A study of an exactly solvable model of two species of identical bosons interacting via harmonic oscillator potential

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A study of an exactly solvable model of two species of identical bosons interacting via harmonic oscillator potential

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Abstract

This thesis studies a three dimensional system containing equal numbers of bosons belong to two different species and interacting via a harmonic oscillator potential. We assume that particles belonging to the same species repel each other, while those belonging to different species attract. The two cases, where the coupling strengths are equal and where the coupling strengths depend on the particle species, are studied. By solving the eigenvalue problem, we reformulated the Hamiltonian of the system in terms of the normal coordinates of the system instead of single particle coordinates.

First, the classical initial value problem is solved, for arbitrary initial conditions for the positions and momenta of the particles, by diagonalizing the classical Hamiltonian of the system and obtaining the trajectories of the particles as functions of time. The quantum system is examined, its complete spectrum of multi-particle eigenstates is obtained. Finally, the statistical mechanical behavior of the system is studied within the framework of the grand canonical ensemble, and the thermodynamic properties of the system and its critical temperature are obtained. It is shown that, the system condenses in one channel when the coupling strengths are identical and in two channels when the coupling strengths are dierent.

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Declaration

The work in this thesis is based on the Ph.D. thesis of Dr. Abdelhamid Abdelhak Galal, carried out at the department of Physics, University of Illinois at Urbana Champaign, 2004.

Contents

List of Figures

Chapter 1

Introduction

Miscibility of gases refers to their ability to mix uniformly with each other in all proportions forming a homogeneous solution. Miscibility of atomic species opens a new attractive research area of physics. Binary mixture of two hyperfine states of the same atomic species [1–10], different isotopes of the same atomic species [11] and different atomic species [12–15] have been realised experimentally. The theoretical aspects of these mixtures have been studied including steady state solutions [16–26], dark-bright solitons [27–31], vortices [32–41] and Finite temperature models [31, 42–48]. This combination of species is very interesting due to the possibility of having both boson-boson and boson-fermion mixtures and introduces new physics not present in the single atomic species.

The mixing of two quantum fluids represents a fundamental property of a two component system and is partially controlled by inter-particle interactions. The achievement of Bose-Einstein condensation (BEC) in dilute-gas and mixtures of ultra-cold quantum gases provides a unique system for studying interacting quantum fluids. The resonant control of two-body interactions in ultracold gases is possible via magnetic-field Feshbach resonances provides a parameter which directly alters the miscibility of the dual-species BEC [49].

The first two-component condensate was produced in different hyperfine states of ^{87}Rb, and showed evidence for repulsive interspecies interactions [1]. Further

work with different hyperfine states of ^{87}Rb enabled the study of the dynamics of inter-penetrating quantum fluids. More recently a dual species BEC of ^{41}K and ^{87}Rb was investigated experimentally where scissors-like collective oscillations were observed as a result of off-axis collisions [50].

1.1 The Bose gas with two body interactions

Much research work has been devoted to investigate the problem of one dimensional non-relativistic Bose gas with two body interaction. The system was firstly studied by summing the perturbation series to different orders to obtain a solution close to the true case. An alternative approach to the problem is to start with the Schroedinger equation and to calculate the eigenvectors and the eigenvalues without introducing any approximation. An important step in this direction was introduced by Girardeau [51], who studied a model of a one-dimensional Bose gas of impenetrable particles.

The drawbacks of the Girardeau treatment have been overcomed by investigating a model of a one-dimensional Bose gas with a delta function potential (quantum non-linear Schroedinger model), which was studied by Lieb and Linger [52], McGuire [53] and Yang [54–56]. The classical inverse scattering method was applied to obtain the exact solution of the classical non-linear Schroedinger model by Zakharov [57], and later, the solution of the quantum non-linear Schroedinger model was obtained using the quantum inverse scattering method [58–62].

1.2 An outline of this thesis

In this thesis, we study a simple exactly solvable model which contains two boson species in three dimensional space interacting via a harmonic oscillator potential. This model is a toy model for studying the miscibility of atomic species. It will also enhance our understanding of the Bose-Einstein condensation.

The study is organized as follows. In chapter 2 we give a brief review of exactly solvable models in classical, quantum and statistical mechanics with finite and infinite number of degrees of freedom. We then discuss briefly the phenomena of BEC and some of its features.

In chapter 3, we consider a boson system consisting of two species A and B of non-relativistic particles having the same mass in three dimensional space. We assume that we have identical number of particles and that particles of the same species repel and those belong to different species attract with the same coupling constant. We solve the classical initial value problem for arbitrary initial conditions of the positions and momenta of the particles, by diagonalizing the classical Hamiltonian of the system and obtaining the trajectories of the particles as functions of time.We then consider the simple case of $N = 3$. Next we study the quantum system and obtain the eigenfunctions, and energy spectrum of the system. Finally we examine the statistical mechanical properties of the system within the framework of the grand canonical ensemble. We obtain an exact expression for the grand canonical partition function $Z(T, V, \mu)$. Using the partition function we examine the thermodynamic properties of the system. We show that the system exhibits BEC and calculate the critical temperature.

In chapter 4, we generalize the model by assuming that the coupling constants depend on the particle species. We again solve the classical initial value problem by diagonalizing the Hamiltonian and show that the system is composed of three sets of uncoupled oscillators vibrating with three different frequencies, two of them depend on the ratio of the coupling constants. Then we examine the quantum system and obtain the eigenfunctions and eigenvalues of the Hamiltonian. Finally we study the statistical mechanical behaviour of the system. We deal with these modes as two independent subsystems with different chemical potentials and show that the system can condense through two channels with different critical temperature.
In chapter 5, we discuss the results obtained in details and comment on further work.

In Appendix A, we compute the solution of the characteristic equation for potential energy matrix V_1 and V_2 obtained in Chapters 3 and 4 respectively .

In Appendix B, we obtain the eigenvalues, eigenvectors of the potential energy matrices and use the eigenvectors to construct the diagonalizing matrices O_1 and O_2.

In Appendix C, we calculate density of states for a single particle in harmonic trap of frequency ω.

Chapter 2

General Review

2.1 Exactly solvable models

Exactly solvable models [63] are very important in physics since they enable us to estimate the accuracy of different approximation methods. The fundamental problem in many fields of theoretical physics is that of solving many body interacting systems and it is rare that we encounter solvable cases. It is generally believed that the classical N body problem is soluble only for $N = 2$, and is not soluble for systems with $N \geq 3$. Exact calculation of physical quantities for any large real system turns out to be difficult, therefore one is forced to make some approximations, such as the Hartree and Hartree-Fock approximations, to simplify the problem or to replace the system by some simple idealization that makes calculation of the quantities of interest possible.

2.1.1 Exactly solvable classical systems

Classical systems with a finite number of degrees of freedom

A classical system of N degrees of freedom can be described by introducing N generalized coordinates q_i and their conjugate momenta p_i and constructing the Hamiltonian function $H(q_i, p_i)$ of the system. The equations of motion of the system

are

$$\begin{aligned} \dot{p}_i &= -\frac{\partial H}{\partial q_i} \\ \dot{q}_i &= \frac{\partial H}{\partial p_i}, \qquad\qquad i = 1, \cdots N \end{aligned}$$

where the dot stands for differentiation with respect to time.

The system is called completely integrable (exactly solvable) if there exist action angle variables $S_k(t), \phi_k, \quad k = 1, \cdots N$ such that,

$$\begin{aligned} S_k(t) &= constant \\ \phi_i(t) &= \phi_i(0) + \omega_i t \end{aligned}$$

One could express the coordinates and momenta in terms of the quantities $S_k(t), \phi_i(t)$. An important class of completely integrable systems with a finite number of degrees of freedom is the 1-D model of particles interacting via a potential of the following types [64],

$$\begin{aligned} V(q) &= g^2 \frac{1}{q^2} \\ V(q) &= g^2 \frac{a^2}{\sin^2(aq)} \\ V(q) &= g^2 \frac{a^2}{\sinh^2(aq)} \\ V(q) &= g^2 (\frac{1}{q^2} + \omega^2 q^2), \end{aligned}$$

where V is the potential between two particles separated by distance q, and g is the coupling constant which gives strength of the interaction.

Classical system with an infinite number of degrees of freedom

An important class of exactly solvable systems with an infinite number of degrees of freedom is described by an equation of the form:

$$\frac{\partial \psi}{\partial t} = \hat{K}\psi,$$

where $\hat{K}$ is a non-linear differential operator. This type of exactly solvable models has two important properties, they possess an infinite number of conservation laws,

and they admit soliton solutions. Such solvable models are described by equations as the non-linear Schroedinger equation, the sine-Gordon equation and Korteweg-deVries equation.

2.1.2 Exactly solvable quantum systems

Quantum systems with a finite number of degrees of freedom

A quantum system with a finite number of degrees of freedom is said to be solvable if we can find a complete set of N commuting operators such that the set of the eigenvalues $\lambda_1, ..., \lambda_N$ defines a one dimensional subspace of the Hilbert space [65].
An important class of exactly solvable quantum systems with a finite number of degrees of freedom is the one-dimensional N particle system described by a Hamiltonian of the form,

$$H = \frac{1}{2}\sum_{i=1}^{N} P_i^2 + g^2 \sum_{i<j} V(q_i - q_j),$$

where P_i is the momentum of the i^{th} particle, and $V(q_i - q_j)$ is a two body interaction of the form mentioned in section (2.1.1)

Quantum system with an infinite number of degrees of freedom

If we consider a free field theory then the full momentum distribution function is conserved and one can construct an infinite number of constants of the motion i.e, moments of the momentum distribution.
In quantum field theory there are several examples of exactly solvable models such that the massive Thirring model [66], the Sine-Gordon model [67] and the SU(2)-Thirring model [68].

2.1.3 Exactly solvable models in statistical mechanics

In statistical mechanics, we have several solvable models which include the anisotropic XXZ model, the symmetric six-vertex model and the symmetric eight-vertex model. A powerful tool for solving these models is the so called the Bethe-ansatez.

The Bethe-ansatz method is used for finding the exact solution of certain one-dimensional quantum many-body models, and setting up the equations which can be used to determine the thermodynamics of these systems. Unfortunately the structure of Bethe-ansatez wave function is very complex especially when the system has additional internal degrees of freedom. In some cases we can write down many-body eigenfunctions which can be represented as a linear combination of $N!$ plane waves with N quasi-momenta. The energy eigenvalue of the lowest energy state in the thermodynamic limit is reduced to a distribution function of the quasi-momenta. In many cases the quasi-momenta are all real numbers for the ground state. But for general eigenstates, quasi-momenta are complex numbers. Fortunately for the delta-function Boson case, quasi-momenta are always real. Yang [54] introduced the thermodynamic theory for this case. The total energy is represented by the distribution function of quasi-momenta, and can be used to calculate all thermodynamic quantities. This method can be extended to other Bethe-ansatz soluble models such as the spin $-\frac{1}{2}$ Heisenberg model. In this case complex quasi-momenta group together to form a string in the rapidity plane in the limit of a big system. The length of the string is dependent on the parameters of the system. Once we accept the string assumption we can construct the equation for the free energy of these models at a given temperature.

2.2 Bose-Einstein condensation

A Bose-Einstein condensate (BEC) is a state of matter in which a large fraction of an ensemble of identical atomic or molecular species occupies the lowest energy quantum state. The indistinguishable nature of the constituent components results in the ensemble displaying collective quantum behaviour on a macroscopic scale.

2.2.1 History

The phenomenon known as Bose-Einstein condensation (BEC) [69,70] was predicted by Einstein 1924 [71] as he reviewed and translated a work of S.N. Bose about the

statistics of photons. Bose derived the famous black-body radiation formula on the basis of the thermodynamic properties of quantized massless harmonic oscillator of some frequencies. Einstein generalized the Bose statistics to arbitrary massive particles finding out that a system of particles satisfying both the Bose statistics and the conservation of the number of particles should undergo a new unknown phase transition at some critical temperature. Below this critical temperature a macroscopic fraction of all particles condenses into one single state of the system, the quantum mechanical ground state. As these condensed particles do not contribute to the entropy of the system any more, Einstein interpreted this phenomenon as a phase transition. That at sufficient low temperature particles in a gas could all reside in the same quantum state.

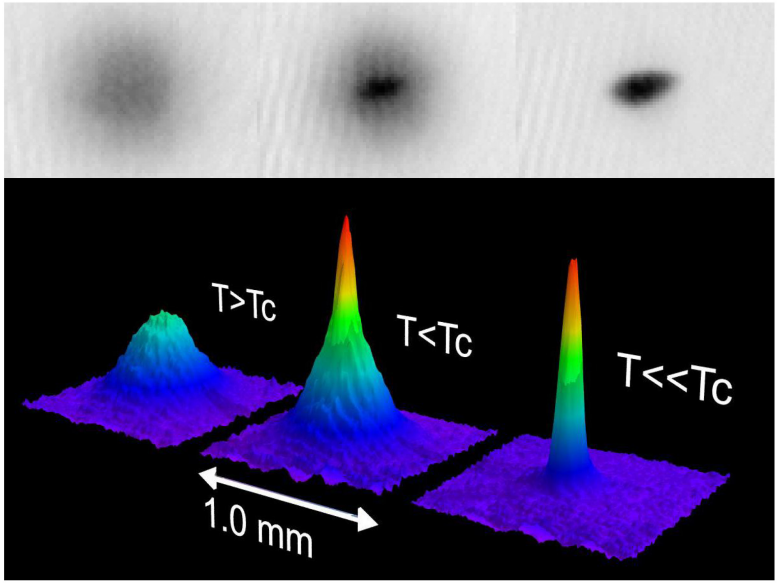

Figure 2.1: The density profile of the condensate after time of flight expansion, giving emphasis to the velocity distribution (Anderson. et al., Science, 269(198),1995)

Immediately after the discovery of superfluidity in liquid helium by Allen [72] and Kapitza [73], London [74], had the intuition that superfluidity could be a manifestation of BEC. In 1947 Bogoliubov developed the first microscopic theory of interacting Bose gases, based on the concept of BEC [75]. After that, intense theoretical work was developed, aimed at a better understanding of the relationship

between BEC and superfluidity. In the same years, the experimental studies on superfluid helium had provided the first measurements of the condensate fraction through the determination of the momentum distribution.

The experimental studies on the dilute atomic gases were developed much later, starting from the 1970s, profiting from the new techniques developed in atomic physics and based on magnetic and optical trapping, and advanced cooling mechanisms. The first studies were focused on spin-polarized hydrogen that was considered, because of its light mass, the most natural candidate for realizing BEC. Hydrogen atoms were first cooled in a dilution refrigerator, then trapped by a magnetic field and further cooled by evaporation, coming very close to BEC. In the 1980s laser-based techniques, such as laser cooling and magneto-optical trapping, were developed to cool and trap neutral atoms. Alkali atoms are well suited to laser-based methods.

In 1995 this peculiar gaseous state (BEC) was observed experimentally in dilute alkali gases using the powerful laser-cooling methods. By combining the different cooling techniques an experimental team at the MIT labs eventually succeeded in reaching the temperature and densities required to observe BEC in vapours of ^{87}Rb [76] and ^{23} Na [77]. Such gases were confined in a magnetic trap and cooled down to extremely low temperatures of the order of fractions of micro-kelvins. The first evidence for the condensation emerged from time-of-flight measurements. The atoms were left to expand by switching off the confining trap and then imaged with optical methods. A sharp peak in the velocity distribution was observed below a certain critical temperature, providing a clear signature for BEC.

One of the most relevant features of these trapped Bose gases is that they are inhomogeneous. This allows for the investigation of a new series of physical quantities which were not accessible with previous experiments on superfluid helium. These specific systems displaying the attractiveness of BEC for researchers. Perhaps the most fascinating aspect of BEC is the possibility of describing thousands to millions of atoms with a single wave function, a macroscopic quantum state. As a consequence of this, quantum effects of a single atomic state which are essentially invisible may be amplified up to a macroscopic level.

2.2.2 What is Bose-Einstein condensation?

In classical mechanics, identical particles are distinguishable. This means that we could in principle follow the trajectory of a particle. Quantum mechanics does not allow this, since their positions and trajectories are known only in a probabilistic sense and therefore particles are indistinguishable.
BEC is based on the indistinguishability and the wave nature of particles, which are the bases of quantum mechanics. The three quantum effects that cause BEC are the indistinguishability of particles, the discrete nature of the energy of each particle, and that several particles are allowed to be in the same state. The first two are a consequence of the wave nature of atoms; the third is only true for bosons. BEC describes a peculiar state of matter that occurs when certain gases are cooled to a few billionths of a degree above absolute zero temperature. It is characterised by all atoms entering the same quantum state losing its individuality, thus merging to form what has been described as one super-atom.

In order to understand this peculiar gaseous state, we should investigate one parameter which characterizes the onset of BEC. This parameter is the phase-space density [78] :

$$n\lambda_T^3 = \frac{Nh^3}{V(2\pi mkT)^{3/2}}, \tag{2.2.1}$$

where n is the particle number density of the ensemble. More precisely, if we put N free bosons in a volume V , the average atomic density is given by $n = N/V$. The quantity λ_T is the particles thermal wavelength

$$\lambda_T = \sqrt{\frac{h^2}{2\pi mkT}} \tag{2.2.2}$$

the thermal wavelength λ_T can be regarded as the position uncertainty associated with the thermal momentum distribution, which increases by lowering the temperature. In fact, the quantity $(n\lambda_T^3)$ can be a very appropriate parameter, in terms of which physics of such systems can be captured in a simple way.
As the phase-space density $(n\lambda_T^3)$ goes to zero, the system behaves in classical manner and doesn't exhibit any quantum feature. For small, but not negligible value

of $(n\lambda_T^3)$ the various quantities of the system can be expanded as a power series in this parameter. Using this expansion we can see the departure from the classical behaviour. But once $(n\lambda_T^3)$ becomes of the order of unity, the behaviour of the system becomes significantly different from the classical regime in which quantum features appear. A study of the system under these circumstances brings us with a phenomena which is unusual to classical statistical mechanics.

