6]

$$\eta^{(1)}(\vec{r},\vec{r}') = \langle \hat{\psi}^{\dagger}(\vec{r})\hat{\psi}(\vec{r}')\rangle \tag{2.1}$$

where $\hat{\Psi}^{\dagger}(\vec{r})$ is the creation operator at position $\vec{r}$ and the $\hat{\Psi}(\vec{r}')$ is the annihilation operator at position $\vec{r}'$. The average is in quantum-statistical sense. This gives the probability amplitude that a particle at $\vec{r}$ is not distinguishable from a particle at $\vec{r}'$. This indistinguishability is not to be confused with the indistinguishability of the bosons. The expression of density matrix for pure and mixed states in terms of N-particle wavefunctions is derived from the above definition in Appendix A.

The density matrix elements can be written as [6]

$$\eta^{(1)}(\vec{r},\vec{r}') = \eta_0 {\phi_0}^*(\vec{r})\phi_0(\vec{r}') + \sum_i \eta_i {\phi_i}^*(\vec{r})\phi_i(\vec{r}') \tag{2.2}$$

where $\phi_i(\vec{r})$ are the eigenfunctions of the single particle reduced density matrix.

In the $N \to \infty$ limit, the sum goes to zero at large distances $s = |\vec{r} - \vec{r'}|$. This shows that the density matrix can have non-zero off-diagonal matrix elements only when a macroscopic occupation of a single particle state is achieved. This is called the Off-Diagonal long range order (ODLRO). This means that ODLRO implies BEC and vice-versa. Therefore, Bose-Einstein condensation is said to occur when the single particle reduced density matrix has a large eigenvalue and the eigenfunction of the reduced density matrix is then defined to be the order parameter or the wavefunction describing the condensate [6].

This is an important and subtle point because this feature of ODLRO is not present in Fermi systems where two-body interactions are essential to show ODLRO [5].

Macroscopic occupation of a single-particle state implies that the condensate wavefunction $\Psi_0(\vec{r})$ completely describes the system [6].

$$\Psi_0(\vec{r}) = |\Psi_0(\vec{r})|e^{i\phi(\vec{r})} \tag{2.3}$$

The modulus determines the contribution of the condensate to the diagonal density. The overall global phase $\phi(\vec{r})$ of the condensate wavefunction can be arbitrary as is reflected by its normalisation condition $\int dx_1...dx_N|\Psi|^2 = N$. Therefore, the phase does not have any physical meaning, but its fluctuations determine the velocity of the condensate [9].

$$v = \frac{\hbar}{m}\nabla\phi(\vec{r}) \tag{2.4}$$

Physically, ODLRO means that a global phase coherence is set up in the condensate system [6]. In fact, an ideal BEC has a globally constant phase throughout the system.

2.2 Gross-Pitaevskii equation

The dynamics of the condensate at zero temperature is generally described by the Gross-Pitaevskii equation which is effectively a mean-field approximation for the

inter-particle interactions [9].

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + g|\psi|^2\right)\psi \tag{2.5}$$

where ψ is a single particle state describing the condensate state where all the particles are accumulated and $g = \frac{4\pi\hbar^2 Na}{m}$ and a is the s-wave scattering length.

It can be derived using the Heisenberg equation for the field operators with the second quantised Hamiltonian and assuming a contact interaction [5]

$$i\hbar\frac{\partial\hat{\Psi}(\vec{r},t)}{\partial t} = \left[\hat{\Psi}(\vec{r},t), \hat{H}\right] \tag{2.6}$$

$$\hat{H} = \int\left[\frac{\hbar^2}{2m}\nabla\hat{\Psi}^\dagger\nabla\hat{\Psi} + \hat{\Psi}^\dagger V_{ext}(\vec{r})\hat{\Psi} + \frac{1}{2}\int\hat{\Psi}^\dagger\hat{\Psi}^{\dagger\prime}V(\vec{r}-\vec{r'})\hat{\Psi}\hat{\Psi}'d\vec{r'}\right]d\vec{r} \tag{2.7}$$

$$V(\vec{r}-\vec{r'}) = \delta^3(\vec{r}-\vec{r'}) \tag{2.8}$$

The Gross-Pitaevskii equation works well in case of dilute systems in which the range of interaction is far lesser than the average inter-particle distance. This diluteness criterion is mathematically written as $n|a|^3 << 1$. This assures that more than two-body scattering can safely be neglected and the actual form of the interaction potential is not important. Therefore,the s-wave scattering length characterizes all the effects of interaction on the physical properties of the gas.

But BEC can be understood even without using the second quantised formalism which seems appropriate to study many-body systems [9]. Bosons, when put in a configuration, get distributed in the energy levels of such a configuration, with an increasing occupation of the states with minimum energy as we lower the temperature. For sufficiently low temperature, an accumulation of particles in the ground state is observed before reaching absolute zero (when that is anyway bound to happen). In this way, they behave as macroscopic fluid with new properties such as superfluidity, etc. To study these properties, it is therefore necessary to concentrate only on the ground state.

Therefore, we need to find eigenvectors for the minimum eigenvalue of the Hamiltonian of our system, which includes all pairwise interactions. The interaction terms as such are difficult to handle rigorously. But when correlations are absent in the gas (i.e., if the gas is dilute), interactions can be approximated by the mean-field approximation.

Now, we derive the time-independent Gross-Pitaevskii equation from a variational approach by using the method of lagrange multiplier [9].

$$\hat{H} = \sum_{i=1}^{N} \left(\frac{\hat{p}^2}{2m} + V_{ext}(\vec{r_i}) \right) + \frac{1}{2} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} V\left(|\vec{r_i} - \vec{r_j}|\right) \tag{2.9}$$

Ground state energy can be found by minimizing the energy with a Lagrange multiplier or equivalently by minimizing the Free energy which can be defined as

$$F = E - \mu N \Rightarrow F = \langle \Psi | \hat{H} | \Psi \rangle - \mu N \langle \Psi | \Psi \rangle \tag{2.10}$$

μ - Lagrange multipier or the chemical potential of the condensate system.

Ψ - N-particle wavefunction of the system.

$$|\Psi\rangle = |\psi\rangle_1 \otimes |\psi\rangle_2 \otimes |\psi\rangle_3 ... \otimes |\psi\rangle_N \tag{2.11}$$

The interaction of a particle in a BEC with all the other $(N-1)$ particles are effectively the same in the mean field approximation since the quantum correlations are small. This is valid only when the gas is dilute otherwise the nearer particles interact more strongly than do the particles far away. So, the N-particle wave function can be approximated as

$$|\Psi\rangle = |\psi\rangle \otimes |\psi\rangle \otimes |\psi\rangle ... \otimes |\psi\rangle \tag{2.12}$$

Therefore, calculating the terms one by one using this approximation

$$\langle\Psi|\sum_{i=1}^{N}\frac{\hat{p}^2}{2m}|\Psi\rangle = \sum_{i=1}^{N}\frac{\hbar^2}{2m}\int\nabla\psi^*(\vec{r_i})\nabla\psi(\vec{r_i})d^3r_i \tag{2.13}$$

$$= -N\frac{\hbar^2}{2m}\int\psi^*(\vec{r})\nabla^2\psi(\vec{r})d^3r \tag{2.14}$$

$$\langle\Psi|\frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\j\neq i}}^{N}V(|\vec{r_i}-\vec{r_j}|)|\Psi\rangle = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\j\neq i}}^{N}\int d^3r_i\int d^3r_j\psi^*(\vec{r_j})\psi^*(\vec{r_i})V(|\vec{r_i}-\vec{r_j}|)\psi(\vec{r_i})\psi(\vec{r_j}) \tag{2.15}$$

$$= \frac{N(N-1)}{2}\int d^3r\psi^*(\vec{r})\left[\int d^3r\prime\psi^*(\vec{r\prime})\psi(\vec{r\prime})V(|\vec{r}-\vec{r\prime}|)\right]\psi(\vec{r}) \tag{2.16}$$

$$\langle\Psi|\sum_{i=1}^{N}V_{ext}(\vec{r_i})|\Psi\rangle = N\int\psi^*(\vec{r})V_{ext}(\vec{r})\psi(\vec{r})d^3r \tag{2.17}$$

$$\mu\langle\Psi|\Psi\rangle = \mu\left(\int d^3r\psi^*(\vec{r})\psi(\vec{r})\right)^N \tag{2.18}$$

Now, we need to minimize $F[\Psi] = E[\Psi] - \mu N\int d^3r\psi^*(\vec{r})\psi(\vec{r})$,

$$\frac{\delta F[\Psi]}{\delta\psi^*} = N\int[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + (N-1)\left(\int|\psi(\vec{r\prime})|^2V(|\vec{r}-\vec{r\prime}|)d^3r\prime\right) - \mu]\psi(\vec{r})\delta\psi^*(\vec{r})d^3r \tag{2.19}$$

For minimizing $F[\Psi]$, $\frac{\delta F[\Psi]}{\delta\psi^*} = 0$

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V_{ext}(\vec{r})\psi(\vec{r}) + N\frac{4\pi\hbar^2}{m}a|\psi(\vec{r})|^2\psi(\vec{r}) = \mu\psi(\vec{r})} \tag{2.20}$$

where $V(|\vec{r}-\vec{r\prime}|)$ is assumed to be a contact interaction.

$$V(|\vec{r}-\vec{r\prime}|) = \frac{4\pi\hbar^2}{m}a\delta(\vec{r}-\vec{r\prime}) \tag{2.21}$$

a - scattering length which measures the intensity of the interactions between the bosons

$a < 0$ means attractive potential

$a > 0$ means repulsive potential

Here we have used the normalization $\langle\Psi|\Psi\rangle = 1$ which means that probability density of finding a boson is $|\Psi|^2$.

We can also use the normalization $\langle\Psi|\Psi\rangle = N$ which means that number density of bosons is $|\Psi|^2$.

An alternative derivation in the language of second quantization is given in Appendix A. The Gross-Pitaevskii equation is a mean-field approximation to study condensates. Some approaches do not consider mean-field approximation, and they are necessary to study strongly correlated systems. But they are increasingly difficult to handle mathematically. For atomic gas BEC, the requirements to justify the mean-field approach is almost always met quite generally [6].

2.3 Fragmentation of Condensates

Due to Bose-statistics, non-interacting bosons always seek the lowest state even though many nearly degenerate states are nearby. Often, interactions do not destroy the condensates but just reduce the particle number in the ground state. The phenomenon of fragmentation of condensates is rare. It is because a single condensate is a state of minimum energy and ground state of a condensate system is non-degenerate given no internal symmetry is present in the system. But the above fact means that whenever there is inherent degeneracy in the system, there will be degenerate states competing for the ground state. This is where fragmentation can happen. In general, larger the degeneracy of the system, greater the probability of having fragmented condensates. But the presence of near degeneracy does not guarantee fragmentation [11].

The definition of condensation and fragmentation (due to Penrose and Onsager) is given in terms of the eigenvalues of the single particle reduced density matrix. When more than one eigenvalue is of the order N, then the state is fragmented. A simple system to study fragmentation of condensates is a symmetric double well potential. A simple two-mode Bose-Hubbard model can be used to model this

system [11]. The Hamiltonian is given by

$$\hat{H} = -t\left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1\right) + \frac{U}{2}\left[\hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2\right] \tag{2.22}$$

where $\hat{a}_i^\dagger$ creates a particle in well i and $\hat{a}_i$ annihilates a particle in well i. U is the interaction parameter. The first term is the tunnelling term and the second is the usual contact interaction. This simple model has wide applicability.

We can solve this model by the Wigner-Schwinger pseudospin representation as given below [11].

$$\hat{J}_x = \frac{1}{2}\left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1\right) \tag{2.23}$$

$$\hat{J}_y = \frac{1}{2i}\left(\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1\right) \tag{2.24}$$

$$\hat{J}_z = \frac{1}{2}\left(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2\right) \tag{2.25}$$

where J_x, J_y, J_z are angular momentum operators.

Computing $\hat{H}$ in this representation gives (Appendix B) [11]

$$\hat{H} = -2t\hat{J}_x + U\left(\hat{J}_z^2 + \hat{J}^2 - N\right) \tag{2.26}$$

$$\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \tag{2.27}$$

The mean field solution looks like [11]

$$|\theta, \phi\rangle = \frac{1}{\sqrt{N!}}\left(u\hat{a}_1^\dagger + v\hat{a}_2^\dagger\right)^N |0\rangle \tag{2.28}$$

$$u = e^{-i\phi/2}\cos(\theta/2), v = e^{i\phi/2}\cos(\theta/2) \tag{2.29}$$

The density matrix for this state (Appendix B) is given by [11]

$$\rho_{\mu\nu} = \begin{bmatrix} N\cos^2(\theta/2) & N\sin(\theta/2)\cos(\theta/2)e^{i\phi} \\ N\sin(\theta/2)\cos(\theta/2)e^{-i\phi} & N\sin^2(\theta/2) \end{bmatrix} \tag{2.30}$$

θ and ϕ characterize the density and phase difference between the bosons in the two wells respectively. In pseudospin language, θ and ϕ are the polar angles subtended by a unit vector in a spherical coordinate, describing the system in the mean field such that $\langle \hat{J} \rangle = (N/2)\hat{n}$.