In a simplified picture, atoms in a gas may be regarded as wave packets with an extension of the order of the thermal de Broglie wavelength λ_T. Atoms become correlated with each other when their related waves overlap, that is when λ_T gets comparable to the inter-atomic separation d: $(\lambda_T \geq d)$. Then, the indistinguishability of particles becomes important, see Fig(2). The particle density of the system n is related to the inter-particles distance d through the equality $d = n^{-1/3}$(i.e $nd^3 = 1$),using the above inequality $\lambda_T \geq d$ one can write

$$n\lambda_T^3 \geq 1 \tag{2.2.3}$$

This equation tells us qualitatively that BEC may occur if the temperature is sufficiently low or the density of particles is sufficiently high.From the last two equations one can obtain a relation between the temperature and the density for condensed phase:

$$T \leq \frac{h^2}{2\pi mk} n^{2/3} \tag{2.2.4}$$

The peculiarity of BEC is that many particles are in the same quantum state. These particles display state coherence which occurs when the particles are strongly correlated with each other. The state coherence may be understood from the above figure, since as the temperature gets lowered the quantum feature appear and uncertainty in particles positions increases. This appears in the widening of the particles wave packets and their overlap. When the temperature reaches zero all particles wave packets form giant matter-wave which is a pure condensed state(coherent state).

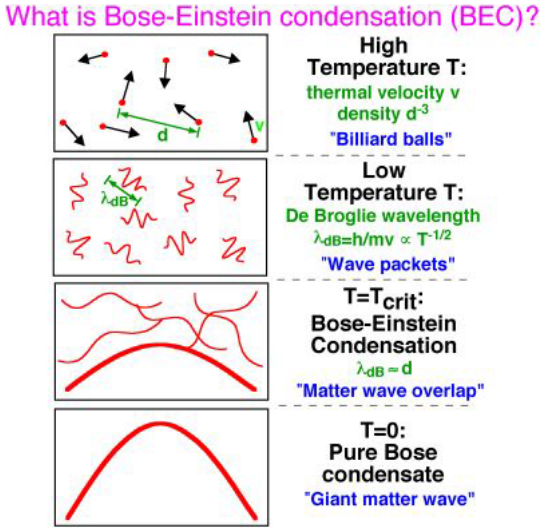

Figure 2.2: A diagram showing the properties of particles in a gas at various temperatures. (Ketterle, Rev. Mod. Phys. 1131(74),2002)

For an ideal (non-interacting, homogeneous) gas of Bosons at thermodynamic equilibrium, the mean number of particles in the grand-canonical ensemble with a single-particle energy ϵ_p of momentum p and a chemical potential μ (the energy required to add a particle to the system) is given, as a function of temperature T, by the Bose distribution.

$$n_p = \frac{1}{e^{(\epsilon_p - \mu)/kT} - 1}, \qquad \epsilon_p = \frac{p^2}{2m} \tag{2.2.5}$$

The total number of particles,

$$N = \sum_p n_p \tag{2.2.6}$$

defines the chemical potential for a given temperature. As the temperature gets below critical temperature T_c, particles are no longer accommodated within the excited states alone but begin to accumulate in the ground state giving rise of the phenomenon of BEC.

$$N = N_e + N_o \qquad T \leq T_c, \tag{2.2.7}$$

where N_o is the number of particles condensed into the lowest energy quantum state which constitutes the Bose-Einstein condensate. N_e represents the number of particles in the excited states and retains a thermal distribution.

Equation (2.2.5) provides the important physical constraint $\mu \leq \epsilon_o$ for the chemical potential of the ideal Bose gas, where ϵ_o is the lowest eigenvalue of the single-particle Hamiltonian. The violation of this inequality would result in a negative value for the occupation number of the states with energy smaller than μ. When $\mu \to \epsilon_o$ the occupation number N_o of the lowest energy state becomes increasingly large. This is actually the mechanism of BEC.
Assuming that the thermodynamic limit, allows the replacement of the summation over p by an integration. We have at the onset of the Bose condensation

$$N = \frac{V}{\lambda_{T_c}^3}\zeta(3/2), \tag{2.2.8}$$

where $\zeta(\nu)$ is Riemann zeta function, which for $\nu = 3/2$ is given by:

$$\zeta(3/2) \approx 2.612$$

For an ideal gas, the condensation into the ground state with $p = 0$ begins, when the chemical potential approaches the ground-state energy $\epsilon_o = 0$. Equation (2.2.8) gives the total number of particles in the system and can be used to determine the transition temperature of the system T_c;

$$T_c = \frac{h^2}{2\pi mk}\left[\frac{N}{V\zeta(3/2)}\right]^{2/3} \tag{2.2.9}$$

This is an interesting result that enables us to choose the transition temperature of our system. We note that T_c is about twice smaller than the right-hand side of the inequality (2.2.4).

The fraction of condensed particles is the ratio between the number of particles occuping the ground state N_o and the total number of particles in the system N. For an ideal bose system this fraction is given by:

$$\frac{N_o}{N} = 1 - \left[\frac{T}{T_c}\right]^{3/2} \tag{2.2.10}$$

From this equation we can see that the condensed fraction is unity when $T = 0$ i.e. all particles of the system occupy the state where $p = 0$, while it is zero when

$T = T_c$ i.e. the condensation has not been built in yet. In an ideal gas, all of the Bose condensed particles occupy the same ground-state wave function, which is the symmetrized product of N_o identical single-particle ground-state wave functions. This product of single-particle wave functions is also called the condensate wave function or the macroscopic wave function. The condensate wave function for a real bose gas is obtained by solving a non-linear Schroedinger equation, the so-called Gross-Pitaevskii equation.

2.2.3 Interactions in BEC

Actually, the ideal gas does not exist since in reality particles usually interact, at least "weakly". Such a system is called a weakly interacting system. In these systems the range r_{int} of the interatomic forces is much smaller than the average distance d between the particles. Then according to $d = n^{-1/3}$, fixed by the density $n = N/V$ of the gas, we can write $nr_{int}^3 \ll 1$, therefore a weakly interacting system is called dilute. This allows one to consider only configurations involving pairs of interacting particles, while configurations with three or more particles interacting simultaneously can be safely neglected. As the particles within a BEC are indistinguishable the condensate may be described by a single wave function $\psi(r)$ normalised to the total particle number. The first order collisions between weakly interacting particles within the condensate are included in the time independent Schroedinger equation using a "mean field" treatment, from which the Gross-Pitaevskii equation(GPE) is obtained

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) + g|\psi(r)|^2\right]\psi(r) = \mu\psi(r), \tag{2.2.11}$$

where m is the mass of the particle, μ the chemical potential and $\hbar$ Planck's constant. The first term accounts for the wave function's kinetic energy and the influence of the external potential (e.g. the presence of a harmonic trap) is included in the second term. Interactions between the particles are accounted for by the non-linear $g|\psi(r)|^2$ coupling term, where:

$$g = \frac{4\pi\hbar^2 a}{m} \tag{2.2.12}$$

The coupling constant g provides a measure of the energy of the condensate due to interactions between its constituent particles. In fact it is the $S-wave$ scattering length "a" which measures this contribution to the energy. The Gross-Pitaevskii equation(GPE) is a mean field equation, which describes the zero-temperature properties of the non-uniform BEC. The state of the BEC can be described by the wave function of the condensate $\psi(r)$ which is obtained by solving Eq.(2.2.11). For a system of this nature, $|\psi(r)|^2$ is interpreted as the particle density, so the total number of atoms is

$$N = \int d\vec{r}|\psi(r)|^2 \tag{2.2.13}$$

GPE is a nonlinear schordinger equation that provides a good description of the exotic behavior of the BEC such as vortices. In a dilute-weakly interacting gas displaying BEC, it is found that the condensate fraction is smaller than unity at zero temperature. This is due to the interaction of particles that depletes the condensate. This phenomenon is termed depletion.

2.2.4 Realisation of Bose-Einstein condensation

There were several trials in the past to achieve BEC in the laboratory but it was difficult because most substances at low temperature do not remain in the gaseous state [79], but they form a solids or liquids as the case of He isotopes and the effect of inter-particle interactions becomes large. In other examples atoms first combine to form molecules which subsequently solidify.

In 1959, Hecht [80] suggested that the spin polarized hydrogen atoms would be a good candidate for weakly interacting Bose gas. In 1980, the experiment was done by Silvera and Walraven in Amsterdam [81]. But although the spin polarized hydrogen atoms don't form a bound states or molecules it will not form a liquid but remain gas to arbitrary low temperature, which was not enough to form BEC. As a consequence of dramatic advances made in laser cooling at the end of eighties [82,83], dilute alkali atoms became attractive candidate for BEC. This is because these neutral atoms

can be easily manipulated by lasers and magnetic fields [76, 77, 84].
Transition to liquids or solids can be avoided at extremely low densities about 10-5 times lower than density of air which is 1019 cm^{-3}. In order to observe BEC of these low density, the temperature must be of order $10^{-7}K$ or less above the absolute zero.

Cooling and trapping of atoms

The advent of laser opened the way to the development of powerful new methods for manipulating and cooling atoms which were exploited in the realization of BEC in alkali atoms vapours.

In 1995, the group of Wolfgang Ketterle in MIT [77] let a beam of sodium atoms emerge from an oven at temperature of $600K$ corresponding to a speed of about $800ms^{-1}$, then they pass through the Zeeman slower where the velocity of the atoms is reduced to $30ms^{-1}$ corresponding to temperature of about $1K$.

In the Zeeman slower, a laser beam propagating in the direction opposite to that of the atomic beam, and the radiation force produced by absorption of photons retards the atoms. The atoms from Zeeman slower are slow enough to be captured by magneto-optical trap (MOT) where they further cooled by the interaction with six laser beams from diode lasers to about $40\mu K$. Even this low temperature is still too high for condensate to form, and the collisions with laser prevents further cooling. The lasers are then turned off and the atoms are held in the trap, by the relatively strong magnetic field. In this trap, they are subjected to evaporative cooling where where the relatively energetic atoms leave the system, thereby lowering the average energy of the remaining atoms. This is the final step for cooling, and when the atoms are cooled to temperatures below $100nK$ BEC achieved.

The Magneto-Optical Trap (MOT)

Magnetic fields are required to confine the atoms in the space while they are being cooled and to keep the cool atoms from falling in the earth's gravitational field. In the MOT this is done with a combination of laser beams(optical molasses) and spa-

tially varying magnetic field. Since the atomic energy levels depend on the magnetic field, the radiation pressure depends on position. The MOT doesn't only trap atoms but also cool them.

By increasing field gradients in MOT, the cloud of atoms can be compressed

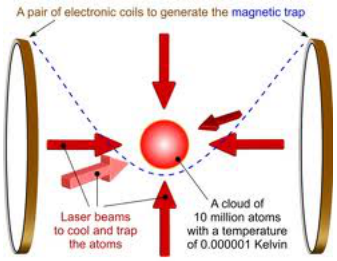

Figure 2.3: Schematic illustration of a magneto-optical trap (MOT). The six laser beams cool the atoms and push them to the intersection point while the magnetic trap (generated with a pair of electronic coils) confines the atoms in a small volume approximately 1 m

by factor 10 (in number density). After sufficiently large number of atoms have accumulated in MOT, laser beams are turned off and the atoms are confined purely by magnetic field, at this stage the gas with phase space density 10^{-6}. Then The final step in achieving BEC is started by evaporative cooling process.

Evaporative cooling

The temperature reached by laser cooling is impressively low $(1 - 0.1\mu K)$, but it is not low enough to produce BEC in gases at the densities that are realizable experimentally. In the experiments performed to date BEC of alkali gases is achieved by using evaporative cooling after laser cooling, it was first suggested by H. F. Hess in 1986 [85]. The basic physical effect in evaporative cooling is that, if particles escaping from a system have energy higher than average energy of particles in the system, the remaining particles are cooled [85].

If one makes a hole in the trap high up in the sides of the trap, only atoms with energy at least equal to the energy of the trap at the hole able to escape. In practice one can make such a hole by applying radio- frequency radiation that flips the spin state of an atom from a low field seeking one to a high field seeking one, thereby

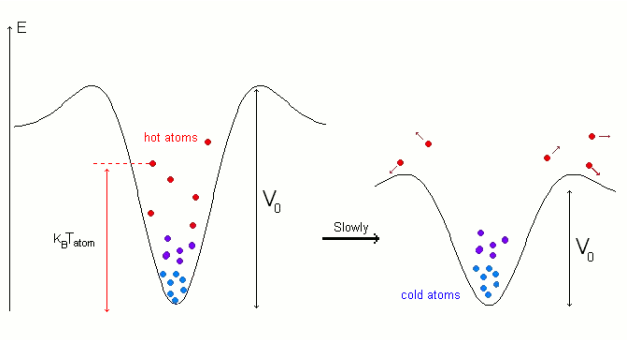

Figure 2.4: illustration of evaporative cooling

expelling the atom from the trap [86]. The position of the hole in the trap may be selected by tuning the frequency of the radio-frequency radiation.

Chapter 3

Two species model

3.1 The physical model

We consider a boson system of two species A and B of non-relativistic particles having the same mass m and moving in three dimensions. We assume that the number of particles of species A is equal to that of species B,

$$N_A = N_B = N,$$

and that two particles belonging to the same species repel each other with a force proportional to their separation

$$\vec{F}^{AA}_{i\to j} = g_{AA}(\vec{r}^{A}_i - \vec{r}^{A}_j) \qquad g_{AA} > 0 \tag{3.1.1}$$

$$\vec{F}^{BB}_{i\to j} = g_{BB}(\vec{r}^{B}_i - \vec{r}^{B}_j) \qquad g_{BB} > 0 \tag{3.1.2}$$

while the attractive force between two particles belonging to two different species is

$$\vec{F}^{AB}_{i\to j} = -g_{AB}(\vec{r}^{A}_i - \vec{r}^{B}_j) \qquad g_{AB} > 0 \tag{3.1.3}$$

The vectors $\vec{r}^{A}_i$ and $\vec{r}^{B}_i$ give the position vector of i^{th} particle of species A and B respectively.

The Hamiltonian of the system is given by:

$$H = H_o + V, \tag{3.1.4}$$

where H_o is the kinetic energy part,

$$H_o = \sum_{i=1}^{N} \left[\frac{(\vec{p}_i^{\,A})^2}{2m} + \frac{(\vec{p}_i^{\,B})^2}{2m} \right], \tag{3.1.5}$$

with $\vec{p}_i^{\,A}$ and $\vec{p}_i^{\,B}$ the momenta for i^{th} particle of species A and B respectively.
The potential energy V is obtained by taking into account all possible interactions between all particles from both species,

$$\begin{aligned} V(\vec{r}_i^{\,A}, \vec{r}_j^{\,B}) &= \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} [g_{AB} (\vec{r}_i^{\,A} - \vec{r}_j^{\,B})^2 - \frac{1}{2} g_{AA} (\vec{r}_i^{\,A} - \vec{r}_j^{\,A})^2 \\ &- \frac{1}{2} g_{BB} (\vec{r}_i^{\,B} - \vec{r}_j^{\,B})^2] \end{aligned} \tag{3.1.6}$$

In this chapter we consider the special case where the coupling constants are equal;

$$g_{AA} = g_{BB} = g_{AB} = g \tag{3.1.7}$$

The general case will be studied in chapter 4.

The potential energy in the special case given by (3.1.7) takes the form:

$$V(\vec{r}_i^{\,A}, \vec{r}_j^{\,B}) = \frac{1}{2} g \sum_{i=1}^{N} \sum_{j=1}^{N} [(\vec{r}_i^{\,A} - \vec{r}_j^{\,B})^2 - \frac{1}{2} (\vec{r}_i^{\,A} - \vec{r}_j^{\,A})^2 - \frac{1}{2} (\vec{r}_i^{\,B} - \vec{r}_j^{\,B})^2] \tag{3.1.8}$$

Exapanding the right hand side we obtain

$$\begin{aligned} V(\vec{r}_i^{\,A}, \vec{r}_j^{\,B}) &= \frac{1}{2} g \sum_{j=1}^{N} \sum_{i=1}^{N} [\vec{r}_i^{\,A} . \vec{r}_j^{\,A} - 2 \vec{r}_i^{\,A} . \vec{r}_j^{\,B} + \vec{r}_i^{\,B} . \vec{r}_j^{\,B}] \\ &= \frac{1}{2} g \left(\sum_{i=1}^{N} \vec{r}_i^{\,A} - \sum_{i=1}^{N} \vec{r}_i^{\,B} \right)^2 \end{aligned} \tag{3.1.9}$$

We can see that the interaction term depends on the separation between the centers of mass of both particle species.

The full Hamiltonian of the system,

$$H = \sum_{i=1}^{N} \left[\frac{(\vec{p}_i^{\,A})^2}{2m} + \frac{(\vec{p}_i^{\,B})^2}{2m} \right] + \frac{1}{2} g \left(\sum_{i=1}^{N} \vec{r}_i^{\,A} - \sum_{i=1}^{N} \vec{r}_j^{\,B} \right)^2 \tag{3.1.10}$$

3.2 Exact solution of the classical system

We are interested in the time evolution of the classical system from the initial configuration:

$$\begin{aligned} \vec{r}_i^{\,A}(t=0) &= \vec{r}_{io}^{\,A} \qquad & \vec{p}_i^{\,A}(t=0) = \vec{p}_{io}^{\,A} \\ \vec{r}_i^{\,B}(t=0) &= \vec{r}_{io}^{\,B} \qquad & \vec{p}_i^{\,B}(t=0) = \vec{p}_{io}^{\,B} \end{aligned} \tag{3.2.1}$$

These conditions give the initial position and the initial momenta of the particles.

To solve the classical initial value problem, we diagonalize the potential energy matrix. Let

$$\vec{r}^{\,A} = \begin{pmatrix} \vec{r}_1^{\,A} \\ \vec{r}_2^{\,A} \\ \vdots \\ \vec{r}_N^{\,A} \end{pmatrix} \qquad \vec{r}^{\,B} = \begin{pmatrix} \vec{r}_1^{\,B} \\ \vec{r}_2^{\,B} \\ \vdots \\ \vec{r}_N^{\,B} \end{pmatrix}$$

and

$$\vec{p}^{\,A} = \begin{pmatrix} \vec{p}_1^{\,A} \\ \vec{p}_2^{\,A} \\ \vdots \\ \vec{p}_N^{\,A} \end{pmatrix} \qquad \vec{p}^{\,B} = \begin{pmatrix} \vec{p}_1^{\,B} \\ \vec{p}_2^{\,B} \\ \vdots \\ \vec{p}_N^{\,B} \end{pmatrix}$$

The linear momentum matrix relates to the position vector by

$$\vec{p}^{\,A} = m\frac{d\vec{r}^{\,A}}{dt}, \qquad \vec{p}^{\,B} = m\frac{d\vec{r}^{\,B}}{dt} \tag{3.2.2}$$

Using the vectors $\vec{r}^{\,A}$ and $\vec{r}^{\,B}$ we rewrite the Hamiltonian in the matrix form

$$\begin{aligned} H &= \frac{1}{2m}\begin{pmatrix} \vec{p}^{\,A} & \vec{p}^{\,B} \end{pmatrix}\left(\begin{array}{c|c} I_N & 0 \\ \hline 0 & I_N \end{array}\right)\begin{pmatrix} \vec{p}^{\,A} \\ \vec{p}^{\,B} \end{pmatrix} \\ &+ \begin{pmatrix} \vec{r}^{\,A} & \vec{r}^{\,B} \end{pmatrix}\left(\begin{array}{c|c} (V_1)_{11} & (V_1)_{12} \\ \hline (V_1)_{21} & (V_1)_{22} \end{array}\right)\begin{pmatrix} \vec{r}^{\,A} \\ \vec{r}^{\,B} \end{pmatrix} \end{aligned} \tag{3.2.3}$$

where I_N is the $(N\times N)$ unit matrix. The potential energy matrix V_1 can be obtained directly from Eq.(3.1.9), namely

$$(V_1)_{11} = (V_1)_{22} = -(V_1)_{12} = -(V_1)_{21} = C \tag{3.2.4}$$

with

$$C = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix}$$

The matrix C is an $(N \times N)$ matrix where the elements are (3×3) unit matrix I_3.

The potential energy matrix is a real symmetric matrix and therefore its eigenvalues are real and its eigenvectors are linearly independent. Furthermore eigenvectors belonging to different eigenvalues are orthogonal.
In Appendix A we show that the characteristic equation for the matrix V_1 is

$$\lambda^{2N} - 2N\lambda^{2N-1} = 0 \tag{3.2.5}$$

The roots of this equation are

$$\lambda = 2N \qquad or \qquad \lambda = 0 \tag{3.2.6}$$

If we consider our vector space to be the configuration space of the system, then $\lambda = 2N$ is a simple eigenvalue while $\lambda = 0$ is a $2N-1$ degenerate eigenvalue. On the other hand if we take our vector space to be R^{3N} then the $\lambda = 2N$ is 3-fold degenerate eigenvalue while $\lambda = 0$ is $3(2N-1)$ degenerate eigenvalue.

In Appendix B we construct 2N orthogonal eigenvectors of the matrix V_1. The (2N-1) eigenvectors corresponding to $\lambda = 0$ are

$$\vec{u}_k = \frac{1}{\sqrt{2}} \Big[\; 0 \;\; \cdots \;\; 0 \;\; 1 \;\; 0 \;\; \cdots \;\; 0 \;\vdots\; 0 \;\; \cdots \;\; 0 \;\; 1 \;\; 0 \;\; \cdots \;\; 0 \Big]^T \qquad k = 1, 2, \cdots, N$$

where T denotes that the transpose of the matrix

$$\vec{u}_{N+k} = \frac{1}{\sqrt{2k(k+1)}} \Big[\; 1 \;\; \cdots \;\; 1 \;\; -k \;\; 0 \;\; \cdots \;\; 0 \;\vdots\; -1 \;\; \cdots \;\; -1 \;\; k \;\; 0 \;\; \cdots \;\; 0 \Big]^T$$
$$k = 1, 2, \cdots, N-1$$

The eigenvector corresponding to the eigenvalue

$$\lambda \;\; = \;\; 2N$$

is given by

$$\vec{u}_{2N} = \frac{1}{\sqrt{2N}}\left[\begin{array}{cccc:cccc} 1 & 1 & \cdots & 1 & -1 & -1 & \cdots & -1 \end{array}\right] \tag{3.2.7}$$

The diagonalizing matrix O_1 is therefore:

$$O_1 = \left[\begin{array}{c|c|c|c|c} \vec{u}_1 & \vec{u}_2 & \cdots & \vec{u}_{2N-1} & \vec{u}_{2N} \end{array}\right] \tag{3.2.8}$$

It is an orthogonal matrix

$$O_1 O_1^T = O_1^T O_1 = I_{2N} \tag{3.2.9}$$

Since the vectors

$$\vec{u}_i \qquad\qquad i = 1, \cdots, N$$

are orthogonal

$$\vec{u}_i . \vec{u}_j = \delta_{ij} \tag{3.2.10}$$

In the same appendix we show that the diagonalizing matrix O_1 can be written in the block form

$$O_1 = \left[\begin{array}{c:c} \frac{1}{\sqrt{2}} I_N & T \\ \hdashline \frac{1}{\sqrt{2}} I_N & -T \end{array}\right] \tag{3.2.11}$$

where the matrix T is given by

$$T_{ij} = \frac{1}{\sqrt{2j(j+1-j\delta_{jN})}} \begin{cases} 1 & i \leq j \\ -j(1-\delta_{jN}) & i = j+1 \\ 0 & i > j+1 \end{cases} \tag{3.2.12}$$

The new coordinate vectors

$$\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{2N}$$

are related to the old coordinate vectors

$$\vec{r}_1^{\,A}, \cdots, \vec{r}_{2N}^{\,A}, \vec{r}_1^{\,B}, \cdots, \vec{r}_{2N}^{\,B}$$

by:

$$\begin{bmatrix} \vec{r}_1 \\ \vec{r}_2 \\ \vdots \\ \vec{r}_{2N} \end{bmatrix} = O_1^T \begin{bmatrix} \vec{r}_1^A \\ \vdots \\ \vec{r}_N^A \\ \vec{r}_1^B \\ \vdots \\ \vec{r}_N^B \end{bmatrix} \tag{3.2.13}$$

Substituting for O_1 we obtain

$$\begin{aligned} \vec{r}_k &= \frac{1}{\sqrt{2}}(\vec{r}_k^A + \vec{r}_k^B) \\ \vec{r}_{N+k} &= \frac{1}{\sqrt{2k(k+1-k\delta_{kN})}} \left[\sum_{j=1}^{k} (\vec{r}_j^A - \vec{r}_j^B) - k(1-\delta_{kN})(\vec{r}_{k+1}^A + \vec{r}_{k+1}^B) \right] \end{aligned} \tag{3.2.14}$$

The inverse transformation is given by

$$\begin{aligned} \vec{r}_k^A &= \frac{1}{\sqrt{N}}\vec{r}_k - \frac{(k-1)}{\sqrt{2k(k-1)}}\vec{r}_{N+k-1} + \sum_{j=k}^{N} \frac{1}{\sqrt{2j(j+1+j\delta_{jN})}}\vec{r}_{N+j} \\ \vec{r}_k^B &= \frac{1}{\sqrt{N}}\vec{r}_k + \frac{(k-1)}{\sqrt{2k(k-1)}}\vec{r}_{N+k-1} - \sum_{j=k}^{N} \frac{1}{\sqrt{2j(j+1+j\delta_{jN})}}\vec{r}_{N+j}, \quad k = 1, \cdots N \end{aligned} \tag{3.2.15}$$

Under the change of coordinates (3.2.13) the matrix for the linear momentum vector

$$\begin{bmatrix} \vec{p}^A \\ \vec{p}^B \end{bmatrix}$$

transforms to

$$\begin{bmatrix} \vec{p}_1^A \\ \vdots \\ \vec{p}_N^A \\ \vec{p}_1^B \\ \vdots \\ \vec{p}_N^B \end{bmatrix} = O_1 \begin{bmatrix} \vec{p}_1 \\ \vec{p}_2 \\ \vdots \\ \vec{p}_{2N} \end{bmatrix} \tag{3.2.16}$$

where

$$\vec{p}_i = m\frac{d\vec{r}_i}{dt} \qquad\qquad i = 1, 2 \cdots, 2N \tag{3.2.17}$$

In the new coordinate system the Hamiltonian is given by:

$$\begin{aligned} H &= \frac{1}{2m}\left[\ \vec{p}_1 \cdots \vec{p}_{2N}\ \right] O_1^T I_{2N} O_1 \begin{bmatrix} \vec{p}_1 \\ \vdots \\ \vec{p}_{2N} \end{bmatrix} \\ &+ \frac{1}{2} g \left[\ \vec{r}_1 \cdots \vec{r}_{2N}\ \right] O_1^T V_1 O_1 \begin{bmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_{2N} \end{bmatrix} \end{aligned} \tag{3.2.18}$$

Since the matrix O_1 is an orthogonal matrix and

$$O_1^T V O_1 = \left[\begin{array}{cccc:c} 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \\ \hdashline 0 & 0 & \cdots & 0 & 2N \end{array}\right] \begin{matrix} \Big\} \\ \\ \\ \\ \Big\} \end{matrix} \begin{matrix} \text{(2N-1)-row} \\ \\ \\ \\ \text{1-row} \end{matrix} \tag{3.2.19}$$

The Hamiltonian takes the simple form:

$$H = \sum_{i=1}^{2N} \frac{\vec{p}_i^{\,2}}{2m} + gN\vec{r}_{2N}^{\,2} \tag{3.2.20}$$

We have (2N-1) translational modes in three dimensions and one mode describing simple harmonic motion.

The Hamilton's equations of motions are:

$$\frac{d\vec{p}_i}{dt} = 0 \qquad i = 1, 2 \cdots (2N-1) \tag{3.2.21}$$

$$\frac{d\vec{p}_{2N}}{dt} = -2Ng\vec{r}_{2N} \tag{3.2.22}$$

and

$$\frac{d\vec{r}_i}{dt} = \frac{\vec{p}_i}{m} \qquad i = 1, 2 \cdots 2N \tag{3.2.23}$$

Eq.(3.2.21) shows that $i = 1, 2 \cdots 2N-1$

$$\vec{p}_i = \vec{A}_i \qquad i = 1, 2 \cdots (2N-1) \tag{3.2.24}$$

where $\vec{A}_i$ are a constant vectors. Inserting this into Eq.(3.2.23) we get

$$\frac{d\vec{r}_i}{dt} = \frac{\vec{A}_i}{m} \qquad i = 1, 2 \cdots (2N-1)$$

or

$$\vec{r}_i = \frac{\vec{A}_i}{m} t + \vec{B}_i \qquad i = 1, 2 \cdots (2N-1) \tag{3.2.25}$$

where $\vec{B}_i$ are constant vectors. For $i = 2N$ we differentiate Eq.(3.2.23) with respect to t.

$$\frac{d^2\vec{r}_{2N}}{dt^2} = \frac{1}{m}\frac{d\vec{p}_{2N}}{dt}$$

and use Eq.(3.2.22)

$$\frac{d^2\vec{r}_{2N}}{dt^2} = -\frac{2gN}{m}\vec{r}_{2N} \tag{3.2.26}$$

This is the equation of a harmonic oscillator of frequency

$$\omega = \sqrt{\frac{2gN}{m}} \tag{3.2.27}$$

The solution of this equation is given by:

$$\vec{r}_{2N} = \frac{\vec{A}_{2N}}{m\omega} \sin\omega t + \vec{B}_{2N} \cos\omega t \tag{3.2.28}$$

We have $2N$ constant $\vec{A}_i$ and $\vec{B}_i$ where $i = 1, 2 \cdots 2N$. They are related to the vectors $\vec{r}_i$ and $\vec{p}_i$

$$\begin{aligned} \vec{r}_i(t=0) &= \vec{B}_i \qquad i = 1, 2 \cdots 2N \\ \vec{p}_i(t=0) &= \vec{A}_i \qquad i = 1, 2 \cdots 2N \end{aligned} \tag{3.2.29}$$

To obtain the position vectors $\vec{r}_i^A$ and $\vec{r}_i^B$ we use the transformation equations (3.2.15). The resulting vectors will depend on $\vec{A}_i$ and $\vec{B}_i$. To express these vectors in term of $\vec{r}_{io}^A$, $\vec{r}_{io}^B$, $\vec{p}_{io}^A$ and $\vec{p}_{io}^B$ we use Eq.(3.2.15) and the inverse of Eq.(3.2.16). This give the complete solution of the problem.

The special case N=3

We consider, in some details, the $N = 3$ case. We have three particles of species A and three particles of species B. The transformation matrix T now reads

$$T = \begin{bmatrix} \frac{1}{\sqrt{4}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{4}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{6}} \\ 0 & -\frac{2}{\sqrt{12}} & \frac{1}{\sqrt{6}} \end{bmatrix} \tag{3.2.30}$$

Also the matrix O_1 is now given by:

$$O_1 = \left[\begin{array}{c|c} \frac{1}{\sqrt{2}} I_3 & T \\ \hline \frac{1}{\sqrt{2}} I_3 & -T \end{array}\right] \tag{3.2.31}$$

Or explicitly

$$O_1 = \frac{1}{\sqrt{2}} \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & 1 & 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & 0 & 1 & 0 & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ \hline 1 & 0 & 0 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} \\ 0 & 1 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} \\ 0 & 0 & 1 & 0 & \frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{3}} \end{array}\right] \tag{3.2.32}$$

The new coordinate vectors are given by:

$$\begin{aligned} \vec{r}_i &= \frac{1}{\sqrt{2}}(\vec{r}_i^{\,A} + \vec{r}_i^{\,B}) \qquad\qquad i = 1, 2, 3 \\ \vec{r}_4 &= \frac{1}{\sqrt{4}}[(\vec{r}_1^{\,A} + \vec{r}_2^{\,B}) - (\vec{r}_2^{\,A} + \vec{r}_1^{\,B})] \\ \vec{r}_5 &= \frac{1}{\sqrt{12}}[(\vec{r}_1^{\,A} + \vec{r}_2^{\,A} + 2\vec{r}_3^{\,B}) - (\vec{r}_1^{\,B} + \vec{r}_2^{\,B} + 2\vec{r}_1^{\,A})] \\ \vec{r}_6 &= \frac{1}{\sqrt{6}}[(\vec{r}_1^{\,A} + \vec{r}_2^{\,A} + \vec{r}_3^{\,A}) - (\vec{r}_1^{\,B} + \vec{r}_2^{\,B} + \vec{r}_3^{\,B})] \end{aligned} \tag{3.2.33}$$

The inverse transformations are also given by

$$\begin{aligned}
\vec{r}_1^{\,A} &= \frac{1}{\sqrt{2}}\vec{r}_1 + \frac{1}{\sqrt{4}}\vec{r}_4 + \frac{1}{\sqrt{12}}\vec{r}_5 + \frac{1}{\sqrt{6}}\vec{r}_6 \\
\vec{r}_2^{\,A} &= \frac{1}{\sqrt{2}}\vec{r}_2 - \frac{1}{\sqrt{4}}\vec{r}_4 + \frac{1}{\sqrt{12}}\vec{r}_5 + \frac{1}{\sqrt{6}}\vec{r}_6 \\
\vec{r}_3^{\,A} &= \frac{1}{\sqrt{2}}\vec{r}_3 - \frac{2}{\sqrt{12}}\vec{r}_5 + \frac{1}{\sqrt{6}}\vec{r}_6 \\
\\
\vec{r}_1^{\,B} &= \frac{1}{\sqrt{2}}\vec{r}_1 - \frac{1}{\sqrt{4}}\vec{r}_4 - \frac{1}{\sqrt{12}}\vec{r}_5 - \frac{1}{\sqrt{6}}\vec{r}_6 \\
\vec{r}_2^{\,B} &= \frac{1}{\sqrt{2}}\vec{r}_2 + \frac{1}{\sqrt{4}}\vec{r}_4 - \frac{1}{\sqrt{12}}\vec{r}_5 - \frac{1}{\sqrt{6}}\vec{r}_6 \\
\vec{r}_3^{\,A} &= \frac{1}{\sqrt{2}}\vec{r}_3 + \frac{2}{\sqrt{12}}\vec{r}_5 - \frac{1}{\sqrt{6}}\vec{r}_6
\end{aligned} \tag{3.2.34}$$