The energy is given by [11]

$$E(\theta, \phi) = \langle \theta, \phi | \hat{H} | \theta, \phi \rangle = -tN \cos\phi \sin\theta + U \left(\frac{N^2}{4} \left(\cos^2\theta + 1 \right) - \frac{N}{2} \right) \tag{2.31}$$

For repulsive interactions, $U > 0$, $E(\theta, \phi)$ is minimum at $\phi = 0$, $\theta = \pi/2$. The mean field approach, therefore, selects the non-interacting ground state as optimal [11].

$$|C\rangle = \frac{1}{\sqrt{2^N N!}} \left(\hat{a}_1^\dagger + \hat{a}_2^\dagger \right)^N |0\rangle \tag{2.32}$$

The density matrix corresponding to this non-interacting state is [11]

$$\rho_{\mu\nu} = \frac{N}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \tag{2.33}$$

This matrix has a single macroscopic eigenvalue $\lambda = N$. Therefore, the non-interacting state is a single condensate.

The above ground state is a linear combination of number states [11]

$$|n_1, n_2\rangle = \frac{1}{\sqrt{n_1!\, n_2!}} \hat{a}_1^{\dagger n_1} \hat{a}_2^{\dagger n_2} |0\rangle \tag{2.34}$$

So, writing it in the number basis (Appendix B) [11]

$$|C\rangle = \sum_{l=-N/2}^{l=N/2} \Psi_l^0 |l\rangle \tag{2.35}$$

$$|l\rangle = |\frac{N}{2} + l, \frac{N}{2} - l\rangle \tag{2.36}$$

$$\Psi_l^0 = \left(\frac{N!}{2^N \left(\frac{N}{2} + l \right)! \left(\frac{N}{2} - l \right)!} \right)^{1/2} \approx \frac{e^{-l^2/N}}{(\pi N/2)^{1/4}} \tag{2.37}$$

This state has a number fluctuation [11]

$$\Delta N \approx \left(\int dl \frac{l^2 e^{-2l^2/N}}{\sqrt{\pi N/2}} \right)^{1/2} = \frac{\sqrt{N}}{2} \tag{2.38}$$

Therefore, the above mean-field solution corresponds to the solution for the non-interacting case ($U = 0$) in the Hamiltonian.

In the interacting case, the Schrödinger equation can be written in the number basis [11] (Appendix B)

$$\hat{H}\Psi = E\Psi \tag{2.39}$$

$$E\Psi_l = -t_{l+1}\Psi_{l+1} - t_l\Psi_{l-1} + Ul^2\Psi_l \tag{2.40}$$

$$t_l = t\sqrt{(N/2+l)(N/2-l+1)} \tag{2.41}$$

For repulsive interaction $U > 0$, the energy is minimized when $l = 0$. The tunnelling term t_l shows that hopping favours wavefunctions Ψ_l with large amplitudes near $l = 0$. [11]

The above analysis shows that repulsive interactions suppress number fluctuations which means that a state with unequal number of bosons in the two wells (like the non-interacting state with a number fluctuation —a Gaussian Ψ_l^0 with a width) is further squeezed (to a sharply peaked Gaussian around $l = 0$).

In the limit of zero fluctuations $\langle(\delta n_1)^2\rangle = \langle(\delta n_1)^2\rangle = 0$, the system becomes the Fock state [11].

$$|F\rangle = \frac{(\hat{a}_1^\dagger)^{N/2}(\hat{a}_1^\dagger)^{N/2}}{(N/2)!}|0\rangle \tag{2.42}$$

This state is clearly fragmented as can be seen from the density matrix for this state. This indicates separate condensation in each well.

$$\rho_{\mu\nu} = \frac{N}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.43}$$

The evolution of the coherent state can be seen from [11]

$$|\Psi_l(\sigma)\rangle = \frac{e^{-l^2/\sigma^2}}{(\pi\sigma^2/2)^{1/4}} \tag{2.44}$$

as σ^2 varies from N to $<< 1$. This transition is due to increase in phase fluctuations, ultimately leading to zero number fluctuations in the limit.

$$|C\rangle \Rightarrow \delta(\phi) \tag{2.45}$$

$$|F\rangle \Rightarrow uniform\ \phi \tag{2.46}$$

In the limit of tunnelling going to zero ($t = 0$), the above model shows that the ground state is again a coherent state (single condensate). It means that when the barrier height or the separation between the two wells is large, the system favours the formation of coherent states.

There can be another kind of fragmented states like Schrödinger cat states in case of attractive interaction. But the density matrix of such a state is identical to that of the Fock state. Therefore, fragmentation cannot be characterised by the single particle reduced density matrix alone, but higher order correlation functions like number fluctuations are also needed.

The phenomenon of fragmentation can be looked upon in a very different framework called the Kramers-Henneberger framework. This is the topic of the next section.

2.4 Kramers-Henneberger Transformation

The interaction of a charged particle with the electromagnetic field in the minimal coupling assumption is given by the Lagrangian [16]

$$L(q, \dot{q} = v) = \frac{1}{2}mv^2 + \frac{e}{c}\vec{A}(t).\vec{\nabla} - e\phi \tag{2.47}$$

where $\vec{A}$ and ϕ are the vector and scalar potentials respectively.

The canonical momentum is given by

$$p = \frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial v} = m\vec{v} + \frac{e}{c}\vec{A} \tag{2.48}$$

Therefore, the classical Hamiltonian for a charged particle in an electromagnetic field is

$$H(q,p) = \frac{\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2}{2m} + e\phi \tag{2.49}$$

In going over to Quantum mechanics, we replace the $\vec{p}$ with $-i\hbar\nabla$ in the position representation. The Schrödinger equation is

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \hat{H}(\vec{r},t)\psi(\vec{r},t) \tag{2.50}$$

When we substitute the Quantum Hamiltonian got above after making the substitution, the Schrödinger equation for an electron in presence of an electromagnetic field becomes

$$\frac{1}{2m}\left[i\hbar\vec{\nabla} + \frac{e}{c}\vec{A}(t)\right]^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t) = i\hbar\frac{\partial\psi}{\partial t}(\vec{r},t) \tag{2.51}$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\nabla^2 + i\hbar\frac{e}{mc}\vec{A}(t).\nabla + \frac{e^2}{2mc^2}\vec{A}^2(t) + V(\vec{r})\right]\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} \tag{2.52}$$

because $\vec{A}$ is a function of t only (assuming dipole approximation [17]) and so commutes with ∇.

But, let us say, we want the time dependent terms only in the potential term of the Schrödinger equation. So, we do a unitary transformation on the system [13]. Physically, it amounts to changing to an accelerated frame of reference moving with the electron and therefore experiencing a time-dependent potential.

$$\Psi = \hat{\Omega}\psi \tag{2.53}$$

where

$$\Omega = \exp\left[\frac{i}{\hbar}\int_{-\infty}^{t}\left\{\frac{i\hbar e}{mc}\vec{A}(\tau).\nabla + \frac{e^2}{2mc}\vec{A}^2(\tau)\right\}d\tau\right] \tag{2.54}$$

Now, due to dipole approximation (the so called long-wavelength approximation)

$$\Omega = \Omega_1\Omega_2 \tag{2.55}$$

$$\Omega_1 = \exp\left[-\int_{-\infty}^{t} \frac{e}{mc}\vec{A}(\tau)d\tau.\nabla\right] \tag{2.56}$$

$$\Omega_2 = \exp\left[\frac{i}{\hbar}\int_{-\infty}^{t} \frac{e^2}{2mc^2}\vec{A}^2(\tau)d\tau\right] \tag{2.57}$$

Now, let us find out the $\hat{H}_{new}$ acting on the transformed wavefunction due to the unitary transformation.

$$i\hbar\frac{\partial\Psi}{\partial t} = i\hbar\frac{\partial\left(\Omega\psi\right)}{\partial t} = i\hbar\frac{\partial\Omega}{\partial t}\psi + \Omega\left(i\hbar\frac{\partial\psi}{\partial t}\right) = \left[i\hbar\frac{\partial\Omega}{\partial t}\Omega^\dagger + \Omega H\Omega^\dagger\right]\Psi \tag{2.58}$$

$$\Rightarrow \hat{H}_{new} = i\hbar\frac{\partial\Omega}{\partial t}\Omega^\dagger + \Omega H\Omega^\dagger \tag{2.59}$$

The $i\hbar\frac{\partial\Omega}{\partial t}\Omega^\dagger$ term cancels the time dependent terms that come from the $\Omega H\Omega^\dagger$. But the term that needs some effort is $\Omega V(\vec{r})\Omega^\dagger$. Let us evaluate it

$$\Omega V(\hat{r})\Omega^\dagger = \Omega_1 V(\hat{r})\Omega_1^\dagger = e^{\hat{\beta}}V(\hat{r})e^{-\hat{\beta}} \tag{2.60}$$

where $\hat{\beta} = -\int_{-\infty}^{t}\frac{e}{mc}d\tau\vec{A}(\tau).\nabla$

The above equation can be written in terms of a series by using the Baker-Campbell-Hausdorff formula which is given by [18]

$$e^{\hat{\beta}}\hat{\gamma}e^{-\hat{\beta}} = \hat{\gamma} + \left[\hat{\beta},\hat{\gamma}\right] + \frac{1}{2!}\left[\hat{\beta},\left[\hat{\beta},\gamma\right]\right] + ... \tag{2.61}$$

Evaluating the commutators one by one

$$\left[\hat{\beta},\hat{\gamma}\right] = -\int_{-\infty}^{t}\frac{e}{mc}d\tau\vec{A}(\tau).\left[\nabla, V(\hat{r})\right] = \left(\vec{\alpha}.\nabla\right)V(\vec{r}) \tag{2.62}$$

$$\frac{1}{2!}\left[\hat{\beta},\left[\hat{\beta},\gamma\right]\right] = \frac{1}{2!}\left(\vec{\alpha}.\nabla\right)^2 V(\vec{r}) \tag{2.63}$$

where

$$\vec{\alpha} = -\int_{-\infty}^{t}\frac{e}{mc}\vec{A}(\tau)d\tau \tag{2.64}$$

$$\Rightarrow \ddot{\vec{\alpha}} = \frac{e}{mc}\vec{E}(t) = \frac{e}{mc}\vec{E}_0\sin\omega t \tag{2.65}$$

$$\Rightarrow \vec{\alpha}(t) = \frac{e\vec{E}_0}{m\omega^2 c}\sin\omega t = \vec{\alpha}_0\sin\omega t \tag{2.66}$$

So, the Baker-Campbell-Hausdorff series actually gives a Taylor's series of $V(\vec{r})$ about $\vec{r}$ and acts as a translation operator and translates the potential by $\vec{\alpha}$. Therefore, the Kramers-Hanneberger transformation leads to the final Schrödinger equation of the form [13]

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r}+\vec{\alpha})\right]\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} \tag{2.67}$$

$$\Rightarrow \left[\frac{-\hbar^2}{2m}\nabla^2 + V^{KH}(\vec{r},t)\right]\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} \tag{2.68}$$

where $V^{KH}(\vec{r},t) = V(\vec{r}+\vec{\alpha})$ is called the Kramers-Henneberger potential.
The above equation has the time dependence only in the potential term as opposed to the original equation we started with. Therefore, one can now attempt to find a time independent approximation to the above equation to solve for the zeroth-order KH state. This state can then serve as a ground state for further perturbative approximations which is justified as opposed to the situation of applying perturbation theory at the outset in a case where the perturbation (intensity) is very high as compared to the ground state Hamiltonian.
The full Kramers-Henneberger potential can be written as [20]

$$V^{KH}(x,t) = V_0(x) + V_{pert}(x,t) \tag{2.69}$$

$$= \frac{\omega}{2\pi}\int_0^{2\pi/\omega} V^{KH}(x,t)dt + \sum_{\substack{m=-\infty \\ m\neq 0}}^{\infty} V_m(x)e^{im\omega t} \tag{2.70}$$

$$= \frac{\omega}{2\pi}\int_0^{2\pi/\omega} V^{KH}(x,t)dt + \frac{\omega}{2\pi}\sum_{\substack{m=-\infty \\ m\neq 0}}^{\infty}\left(\int_0^{2\pi/\omega} V^{KH}(x,t')e^{-im\omega t'}dt'\right)e^{im\omega t} \tag{2.71}$$

This effective potential (averaged out potential) in the quantum picture analogous to the classical Kapitza problem was defined by Gillary and Moiseyev. There can be found more time-independent terms like this as shown below.

The Schrödinger equation in the Kramer-Henneberger frame is given by

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \left[\frac{\hat{p}^2}{2m} + V_0^{KH}(\vec{r}) + \sum_{\substack{n=-\infty \\ n\neq 0}}^{n=\infty} V_n(\vec{r})e^{in\omega t}\right]\psi_0^{KH}(\vec{r},t) \tag{2.72}$$

To remove the time dependent harmonics from the Hamiltonian we apply the unitary transformation

$$\hat{U}_{(1)}(\vec{r},t) = \exp\left[\sum_{\substack{n=-\infty \\ n\neq 0}}^{n=\infty} \frac{1}{\hbar n\omega} V_n(\vec{r})e^{in\omega t}\right] = e^{S(\vec{r},t)} \tag{2.73}$$

Now the new Hamiltonian is given by

$$\hat{H}_{new} = i\hbar\frac{\partial\hat{U}_{(1)}}{\partial t}\hat{U}_{(1)}^{\dagger} + \hat{U}_{(1)}\hat{H}\hat{U}_{(1)}^{\dagger} \tag{2.74}$$

$$\Rightarrow \hat{H}_{new} = -\frac{\hbar^2}{m}\left[\frac{\nabla^2}{2m} + \frac{1}{2}\nabla^2\hat{S} + \nabla\hat{S}.\nabla - \frac{1}{2}\nabla\hat{S}.\nabla\hat{S}\right] + \hat{V}_0^{KH} \tag{2.75}$$

The extra time-independent term comes only from the fourth term in the parenthesis. The time-independent Hamiltonian is given by

$$\hat{H}(\vec{r}) = -\frac{\hbar^2}{2m}\left[\nabla^2 - \frac{1}{(\hbar\omega)^2}\sum_{\substack{n=-\infty \\ n\neq 0}}^{n=\infty} \frac{\nabla V_n.\nabla V_{-n}}{n^2}\right] + \hat{V}_0^{KH} \tag{2.76}$$

$$\nabla V_n = \frac{\omega}{2\pi}\int_0^{2\pi/\omega} \left(\nabla V^{KH}(x,t')\right) e^{-in\omega t'}dt' \tag{2.77}$$

The Kramers-Henneberger transformation was motivated by the situation of a charged particle in an electromagnetic field. But the argument presented can be used in a very general way. A charged particle in an electromagnetic field (plane wave) is in no way different, in principle, from a particle in an oscillating trap. Therefore, the same transformation can be applied in the other case.

If the frequency of the oscillation is sufficiently large, the time-dependent terms do not make a significant contribution because of their increasingly oscillating behaviour. The zeroth order time-independent potential can then describe the

system very well under high-frequency conditions. So, a time-dependent problem becomes a time-independent problem.

To go back to the lab frame, we need to back transform the wavefunction obtained by solving the time-independent problem in the KH frame. But the probability density remains unaffected. Therefore, the original time-dependent problem can be more easily solved by a time-independent approach by the Kramers-Henneberger transformation when the frequency is sufficiently high.

2.5 Calculation of time-independent Kramers-Henneberger potential

We choose a harmonic potential with an upper bound of the form [10]

$$V(x,y,z) = \left\{ \begin{array}{cc} \frac{1}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right) & V < V_c \\ V_c & V \geq V_c \end{array} \right\} \tag{2.78}$$

The trap is assumed to be highly anisotropic such that that ω_x and ω_y are much larger than ω_z. Therefore, the system is quasi-one dimensional, i.e., we assume that the transverse excitations are absent when trap oscillations are in the z-direction. For this trap potential, the time-independent Kramers-Henneberger potential can be found, as discussed above, by integrating (numerically) the full KH-potential

$$V_0^{KH}(x) = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} V^{KH}(x,t)dt \tag{2.79}$$

We perform this integration using the Gauss-Legendre Quadrature in a Discrete Variable Representaion (DVR) grid. The time-independent KH potential for different values of the oscillation parameter α_0 is shown below.

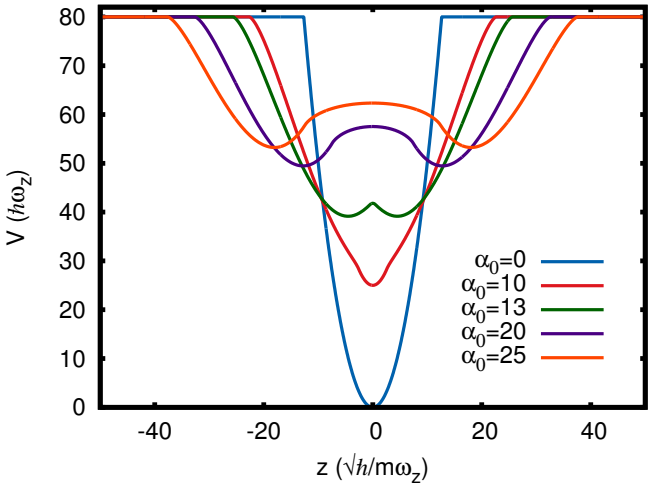

FIGURE 2.1: Effective time-independent potential

Therefore, the fast oscillation of the trap is forming a double well out of a single well given the amplitude is sufficiently high. It means that this mechanism can lead to the formation of stable dichotomic states which further means that we can get fragmented condensates out of a single condensate when the condensate formed in the single well trap is driven by fast oscillations of the trap. But the oscillations has to be switched on adiabatically so that the ground state of the condensate system evolves to the ground state of the transformed Hamiltonian. We show this by numerically solving the Gross-Pitaevskii equation for the time-independent KH-potential shown above in the DVR grid.

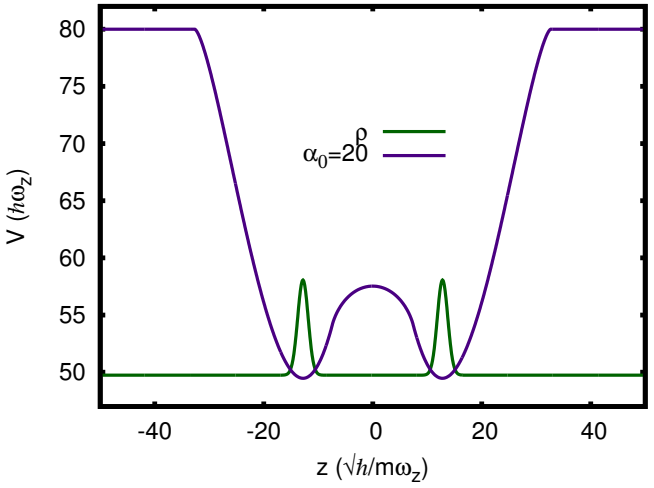

FIGURE 2.2: Dichotomy of the condensate density

This kind of probability densities which has sharp peaks with wide gaps in between is vulnerable to giving nonsensical results when the variance of the position operator is used as an indicator of the uncertainty in the measurement of the position of the particle. This is because variance depends upon the gap in between the peaks and increases with it indicative of the fact that the uncertainty in the measurement of the variable is increasing. But as the gap increases, the peaks themselves get sharpened individually meaning that the uncertainty in the measurement of the position gets smaller. It means that using variances to compute the uncertainties is not a good measure in these situations.

Entropic uncertainties are free from this defect, and hence they are a better, if not the best, measure of uncertainties especially for these kinds of distributions [19]. The entropic uncertainty relations are the topic of the next section where the idea is elaborated.

2.6 Entropic Uncertainty Relations

There are many measures of Uncertainty in Quantum Mechanics. Variance is a standard measure of uncertainty as in Heisenberg's Uncertainty Principle. Likewise, Information Entropy is also a measure of Uncertainty. There are several ways to define Information Entropy. One of the famous and simple ways was given by Shannon. For discrete probabilities, Shannon Information entropy is defined as [19]

$$S = -\sum_i p_i \ln p_i \tag{2.80}$$

given the following conditions

1. $0 \leq p_i \leq 1$
2. $\sum_i p_i = 1$

The definition can be understood as follows [19]

1. The negative sign in the definition implies that uncertainty in measurement is related to the missing information about the variable.
2. When the probability of a certain event occurring is 1, i.e., the event is certain to happen, then $S = 0$. This shows that the uncertainty in the measurement of the variable is zero as expected.
3. When the probability distribution is uniform, S is maximum. This shows that the uncertainty in the measurement of the variable is maximum is such a case.
4. Sharper the distribution, lesser is the uncertainty.

For continuous position and momentum probability distributions, Shannon Information Entropies are defined as

$$S[\rho] = S_\rho = -\int d\rho \rho(\vec{r}) \ln \rho(\vec{r}) \tag{2.81}$$

$$S[\gamma] = S_\gamma = -\int d\gamma \gamma(\vec{k}) \ln \gamma(\vec{k}) \tag{2.82}$$

where $\rho(\vec{r})$ and $\gamma(\vec{k})$ are position and momentum space probability distributions. The fourth feature of the entropic measure of uncertainty remains valid even when the distribution is such that there exist wide gaps between sharp peaks. This is not the case with variance being used as a measure of uncertainty. Therefore, our use of entropic uncertainty to study the probability distributions in case of double well bosonic systems is well justified.

A generalized uncertainty relation in terms of the dual space information entropies of probability distributions was given by Białynickii-Birula and Mycielski [14]

$$S_\rho + S_\gamma \geqslant n\,(1 + ln\pi) \tag{2.83}$$

This relation is a part of a general relation which also gives Heisenberg's uncertainty relation as a by-product.

$$\frac{2}{n}\langle(\vec{k} - \langle\vec{k}\rangle)^2\rangle \geq (e\pi)^{-1} \exp\left(\frac{2}{n}S_\gamma\right) \geq (e\pi) \exp\left(-\frac{2}{n}S_\rho\right) \geq \frac{n}{2}(\langle(\vec{r} - \langle\vec{r}\rangle)^2\rangle)^{-1} \tag{2.84}$$

The first and the last term in this relation gives the Heisenberg's uncertainty relation. The mid-two terms gives the entropic uncertainty relation. The derivation of the above uncertainty relation is given in Appendix C.

Let us see some important features of Fourier transforms of some special kinds of wavefunctions relevant to our study before presenting the results of $\rho(z)$, $\gamma(k_z)$, S_ρ and S_γ.

2.7 Fourier Transforms

1. Gaussian wavefunction

$$\psi(x) = A\exp\left(-\frac{1}{2}\left(\frac{x-\alpha}{\beta}\right)^2\right) \tag{2.85}$$

$$\tilde{\psi}(k) = \frac{A}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx e^{ikx}\exp\left(-\frac{1}{2}\left(\frac{x-\alpha}{\beta}\right)^2\right) \tag{2.86}$$

The normalized probability densities corresponding to these wavefunctions are

$$\rho(x) = \frac{1}{\beta\sqrt{\pi}}\exp\left(-\left(\frac{x-\alpha}{\beta}\right)^2\right) \tag{2.87}$$

$$\gamma(k) = \frac{\beta}{\sqrt{\pi}}e^{-\beta^2k^2} \tag{2.88}$$

2. Double Gaussian wavefunction

$$\psi(x) = A\left[\exp\left(-\frac{1}{2}\left(\frac{x-\alpha}{\beta}\right)^2\right) + \exp\left(-\frac{1}{2}\left(\frac{x+\alpha}{\beta}\right)^2\right)\right] \tag{2.89}$$

$$\tilde{\psi}(k) = A\int_{-\infty}^{\infty} dx e^{ikx}\left[\exp\left(-\frac{1}{2}\left(\frac{x-\alpha}{\beta}\right)^2\right) + \exp\left(-\frac{1}{2}\left(\frac{x+\alpha}{\beta}\right)^2\right)\right] \tag{2.90}$$

The normalized probability densities corresponding to these wavefunctions are (shown in Appendix C)

$$\rho(x) = \frac{1}{2\beta\sqrt{\pi}\,(1+e^{-\alpha^2/\beta^2})}\{\exp\left(-\left(\frac{x-\alpha}{\beta}\right)^2\right)$$

$$+\exp\left(-\left(\frac{x+\alpha}{\beta}\right)^2\right)+2\exp\left(-\frac{x^2+\alpha^2}{\beta^2}\right)\} \tag{2.91}$$

$$\gamma(k) = \frac{2\beta}{\sqrt{\pi}\,(1+e^{-\alpha^2/\beta^2})}e^{-\beta^2k^2}\cos^2(k\alpha) \tag{2.92}$$

Now, let us see some general remarks on Fourier transforms. This follows from the above and similar calculations.