The constants $\vec{A}_i, \vec{B}_i \quad i = 1, 2, 3$ are related to $\vec{r}_{io}^{\,A}, \vec{r}_{io}^{\,B}, \vec{p}_{io}^{\,A} \quad and \quad \vec{p}_{io}^{\,B}$ through

$$\begin{aligned}
\vec{A}_i &= \frac{1}{\sqrt{2}}(\vec{p}_{io}^{\,A} + \vec{p}_{io}^{\,B}) \qquad\qquad i = 1, 2, 3 \\
\vec{A}_4 &= \frac{1}{\sqrt{4}}[(\vec{p}_{1o}^{\,A} + \vec{p}_{2o}^{\,B}) - (\vec{p}_{2o}^{\,A} + \vec{p}_{1o}^{\,B})] \\
\vec{A}_5 &= \frac{1}{\sqrt{12}}[(\vec{p}_{1o}^{\,A} + \vec{p}_{2o}^{\,A} + 2\vec{p}_{3o}^{\,B}) - (\vec{p}_{1o}^{\,B} + \vec{p}_{2o}^{\,B} + 2\vec{p}_{3o}^{\,A})] \\
\vec{A}_6 &= \frac{1}{\sqrt{6}}[(\vec{p}_{1o}^{\,A} + \vec{p}_{2o}^{\,A} + \vec{p}_{3o}^{\,A}) - (\vec{p}_{1o}^{\,B} + \vec{p}_{2o}^{\,B} + \vec{p}_{3o}^{\,B})]
\end{aligned} \tag{3.2.35}$$

and

$$\begin{aligned}
\vec{B}_i &= \frac{1}{\sqrt{2}}(\vec{r}_{io}^{\,A} + \vec{r}_{io}^{\,B}) \qquad\qquad i = 1, 2, 3 \\
\vec{B}_4 &= \frac{1}{\sqrt{4}}[(\vec{r}_{1o}^{\,A} + \vec{r}_{2o}^{\,B}) - (\vec{r}_{2o}^{\,A} + \vec{r}_{1o}^{\,B})] \\
\vec{B}_5 &= \frac{1}{\sqrt{12}}[(\vec{r}_{1o}^{\,A} + \vec{r}_{2o}^{\,A} + 2\vec{r}_{3o}^{\,B}) - (\vec{r}_{1o}^{\,B} + \vec{r}_{2o}^{\,B} + 2\vec{r}_{3o}^{\,A})] \\
\vec{B}_6 &= \frac{1}{\sqrt{6}}[(\vec{r}_{1o}^{\,A} + \vec{r}_{2o}^{\,A} + \vec{r}_{3o}^{\,A}) - (\vec{r}_{1o}^{\,B} + \vec{r}_{2o}^{\,B} + \vec{r}_{3o}^{\,B})]
\end{aligned} \tag{3.2.36}$$

The vectors $\vec{r}_i$ are then

$$\begin{aligned}
\vec{r}_i &= \frac{\vec{A}_i}{m}t + \vec{B}_i \qquad\qquad i = 1, 2, \cdots 5 \\
\vec{r}_6 &= \frac{\vec{A}_6}{m\omega}\sin\omega t + \vec{B}_6\cos\omega t
\end{aligned} \tag{3.2.37}$$

Using Eq.(3.2.35) with Eq.(3.2.38) we obtain

$$\begin{aligned}
\vec{r}_i^{\,A} &= \frac{1}{\sqrt{2}}[(\vec{B}_i + \frac{\vec{A}_i}{m}t) - \frac{(i-1)}{\sqrt{i(i-1)}}(\vec{B}_{i+2} + \frac{\vec{A}_{i+2}}{m}t) \\
&+ \sum_{j=i}^{3} \frac{1}{\sqrt{j(j+1-j\delta_{j3})}}(\vec{B}_{j+3}\cos\omega t + \frac{\vec{A}_{j+3}}{m\omega}\sin\omega t) \\
\vec{r}_i^{\,B} &= \frac{1}{\sqrt{2}}[(\vec{B}_i + \frac{\vec{A}_i}{m}t) + \frac{(i-1)}{\sqrt{i(i-1)}}(\vec{B}_{i+2} + \frac{\vec{A}_{i+2}}{m}t) \\
&- \sum_{j=i}^{3} \frac{1}{\sqrt{j(j+1-j\delta_{j3})}}(\vec{B}_{j+3}\cos\omega t + \frac{\vec{A}_{j+3}}{m\omega}\sin\omega t), \quad i = 1, \cdots 3
\end{aligned}$$

These equations express $\vec{r}_i^{\,A} \quad and \quad \vec{r}_i^{\,B}, \quad i = 1, 2, 3$ in terms of $\vec{A}_i, \vec{B}_i$,
we use Eqs.(3.2.36),(3.2.37) to obtain the position vectors in terms of the initial positions and momenta of the particles

$$\begin{aligned}
\vec{r}_j^{\,A}(t) &= \frac{1}{6}[(5\vec{r}_{jo}^{\,A} - \sum_{i\neq j}\vec{r}_{io}^{\,A} + \sum_{i=1,2,3}\vec{r}_{io}^{\,B}) + \frac{1}{m}(5\vec{p}_{jo}^{\,A} - \sum_{i\neq j}\vec{p}_{io}^{\,A} + \sum_{i=1,2,3}\vec{p}_{io}^{\,B})t \\
&+ \sum_{i=1,2,3}[\frac{1}{m\omega}(\vec{p}_{io}^{\,A} - \vec{p}_{io}^{\,B})\sin\omega t + (\vec{r}_{io}^{\,A} - \vec{r}_{io}^{\,B})\cos\omega t]] \\
\vec{r}_j^{\,B}(t) &= \frac{1}{6}[(5\vec{r}_{jo}^{\,B} - \sum_{i\neq j}\vec{r}_{io}^{\,B} + \sum_{i=1,2,3}\vec{r}_{io}^{\,A}) + \frac{1}{m}(5\vec{p}_{jo}^{\,B} - \sum_{i\neq j}\vec{p}_{io}^{\,B} + \sum_{i=1,2,3}\vec{p}_{io}^{\,A})t \\
&- \sum_{i=1,2,3}[\frac{1}{m\omega}(\vec{p}_{io}^{\,A} - \vec{p}_{io}^{\,B})\sin\omega t + (\vec{r}_{io}^{\,A} - \vec{r}_{io}^{\,B})\cos\omega t]] \qquad i = 1, 2, 3 \quad (3.2.38)
\end{aligned}$$

Thus each particle preforms harmonic oscillator about a center which moves with constant velocity. For a particle of species A, its velocity is given by:

$$\frac{1}{m}\vec{p}_{jo}^{\,A} - \frac{1}{2}[\frac{1}{3m}\sum_{i=1,2,3}\vec{p}_{io}^{\,A} - \frac{1}{3m}\sum_{i=1,2,3}\vec{p}_{io}^{\,B}]$$

The quantity in the square brackets gives the difference between the average velocities of the three particles of species A and the three particles of species B.
The velocity of the center of oscillation of the particle of species B is also

$$\frac{1}{m}\vec{p}_{jo}^{\,B} - \frac{1}{2}[\frac{1}{3m}\sum_{i=1,2,3}\vec{p}_{io}^{\,B} - \frac{1}{3m}\sum_{i=1,2,3}\vec{p}_{io}^{\,A}]$$

This can also be obtained by replacing each A-label by B-label.

The classical motion is described as follows: Each particle oscillates with the same frequency

$$\omega = \sqrt{\frac{2gN}{m}}$$

about a center which moves with uniform velocity. This velocity depends on the particles initial position and momentum.

3.3 Exact solution of the quantum system

The quantum mechanical behaviour of the system is determined by the quantum Hamiltonian operator $\hat{H}$ which is obtained from the classical Hamiltonian by replacing the dynamical variables by operators. In the coordinate representation we have:

$$\begin{aligned} \vec{r}_i^A &\rightarrow \vec{r}_i^A \qquad \vec{r}_i^B \rightarrow \vec{r}_i^B \\ \vec{p}_i^A &\rightarrow \frac{\hbar}{i}\vec{\nabla}_i^A \qquad \vec{p}_i^B \rightarrow \frac{\hbar}{i}\vec{\nabla}_i^B \qquad i = 1, 2, \cdots N \end{aligned} \tag{3.3.1}$$

Subsituting Eq.(3.3.1) into Eq.(3.1.10) we get

$$\hat{H} = \sum_{i=1}^{N} \frac{1}{2m}[(\vec{\nabla}_i^A)^2 + (\vec{\nabla}_i^B)^2] + \frac{1}{2}g\left(\sum_{i=1}^{N}\vec{r}_i^A - \sum_{i=1}^{N}\vec{r}_i^B\right)^2 \tag{3.3.2}$$

The wave function of the system

$$\psi = \psi(t, \vec{r}_i^A, \vec{r}_i^B) \tag{3.3.3}$$

is the solution of the time dependent Schroedinger equation

$$i\hbar\frac{\partial\psi(t, \vec{r}_i^A, \vec{r}_i^B)}{\partial t} = \hat{H}\psi(t, \vec{r}_i^A, \vec{r}_i^B) \tag{3.3.4}$$

Since the Hamiltonian doesn't depend explicitly on time, the time evolution of the system is given by;

$$\psi(t, \vec{r}_i^A, \vec{r}_i^B) = e^{i\frac{Et}{\hbar}}\psi_E(\vec{r}_i, \vec{r}_j) \tag{3.3.5}$$

where $\psi_E(\vec{r}_i, \vec{r}_j)$ is the solution of the time independent Schroedinger equation

$$\hat{H}\psi_E(\vec{r}_i, \vec{r}_j) = E\psi_E(\vec{r}_i, \vec{r}_j) \tag{3.3.6}$$

Under the transformation of coordinates given by Eq.(3.2.15) the Hamiltonian operator takes the simple form:

$$\hat{H} = \sum_{i=1}^{2N} \frac{-\hbar^2}{2m}(\vec{\nabla}_i)^2 + gN\vec{r}_{2N}^2 \tag{3.3.7}$$

The Hamiltonian operator split up into the single particle Hamiltonians:

$$\begin{aligned} \hat{h}_i &= \frac{-\hbar^2}{2m}\vec{\nabla}_i^2 \qquad i = 1, 2, \cdots 2N-1 \\ \hat{h}_{2N} &= \frac{-\hbar^2}{2m}\vec{\nabla}_{2N}^2 + gN\vec{r}_{2N}^2 \end{aligned} \tag{3.3.8}$$

so that the total Hamiltonian is;

$$\hat{H} = \sum_{i=1}^{2N-1} \hat{h}_i + \hat{h}_{2N} \tag{3.3.9}$$

Inserting the Hamiltonian $\hat{H}$ into the Schroedinger equation, we obtain

$$\left(\sum_{i=1}^{2N-1} \hat{h}_i + \hat{h}_{2N} \right) \psi_E(\vec{r}_1, \cdots \vec{r}_{2N}) = E\psi_E(\vec{r}_1, \cdots \vec{r}_{2N}) \tag{3.3.10}$$

The wave function ψ_E of the total system can be expressed as a product of wave functions each of which depends on the variables of a single particle

$$\psi_E(\vec{r}_1, \cdots \vec{r}_{2N}) = \Phi(\vec{r}_{2N}) \prod_{i=1}^{2N-1} \phi_i(\vec{r}_i) \tag{3.3.11}$$

where

$$\begin{aligned} \hat{h}_i\phi_i(\vec{r}_i) &= \varepsilon_i\phi_i(\vec{r}_i) \qquad i = 1, \cdots 2N-1 \\ \hat{h}_{2N}\phi(\vec{r}_{2N}) &= \varepsilon_{2N}\phi(\vec{r}_{2N}) \end{aligned} \tag{3.3.12}$$

The total energy of the system is the sum of energies ε_i

$$E = \sum_{i=1}^{2N} \varepsilon_i \tag{3.3.13}$$

Substituting for $\hat{h}_i$ we get

$$-\frac{\hbar^2}{2m}\vec{\nabla}_i^2\phi(\vec{r}_i) = \varepsilon_i\phi(\vec{r}_i) \qquad i = 1, \cdots 2N-1 \tag{3.3.14}$$

$$\left(-\frac{\hbar^2}{2m}\vec{\nabla}_{2N}^2 + gN\vec{r}_{2N}^2 \right) \Phi(\vec{r}_{2N}) = \varepsilon_{2N}\Phi(\vec{r}_{2N}) \tag{3.3.15}$$

Eq.(3.3.14) is the Schroedinger equation for a free particle of energy ε_i.

To solve Eq.(3.3.14), we imagine the system to be in a very large cubic box of volume

$$V = L^3$$

and impose periodic boundary conditions on the function ϕ

$$\begin{aligned} \phi(x_i + L, y_i, z_i) &= \phi(x_i, y_i, z_i) \\ \phi(x_i, y_i + L, z_i) &= \phi(x_i, y_i, z_i) \\ \phi(x_i, y_i, z_i + L) &= \phi(x_i, y_i, z_i) \qquad i = 1, 2, \cdots 2N-1 \end{aligned} \tag{3.3.16}$$

Then the free particle solution is

$$\phi_i(\vec{r}_1) = \frac{1}{\sqrt{V}} e^{ik.\vec{r}_i} \qquad i = 1, 2, \cdots 2N-1 \tag{3.3.17}$$

Using Eq.(3.3.16) we obtain

$$k_i = \frac{2\pi}{L}(n_{ix}, n_{iy}, n_{iz}) \qquad n_{ix}, n_{iy}, n_{iz} = 0, \pm 1, \pm 2, \cdots \tag{3.3.18}$$

The energy of the free particle is given by:

$$\varepsilon_i \;\; = \;\; \frac{\hbar^2 \vec{k}_i^2}{2m} \tag{3.3.19}$$

Eq.(3.3.15) is the Schordinger equation for a three dimensional harmonic oscillator of a mass m and force constant $2gN$. The solution of this equation is the product of the wave functions of three one-dimensional oscillators, one in $x-$, one in $y-$ and one in $z-$direction. The wave function of the one-dimensional oscillator is given by:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left[\frac{m\omega}{\pi\hbar}\right]^{1/4} H_n(\sqrt{\frac{m\omega}{\pi\hbar}}x) e^{-m\omega x^2/2\hbar} \tag{3.3.20}$$

and the corresponding energy eigenvalue is

$$E_n = \hbar\omega(n + 1/2) \tag{3.3.21}$$

Using Eq.(3.3.20) we build the wave function $\Phi(\vec{r}_{2N})$ of the three dimensional harmonic oscillator

$$\Phi_{n_{2N,x}, n_{2N,y}, n_{2N,z}} = \prod_{\sigma=x,y,z} \left[(\sqrt{2^{n_{2N,\sigma}}(n_{2N,\sigma})!})^{-1/2} \left[\frac{m\omega}{\pi\hbar}\right]^{3/4} H_{n_{2N,\sigma}}(\sqrt{\frac{m\omega}{\pi\hbar}}\sigma) e^{-m\omega\sigma^2/2\hbar} \right] \tag{3.3.22}$$

The energy eigenvalue of the 3-dimensional oscillator

$$E_{n_{2N,x}, n_{2N,y}, n_{2N,z}} = \hbar\omega(n_{2N,x} + n_{2N,y} + n_{2N,z} + 3/2) \tag{3.3.23}$$

To construct the wave function of the system we need to determine the maximal number of commuting operators which commute with the Hamiltonian of the system. The exchange operators

$$\hat{P}_{ij} \qquad i, j = 1, 2, \cdots 2N-1$$

are defined by

$$\hat{P}_{ij}\psi_E(\cdots\vec{r}_i\cdots\vec{r}_j\cdots) = \psi_E(\cdots\vec{r}_j\cdots\vec{r}_i\cdots) \tag{3.3.24}$$

These operators commute with each other:

$$\left[\hat{P}_{ij},\hat{P}_{kl}\right] = 0 \tag{3.3.25}$$

They also commute with the Hamiltonian (3.3.9)

$$\left[\hat{P}_{ij},\hat{H}\right] = 0 \qquad i,j=1,2,\cdots 2N-1 \tag{3.3.26}$$

The wave function

$$\psi(\vec{r}_1\cdots\vec{r}_{2N})$$

should be an eigenfunction of the operator $\hat{P}_{ij}$. since we have a system of bosons

$$\hat{P}_{ij}\psi_E(\vec{r}_1,\cdots\vec{r}_i,\cdots\vec{r}_j,\cdots\vec{r}_{2N-1};\vec{r}_{2N}) = \psi_E(\vec{r}_1,\cdots\vec{r}_j,\cdots\vec{r}_i,\cdots\vec{r}_{2N-1};\vec{r}_{2N}) \tag{3.3.27}$$

with $i,j=1,2,\cdots 2N-1$. Thus the wave function should be symmetric with respect to a change of coordinates and momenta of the first $2N-1$ modes. This gives

$$\psi_E(r_1..r_{2N}) = \frac{1}{\sqrt{(2N-1)S!}}\sum_P \hat{P}[\phi_{k_1}(r_1)\phi_{k_1}(r_1)...\phi_{k_{2N-1}}(r_{2N-1})]\times\Phi_{2N,x;2N,y;2N,z} \tag{3.3.28}$$

where S is an additional normalization constant, and the sum is over all permutations

$$\hat{P}_1,\hat{P}_2,\cdots\hat{P}_{2N-1}$$

of

$$1,2,\cdots 2N-1$$

in the argument of the one-particle wave function

$$\phi_{\vec{k}_i}(\vec{r}_i)$$

The total energy of the system is given according to Eq.(3.3.13) by:

$$E = \sum_{i=1}^{2N-1} \frac{\hbar^2 \vec{k}_i^2}{2m} + \hbar\omega(n_{2N,x} + n_{2N,y} + n_{2N,z} + 3/2) \tag{3.3.29}$$

Where the $\vec{k}_i$ are given by Eq.(3.3.18). The total energy of the system is the sum of the translational energy of the $(2N-1)$ modes plus the energy of the three dimensional harmonic oscillators.