1. The probability density corresponding to the Fourier transform of a Gaussian wavefunction is again a Gaussian with an inverse width.

2. The probability density of a Double Gaussian wavefunction is in general a double Gaussian with an extra modulated Gaussian profile in the centre. This will be prominent when we plot the solutions of the Gross-Pitaevskii equation for different oscillation parameters corresponding to different α's.

3. The probability density corresponding to the Fourier transform of a Double Gaussian wavefunction is an Oscillatory Gaussian. This will also be clear when we plot the results of the calculations with the Gross-Pitaevskii equation.

4. Increasing the distance between the peaks in the position space density leads to increase in oscillations in the momentum space densities.

5. If the position space probability distribution function $\rho(x)$ is oscillatory, the momentum space probability distribution function $\gamma(k)$ is two separated oscillatory Gaussians.

6. More oscillations in $\rho(x)$ does not increase the separation between the Oscillatory Gaussians in $\gamma(k)$ but increase the oscillations in the Gaussians individually and also squeeze them more.

Chapter 3

Results and Discussion

3.1 Solving the Gross-Pitaevskii equation

Time-independent Gross-Pitaevskii equation is solved for the cut harmonic potential trap [10].

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + g|\psi|^2\right)\psi = \mu\psi \tag{3.1}$$

where $g = \dfrac{4\pi\hbar^2 Na}{m}$ and a is the s-wave scattering length.

$$\begin{aligned} V_{ext}(x,y,z) &= \frac{1}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right) && V < V_c \\ &= V_c && V \geq V_c \end{aligned}$$

To solve this equation, we first do a rescaling of the original equation to dimensionless units [22] as shown below.

$$\vec{r} = a_z \vec{r_1} \tag{3.2}$$

$$E = h\omega_z E_1 \tag{3.3}$$

$$\psi(\vec{r}) = \sqrt{\frac{N}{a_z^3}}\psi_1(\vec{r_1}) \tag{3.4}$$

$$\mu = \hbar\omega_z \mu_1 \tag{3.5}$$

where $a_z = \left(\frac{\hbar}{m\omega_z}\right)^{1/2}$ and $\hbar\omega_z$ are the characteristic length scale and energy scale of the problem.

The equation in rescaled dimensionless units in one dimension looks as follows

$$\left(-\frac{1}{2}\nabla_1^2 + V_{ext}(\vec{r}_1) + \frac{4\pi aN}{a_z}|\psi_1|^2\right)\psi_1 = \mu_1\psi_1 \tag{3.6}$$

The assumption used in solving this equation as already discussed previously is that the potential is very anisotropic so that the transverse excitations are absent and hence the system is effectively one-dimensional. The one-dimensional equation in rescaled units looks as follows

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial z_1^2} + V_{ext}(z_1) + \frac{4\pi aN}{a_z}|\psi_1|^2\right)\psi_1 = \mu_1\psi_1 \tag{3.7}$$

This equation is solved by the grid-based approach. We make a Discrete Variable Representation (DVR) grid [17] using the 'particle in a box eigenfunctions' [21]. In this method, the potential energy and the non-linear term is a local operator due to which they are diagonal matrices with the diagonal entries corresponding to their values at the grid points. But the Kinetic energy matrix has to be found. The kinetic energy matrix evaluation has already been done by Colbert and Miller (1991) [21] and the kinetic energy matrix for a grid $z \to (-\infty, \infty)$ is shown to be (Appendix A)

$$T_{ii'} = \frac{\hbar^2}{2m\Delta z^2}(-1)^{i-i'}\left\{\begin{array}{ll} \pi^2/3, & i = i' \\ \dfrac{2}{(i-i')^2}, & i \neq i' \end{array}\right\} \tag{3.8}$$

where grid spacing $\Delta z = \dfrac{b-a}{N}$ with $a \to -\infty$, $b \to \infty$ and $N \to \infty$ being finite. The trap V_{ext} that we use is the zeroth order Kramers-Henneberger potential for the cut harmonic trap as already discussed in the previous chapter. We diagonalize the resulting Hamiltonian in the DVR grid iteratively. The converged eigenvalues and the corresponding eigenfunctions are the solutions to the time-independent Gross-Pitaevskii equation for different oscillation parameters α_0.

Finally, we do Fourier transformation of the obtained eigenfunctions thereby getting both the probability densities $\rho(\vec{r})$ and $\gamma(\vec{k})$ from which the S_ρ and S_γ can be calculated by numerical integration for which we use Simpson's integration rule.

3.2 Merging Dynamics

The fragmentation of condensates in the presence of fast and wide oscillations can also be understood if we consider the exactly opposite phenomenon of merging of two separated condensates. In this case, two separately prepared condensates are brought together by merging the traps [27], which can again be understood via the Kramers-Henneberger frame which says that the time-averaged effect of fast oscillations of a double well leads to a single well. The fragmented (separated) condensate is the eigenstate of the double well potential which evolves to a single condensate which is the eigenstate of the single well trap. This can be well understood in the light of the adiabatic theorem in quantum mechanics in the limit of adiabatic switching of the trap oscillation. But even if the merging is non-adiabatic as the real case may be, the high differences in the energy eigenstates of the Hamiltonian is shown to limit the occupation of only a few low-lying levels, and this ultimately leads to the formation of a state with the dominant number of particles in the condensate mode [27]. This fixing of the phase difference between the initially separated condensates with ambiguous phase relationship enhances the fraction of particles in the condensate mode making it a potentially useful way to build a continuous atom laser [27].

The Gross-Pitaevskii equation assumes that all the particles of the condensate occupy the same (ground) state whereas the multi-configurational Hartree equations go beyond the mean-field approach and do not assume the occupancy of only a single state. It allows for the occupancy of more than one state in the condensed mode. The MCTDHB package can solve the time-dependent Gross-Pitaevskii equation as well as multi-configurational Hartree equations for bosons. The merging dynamics is shown later in the next section.

3.3 Results and Discussion

3.3.1 Dual space probability densities and entropy

We first show the plots for $\rho(z)$ and $\gamma(k_z)$ for different α_0 and explain their behaviour as α_0 increases. Later, we also show $S_\rho + S_\gamma$ as a function of α_0.
As α_0 increases beyond the point where the upper cut of the harmonic trap is located, $\gamma(k_z)$ starts becoming sharper than $\rho(z)$.

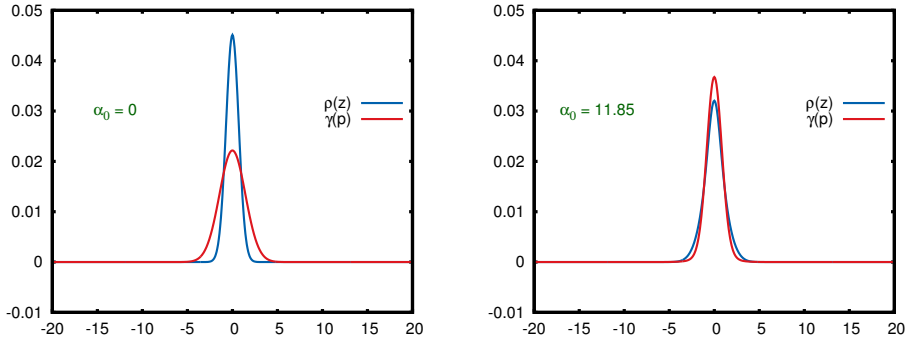

FIGURE 3.1: $\rho(z)$ & $\gamma(p)$ **(3.1a)** $\alpha_0 = 00.000$ **(3.1b)** $\alpha_0 = 11.850$

On increasing α_0, ρ_z becomes much more dispersed thus leading to a sharp increase in S_ρ. This also makes $\gamma(k_z)$ more squeezed leading to sharp increase in S_γ. Further increasing α_0 makes the modulated Gaussian at the center prominent and therefore $\gamma(k_z)$ starts picking oscillations as was discussed in the section on Fourier transforms of Double Gaussian (point 2).

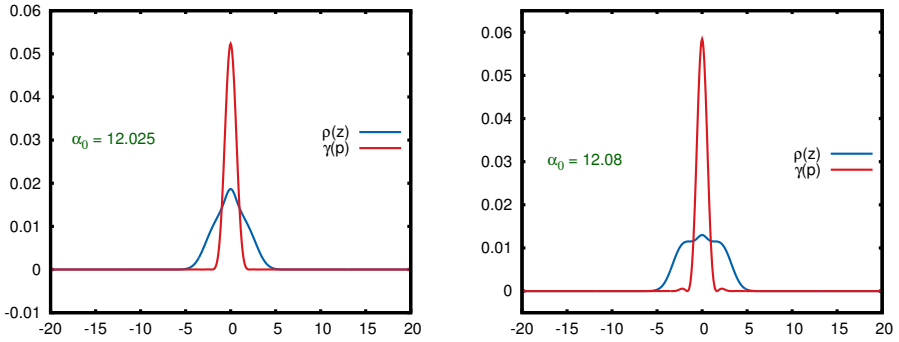

FIGURE 3.2: $\rho(z)$ & $\gamma(p)$ **(3.2a)** $\alpha_0 = 12.025$ **(3.2b)** $\alpha_0 = 12.080$

Increasing α_0 further would start reducing the central bump in S_ρ as can be seen below.

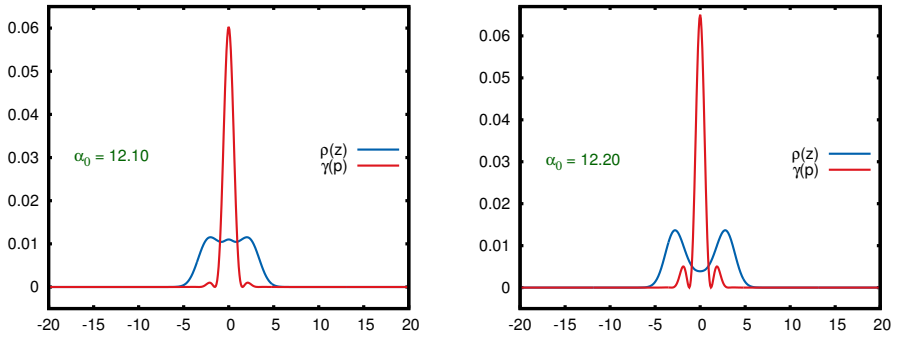

FIGURE 3.3: $\rho(z)$ & $\gamma(p)$ **(3.3a)** $\alpha_0 = 12.100$ **(3.3b)** $\alpha_0 = 12.200$

As we increase the α_0 further, ρ_z begins to move towards a fragmented state and more oscillations set in $\gamma(k_z)$. ρ_z starts becoming dichotomic and therefore S_ρ starts to decrease and due to increasing oscillations S_γ increases more.

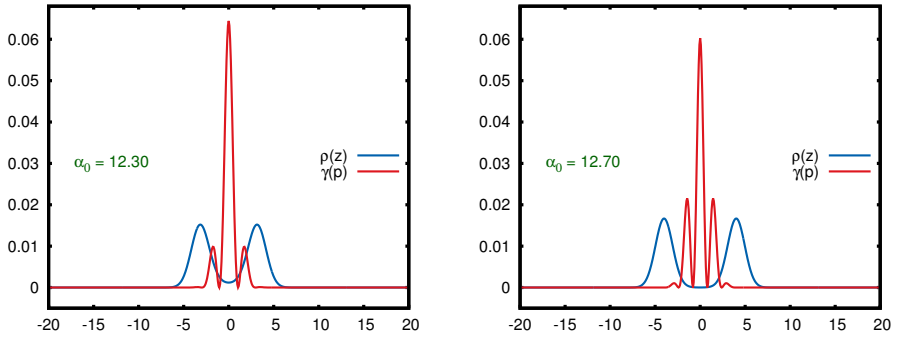

FIGURE 3.4: $\rho(z)$ & $\gamma(p)$ **(3.4a)** $\alpha_0 = 12.300$ **(3.4b)** $\alpha_0 = 12.700$

The separation between the two lobes increases with the lobes individually getting more squeezed, due to which S_ρ decreases further. $\gamma(k_z)$ gets more oscillatory due to this as discussed in the section on Fourier transforms thus increasing S_γ.

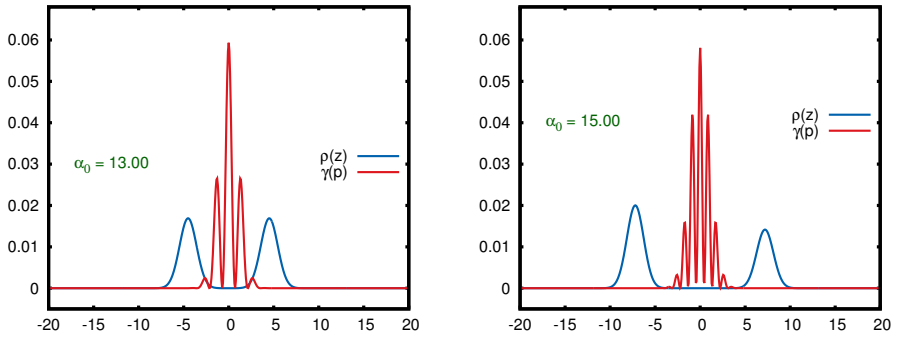

FIGURE 3.5: $\rho(z)$ & $\gamma(p)$ **(3.5a)** $\alpha_0 = 13.000$ **(3.5b)** $\alpha_0 = 15.000$

Increasing the α_0 further shows the same trend and both S_ρ and S_γ begins to saturate as $\rho(z)$ becomes more and more squeezed in the individual lobes and $\gamma(k_z)$ becomes more and more oscillatory. The interesting feature that comes out further at this point is that $\rho(z)$ is not anymore a state with an equal number of particles in the two wells. This feature is expected and already discussed in the section on fragmented condensates. Therefore, the state will again evolve towards a single condensate. Both the kind of states as shown below are equally probable because they are nearly degenerate in this range of α_0.

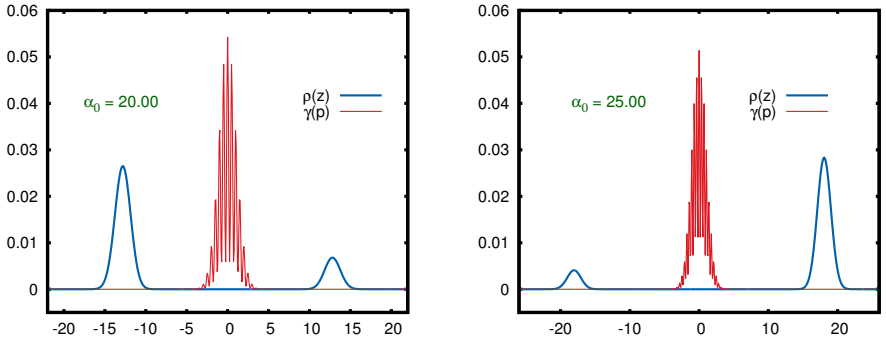

FIGURE 3.6: $\rho(z)$ & $\gamma(p)$ **(3.6a)** $\alpha_0 = 20.000$ **(3.6b)** $\alpha_0 = 25.000$

The result of entropy calculation S_ρ and S_γ is shown below. The behaviour of S_ρ and S_γ is already discussed above.

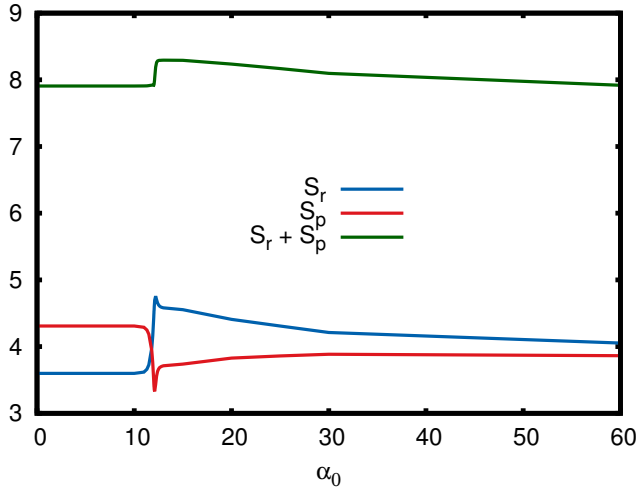

FIGURE 3.7: S_r and S_p

3.3.2 Merging the condensates

The initial state is a fragmented condensate which is prepared by solving the Gross-Pitaevskii equation or the multi-configurational Hartree equations for bosons through the MCTDHB package with a double well potential of the form

$$V(x) = Ax^4 - Bx^2, \qquad A = 1, B = 5 \tag{3.9}$$

This state is then propagated by a Hamiltonian with potential of the form

$$V(x) = A\left[x - \alpha_0 \sin^2\left(\frac{\pi}{2}\frac{t}{t_{on}}\right)\sin\omega t\right]^4 - B\left[x - \alpha_0 \sin^2\left(\frac{\pi}{2}\frac{t}{t_{on}}\right)\sin\omega t\right]^2 \tag{3.10}$$

where $A = 1$, $B = 5$, $\omega = 25$ units, $\alpha_0 = 4.3245$ units, $t_{on} = 100$.

The software shows the dynamics as a 'gif' file. We are pasting the screenshots at different times of the 'gif' file created through MCTDHB package.

The screenshots at different times of the 'gif' files for Gross-Pitaevskii equation and multi-confiurational ($M = 2$) Hartree equations are shown.

3.4 Conclusion

1. The dual space entropy sum is close to its minimum value at the beginning itself because of the state there being very close to the Gaussian nature. In our calculations, we don't find an α_0 further which globally minimises $S_\rho + S_\gamma$. Therefore, our conclusion remains that wide and fast oscillation of the potential trap do lead to fragmentation, but the fragmentation of the state does not bear a simple, direct relationship with the minimum of the dual space information entropy.

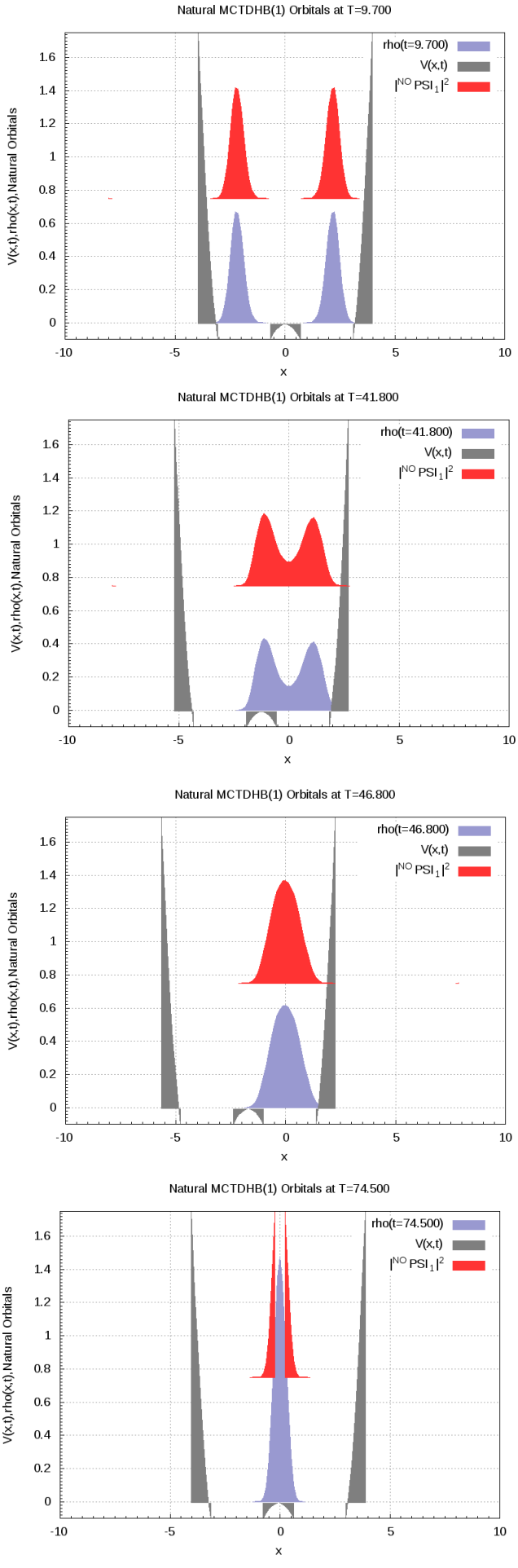

FIGURE 3.8: Dynamics for M=1 or Gross-Pitaevskii

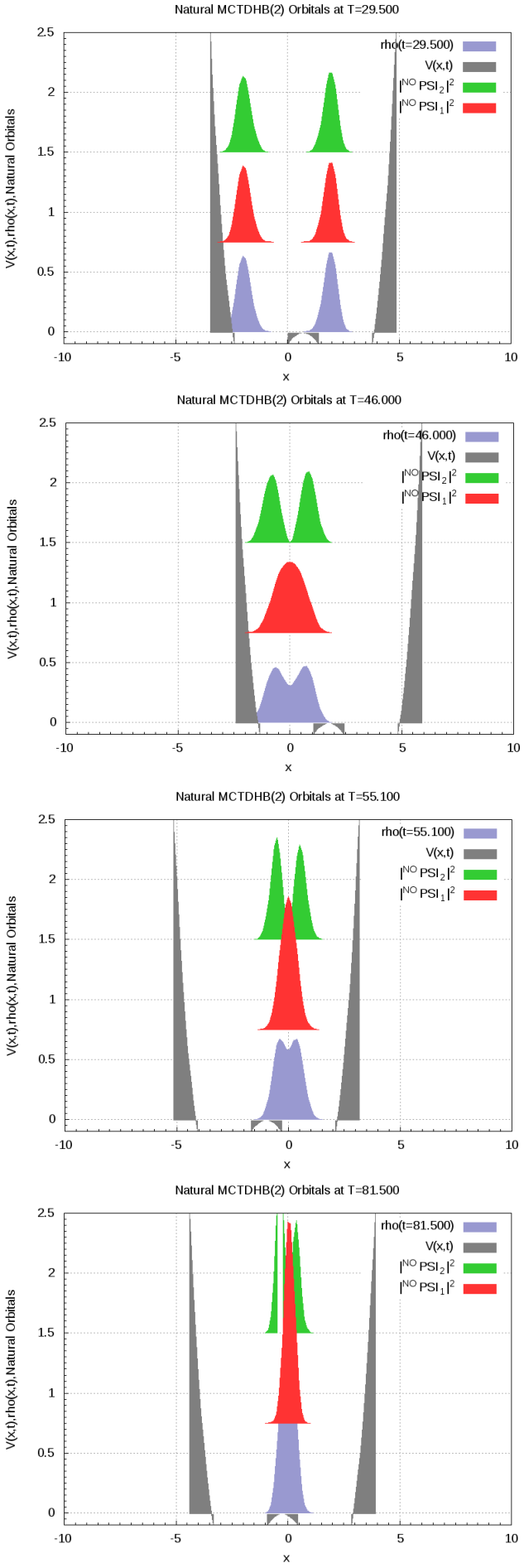

FIGURE 3.9: Dynamics for M=2

2. The merging dynamics clearly shows that as the oscillation of the trap is switched on adiabatically, the double well becomes a single well and the condensates (ground state of the system) merge adiabatically. Hence, the adiabatic evolution of the ground state takes the fragmented state to a single condensate. This feature is just the opposite of what happens when a single well with an uppercut oscillates and a fragmented state emerges from a single condensate.

References

[1] A. Pais, *Subtle is the Lord ... The Science and the Life of Albert Einstein*, (Oxford University Press, New York, (1982).

[2] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell *Science* **269**, 198201 (1995)

[3] C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, *Phys. Rev. Lett.* **75**, 16871690 (1995).

[4] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Phys. Rev. Lett.* **75**, 39693973 (1995).

[5] Masahito Ueda, *Fundamentals and New Frontiers of Bose-Einstein Condensation*, World Scientific, (2010).

[6] L. P. Pitaevskii and S. Stringari, *Bose-Einstein Condensation*, Clarendon Press , (2003).

[7] Richard P. Feynman, *Statistical Mechanics*, Levant Books, Kolkata (2008).

[8] M. R. Andrews, C. G. Townsend, H.-J. Miesner, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Science* **275**, 637641 (1997).

[9] J Rogel Salazar, *Eur. J . Phys.* **34**, 247 (2013).

[10] R. Dum, A. Sanpera, K.A. Suominen, M. Brewczyk, M. Kuś, K. Rzażewski, M. Lewenstein, *Phys. Rev. Lett.*, **80**, 3899 (1998).

[11] Erich J. Mueller, Tin-Liu Ho, Masahito Ueda, Gordon Baym, *Phys. Rev. A* **74**, 033612 (2006).

[12] Feynman, Leighton and Sands, *The Feynman Lectures on Physics* 3, Pearson Education, (2012).

[13] W.C. Henneberger, *Phys. Rev. Lett*, **21**, 838 (1968).

[14] I. Białynickii-Birula & J. Mycielski, *Commun. Math. Phys.* **44**, 129-132 (1975).

[15] W. Ketterle and H.J. Miesner, *Phys. Rev. A* **56**, 3291 (1997).