3.4 Exact solution of the statistical mechanical system

For the two species system to have well defined thermodynamic parameters such as the pressure P, the temperature T and the entropy S, the number of particle of each species N as well as volume V occupied by the system should be very large such that we can take the thermodynamic limit

$$N \to \infty, \qquad V \to \infty, \qquad \frac{N}{V} \to \text{finite number} \tag{3.4.1}$$

3.4.1 Determination of the grand canonical partition function

We study the quantum statistical behaviour of the system within the frame work of the grand canonical ensemble. The fundamental physical quantity in the grand canonical description of the system is the grand canonical partition function Z which is defined by [78, 87]:

$$Z(T, V, \mu) = Tr\left\{e^{-\beta(\hat{H}-\mu\hat{N})}\right\} \tag{3.4.2}$$

On the right hand side we have the Hamiltonian of the system $\hat{H}$ and the particle number operator $\hat{N}$ which describe the system from a microscopic point of view. On the left hand side we have Z which depends on the thermodynamic parameters T, V, μ. These parameters give the macroscopic description of the system. The partition function provides the transition from the microscopic to the macroscopic description of the system. Eq.(3.4.2) shows that to obtain Z we need to calculate the trace of the operators in right hand side. Using the grand canonical partition function, we obtain the grand canonical potential

$$\Phi(T, V, \mu) \;=\; -kT \ln Z(T, V, \mu), \tag{3.4.3}$$

which is equivalent to the thermodynamical definition for the grand canonical potential of the system through the relation

$$\Phi(T, V, \mu) \;=\; U - TS - \mu N, \tag{3.4.4}$$

where μ is the chemical potential. The pressure, entropy and number of particles in the system are obtained from the grand potential using the relations:

$$S = -\frac{\partial \Phi}{\partial T} \mid_{V,\mu}, \qquad P = -\frac{\partial \Phi}{\partial V} \mid_{T,\mu}, \qquad N = -\frac{\partial \Phi}{\partial \mu} \mid_{T,V} \tag{3.4.5}$$

To calculate the trace of the operator on the right hand side of Eq.(3.4.2) we have to choose a basis for the Hilbert space of the system. A suitable basis is given by;

$$\left\{ \mid \vec{k}_1, \cdots, \vec{k}_{2N-1} \rangle^s \otimes \mid n_{2N,x}, n_{2N,y}, n_{2N,z} \rangle \right\} \tag{3.4.6}$$

$$\mid \vec{k}_1, \cdots, \vec{k}_{2N-1} \rangle^s = \frac{1}{\sqrt{(2N-1)S!}} \sum_P \hat{P} \mid \vec{k}_1, \cdots, \vec{k}_{2N-1} \rangle \tag{3.4.7}$$

and S is an additional normalization.

The wave function in Eq.(3.3.28) is a coordinate representation of the state vectors. Thus

$$\begin{aligned} \psi(\vec{r}_1, \cdots \vec{r}_{2N-1}, \vec{r}_{2N}) &= ({}^s\langle \vec{r}_1, \cdots \vec{r}_{2N-1} \mid \otimes \langle \vec{r}_{2N} \mid)(\mid \vec{k}_1, \cdots, \vec{k}_{2N-1} \rangle^s \\ &\otimes \mid n_{2N,x}, n_{2N,y}, n_{2N,z} \rangle) \\ &= {}^s\langle \vec{r}_1, \cdots \vec{r}_{2N-1} \mid \vec{k}_1, \cdots, \vec{k}_{2N-1} \rangle^s \\ &\langle \vec{r}_{2N} \mid n_{2N,x}, n_{2N,y}, n_{2N,z} \rangle \end{aligned} \tag{3.4.8}$$

From Eq.(3.4.7) we see that

$${}^s\langle \vec{r}_1, \cdots \vec{r}_{2N-1} \mid \vec{k}_1, \cdots, \vec{k}_{2N-1} \rangle^s = \frac{1}{\sqrt{(2N-1)S!}} \sum_P \hat{P} \mid \phi_{\vec{k}_1}(\vec{r}_1), \cdots, \phi_{\vec{k}_{2N-1}}(\vec{r}_{2N-1}) \rangle \tag{3.4.9}$$

and

$$\langle \vec{r}_{2N} \mid n_{2N,x}, n_{2N,y}, n_{2N,z} \rangle = \Phi_{n_{2N,x}, n_{2N,y}, n_{2N,z}}(\vec{r}_{2N}) \tag{3.4.10}$$

The state vectors

$$\mid \vec{k}_1, \cdots \vec{k}_{2N-1} \rangle^s$$

can also be characterized by the occupation numbers instead of the quantum numbers of the occupied state

$$\mid n_1, n_2, \cdots \rangle^s \equiv \mid \vec{k}_1, \cdots \vec{k}_{2N-1} \rangle^s \tag{3.4.11}$$

These state vectors are orthogonal

$${}^s\langle n_1', n_2', \cdots \mid n_1, n_2, \cdots \rangle^s = \delta_{n_1,n_1'}\delta_{n_2,n_2'}\cdots \tag{3.4.12}$$

The occupation number representation is useful since the Hamiltonian and the occupation number operators are diagonal in this representation

$$\hat{H} \mid n_1, n_2, \cdots \rangle^s = E \mid n_1, n_2, \cdots \rangle^s \tag{3.4.13}$$

$$\hat{N} \mid n_1, n_2, \cdots \rangle^s = N \mid n_1, n_2, \cdots \rangle^s \tag{3.4.14}$$

Where

$$E = \sum_{k=1}^{\infty} n_k \epsilon_k, \qquad N = \sum_{k=1}^{\infty} n_k \tag{3.4.15}$$

The basis vectors (3.4.6) now take the form

$$\{\mid n_1, n_2 \cdots \rangle^s \otimes \mid n_{2N,x}, n_{2N,y}, n_{2N,z} \rangle\} \tag{3.4.16}$$

We will use these basis vectors to calculate the trace in Eq.(3.4.2)

$$\begin{aligned} Z(T,V,\mu) = & \sum_{n_k} \sum_{n_{2N,x}, n_{2N,y}, n_{2N,z}} \langle n_{2N,x}, n_{2N,y}, n_{2N,z} \mid \otimes^s \langle n_1, n_2 \cdots \mid \\ & e^{-\beta(\hat{H}-\mu\hat{N})} \mid n_1, n_2 \cdots \rangle^s \otimes \mid n_{2N,x}, n_{2N,y}, n_{2N,z} \rangle \end{aligned} \tag{3.4.17}$$

We split the Hamiltonian into two parts:

$$\hat{H} = \hat{H}_{2N-1} + \hat{h}_{2N} \tag{3.4.18}$$

where

$$\hat{H}_{2N-1} = \sum_{i=1}^{2N-1} h_i \tag{3.4.19}$$

Similarly we let

$$\mu = \mu_{2N-1} + \mu_{2N} \tag{3.4.20}$$

Since

$$\begin{aligned}\left[\hat{H}_{2N-1}, \hat{h}_{2N}\right] &= 0 \\ \left[\hat{N}, \hat{H}_{2N-1}\right] &= 0 \\ \left[\hat{N}, \hat{h}_{2N}\right] &= 0\end{aligned}$$

$$e^{-\beta(\hat{H}-\mu\hat{N})} = e^{-\beta(\hat{H}_{2N-1}-\mu_{2N-1}\hat{N})}e^{-\beta(\hat{h}_{2N}-\mu_{2N}\hat{N})} \tag{3.4.21}$$

The matrix element on the right hand side of Eq.(3.4.17) is now very easy to evaluate

$$\begin{aligned}&\langle \quad n_{2N,x}, n_{2N,y}, n_{2N,z} \mid \otimes^s \langle n_1, n_2 \cdots \mid e^{-\beta(\hat{H}-\mu\hat{N})} \mid n_1, n_2 \cdots \rangle^s \otimes \mid n_{2N,x}, n_{2N,y}, n_{2N,z} \rangle \\ &= \quad e^{-\beta\sum_{k=1}^{\infty} n_k(\epsilon_k-\mu_{2N-1})} e^{-\beta[\hbar\omega(n_{2N,x}+n_{2N,y}+n_{2N,z}+\frac{3}{2})-\mu_{2N}]}\end{aligned} \tag{3.4.22}$$

where we used Eqs.(3.4.13),(3.4.14) and the orthogonality condition (3.4.12).
We choose

$$\mu_{2N} = 0 \tag{3.4.23}$$

and denote μ_{2N-1} by μ

$$\mu_{2N-1} \equiv \mu \tag{3.4.24}$$

$$Z(T,V,\mu) = \left[\sum_{n_k} e^{-\beta[\sum_{k=1}^{\infty} n_k(\epsilon_k-\mu)]}\right] \times \left[e^{-\frac{3}{2}\beta\hbar\omega}\left(\sum_{n=0}^{\infty} e^{-n\beta\hbar\omega}\right)^3\right] \tag{3.4.25}$$

The grand canonical partition function splits into two parts, the first part associated with the translational modes of the system while the second associated with the vibrational mode.

$$Z(T,V,\mu) = Z_{tr}(T,V,\mu) \times Z_{vib}(T,V) \tag{3.4.26}$$

where

$$Z_{tr}(T,V,\mu) = \sum_{n_k} e^{-\beta[\sum_{k=1}^{\infty} n_k(\epsilon_k-\mu)]} \tag{3.4.27}$$

and

$$Z_{vib}(T,V) = e^{-\frac{3}{2}\beta\hbar\omega}\left(\sum_{n=0}^{\infty} e^{-n\beta\hbar\omega}\right)^3 \tag{3.4.28}$$

The partition function $Z_{vib}(T,V)$ is the canonical partition function for the three dimensional harmonic oscillator. The sum of the geometric series in Eq.(3.4.28) is

$$\sum_{n=0}^{\infty} e^{n\beta\hbar\omega} = \frac{1}{(1-e^{-\beta\hbar\omega})} \tag{3.4.29}$$

Therefore

$$Z_{vib}(T,V) = \frac{e^{-\frac{3}{2}\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^3} \tag{3.4.30}$$

The partition function Z_{tr} can be rearranged in the form:

$$Z_{tr}(T,V,\mu) = \prod_{k=1}^{\infty}\sum_{n_k}\left[e^{-\beta(\epsilon_k-\mu)}\right]^{n_k} \tag{3.4.31}$$

Since we have a system of bosons, any quantum state can be occupied by any number of bosons i.e. $n_k = 0, 1, 2....$ Therefore

$$\sum_{n_k}\left[e^{-\beta(\epsilon_k-\mu)}\right]^{n_k} = \frac{1}{1-ze^{-\beta\epsilon_k}} \tag{3.4.32}$$

where

$$z = e^{\beta\mu} \tag{3.4.33}$$

is the fugicity of the system. Inserting Eq.(3.4.32) into Eq.(3.4.31) we obtain

$$Z_{tr}(T,V,\mu) = \prod_{k=1}^{\infty}\frac{1}{1-ze^{-\beta\epsilon_k}} \tag{3.4.34}$$

where $z = e^{\beta}\mu$ is the fugacity Then the total partition function of the system is,

$$Z(T,V,\mu) = \left[\prod_{k=1}^{\infty}\left(\frac{1}{1-ze^{-\beta\epsilon_k}}\right)\right]\frac{e^{-\frac{3}{2}\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^3} \tag{3.4.35}$$

We can now obtain the grand canonical potential

$$\Phi(T,V,\mu) = kT\sum_{k=0}^{\infty}\ln(1-ze^{-\beta\epsilon_k}) + 3kT\left[\ln(1-e^{-\beta\hbar\omega}) + \frac{1}{2}\beta\hbar\omega\right] \tag{3.4.36}$$

3.4.2 Thermodynamical parameters of the system

The thermodynamic parameters of the system are obtained from the grand canonical potential using Eq.(3.4.5).

The number of the particles is given by

$$2N-1 = \sum_{\vec{k}=0}^{\infty} \frac{1}{z^{-1}e^{\beta\epsilon_k}-1} \tag{3.4.37}$$

Since

$$N \gg 1$$

we have

$$2N = \sum_{\vec{k}=0}^{\infty} \frac{1}{z^{-1}e^{\beta\epsilon_k}-1} \tag{3.4.38}$$

We split the sum over $\vec{k}$ into two parts, the $\vec{k}=0$ and the $\vec{k}\neq 0$ states. Since

$$\vec{k}=0 \Longrightarrow \varepsilon_o = 0$$

we have

$$2N = \frac{z}{1-z} + \sum_{k\neq 0}^{\infty} \frac{1}{z^{-1}e^{\beta\epsilon_{\vec{k}}}-1} \tag{3.4.39}$$

The first term gives the contribution of the ground state energy to the total number of the particles

$$N_o = \frac{z}{1-z} \tag{3.4.40}$$

The second term gives the number of the particle N_e in the excited state

$$N_e = \sum_{\vec{k}\neq 0}^{\infty} \frac{1}{z^{-1}e^{\beta\epsilon_k}-1} \tag{3.4.41}$$

For a large volume, the sum over the one-particle states can be approximated by an integral

$$\sum_{\vec{k}\neq 0} f(\vec{k}) \longrightarrow \frac{V}{(2\pi)^3}\int d^3\vec{k} f(\vec{k}) \tag{3.4.42}$$

The energy of the single particle state is related to the wave vector $\vec{k}$ by

$$\varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}}{2m} \tag{3.4.43}$$

Transforming the integral in Eq.(3.4.42) into an integral over energy we obtain

$$\sum_{\vec{k}\neq 0} f(\vec{k}) = \frac{2\pi V}{h^3}(2m)^{3/2}\int_0^\infty \varepsilon^{1/2} f(\varepsilon)d\varepsilon \tag{3.4.44}$$

Using this equation we can express the number of particles in the excited states in terms of an integral over the energy ε of the single particle state,

$$N_e(T,V,z) = \frac{2\pi V}{h^3}(2m)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}}{z^{-1}e^{\beta\epsilon_k}-1}d\varepsilon \tag{3.4.45}$$

We introduce the bose function $g_n(z)$ of order n

$$g_n(z) = \frac{1}{\Gamma(n)}\int_0^\infty \frac{x^{n-1}dx}{z^{-1}e^x - 1} \qquad 0 \leqslant z \leqslant 1 \tag{3.4.46}$$

The function $g_n(z)$ is a monotonically increasing function of z and its derivatives is given by:

$$\frac{dg_n(z)}{dz} = \frac{1}{z}g_{n-1}(z) \tag{3.4.47}$$

For $z = 1$, $g_n(z)$ goes to the Reimann $\zeta-$function of order n

$$g_n(1) = \zeta(n) \tag{3.4.48}$$

The number of particles in the excited states is therefore

$$N_e(T,V,z) = \frac{V}{\lambda_T^3}g_{\frac{3}{2}}(z) \tag{3.4.49}$$

where

$$\lambda_T = \left(\frac{h^2}{2\pi mkT}\right)^{1/2} \tag{3.4.50}$$

is the thermal wave length of the particle. Substituting Eq.(3.4.49) into Eq.(3.4.39) we obtain

$$2N = \frac{z}{1-z} + \frac{V}{\lambda_T^3}g_{\frac{3}{2}}(z) \tag{3.4.51}$$

Since

$$0 \leqslant g_{\frac{3}{2}}(z) \leqslant g_{\frac{3}{2}}(1) = \zeta(\frac{3}{2}) \tag{3.4.52}$$

The maximum number of the particles in excited state is

$$N_c = N_e^{max} = \frac{V}{\lambda_T^3}\zeta(\frac{3}{2}) \tag{3.4.53}$$

Therefore the number of particles condensed in the ground state

$$N_o = 2N - N_e^{max} \tag{3.4.54}$$

The fraction of particle condensed in the ground state is

$$\frac{N_o}{2N} = 1 - \frac{V}{2N\lambda_T^3}\zeta(\frac{3}{2}) \tag{3.4.55}$$

The onset of condensation occurs when

$$N_o = 0$$

That is

$$\frac{2N\lambda_{T_c}^3}{V} = \zeta(\frac{3}{2}) \tag{3.4.56}$$

This equation defines the critical temperature T_c, below which the condensation sets in

$$kT_c = \left(\frac{2N}{V}\right)^{2/3} \frac{h^2}{2\pi m \left[\zeta(3/2)\right]^{2/3}} \tag{3.4.57}$$

The critical temperature is independent of the coupling constant g since it is associated with the translational mode. If we consider the two species system at a given particle density $\frac{2N}{V}$ as a function of temperature, the fraction of particles condensed in the ground state

$$\frac{N_o}{2N} = \begin{cases} 0 & T \geqslant T_c \\ 1 - \left(\frac{T}{T_c}\right)^{3/2} & T < T_c \end{cases} \tag{3.4.58}$$

while the fraction of particles in the excited states

$$\frac{N_e}{2N} = \begin{cases} 1 & T \geqslant T_c \\ \left(\frac{T}{T_c}\right)^{3/2} & T < T_c \end{cases} \tag{3.4.59}$$

The translational modes of the system exhibit the standard behaviour of an ideal bose gas. Using the boson function $g_n(z)$, we can express the grand canonical potential in the form

$$\begin{aligned}\Phi &= -kT\frac{V}{\lambda^3}g_{\frac{5}{2}}(z) + kT\ln(1-z) \\ &+ 3kT\left[\ln(1-e^{-\beta\hbar\omega}) + \frac{1}{2}\beta\hbar\omega\right] \end{aligned} \tag{3.4.60}$$

The pressure of the system is given by,

$$P = -\frac{\partial\Phi}{\partial V}\mid_{T,\mu} \tag{3.4.61}$$

or

$$\begin{aligned}P &= \frac{kT}{\lambda_T^3}g_{\frac{5}{2}}(z) - \frac{kT}{V}\ln(1-z) \\ &- \frac{3kT}{V}\left[\ln(1-e^{-\beta\hbar\omega}) + \frac{1}{2}\beta\hbar\omega\right] \end{aligned} \tag{3.4.62}$$

In the thermodynamic limit, the third limit goes to zero as $V \to \infty$. The behaviour of the second term in the thermodynamic limit can be obtained by considering the $T > T_c$ and the $T < T_c$ cases. For $T > T_c$, $z < 1$ and $\ln(1-z)$ is a finite number. Thus this term goes to zero as $V \to \infty$. For $T < T_c$, $z \to 1$ and from Eq.(3.4.40) we have

$$\ln(1-z) = -\ln(N_o + 1)$$

But the number of the particle condensed in the ground state is a finite fraction of the total number of particle

$$N_o = \alpha'(2N-1) = \alpha N$$

since $N \gg 1$. Then

$$\begin{aligned}\lim_{N,V\to\infty}\frac{-kT}{V}\ln(1-z) &= \lim_{N,V\to\infty}\frac{kT}{V}\ln(1+\alpha N) \\ &= nkT\lim_{N\to\infty}\frac{\ln(1+\alpha N)}{2N} \\ &= 0\end{aligned}$$

where n is the particle density which is finite. So for $T < T_c$ the second term is also vanishes. Therefore the pressure is given by:

$$P = \frac{kT}{\lambda_T^3} g_{\frac{5}{2}}(z) \tag{3.4.63}$$

The pressure is independent of the volume and number of particles. The oscillatory mode as well as the particles condensed in the ground state do not contribute to the pressure.