[16] L.D. Landau & E.M. Lifschitz *The Classical Theory of Fields*, 7th Edition, Butterworh Heinemann, 1987

[17] D.J. Tannor, *Introduction to Quantum Mechanics*, University Science Books, 2007

[18] G.B. Arfken, H.J. Weber & F.E. Harris *Mathematical Methods For Physicists*, 7th Edition, Elsevier, 2013

[19] I. Białynickii-Birula & L. Rudnicki, *Statistical Complexity*, Springer, 2011, Ch. 1 `arXiv:1001.4668v2`

[20] Ido Gillary and N. Moiseyev, *Phys. Rev. A* **66**, 063415 (2002)

[21] D.T. Colbert, W.H. Miller, *J. Chem. Phys*, **96** (3), 1992

[22] F. Dalfovo and S. Stringari, *Phys. Rev. A* **53**, 2477 (1996)

[23] B.I. Schneider and D.L. Feder, *Phys. Rev. A* **59**, 2232 (1999)

[24] V Majerník and T Opatrný *J. Phys. A: Math Gen* **29**, 2187 (1996)

[25] V Majernik, R Charvot and E Majerníková, *J. Phys. A: Math Gen* **32**, 2207 (1999)

[26] Shachar Klaiman, Alexej I. Streltsov, Ofir E. Alon, *Phys. Rev. A* **93**, 023605 (2016)

[27] W. Yi and L.-M. Duan, *Phys. Rev. A* **71**, 043607 (2005)

[28] Alexej. I. Streltsov and Ofir. E. Alon **MCTDHB** Package

Appendix A

Second Quantisation and DVR

A.1 Density matrix

$$|\psi_n\rangle = \int d\vec{r}_1 ... d\vec{r}_n |\vec{r}_1 ... \vec{r}_n\rangle\langle\vec{r}_1 ... \vec{r}_n|\psi\rangle \tag{A.1}$$

$$\Rightarrow \hat{a}\langle\vec{r}'|\psi_n\rangle = \int d\vec{r}_1 ... d\vec{r}_n \hat{a}\langle\vec{r}'|\vec{r}_1 ... \vec{r}_n\rangle\psi_n(\vec{r}_1 ... \vec{r}_n) \tag{A.2}$$

$$\Rightarrow \hat{a}\langle\vec{r}'|\psi_n\rangle = \int d\vec{r}_1 ... d\vec{r}_n \sum_{k=1}^{N} \zeta^{k-1}\langle\vec{r}'|\vec{r}_k\rangle|\vec{r}_1 ... \vec{r}_{k-1}, \vec{r}_{k+1} ... \vec{r}_n\rangle\psi_n(\vec{r}_1 ... \vec{r}_k ... \vec{r}_n) \tag{A.3}$$

$$\Rightarrow \hat{a}^\dagger|\vec{r}\rangle\hat{a}\langle\vec{r}'|\psi_n\rangle = \sum_{k=1}^{N} \int d\vec{r}_1 ... d\vec{r}_n \delta^3(\vec{r}' - \vec{r}_k)|\vec{r}_1 ... \vec{r} ... \vec{r}_n\rangle\psi_n(\vec{r}_1 ... \vec{r}_k ... \vec{r}_n) \tag{A.4}$$

$$\Rightarrow \langle\psi_n|\hat{a}^\dagger(\vec{r})\hat{a}(\vec{r}')|\psi_n\rangle = \sum_{k=1}^{N} \int d\vec{r}_1 ... d\vec{r}_{k-1}, d\vec{r}_{k+1} ... d\vec{r}_n \psi_n^\star(\vec{r}_1 ... \vec{r} ... \vec{r}_n)\psi_n(\vec{r}_1 ... \vec{r}' ... \vec{r}_n) \tag{A.5}$$

For pure state

$$n^{(1)}(\vec{r}, \vec{r}') = N \int d\vec{r}_2 ... d\vec{r}_n \psi_n^\star(\vec{r}, \vec{r}_2 ... \vec{r}_n)\psi_n(\vec{r}', \vec{r}^2 ... \vec{r}_n) \tag{A.6}$$

For mixed state

$$\rho^{(1)}(\vec{r}, \vec{r}') = \frac{1}{Q} \sum_{n=1}^{N} e^{-\beta E_n} n^{(1)}(\vec{r}, \vec{r}') \tag{A.7}$$

where Q is the canonical partition function.

A.2 Derivation of Gross-Pitaevskii equation

The field operator follows the Heisenberg equation as shown below.

$$\hat{\psi}(\vec{r},t) = \hat{U}^{\dagger}(t)\hat{\psi}(\vec{r},0)\hat{U}(t) \tag{A.8}$$

$$\frac{\partial\hat{\psi}(\vec{r},t)}{\partial t} = \frac{\partial\hat{U}^{\dagger}(t)}{\partial t}\hat{\psi}(\vec{r},0)\hat{U}(t) + \hat{U}^{\dagger}\hat{\psi}(\vec{r},0)\frac{\partial\hat{U}(t)}{\partial t} \tag{A.9}$$

$$= -\frac{1}{i\hbar}\hat{U}^{\dagger}(t)\hat{H}\hat{\psi}(\vec{r},0)\hat{U}(t) + \frac{1}{i\hbar}\hat{U}^{\dagger}(t)\hat{\psi}(\vec{r},0)\hat{H}\hat{U}(t) \tag{A.10}$$

$$= \frac{1}{i\hbar}\hat{U}^{\dagger}(t)\left[\hat{\psi}(\vec{r},0),\hat{H}\right]\hat{U}(t) \tag{A.11}$$

$$i\hbar\frac{\partial\hat{\psi}(\vec{r},t)}{\partial t} = \left[\hat{\psi}(\vec{r},t),\hat{H}\right] \tag{A.12}$$

The Hamiltonian in the second quantised formalism is given as

$$\hat{H} = \int\left(-\frac{\hbar^2}{2m}\hat{\Psi}^{\dagger}\nabla^2\hat{\Psi} + \hat{\Psi}^{\dagger}V_{ext}(\vec{r})\hat{\Psi} + \frac{1}{2}\int\hat{\Psi}^{\dagger}\hat{\Psi}^{\dagger\prime}V(\vec{r}-\vec{r'})\hat{\Psi}\hat{\Psi}'d^3\vec{r'}\right)d^3\vec{r} \tag{A.13}$$

Evaluating the commutator one by one as shown below.

The kinetic energy term gives

$$\left[\hat{\psi}(\vec{r},t),\int d^3\vec{r}'\hat{\Psi}^{\dagger}(\vec{r}',t)\nabla'^2\hat{\Psi}(\vec{r}',t)\right] = \int d^3\vec{r}'\Big(\left[\hat{\psi}(\vec{r},t),\hat{\Psi}^{\dagger}(\vec{r}',t)\right]\nabla'^2\hat{\Psi}(\vec{r}',t)$$

$$+\hat{\Psi}^{\dagger}(\vec{r}',t)\nabla'^2\left[\hat{\psi}(\vec{r},t),\hat{\Psi}(\vec{r}',t)\right]\Big) \tag{A.14}$$

$$\Rightarrow\left[\hat{\psi}(\vec{r},t),\int d^3\vec{r}'\hat{\Psi}^{\dagger}(\vec{r}',t)\nabla'^2\hat{\Psi}(\vec{r}',t)\right] = \nabla^2\hat{\Psi}(\vec{r},t) \tag{A.15}$$

The potential energy due to trap gives

$$\left[\hat{\psi}(\vec{r},t),\int d^3\vec{r}'\hat{\Psi}^{\dagger}(\vec{r}',t)V_{ext}(\vec{r}')\hat{\Psi}(\vec{r}',t)\right] = \int d^3\vec{r}'\Big(\left[\hat{\psi}(\vec{r},t),\hat{\Psi}^{\dagger}(\vec{r}',t)\right]V_{ext}(\vec{r}')\hat{\Psi}(\vec{r}',t)$$

$$+\hat{\Psi}^{\dagger}(\vec{r}',t)V_{ext}(\vec{r}')\left[\hat{\psi}(\vec{r},t),\hat{\Psi}(\vec{r}',t)\right]\Big) \tag{A.16}$$

$$\Rightarrow\left[\hat{\psi}(\vec{r},t),\int d^3\vec{r}'\hat{\Psi}^{\dagger}(\vec{r}',t)V_{ext}(\vec{r}')\hat{\Psi}(\vec{r}',t)\right] = V_{ext}(\vec{r})\hat{\Psi}(\vec{r},t) \tag{A.17}$$

The potential energy due to interaction gives

$$\left[\hat{\psi}(\vec{r},t),\frac{1}{2}\int d^3\vec{r}_1d^3\vec{r}_2\hat{\Psi}^{\dagger}(\vec{r}_1)\hat{\Psi}^{\dagger}(\vec{r}_2)V^{(2)}(\vec{r}_1-\vec{r}_2)\hat{\Psi}(\vec{r}_1)\hat{\Psi}(\vec{r}_2)\right]$$

$$= \frac{1}{2}\int d^3\vec{r}_1 d^3\vec{r}_2 \left[\hat{\psi}(\vec{r},t), \hat{\Psi}^\dagger(\vec{r}_1)\right] \hat{\Psi}^\dagger(\vec{r}_2) V^{(2)}(\vec{r}_1 - \vec{r}_2)\hat{\Psi}(\vec{r}_1)\hat{\Psi}(\vec{r}_2) + ... \quad \text{(A.18)}$$

$$= \frac{1}{2}\int d^3\vec{r}_1 d^3\vec{r}_2 \delta^3(\vec{r} - \vec{r}_1)\hat{\Psi}^\dagger(\vec{r}_2) V^{(2)}(\vec{r}_1 - \vec{r}_2)\hat{\Psi}(\vec{r}_1)\hat{\Psi}(\vec{r}_2) + ... \quad \text{(A.19)}$$

$$= \left[\int d^3\vec{r}' \hat{\Psi}^\dagger(\vec{r}') V^{(2)}(\vec{r} - \vec{r}')\hat{\Psi}(\vec{r}')\right] \hat{\Psi}(\vec{r}) \quad \text{(A.20)}$$

Therefore, the Heisenberg equation for the field operators becomes

$$i\hbar\frac{\partial\hat{\psi}(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + \left(\int d^3\vec{r}' \hat{\Psi}^\dagger(\vec{r}') V^{(2)}(\vec{r} - \vec{r}')\hat{\Psi}(\vec{r}')\right)\right] \hat{\Psi}(\vec{r}) \quad \text{(A.21)}$$

The exact form of the interaction potential does not matter in low energy scattering as in the case of Bose-Einstein condensate because all the interaction effects are described by the scattering length. Therefore, $V^{(2)}(\vec{r} - \vec{r}')$ can be replaced by a soft potential V_{eff} to which Born approximation can be applied. Then it is safe to replace $\hat{\psi}(\vec{r},t)$ by $\psi_0(\vec{r},t)$ and assume $V^{(2)}(\vec{r} - \vec{r}') = g\delta^3(\vec{r} - \vec{r}')$ where g depends on the scattering length. The equation then becomes

$$i\hbar\frac{\partial\psi_0(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + g|\psi_0(\vec{r},t)|^2\right] \psi_0(\vec{r},t) \quad \text{(A.22)}$$

$\psi_0(\vec{r},t)$ is the condensate wavefunction and the above equation is the time-dependent Gross-Pitaevskii equation.

A.3 Sinc DVR Method

The Discrete Variable Represntation (DVR) introduced by Light and coworkers, is a powerful technique which can used for solving both time-independent and time-dependent quantum mechanical problems. A convenient analytical expression developed by Corbert and Miller [1] to solve for the matrix elements of a derivative operator in quantum mechanics is discussed here.