The internal energy of the system is related to the partition function by

$$\begin{aligned} U &= -\frac{\partial}{\partial\beta} \ln Z(T, V, \mu) \mid_{z,V} \\ &= -\frac{\partial}{\partial\beta} \left(\frac{\Phi}{-kT} \right) \mid_{z,V} \end{aligned} \tag{3.4.64}$$

Using Eq.(3.4.60) we obtain,

$$U = \frac{3}{2} kT \frac{v}{\lambda_T^3} g_{\frac{5}{2}}(z) + \frac{3}{2}\hbar\omega + \frac{3\hbar\omega}{e^{\beta\hbar\omega} - 1} \tag{3.4.65}$$

For $T > T_c$, $\quad z < 1 \quad$ and $\quad N_o \approx 0$

$$2N = \frac{V}{\lambda_T^3} g_{\frac{3}{2}}(z) \qquad for \quad z < 1 \tag{3.4.66}$$

The internal energy is given by

$$U = 3NkT \left\{ \frac{g_{\frac{5}{2}}(z)}{g_{\frac{3}{2}}(z)} \right\} + \frac{3\hbar\omega}{e^{\beta\hbar\omega} - 1} + \frac{3}{2}\hbar\omega \tag{3.4.67}$$

The internal energy is the sum of two parts: A part associated with the translational motion of the system and is represented by the first term and a part due to the 3-dimensional oscillatory motion of the system. Figure(3.1[a]) shows that, above the transition temperature and for $N > N_c$ the oscillator mode doesn't contribute to the internal energy of the system. The major contribution comes from the translational modes i.e. the system behaves essentially as a system of free particles. Since the coupling constant g appears only in ω, the internal energy above T_c and for $N > N_c$ doesn't depend on g. This is shown in Fig.(3.1[b]).

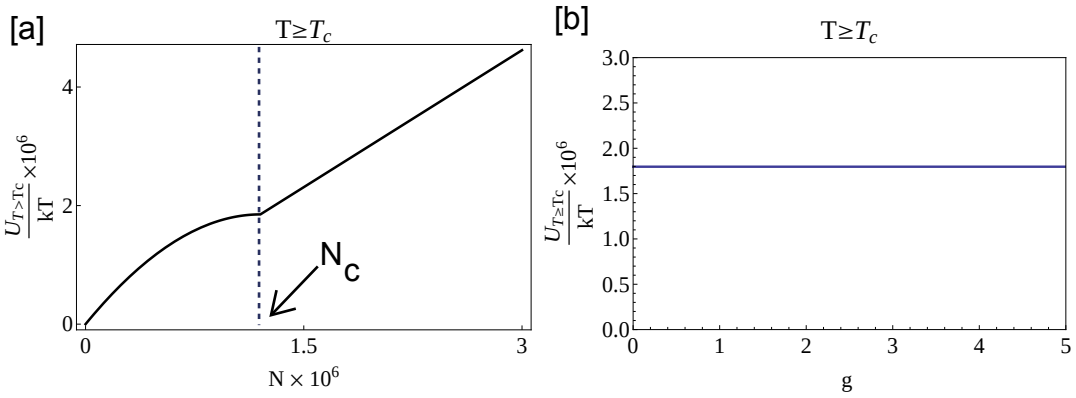

Figure 3.1: Total internal energy above transition temperature T_c in unit of kT. [a] variation of total internal energy with particle numbers with $g = 0.5$. [b]variation of total internal energy with coupling strength with $N = 10^6$.

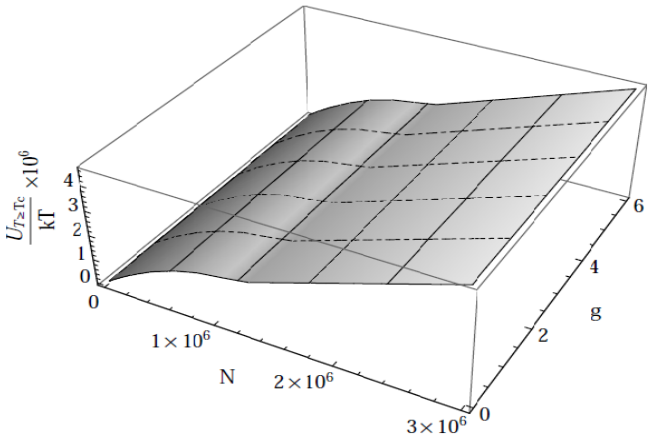

Figure 3.2: Total internal energy above transition temperature T_c in unit of kT

The kink appear in Fig.(3.1[a]) shows that the system exhibits a phase transition $N > N_c$.

For $T < T_c$, $z \to 1$ and we obtain from Eq.(3.4.65)

$$U = \frac{3}{2}kT\frac{V}{\lambda_T^3}\zeta(\frac{5}{2}) + \frac{3\hbar\omega}{e^{\beta\hbar\omega}-1} + \frac{3}{2}\hbar\omega \tag{3.4.68}$$

Below T_c a macroscopic fraction of the number of particles condenses in the ground state. This in turn gives a chance to the oscillator mode to contribute to the total energy. For N of order 10^4 the total energy of the system is constant which implies that the behaviour is mainly due to the translational modes Fig(3.3[a]). But as N increases above this value the effect of the vibrational mode begins to appear Fig(3.3[b]). Fig.(3.4) illustrates the relationship between the total energy of the

system below T_c and the coupling constant at different particle numbers. The contribution of oscillator mode is enhanced by increasing particle number. The curve shoots as N increases. Fig(3.5) shows the dependence of the internal energy of the system on both the number of particles of the system N and the coupling strengths for temperature below T_c. The internal energy surface rises up as N or g increases.

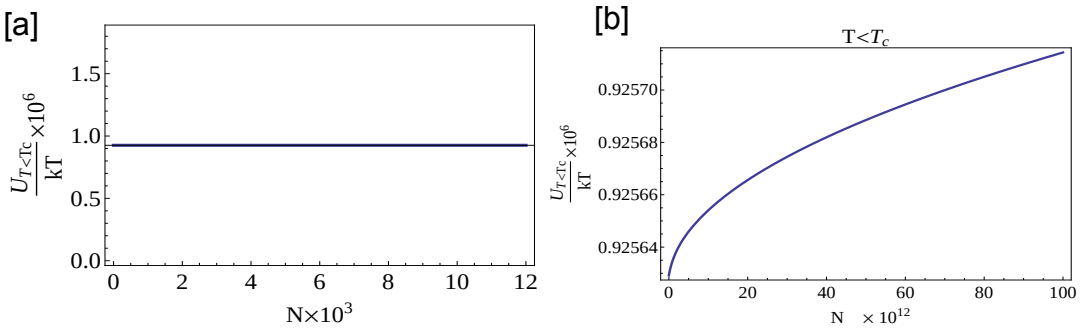

Figure 3.3: Total internal energy below transition temperature T_c in unit of kT [a]variation of total internal energy with particle number with $g = 0.5$. [b]variation of total internal energy with particle number with $g = 0.5$

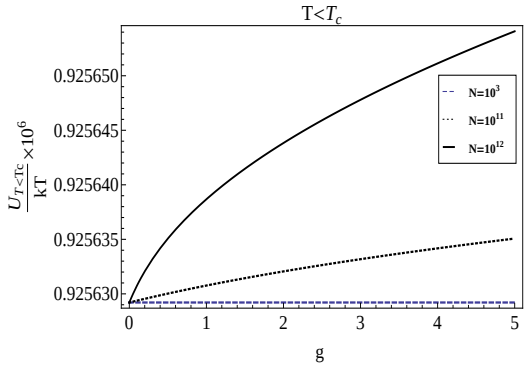

Figure 3.4: Total internal energy versus coupling strength below transition temperature T_c in unit of kT

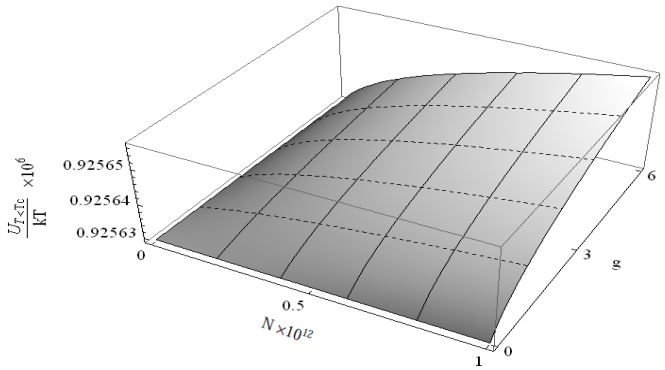

Figure 3.5: Total internal energy versus N and g below transition temperature T_c in unit of kT

We next calculate the specific heat capacity C_V of the system

$$C_V = \frac{\partial U}{\partial T}\,|_{V,N} \tag{3.4.69}$$

For $T > T_c$ we use the expression for U given in (3.4.67), this gives

$$\frac{C_V}{2Nk} = \frac{15}{4}\frac{g_{\frac{5}{2}}(z)}{g_{\frac{3}{2}}(z)} - \frac{9}{4}\frac{g_{3/2}(z)}{g_{1/2}(z)} + 3(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} \qquad T > T_c \tag{3.4.70}$$

where we have used the result

$$\frac{\partial z}{\partial T} = -\frac{3}{2}\frac{z}{T}\frac{g_{3/2}(z)}{g_{1/2}(z)} \tag{3.4.71}$$

In deriving Eq.(3.4.71) we used the expression for the derivative of the boson function $g_n(z)$ given in Eq.(3.4.47).

For $T < T_c$ we use the expression for U given in Eq.(3.4.68). The specific heat capacity is then

$$\frac{C_V}{2Nk} = \frac{15}{4}\frac{V}{2N}\frac{1}{\lambda_T^3}\zeta(\frac{5}{2}) + 3(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} \qquad T < T_c \tag{3.4.72}$$

Subtracting Eq.(3.4.72) from Eq.(3.4.70) we have

$$\left(\frac{C_V}{2Nk}\right)_{T>T_c} - \left(\frac{C_V}{2Nk}\right)_{T<T_c} = \frac{15}{4}\left[\frac{g_{\frac{5}{2}}(z)}{g_{\frac{3}{2}}(z)} - \frac{V}{2N}\frac{1}{\lambda_T^3}\zeta(\frac{5}{2})\right] \tag{3.4.73}$$

Taking the limit $T \to T_c$ i.e. $z \to 1$ and using Eq.(3.4.56) we obtain

$$(C_V)_{T_c+0} = (C_V)_{T_c-0} \tag{3.4.74}$$

The specific heat capacity is a continuous function of temperature. It increases to the maximum value at

$$T = T_c$$

where a spike appears. The appearance of a spike in the specific heat is an indication that the system undergoes a second order phase transition.

To obtain the entropy of the system, we rearrange Eq.(3.4.4) in the form

$$TS = U - \Phi - 2\mu N$$

and substitute for U, Φ and $\mu = kT \ln z$. This gives

$$\frac{S}{k} = \frac{5}{2}\frac{V}{\lambda_T^3} g_{\frac{5}{2}}(z) - 2N \ln z - \ln(1-z) - 3\ln(1-e^{-\beta\hbar\omega}) + \frac{3\beta\hbar\omega}{e^{\beta\hbar\omega}-1} \quad (3.4.75)$$

We first show that the third term is very much smaller than the second term. The contribution of the particles, condensed in ground state to the entropy, is negligible. For $T < T_c$ we have as before (see page 45):

$$\ln(1-z) = \ln(1+\alpha N)$$

Therefore

$$\begin{aligned} 2N \ln z + \ln(1-z) &= 2N \ln\left(\frac{\alpha N}{1+\alpha N}\right) + \ln(1+\alpha N) \\ &= \ln\left[\frac{(\alpha N)^{2N}}{(1+\alpha N)^{2N-1}}\right] \\ &= \ln\left(\frac{(\alpha N)}{(1+\alpha N)}\right)^{2N} \\ &= 2N \ln z \end{aligned}$$

since $N \gg 1$. For $T < T_c$, $z < 1$

and $$2N \ln z \gg \ln(1-z)$$

Since N is very large. Hence

$$\frac{S}{k} = \frac{5}{2}\frac{V}{\lambda_T^3} g_{\frac{5}{2}}(z) - 2N \ln z - 3\ln(1-e^{-\beta\hbar\omega}) + \frac{3\beta\hbar\omega}{e^{\beta\hbar\omega}-1} \quad (3.4.76)$$

The first two terms give the contribution of the translational motion of the system to the entropy while the last two terms give the contribution of the 3-dimensional oscillatory motion to the entropy.

For $T < T_c$, $z < 1$, the first term on the right hand side is

$$\frac{5}{2}\frac{V}{\lambda_T^3}\zeta(\frac{5}{2})$$

To calculate the limit of the second term as $z \to 1$ we use Eq.(3.4.51)

$$\lim_{z\to 1} 2N \ln z = \lim_{z\to 1}\left[\frac{z}{1-z}\ln z + \frac{V}{\lambda_T^3} g_{\frac{3}{2}}(z) \ln z\right]$$

The second term goes to zero as $z \to 1$. The limit of the first term can be obtained by introducing a variable x defined by

$$x = 1 - z \qquad x \ll 1$$

$$\ln z = \ln(1-x) \approx -x \tag{3.4.77}$$

So that

$$\lim_{z\to 1} \frac{z \ln z}{1-z} = \lim_{x\to 0}(1-x) = -1 \tag{3.4.78}$$

Below the critical temperature, the entropy of the system is

$$\frac{S}{k} = \frac{5}{2}\frac{V}{\lambda_T^3}\zeta(\frac{5}{2}) + 1 - 3\ln(1-e^{-\beta\hbar\omega}) + \frac{3\beta\hbar\omega}{e^{\beta\hbar\omega}-1} \tag{3.4.79}$$

For $T > T_c$ the entropy is:

$$\frac{S}{k} = 5N\left[\frac{g_{(\frac{5}{2})}(z)}{g_{(\frac{3}{2})}(z)}\right] - 2N\ln z - 3\ln(1-e^{-\beta\hbar\omega}) + \frac{3\beta\hbar\omega}{e^{\beta\hbar\omega}-1} \tag{3.4.80}$$

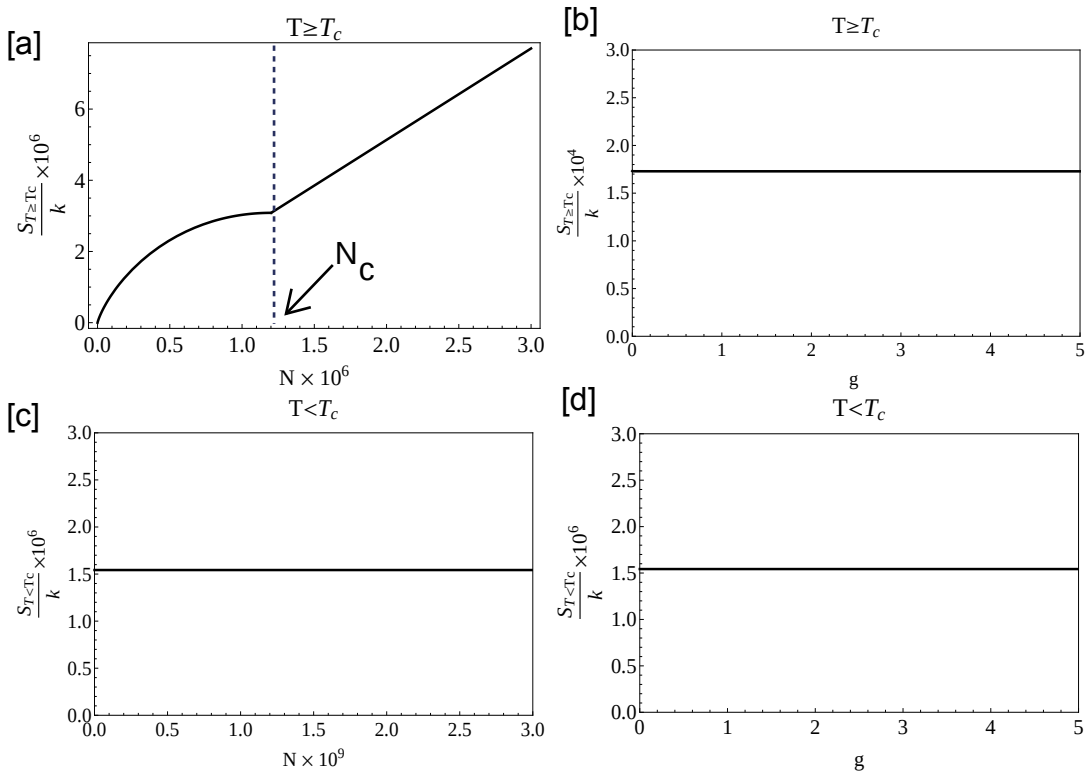

Figure 3.6: The entropy of the system in unit of k [a] variation of entropy with particle number above T_c for $g = 1$. [b] variation of entropy with coupling strength above T_c for $N = 5 \times 10^3$. [c] variation of entropy with particle number below T_c for $g = 0.5$. [d] variation of entropy with coupling strength above T_c for $N = 10^3$.

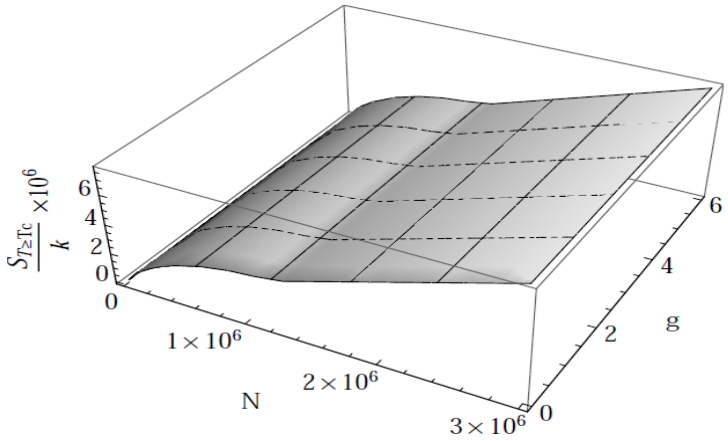

Figure 3.7: The entropy of the system versus particle number and coupling strength above transition temperature T_c in unit of k

The entropy of a system is a measure of the degree of disorder of the system. This implies that the contribution of the oscillator mode is negligible compared to that of the highly degenerate translational modes. Figure(3.6) illustrates the variation of entropy of the system above and below T_c with particle number N and coupling strength g. Fig(3.6[a]) shows that above T_c the entropy is due to the $2N-1$ free modes, it exhibits a phase transition at $N_e^{max} = N_c$ given by Eq.(3.4.53). Below T_c a macroscopic fraction of those modes occupy the ground state of the system and does not contribute to entropy of the system. Therefore the entropy of the system is approximately constant as shown in Fig.(3.6[c]). The entropy of such a system no longer depends on the coupling strength above and below T_c.

We next calculate the free energy of the system. The Helmholtz free energy F given by

$$F = U - TS = \Phi + 2\mu N$$

Substituting for Φ from Eq.(3.4.60) and neglecting the term

$$kT\ln(1-z)$$

we obtain

$$F = 2NkT\left[\ln z - \frac{V}{2\lambda_T^3 N} g_{(\frac{5}{2})}(z)\right] + 3kT\ln(1-e^{-\beta\hbar\omega}) + \frac{3}{2}\hbar\omega \quad (3.4.81)$$

For $T < T_c$

$$2N = \frac{V}{\lambda_{T_c}^3}\zeta(\frac{3}{2})$$

and $z \approx 1$. Hence

$$F = -\frac{VkT}{\lambda_T^3}g_{(\frac{5}{2})}(1) + 3kT\ln(1-e^{-\beta\hbar\omega}) + \frac{3}{2}\hbar\omega \tag{3.4.82}$$

where $\lambda_c^3 = \frac{h^2}{2\pi mkT_c}$. For $T > T_c$

$$2N = \frac{V}{\lambda^3}g_{\frac{3}{2}}(z)$$

$$F = 2NkT\left[\ln z - \frac{g_{(\frac{5}{2})}(z)}{g_{(\frac{3}{2})}(z)}\right] + 3\ln(1-e^{-\beta\hbar\omega}) + \frac{3}{2}\hbar\omega \tag{3.4.83}$$

Gibbs free energy G given by

$$\begin{aligned} G &= F + PV \\ &= U - TS - \Phi \\ &= 2\mu N \end{aligned}$$

$$G = 2NkT\ln z \tag{3.4.84}$$

The free energy shows a kink at a number of particles equal to N_c which is independent of the coupling strength g. Variation of the Gibbs free energy with particle number shows that the system has a stable minima at $N \approx 2.5 \times 10^5$. By increasing the particle number G increase till reach to zero at particle number corresponding to the maximum capacity of the excited states $N_c \approx 1.2 \times 10^6$.

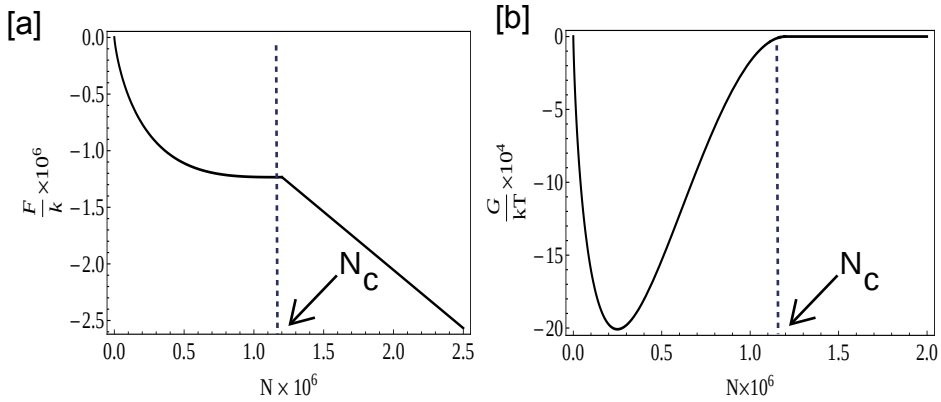

Figure 3.8: [a]Helmholtz free energy F in unit of kT with number of particles for $g = 1$. [b]Gibbs free energy G versus number of particles in unit of kT

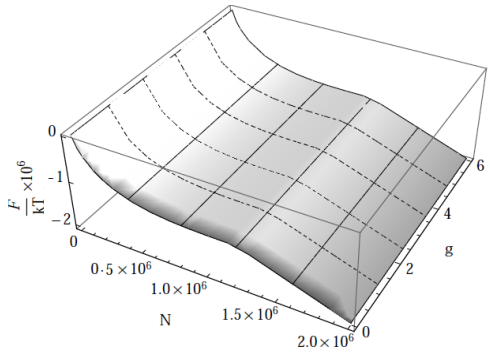

Figure 3.9: Helmholtz free energy F in unit of kT

All thermodynamic parameters of the system with the exception of the pressure of the system, is the sum of two terms one describing the translational motion and the other describing the 3-dimensional vibrational motion of the system.

Chapter 4

Extension of the model

4.1 The physical model

In this chapter we study the two species model of Sec.(3.1), assuming that the coupling constants are different

$$g_{AA} \neq g_{BB} \neq g_{AB}$$

Our objective is to underatand how the system behaves as the coupling strength is varied.

We have seen in Chapter 3 that the Hamiltonian of the system is given by:

$$H = H_o + V_2, \tag{4.1.1}$$

where H_o is kinetic energy part,

$$H_o = \sum_{i=1}^{N} \left[\frac{(\vec{p}_i^{\,A})^2}{2m} + \frac{(\vec{p}_i^{\,B})^2}{2m} \right] \tag{4.1.2}$$

with $\vec{p}_i^{\,A}$ and $\vec{p}_i^{\,B}$ the momenta for i^{th} particle of species A and B respectively and V_2 the potential energy given by Eq.(3.1.6)

$$V_2 = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} [g_{AB}(\vec{r}_i^{\,A} - \vec{r}_j^{\,B})^2 - \frac{1}{2} g_{AA}(\vec{r}_i^{\,A} - \vec{r}_j^{\,A})^2 - \frac{1}{2} g_{BB}(\vec{r}_i^{\,B} - \vec{r}_j^{\,B})^2]$$

Exapanding the right hand side and simplifying we obtain

$$\begin{aligned} V_2 &= \frac{1}{2}Ng_{AB}(1-\frac{g_{AA}}{g_{AB}})\sum_{i=1}^{N}(\vec{r}_i^{\,A})^2+\frac{1}{2}Ng_{AB}(1-\frac{g_{BB}}{g_{AB}})\sum_{j=1}^{N}(\vec{r}_j^{\,B})^2 \\ &+ \frac{1}{2}g_{AB}\sum_{i=1}^{N}\sum_{j=1}^{N}(\frac{g_{AA}}{g_{AB}}\vec{r}_i^{\,A}.\vec{r}_j^{\,A}-2\vec{r}_i^{\,A}.\vec{r}_j^{\,B}+\frac{g_{BB}}{g_{AB}}\vec{r}_i^{\,B}.\vec{r}_j^{\,B}) \end{aligned} \tag{4.1.3}$$

We introduce the notations:

$$\alpha=\frac{g_{AA}}{g_{AB}}, \qquad \gamma=\frac{g_{BB}}{g_{AB}}$$

and assume that

$$0<\alpha\leq 1, \quad and \quad 0<\gamma\leq 1$$

Eq.(4.1.3) becomes

$$\begin{aligned} V_2 &= \frac{1}{2}Ng_{AB}(1-\alpha)\sum_{i=1}^{N}(\vec{r}_i^{\,A})^2+\frac{1}{2}Ng_{AB}(1-\gamma)\sum_{j=1}^{N}(\vec{r}_j^{\,B})^2 \\ &+ \frac{1}{2}g_{AB}\sum_{i=1}^{N}\sum_{j=1}^{N}(\alpha\vec{r}_i^{\,A}.\vec{r}_j^{\,A}-2\vec{r}_i^{\,A}.\vec{r}_j^{\,B}+\gamma\vec{r}_i^{\,B}.\vec{r}_j^{\,B}) \end{aligned} \tag{4.1.4}$$

The full Hamiltonian of the system,

$$\begin{aligned} H &= \sum_{i=1}^{N}\left[\frac{(\vec{p}_i^{\,A})^2}{2m}+\frac{(\vec{p}_i^{\,B})^2}{2m}\right]+\frac{1}{2}Ng_{AB}(1-\alpha)\sum_{i=1}^{N}(\vec{r}_i^{\,A})^2+\frac{1}{2}Ng_{AB}(1-\gamma)\sum_{j=1}^{N}(\vec{r}_j^{\,B})^2 \\ &+ \frac{1}{2}g_{AB}\sum_{i=1}^{N}\sum_{j=1}^{N}(\alpha\vec{r}_i^{\,A}.\vec{r}_j^{\,A}-2\vec{r}_i^{\,A}.\vec{r}_j^{\,B}+\gamma\vec{r}_i^{\,B}.\vec{r}_j^{\,B})] \end{aligned} \tag{4.1.5}$$

We next proceed as in chapter 3 to study the system. We begin with the classical solution.

4.2 Exact solution of the classical system

Assuming that the initial configuration of the system is given by:

$$\begin{aligned} \vec{r}_i^{\,A}(t=0) &= \vec{r}_{io}^{\,A} \qquad & \vec{p}_i^{\,A}(t=0) = \vec{p}_{io}^{\,A} \\ \vec{r}_i^{\,B}(t=0) &= \vec{r}_{io}^{\,B} \qquad & \vec{p}_i^{\,B}(t=0) = \vec{p}_{io}^{\,B} \end{aligned} \tag{4.2.1}$$

These conditions give the initial position and initial momenta of the particles.
We are interested in the time evolution of the classical system from the initial configuration (4.2.1).
To solve the classical initial value problem we diagonalize the potential energy matrix. Again we let

$$\vec{r}^{\,A} = \begin{bmatrix} \vec{r}_1^{\,A} \\ \vec{r}_2^{\,A} \\ \vdots \\ \vec{r}_N^{\,A} \end{bmatrix} \qquad \vec{r}^{\,B} = \begin{bmatrix} \vec{r}_1^{\,B} \\ \vec{r}_2^{\,B} \\ \vdots \\ \vec{r}_N^{\,B} \end{bmatrix}$$

and

$$\vec{p}^{\,A} = \begin{bmatrix} \vec{p}_1^{\,A} \\ \vec{p}_2^{\,A} \\ \vdots \\ \vec{p}_N^{\,A} \end{bmatrix} \qquad \vec{p}^{\,B} = \begin{bmatrix} \vec{p}_1^{\,B} \\ \vec{p}_2^{\,B} \\ \vdots \\ \vec{p}_N^{\,B} \end{bmatrix}$$

with

$$\vec{p}^{\,A} = m\frac{d\vec{r}^{\,A}}{dt}, \qquad \vec{p}^{\,B} = m\frac{d\vec{r}^{\,B}}{dt} \tag{4.2.2}$$

Using the vectors $\vec{r}^{\,A}$ and $\vec{r}^{\,B}$ we rewrite the Hamiltonian in the matrix form

$$\begin{aligned} H &= \frac{1}{2m}\begin{bmatrix} \vec{p}^{\,A} & \vec{p}^{\,B} \end{bmatrix}\left[\begin{array}{c|c} I_N & 0 \\ \hline 0 & I_N \end{array}\right]\begin{bmatrix} \vec{p}^{\,A} \\ \vec{p}^{\,B} \end{bmatrix} \\ &+ \frac{1}{2}g_{AB}\begin{bmatrix} \vec{r}^{\,A} & \vec{r}^{\,B} \end{bmatrix}\left[\begin{array}{c|c} (V_2)_{11} & (V_2)_{12} \\ \hline (V_2)_{21} & (V_2)_{22} \end{array}\right]\begin{bmatrix} \vec{r}^{\,A} \\ \vec{r}^{\,B} \end{bmatrix} \end{aligned} \tag{4.2.3}$$

where I_N is the $(N\times N)$ unit matrix. The potential energy matrix V_2 can be obtained

directly from Eq.(4.1.4), namely

$$\begin{aligned}(V_2)_{11} &= N(1-\alpha)I_N + \alpha C \\ (V_2)_{12} &= (V_2)_{21} = -C \\ (V_2)_{22} &= N(1-\gamma)I_N + \gamma C \end{aligned} \tag{4.2.4}$$

with

$$C = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{bmatrix} \tag{4.2.5}$$

The matrix C is an $(N \times N)$ matrix whose elements are the (3×3) unit matrix I_3. In Appendix A, we show that the characteristic equation for the matrix V_2 is

$$\lambda(\lambda - 2N)[\lambda - N(1-\alpha)]^{N-1}[\lambda - N(1-\gamma)]^{N-1} = 0 \tag{4.2.6}$$

We have two simple eigenvalues

$$\lambda = 0 \qquad \textit{and} \qquad \lambda = 2N \tag{4.2.7}$$

and two eigenvalues

$$\lambda = N(1-\alpha) \qquad \textit{and} \qquad \lambda = N(1-\gamma) \tag{4.2.8}$$

of multiplicity $(N-1)$.