[1] Daniel T. Colbert and William H. Miller, J. Chem. Phys., 96, 1982 (1992)

The kinetic energy operator for a one-dimensional quantum system with coordinate x restricted to the interval (a, b) can be written as

$$T = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \tag{A.23}$$

It is assumed here that the wavefunction vanish at the endpoints a and b. The wavefunction can be expanded in an orthonormal basis set defined on a grid. The grid x_i in DVR is equally spaced.

$$x_i = a + (b-a)i/N, \qquad i = 1, ..., N-1 \tag{A.24}$$

and the associated functions for a uniform grid are fourier functions (i.e., particle in a box eigenfunctions).

$$\phi_n(x) = \left(\frac{2}{b-a}\right)^{1/2} sin\left[\frac{n\pi(x-a)}{b-a}\right], \qquad n = 1, ..., N-1 \tag{A.25}$$

As $\phi_n(x_o \equiv a) = \phi_n(x_N \equiv b) = 0$, there are thus $N-1$ functions and $N-1$ points. Within the Fourier-basis DVR formalism, the grid point representation of kinetic energy is then given by

$$T_{ii'} = \frac{-\hbar^2}{2m}\left(\frac{\pi}{b-a}\right)^2 \frac{2}{N}\sum_{n=1}^{N-1} n^2 sin\left(\frac{n\pi i}{N}\right) sin\left(\frac{n\pi i'}{N}\right) \tag{A.26}$$

The sum over n can be evaluated analytically which gives

$$T_{ii'} = \frac{\hbar^2}{2m}\frac{(-1)^{i-i'}}{(b-a)^2}\frac{\pi^2}{2}\frac{1}{sin^2[\pi(i-i')/2N]} - \frac{1}{sin^2[\pi(i-i')/2N]} \tag{A.27}$$

for $i \neq i\prime$ and

$$T_{ii'} = \frac{\hbar^2}{2m}\frac{1}{(b-a)^2}\frac{\pi^2}{2}[(2N^2 + 1/3 - \frac{1}{sin^2(\pi i/N)}] \tag{A.28}$$

for $i = i'$

For the case where a $= -\infty$ to b $= \infty$. The grid spacing $\Delta x = (b-a)/N$ requires that $N \to \infty$ also. Thus equation becomes

$$T_{ii'} = \frac{\hbar^2}{2m \triangle x^2}(-1)^{i-i'} \begin{cases} \pi^2/3 & \text{if } i = i' \\ \frac{2}{(i-i')^2} & \text{if } i \neq i' \end{cases}$$

and the grid is now specified as $x_i = i\Delta x, \quad i = 0, \pm 1, \pm 2, \ldots$.

Appendix B

Double well model

B.1 Hamiltonian in Schwinger representation

$$\hat{H}^{1} = -t\left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1\right) + \frac{U}{2}\left[\hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2\right] \tag{B.1}$$

where $\hat{a}_i^\dagger$ creates a particle in well i and $\hat{a}_i$ annihilates a particle in well i. The first term is the tunnelling term and the second is the usual contact interaction. Evaluating the Hamiltonian in Schwinger representation

$$\hat{J}_x = \frac{1}{2}\left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1\right) \tag{B.2}$$

$$\hat{J}_y = \frac{1}{2i}\left(\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1\right) \tag{B.3}$$

$$\hat{J}_z = \frac{1}{2}\left(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2\right) \tag{B.4}$$

where $\hat{a}_i^\dagger \hat{a}_i = n_i$ and $n_1 + n_2 = N$.

In this representation, the Hamiltonian becomes

$$\hat{H} = -2t\hat{J}_x + \frac{U}{4}\left[(n_1 - n_2)^2 + N^2 - 2N\right] \tag{B.5}$$

[1] Erich J. Mueller, Tin-Liu Ho, Masahito Ueda, Gordon Baym, *Phys. Rev. A* **74**, 033612 (2006)

$$\hat{J}_x^2 = \frac{1}{4}\left[\hat{a}_1^\dagger\hat{a}_2\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_1^\dagger\hat{a}_2\hat{a}_2^\dagger\hat{a}_1 + \hat{a}_2^\dagger\hat{a}_1\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1\hat{a}_2^\dagger\hat{a}_1\right] \quad \text{(B.6)}$$

$$\hat{J}_y^2 = -\frac{1}{4}\left[\hat{a}_1^\dagger\hat{a}_2\hat{a}_1^\dagger\hat{a}_2 - \hat{a}_1^\dagger\hat{a}_2\hat{a}_2^\dagger\hat{a}_1 - \hat{a}_2^\dagger\hat{a}_1\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1\hat{a}_2^\dagger\hat{a}_1\right] \quad \text{(B.7)}$$

$$\hat{J}_z^2 = \frac{1}{4}\left[\hat{a}_1^\dagger\hat{a}_1\hat{a}_1^\dagger\hat{a}_1 + \hat{a}_2^\dagger\hat{a}_2\hat{a}_2^\dagger\hat{a}_2 - 2\hat{a}_1^\dagger\hat{a}_1\hat{a}_2^\dagger\hat{a}_2\right] \quad \text{(B.8)}$$

$$\hat{J}^2 = \frac{N}{2}\left(\frac{N}{2}+1\right) \quad \text{(B.9)}$$

$$\hat{J}^2 + \hat{J}_z^2 - N = \frac{1}{4}\left[(n_1-n_2)^2 + N^2 - 2N\right] \quad \text{(B.10)}$$

Therefore, the Hamiltonian becomes

$$\hat{H} = -2t\hat{J}_x + U\left(\hat{J}^2 + \hat{J}_z^2 - N\right) \quad \text{(B.11)}$$

B.2 Schrodinger equation in the interacting double well model

$$\hat{H} = -t\left(\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1\right) + \frac{U}{4}\left[(n_1-n_2)^2 + N^2 - 2N\right] \quad \text{(B.12)}$$

In number basis, a state can be written as

$$|\psi\rangle = \sum_{l=-N/2}^{N/2}\psi_l|l\rangle = \sum_{l=-N/2}^{N/2}\psi_l|\frac{N}{2}+l, \frac{N}{2}-l\rangle \quad \text{(B.13)}$$

$$\hat{H}_t|\psi\rangle = -t\left(\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1\right)\sum_{l=-N/2}^{N/2}\psi_l|\frac{N}{2}+l, \frac{N}{2}-l\rangle \quad \text{(B.14)}$$

$$= -t\sum_{l=-N/2}^{N/2}\sqrt{\left(\frac{N}{2}+l+1\right)\left(\frac{N}{2}-l\right)}\psi_l|\frac{N}{2}+l+1, \frac{N}{2}-l-1\rangle$$

$$-t\sum_{l=-N/2}^{N/2}\sqrt{\left(\frac{N}{2}-l+1\right)\left(\frac{N}{2}+l\right)}\psi_l|\frac{N}{2}+l-1, \frac{N}{2}-l+1\rangle \quad \text{(B.15)}$$

$$\frac{U}{2}\left[n_1(n_1-1)+n_2(n_2-1)\right]\sum_{l=-N/2}^{N/2}\psi_l|\frac{N}{2}+l,\frac{N}{2}-l\rangle =$$

$$\frac{U}{2}\sum_{l=-N/2}^{N/2}\left[\left(\frac{N}{2}+l-1\right)\left(\frac{N}{2}+l\right)+\left(\frac{N}{2}-l-1\right)\left(\frac{N}{2}-l\right)\psi_l|\frac{N}{2}+l,\frac{N}{2}-l\rangle\right] \tag{B.16}$$

$$\Rightarrow \langle l|\hat{H}|\psi\rangle = -t_l\psi_{l-1}-t_{l+1}\psi_{l+1}+Ul^2+U\left(\frac{N^2}{4}-\frac{N}{2}\right) \tag{B.17}$$

The last term in the equation does not matter because it is a constant.

$$\Rightarrow E\psi_l = -t_l\psi_{l-1}-t_{l+1}\psi_{l+1}+Ul^2\psi_l \tag{B.18}$$

B.3 Density matrix for the mean-field solution

$$|\theta,\phi\rangle = \frac{1}{\sqrt{N}}\left(u\hat{a}_1^\dagger+v\hat{a}_2^\dagger\right)^N|0\rangle \tag{B.19}$$

$$\langle\theta,\phi|\hat{a}_1^\dagger\hat{a}_2|\theta,\phi\rangle = \frac{1}{N!}\langle 0|(u^\star\hat{a}_1+v^\star\hat{a}_2)^N\,|\hat{a}_1^\dagger\hat{a}_2|(u\hat{a}_1^\dagger+v\hat{a}_2^\dagger)^N|0\rangle \tag{B.20}$$

$$\begin{aligned}= \frac{1}{N!}\quad &\langle 0|\left[\textstyle\sum_j\binom{N}{j}\left(e^{i\phi/2}\cos\frac{\theta}{2}\hat{a}_1\right)^{N-j}\left(e^{-i\phi/2}\sin\frac{\theta}{2}\hat{a}_2\right)^j\right](\hat{a}_1^\dagger\hat{a}_2)\\ &\left[\textstyle\sum_k\binom{N}{k}\left(e^{-i\phi/2}\cos\frac{\theta}{2}\hat{a}_1^\dagger\right)^{N-k}\left(e^{i\phi/2}\sin\frac{\theta}{2}\hat{a}_2^\dagger\right)^k\right]|0\rangle\end{aligned} \tag{B.21}$$

$$\begin{aligned}= \frac{1}{N!}\sum_j\sum_k\binom{N}{j}\binom{N}{k}e^{i\phi(k-j)}&\left(\cos\frac{\theta}{2}\right)^{(2N-j-k)}\left(\sin\frac{\theta}{2}\right)^{(j+k)}\\ &\langle 0|\hat{a}_1^{(N-j)}\left(\hat{a}_1^\dagger\right)^{(N-k+1)}\hat{a}_2^{(j+1)}\left(\hat{a}_2^\dagger\right)^{(N-j)}|0\rangle\end{aligned} \tag{B.22}$$

The terms with non-zero value must have $k = j+1$.

$$= N\cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{i\phi}\sum_j\binom{N-1}{j}\left(\cos^2\frac{\theta}{2}\right)^{(N-1-j)}\left(\sin^2\frac{\theta}{2}\right)^j \tag{B.23}$$

$$= N\cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{i\phi}\left(\sin^2\frac{\theta}{2}+\cos^2\frac{\theta}{2}\right)^{(N-1)} \tag{B.24}$$

$$= N\cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{i\phi} \tag{B.25}$$

$$\therefore \langle \hat{a}_1^\dagger \hat{a}_2 \rangle = N \cos\frac{\theta}{2} \sin\frac{\theta}{2} e^{i\phi} \tag{B.26}$$

$$\langle \hat{a}_2^\dagger \hat{a}_1 \rangle = N \cos\frac{\theta}{2} \sin\frac{\theta}{2} e^{-i\phi} \tag{B.27}$$

$$\langle \hat{a}_1^\dagger \hat{a}_1 \rangle = N \cos^2\frac{\theta}{2} \tag{B.28}$$

$$\langle \hat{a}_2^\dagger \hat{a}_2 \rangle = N \sin^2\frac{\theta}{2} \tag{B.29}$$

Therefore, the density matrix for this state is given by

$$\rho_{\mu\nu} = \begin{bmatrix} N\cos^2(\theta/2) & N\sin(\theta/2)\cos(\theta/2)e^{i\phi} \\ N\sin(\theta/2)\cos(\theta/2)e^{-i\phi} & N\sin^2(\theta/2) \end{bmatrix} \tag{B.30}$$

B.4 Coherent state in number basis

$$|C\rangle = \sum_{l=-N/2}^{N/2} \psi_l |\frac{N}{2}+l, \frac{N}{2}-l\rangle = \sum_{l=-N/2}^{N/2} \psi_l |l\rangle = \frac{1}{\sqrt{2^N N!}} \left(\hat{a}_1^\dagger + \hat{a}_2^\dagger\right)^N |0\rangle \tag{B.31}$$

$$\Rightarrow \psi_l = \frac{1}{2^N N!} \frac{N!}{\left(\frac{N}{2}+l\right)!\left(\frac{N}{2}-l\right)!} \sqrt{\left(\frac{N}{2}+l\right)!\left(\frac{N}{2}-l\right)!} \tag{B.32}$$

$$\Rightarrow \psi_l = \left(\frac{N!}{2^N \left(\frac{N}{2}+l\right)!\left(\frac{N}{2}-l\right)!} \right)^{1/2} \tag{B.33}$$

$$\begin{aligned} \Rightarrow \ln\psi_l = \frac{1}{2}[N\ln\frac{N}{2} &- \left(\frac{N}{2}+l\right)\left\{\ln\frac{N}{2} + \ln\left(1+\frac{2l}{N}\right)\right\} \\ &- \left(\frac{N}{2}-l\right)\left\{\ln\frac{N}{2} + \ln\left(1-\frac{2l}{N}\right)\right\} \\ &+ \frac{1}{2}\left\{\ln(2\pi N) - \ln\left(2\pi\left(\frac{N}{2}+l\right)\right) - \ln\left(2\pi\left(\frac{N}{2}-l\right)\right)\right\}] \end{aligned} \tag{B.34}$$

$$\Rightarrow \psi_l = \frac{e^{-l^2/N}}{(\pi N/2)^{1/4}} \tag{B.35}$$

$$\Rightarrow \psi_l = \int \frac{l^2 e^{-2l^2/N}}{(\pi N/2)^{1/2}} = \frac{N}{4} \tag{B.36}$$

Appendix C

Derivation of Entropic Uncertainty Relations and Fourier Transforms

C.1 Derivation of EUR

The BBM inequality comes from an inequality theorem in Fourier Analysis on R^n called the Babenko-Beckner inequality. This inequality relates the norm of an integrable function in L^p to the norm of its Fourier transform. The theorem states that

The (p, q) norm of the Fourier transformation follows the inequality

$$\|\tilde{\psi}\|_q \leq k(p,q)\|\psi\|_p \tag{C.1}$$

where $\|\psi\|_p = \left(\int d^n r|\psi|^p\right)^{1/p}$, $\frac{1}{p}+\frac{1}{q}=1$, $q \geq 2$ and

$$k(p,q) = \left(\frac{2\pi}{q}\right)^{n/2q}\left(\frac{2\pi}{p}\right)^{-n/2p} \tag{C.2}$$

Let us define a function

$$W(q) \equiv k(p,q)\|\psi\|_p - \|\tilde{\psi}\|_q \tag{C.3}$$

$$\Rightarrow W(q) \geq 0 \tag{C.4}$$

Let us now look at a theorem which will be useful to us for deriving the EUR.

$$A(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\tilde{A}(k')e^{ik'x}dk' \tag{C.5}$$

$$B(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\tilde{B}(k')e^{ik'x}dk' \tag{C.6}$$

$$\Rightarrow \overline{B(x)} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\overline{\tilde{B}(k')}e^{ik'x}dk' \tag{C.7}$$

$$\int_{-\infty}^{\infty}A(x)\overline{B(x)}dx = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\tilde{A}(k)\overline{\tilde{B}(k')}e^{i(k-k')x}dkdk'\right]dx \tag{C.8}$$

$$\Rightarrow \boxed{\int_{-\infty}^{\infty}A(x)\overline{B(x)}dx = \frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{A}(k)\overline{\tilde{B}(k)}dk} \tag{C.9}$$

This is the Parseval-Plancheral theorem. This implies

$$\int_{-\infty}^{\infty}|A(x)|^2dx = \frac{1}{2\pi}\int_{-\infty}^{\infty}|\tilde{A}(k)|^2dk \tag{C.10}$$

$$\Rightarrow W(2) = 0 \tag{C.11}$$

$$\Rightarrow \left(\frac{dW}{dq}\right)_{q=2} \geq 0 \tag{C.12}$$

$$\frac{dW}{dq} = \frac{dk}{dq}\|\psi\|_p + k(p,q)\frac{d}{dq}\|\psi\|_p - \frac{d}{dq}\|\tilde{\psi}\|_q \tag{C.13}$$

Let us now compute $\dfrac{dW}{dq}$ term by term.

$$\left(\frac{dk}{dq}\right)_{q=2} = \frac{d}{dq}\left[\left(\frac{2\pi}{q}\right)^{n/2q}\cdot\left(\frac{2\pi}{p}\right)^{-n/2p}\right]_{q=2} = -\frac{n}{4}(1+\ln\pi) \tag{C.14}$$

$$\left(\frac{d\|\tilde{\psi}\|_q}{dq}\right)_{q=2} = \left[\frac{d}{dq}\left(\int d^n\vec{k}\|\tilde{\psi}\|^q\right)^{1/q}\right]_{q=2} = \frac{1}{2N}\int d^n\vec{k}\|\tilde{\psi}\|^2\ln\|\tilde{\psi}\| - \frac{1}{4}N\ln N \tag{C.15}$$

$$\left(\frac{d}{dq}\|\psi\|_p\right)_{q=2} = -\frac{1}{2N}\int d^n\vec{r}\|\psi\|^2\ln\|\psi\| + \frac{1}{4}N\ln N \tag{C.16}$$

where $N = \int d^n\vec{r}\|\psi\|^2 = \int d^n\vec{k}\|\tilde{\psi}\|^2$.

$$\therefore \left(\frac{dW(q)}{dq}\right)_{q=2} =$$

$$-\frac{1}{2N}\int d^n\vec{r}\|\psi\|^2\ln\|\psi\| - \frac{1}{2N}\int d^n\vec{k}\|\tilde{\psi}\|^2\ln\|\tilde{\psi}\| + \frac{N}{2}\ln N - \frac{nN}{4}(1+\ln\pi) \geq 0$$

$$\Rightarrow \boxed{-\langle\ln\rho\rangle - \langle\ln\gamma\rangle \geq n(1+\ln\pi)} \tag{C.17}$$

Now, we need to maximize $-\langle\ln\rho\rangle$ subject to the two following constraints $\rho(\vec{r}) = \int d^n\vec{r}\|\psi\|^2 = 1$ and $\langle(\vec{r} - \langle\vec{r}\rangle)^2\rangle = r_0^2$.

$$\frac{d}{d\rho}\left[-\int d^n\vec{r}\rho\ln\rho - \lambda\left(\int d^n\vec{r}\rho - 1\right) - \mu\left(\int r^2\rho d^n\vec{r} - (r\rho d^n\vec{r})^2 - r_0^2\right)\right] = 0 \tag{C.18}$$

$$\Rightarrow \int d^n\vec{r}\left[-\ln\rho - 1 - \lambda - \mu r^2 + \mu\langle\vec{r}\rangle.\vec{r}\right] = 0 \tag{C.19}$$

$$\Rightarrow \rho(\vec{r}) = e^{-(1+\lambda)}e^{-\mu(r^2 - 2\langle\vec{r}\rangle.\vec{r})} \tag{C.20}$$

$$\int \rho(\vec{r})d^n\vec{r} = e^{-(1+\lambda)}\left[\int e^{-\mu(x^2 - 2x.\overline{x} + \overline{x}^2)}dx\right]^n e^{\mu(\overline{x}^2 + \overline{y}^2 + \ldots)} \tag{C.21}$$

$$\Rightarrow 1 = e^{-(1+\lambda)}\left(\int e^{-\mu x'^2}dx'\right)^n e^{\mu\overline{r}^2} \tag{C.22}$$

$$\Rightarrow e^{(1+\lambda)} = \left(\frac{\pi}{\mu}\right)^{n/2} e^{\mu\langle\vec{r}\rangle^2} \tag{C.23}$$

$$\Rightarrow \rho(\vec{r}) = \left(\frac{\mu}{\pi}\right)^{n/2} e^{-\mu(\vec{r} - \langle\vec{r}\rangle)^2} \tag{C.24}$$

For $\rho_{max}(\vec{r})$, $\dfrac{d\rho(\vec{r})}{d\mu} = 0$.

$$\Rightarrow \frac{n}{2\mu} = (\vec{r} - \langle\vec{r}\rangle)^2 \tag{C.25}$$

$$\Rightarrow \frac{n}{2\mu}\int \rho(\vec{r})d^n\vec{r} = \langle(\vec{r} - \langle\vec{r}\rangle)^2\rangle = r_0^2 \tag{C.26}$$

$$\Rightarrow \mu = \frac{n}{2r_0^2} \tag{C.27}$$

$$\Rightarrow \rho_{max}(\vec{r}) = \left(\frac{n}{2\pi r_0^2}\right)^{n/2} e^{-n(\vec{r}-\langle\vec{r}\rangle)^2/2r_0^2} \tag{C.28}$$

$$\Rightarrow -\ln(\rho_{max}(\vec{r})) = \frac{n}{2r_0^2}(\vec{r}-\langle\vec{r}\rangle)^2 + \frac{n}{2}\ln\left(\frac{2\pi r_0^2}{n}\right) \tag{C.29}$$

$$\Rightarrow -\ln\rho(\vec{r}) \leq \frac{n}{2r_0^2}(\vec{r}-\langle\vec{r}\rangle)^2 + \frac{n}{2}\ln\left(\frac{2\pi r_0^2}{n}\right) \tag{C.30}$$

$$\Rightarrow -\ln\rho(\vec{r}) \leq \frac{n}{2}\ln\left(\frac{2\pi e r_0^2}{n}\right) \tag{C.31}$$

$$\Rightarrow e\pi\left[\exp\left(\frac{2}{n}\langle\ln\rho\rangle\right)\right] \geq \frac{n}{2}\langle(\vec{r}-\langle\vec{r}\rangle)^2\rangle^{-1} \tag{C.32}$$

$$\Rightarrow \frac{2}{n}\langle(\vec{k}-\langle\vec{k}\rangle)^2\rangle \geq (e\pi)^{-1}\exp\left(\frac{2}{n}\langle\ln\gamma\rangle\right) \tag{C.33}$$

From the BBM inequality, we have

$$-\langle\ln\rho\rangle - \langle\ln\gamma\rangle \geq n(1+\ln\pi) = \frac{n}{2}\ln(\pi e)^2 \tag{C.34}$$

$$\Rightarrow e\pi\left[\exp\left(\frac{2}{n}\langle\ln\rho\rangle\right)\right] \leq (e\pi)^{-1}\exp\left(\frac{2}{n}\langle\ln\gamma\rangle\right) \tag{C.35}$$

$$\therefore \boxed{\frac{n}{2}\langle(\vec{r}-\langle\vec{r}\rangle)^2\rangle^{-1} \leq e\pi\left[\exp\left(\frac{2}{n}\langle\ln\rho\rangle\right)\right] \leq (e\pi)^{-1}\exp\left(\frac{2}{n}\langle\ln\gamma\rangle\right) \leq \frac{2}{n}\langle(\vec{k}-\langle\vec{k}\rangle)^2\rangle} \tag{C.36}$$

A single Gaussian saturates this string of inequality.

C.2 Fourier Transform of Double Gaussian

$$\psi(x) = A\left[\exp\left\{-\frac{1}{2}\left(\frac{x-\alpha}{\beta}\right)^2\right\} + \exp\left\{-\frac{1}{2}\left(\frac{x+\alpha}{\beta}\right)^2\right\}\right] \tag{C.37}$$

$$\Rightarrow \int|\psi(x)|^2dx = 2|A|^2\beta\sqrt{\pi}\left(1+e^{-\alpha^2/\beta^2}\right) = 1 \tag{C.38}$$

$$\Rightarrow |A|^2 = \frac{1}{2\beta\sqrt{\pi}\left(1+e^{-\alpha^2/\beta^2}\right)} \tag{C.39}$$

$$\tilde{\psi}(k) = \int e^{ikx}\left[\exp\left\{-\frac{1}{2}\left(\frac{x-\alpha}{\beta}\right)^2\right\} + \exp\left\{-\frac{1}{2}\left(\frac{x+\alpha}{\beta}\right)^2\right\}\right]dx \tag{C.40}$$

$$\Rightarrow |\tilde{\psi}(k)|^2 = e^{-ik\alpha}e^{-\beta^2k^2/2} + e^{ik\alpha}e^{-\beta^2k^2/2} = 2e^{-\beta^2k^2/2}(1+\cos(2k\alpha)) \tag{C.41}$$

$$\Rightarrow \int |\tilde{\psi}(k)|^2 dx = \frac{2|B|^2\sqrt{\pi}}{\beta}\left(1+e^{-\alpha^2/\beta^2}\right) \tag{C.42}$$

$$\Rightarrow |B|^2 = \frac{\beta}{2\sqrt{\pi}\left(1+e^{-\alpha^2/\beta^2}\right)} \tag{C.43}$$

Therefore, the position-space and momentum-space probability densities for a double Gaussian are given by

$$\rho(x) = \frac{1}{2\beta\sqrt{\pi}\left(1+e^{-\alpha^2/\beta^2}\right)}\left[\exp\left\{-\frac{1}{2}\left(\frac{x-\alpha}{\beta}\right)^2\right\} + \exp\left\{-\frac{1}{2}\left(\frac{x+\alpha}{\beta}\right)^2\right\}\right] \tag{C.44}$$

$$\gamma(k) = \frac{\beta}{\sqrt{\pi}\left(1+e^{-\alpha^2/\beta^2}\right)}e^{-\beta^2k^2/2}(1+\cos(2k\alpha)) \tag{C.45}$$

C.3 Entropy of Gaussian distributions

$$\rho(x) = \frac{1}{\beta\sqrt{\pi}}\exp\left\{-\frac{1}{2}\left(\frac{x-\alpha}{\beta}\right)^2\right\} \tag{C.46}$$

$$\Rightarrow S_\rho = -\int dx\rho\ln\rho = \frac{1}{2}(1+\ln\pi\beta^2) \tag{C.47}$$

$$\gamma(k) = \frac{\beta}{\sqrt{\pi}}e^{-\beta^2k^2/2} \tag{C.48}$$

$$\Rightarrow S_\gamma = -\int dk\gamma\ln\gamma = \frac{1}{2}(1+\ln\frac{\pi}{\beta^2}) \tag{C.49}$$

$$\Rightarrow S_\rho + S_\gamma = 1+\ln\pi \tag{C.50}$$

Thus, a single Gaussian saturates the BBM inequality as it saturates the Heisenberg inequality.