In Appendix B, we construct $2N$ orthogonal eigenvectors of the matrix V_2. The $(N-1)$ eigenvectors corresponding to $\lambda = N(1-\alpha)$ are

$$\vec{u}_k = \frac{1}{\sqrt{k(k+1)}} \Big[\underbrace{1 \quad \cdots \quad 1 \quad -k}_{\text{k}} \quad 0 \quad \cdots \quad 0 \;\vdots\; 0 \quad \cdots \quad 0 \Big]^T \qquad k = 1, 2, \cdots, N-1$$

Finally the eigenvector corresponding to the eigenvalue $\lambda = 0$ is given by:

$$\vec{u}_N = \frac{1}{2N} \Big[1 \quad \cdots \quad 1 \;\vdots\; 1 \quad \cdots \quad 1 \Big]^T,$$

whereas the eigenvectors belonging to the eigenvalue $\lambda = N(1-\gamma)$ are

$$\vec{u}_{N+k} = \frac{1}{\sqrt{k(k+1)}} \Big[\underbrace{0 \quad \cdots \quad 0}_{} \; \underbrace{1 \quad \cdots \quad 1}_{\text{k}} \quad -k \quad 0 \quad 0 \Big]^T \qquad k = 1, 2, \cdots, N-1$$

The eigenvector belonging to the eigenvalue $\lambda = 2N$ is

$$\vec{u}_N = \frac{1}{2N} \Big[-1 \quad \cdots \quad -1 \;\vdots\; 1 \quad \cdots \quad 1 \Big]^T,$$

The diagonalizing matrix O_2 is obtained by grouping together the orthogonal eigenvectors:

$$O_2 \;=\; \Big(\vec{u}_1 \,\Big|\, \vec{u}_2 \,\Big|\, \cdots \,\Big|\, \vec{u}_{2N-1} \,\Big|\, \vec{u}_{2N} \Big) \tag{4.2.9}$$

It is an orthogonal matrix

$$O_2 O_2^T = O^T O = I_{2N},$$

since the vectors

$$\vec{u}_i \qquad\qquad i = 1, \cdots, 2N$$

are orthonormal

$$\vec{u}_i . \vec{u}_j = \delta_{ij}$$

In the same appendix we show that the diagonalizing matrix O_2 can be written in the form

$$O_2 \;=\; \left[\begin{array}{c:c} S & -\frac{1}{\sqrt{2N}} D \\ \hdashline \frac{1}{\sqrt{2N}} D & S \end{array} \right] \tag{4.2.10}$$

where

$$D_{ij} = \delta_{jN} \qquad\qquad i, j = 1, 2, \cdots, N \tag{4.2.11}$$

and the elements S_{ij} is given by:

$$S_{ij} = \frac{1}{\sqrt{j(j+1+(1-j)\delta_{jN})}} \begin{cases} 1 & i \leq j \\ -j(1-\delta_{jN}) & i = j+1 \\ 0 & i > j+1 \end{cases} \tag{4.2.12}$$

The new coordinates vectors

$$\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{2N}$$

are related to the single particle coordinate vectors

$$\vec{r}_1^{\,A}, \cdots, \vec{r}_{2N}^{\,A}, \vec{r}_1^{\,B}, \cdots, \vec{r}_{2N}^{\,B}$$

by:

$$\begin{bmatrix} \vec{r}_1 \\ \vec{r}_2 \\ \vdots \\ \vec{r}_{2N} \end{bmatrix} = O^T \begin{bmatrix} \vec{r}_1^{\,A} \\ \vdots \\ \vec{r}_{2N}^{\,A} \\ \vec{r}_1^{\,B} \\ \vdots \\ \vec{r}_{2N}^{\,B} \end{bmatrix} \tag{4.2.13}$$

Substituting for O_2 we obtain

$$\begin{aligned} \vec{r}_k &= \frac{1}{\sqrt{k(k+1+(1-k)\delta_{kN})}}[\sum_{j=1}^{k} \vec{r}_j^{\,A} - k(1-\delta_{kN})\vec{r}_{k+1}^{\,A}] + \frac{1}{\sqrt{2N}}\delta_{kN}\sum_{j=1}^{N}\vec{r}_j^{\,B} \\ \vec{r}_{N+k} &= \frac{1}{\sqrt{k(k+1+(1-k)\delta_{kN})}}[\sum_{j=1}^{k} \vec{r}_j^{\,B} - k(1-\delta_{kN})\vec{r}_{k+1}^{\,B}] - \frac{1}{\sqrt{2N}}\delta_{kN}\sum_{j=1}^{N}\vec{r}_j^{\,A} \quad k = 1, \cdots, N \end{aligned} \tag{4.2.14}$$

We notice that the position vector $\vec{r}_N$ describes the translational mode and is proportional to the position vector of the center of mass.

The inverse transformation is given by

$$\begin{aligned} \vec{r}_k^{\,A} &= \sum_{k=j}^{N} \frac{1}{\sqrt{j(j+1+(1-j)\delta_{jN})}}\vec{r}_j - \frac{(k-1)}{\sqrt{k(k-1)}}\vec{r}_{k-1} - \frac{1}{\sqrt{2N}}\vec{r}_{2N} \\ \vec{r}_k^{\,B} &= \sum_{k=j}^{N} \frac{1}{\sqrt{j(j+1+(1-j)\delta_{jN})}}\vec{r}_{N+j} - \frac{(k-1)}{\sqrt{k(k-1)}}\vec{r}_{N+k-1} + \frac{1}{\sqrt{2N}}\vec{r}_{2N} \end{aligned} \tag{4.2.15}$$

We remark that in the term

$$-\frac{(k-1)}{\sqrt{k(k-1)}}\vec{r}_{k-1}$$

the case $k = 1$ is considered as a limiting case which gives zero.

Under the change of coordinates (4.2.13) the matrix for the linear momentum vector

$$\begin{bmatrix} \vec{p}^{\,A} \\ \vec{p}^{\,B} \end{bmatrix}$$

transforms to

$$\begin{bmatrix} \vec{p}_1^{\,A} \\ \vdots \\ \vec{p}_{2N}^{\,A} \\ \hdashline \vec{p}_1^{\,B} \\ \vdots \\ \vec{p}_{2N}^{\,B} \end{bmatrix} = O_2 \begin{bmatrix} \vec{p}_1 \\ \vec{p}_2 \\ \vdots \\ \vec{p}_{2N} \end{bmatrix} \tag{4.2.16}$$

where

$$\vec{p}_i = m\frac{d\vec{r}_i}{dt} \qquad\qquad i = 1, 2\cdots, 2N$$

In the new coordinate system the Hamiltonian is given by:

$$\begin{aligned} H &= \frac{1}{2m}\begin{bmatrix} \vec{p}_1 \cdots \vec{p}_{2N} \end{bmatrix} O_2^T I_{2N} O_2 \begin{bmatrix} \vec{p}_1 \\ \vdots \\ \vec{p}_{2N} \end{bmatrix} \\ &+ \frac{1}{2}g_{AB}\begin{bmatrix} \vec{r}_1 \cdots \vec{r}_{2N} \end{bmatrix} O_2^T V_2 O_2 \begin{bmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_{2N} \end{bmatrix} \end{aligned} \tag{4.2.17}$$

Since the matrix O_2 is an orthogonal matrix and

$$O_2^T V_2 O_2 = \left[\begin{array}{cccc:c:cccc:c} N(1-\alpha) & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & N(1-\alpha) & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & N(1-\alpha) & 0 & 0 & 0 & \cdots & 0 & 0 \\ \hdashline 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \hdashline 0 & 0 & \cdots & 0 & 0 & N(1-\gamma) & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & N(1-\gamma) & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & N(1-\gamma) & 0 \\ \hdashline 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 2N \end{array}\right] \begin{matrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{matrix}$$

$$\underbrace{\qquad\qquad}_{\text{(N-1)-col.}}\ \underbrace{\quad}_{\text{1-col.}}\ \underbrace{\qquad\qquad}_{\text{(N-1)-col.}}\ \underbrace{\quad}_{\text{1-col.}}$$

The Hamiltonian takes the simple form:

$$H = \sum_{i=1}^{2N}\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}g_{AB}N(1-\alpha)\sum_{i=1}^{N-1} r_i^2 + \frac{1}{2}g_{AB}N(1-\gamma)\sum_{i=1}^{N-1} r_{i+N}^2 + g_{AB}N\vec{r}_{2N}^{\,2} \tag{4.2.18}$$

We have one translational-mode in three dimensions and $(2N-1)$ modes which execute simple harmonic motion.

Hamilton's equations of motion give:

$$\frac{d\vec{p}_i}{dt} = -Ng_{AB}(1-\alpha)\vec{r}_i \qquad i = 1, 2\cdots(N-1) \tag{4.2.19}$$

$$\frac{d\vec{p}_N}{dt} = 0 \tag{4.2.20}$$

$$\frac{d\vec{p}_{i+N}}{dt} = -Ng_{AB}(1-\gamma)\vec{r}_{i+N} \qquad i = 1, 2\cdots(N-1) \tag{4.2.21}$$

$$\frac{d\vec{p}_{2N}}{dt} = -2Ng_{AB}\vec{r}_{2N} \tag{4.2.22}$$

and

$$\frac{d\vec{r}_i}{dt} = \frac{\vec{p}_i}{m} \qquad i = 1, 2\cdots 2N \tag{4.2.23}$$

We differentiate Eq.(4.2.23) with respect to t.

$$\frac{d^2\vec{r}_i}{dt^2} = \frac{1}{m}\frac{d\vec{p}_i}{dt} \tag{4.2.24}$$

For $i = 1, \cdots, (N-1)$ use Eq.(4.2.19) we obtain

$$\frac{d^2\vec{r}_i}{dt^2} = -\frac{g_{AB}N(1-\alpha)}{m}\vec{r}_i \tag{4.2.25}$$

This is the equation of a harmonic oscillator of frequency

$$\omega_\alpha = \sqrt{\frac{g_{AB}N(1-\alpha)}{m}} \tag{4.2.26}$$

The solution of this equation is given by:

$$\vec{r}_i = \frac{\vec{A}_i}{m\omega_\alpha}\sin\omega_\alpha t + \vec{B}_i\cos\omega_\alpha t \qquad i = 1, \cdots, N-1 \tag{4.2.27}$$

where $\vec{A}_i, \vec{B}_i$ are constant vectors. Now for $i = N$

$$\frac{d\vec{r}_N}{dt} = \frac{\vec{A}_N}{m} \tag{4.2.28}$$

Integrating we obtain

$$\vec{r}_N = \frac{\vec{A}_N}{m}t + \vec{B}_N \tag{4.2.29}$$

where $\vec{A}_N, \vec{B}_N$ are constant vectors. For $r_{N+1}, \cdots, r_{2N-1}$ we have

$$\frac{d^2\vec{r}_{i+N}}{dt^2} = \frac{1}{m}\frac{d\vec{p}_{i+N}}{dt} \qquad i = 1, \cdots, N-1 \tag{4.2.30}$$

and using Eq.(4.2.21)

$$\frac{d^2\vec{r}_{i+N}}{dt^2} = -\frac{g_{AB}N(1-\gamma)}{m}\vec{r}_{i+N} \tag{4.2.31}$$

This is the equation of a harmonic oscillator of frequency

$$\omega_\gamma = \sqrt{\frac{g_{AB}N(1-\gamma)}{m}} \tag{4.2.32}$$

The solution of this equation is given by:

$$\vec{r}_{i+N} = \frac{\vec{A}_{i+N}}{m\omega_\gamma}\sin\omega_\gamma t + \vec{B}_{i+N}\cos\omega_\gamma t \qquad i = 1, \cdots, N-1 \tag{4.2.33}$$

For the vibrational mode corresponding to $\lambda = 2N$

$$\frac{d^2\vec{r}_{2N}}{dt^2} = \frac{1}{m}\frac{d\vec{p}_{2N}}{dt} \tag{4.2.34}$$

and using Eq.(4.2.22)

$$\frac{d^2\vec{r}_{2N}}{dt^2} = -\frac{2gN}{m}\vec{r}_{2N} \tag{4.2.35}$$

This is the equation of a harmonic oscillator of frequency

$$\omega = \sqrt{\frac{2g_{AB}N}{m}} \tag{4.2.36}$$

The solution of this equation is given by:

$$\vec{r}_{2N} = \frac{\vec{A}_{2N}}{m\omega}\sin\omega t + \vec{B}_{2N}\cos\omega t \tag{4.2.37}$$

We have $2N$ constants $\vec{A}_i$ and $\vec{B}_i$ where $i = 1, 2\cdots 2N$. They are related to the vectors $\vec{r}_i$ and $\vec{p}_i$

$$\vec{r}_i(t=0) = \vec{B}_i \qquad i = 1, 2\cdots 2N \tag{4.2.38}$$

$$\vec{p}_i(t=0) = \vec{A}_i \qquad i = 1, 2\cdots 2N \tag{4.2.39}$$

The special case N=3

As we did in chapter 3, we consider, in some details, the $N = 3$ case. We have three particles of species A and three particles of species B. The transformation matrix S now reads

$$S = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{bmatrix} \tag{4.2.40}$$

The matrix O_2 is now given by:

$$O_2 = \left(\begin{array}{c|c} S & -\frac{1}{\sqrt{6}}D_3 \\ \hline \frac{1}{\sqrt{6}}D_3 & S \end{array}\right) \tag{4.2.41}$$

Or explicitly

$$O_2 = \frac{1}{\sqrt{2}} \left[\begin{array}{ccc|ccc} 1 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 & -\frac{1}{\sqrt{3}} \\ -1 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 & -\frac{1}{\sqrt{3}} \\ 0 & -\frac{2}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 & -\frac{1}{\sqrt{3}} \\ \hline 0 & 0 & \frac{1}{\sqrt{3}} & 1 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & 0 & \frac{1}{\sqrt{3}} & -1 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 & -\frac{2}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{array}\right] \tag{4.2.42}$$

The new coordinate vectors are given by:

$$\begin{aligned} \vec{r}_1 &= \frac{1}{\sqrt{2}}(\vec{r}_1^{\,A} - \vec{r}_2^{\,A}) \\ \vec{r}_2 &= \frac{1}{\sqrt{6}}(\vec{r}_1^{\,A} + \vec{r}_2^{\,A} - 2\vec{r}_3^{\,A}) \\ \vec{r}_3 &= \frac{1}{\sqrt{6}}[(\vec{r}_1^{\,A} + \vec{r}_2^{\,A} + \vec{r}_3^{\,A}) + (\vec{r}_1^{\,B} + \vec{r}_2^{\,B} + \vec{r}_3^{\,B})] \\ \vec{r}_4 &= \frac{1}{\sqrt{2}}(\vec{r}_1^{\,B} - \vec{r}_2^{\,B}) \\ \vec{r}_5 &= \frac{1}{\sqrt{6}}(\vec{r}_1^{\,B} + \vec{r}_2^{\,B} - 2\vec{r}_3^{\,B}) \\ \vec{r}_6 &= \frac{1}{\sqrt{6}}[(\vec{r}_1^{\,B} + \vec{r}_2^{\,B} + \vec{r}_3^{\,B}) - (\vec{r}_1^{\,A} + \vec{r}_2^{\,A} + \vec{r}_3^{\,A})] \end{aligned}$$

To obtain the position vectors $\vec{r}_i^A$ and $\vec{r}_i^B$ we use the inverse transformation equations (4.2.15).

$$\begin{aligned}
\vec{r}_1^A &= \frac{1}{\sqrt{2}}[\vec{r}_1 + \frac{1}{\sqrt{3}}(\vec{r}_2 + \vec{r}_3 - \vec{r}_6)] \\
\vec{r}_2^A &= \frac{1}{\sqrt{2}}[-\vec{r}_1 + \frac{1}{\sqrt{3}}(\vec{r}_2 + \vec{r}_3 - \vec{r}_6)] \\
\vec{r}_3^A &= \frac{1}{\sqrt{6}}(-2\vec{r}_2 + \vec{r}_3 - \vec{r}_6) \\
\vec{r}_1^B &= \frac{1}{\sqrt{2}}[\frac{1}{\sqrt{3}}\vec{r}_3 + \vec{r}_4 + \frac{1}{\sqrt{3}}(\vec{r}_5 + \vec{r}_6)] \\
\vec{r}_2^B &= \frac{1}{\sqrt{2}}[\frac{1}{\sqrt{3}}\vec{r}_3 - \vec{r}_4 + \frac{1}{\sqrt{3}}(\vec{r}_5 + \vec{r}_6)] \\
\vec{r}_3^B &= \frac{1}{\sqrt{6}}(\vec{r}_3 - 2\vec{r}_5 + \vec{r}_6)
\end{aligned} \tag{4.2.43}$$

The constants $\vec{A}_i, \vec{B}_i \quad i = 1, \cdots, 6$ are related to $\vec{r}_{io}^A, \vec{r}_{io}^B, \vec{p}_{io}^A \quad and \quad \vec{p}_{io}^B$ through

$$\begin{aligned}
\vec{A}_1 &= \frac{1}{\sqrt{2}}(\vec{p}_{1o}^A - \vec{p}_{2o}^A) \\
\vec{A}_2 &= \frac{1}{\sqrt{6}}(\vec{p}_{1o}^A + \vec{p}_{2o}^A - 2\vec{p}_{3o}^A) \\
\vec{A}_3 &= \frac{1}{\sqrt{6}}[(\vec{p}_{1o}^A + \vec{p}_{2o}^A + \vec{p}_{3o}^A) + (\vec{p}_{1o}^B + \vec{p}_{2o}^B + \vec{p}_{3o}^B)] \\
\vec{A}_4 &= \frac{1}{\sqrt{2}}(\vec{p}_{1o}^B - \vec{p}_{2o}^B) \\
\vec{A}_5 &= \frac{1}{\sqrt{6}}(\vec{p}_{1o}^B + \vec{p}_{2o}^B - 2\vec{p}_{3o}^B) \\
\vec{A}_6 &= \frac{1}{\sqrt{6}}[(\vec{p}_{1o}^B + \vec{p}_{2o}^B + \vec{p}_{3o}^B) - (\vec{p}_{1o}^A + \vec{p}_{2o}^A + \vec{p}_{3o}^A)]
\end{aligned} \tag{4.2.44}$$

and $r_i(t=0) = B_i$

$$\begin{aligned}
\vec{B}_1 &= \frac{1}{\sqrt{2}}(\vec{r}^{\,A}_{1o} - \vec{r}^{\,A}_{2o}) \\
\vec{B}_2 &= \frac{1}{\sqrt{6}}(\vec{r}^{\,A}_{1o} + \vec{r}^{\,A}_{2o} - 2\vec{r}^{\,A}_{3o}) \\
\vec{B}_3 &= \frac{1}{\sqrt{6}}[(\vec{r}^{\,A}_{1o} + \vec{r}^{\,A}_{2o} + \vec{r}^{\,A}_{3o}) + (\vec{r}^{\,B}_{1o} + \vec{r}^{\,B}_{2o} + \vec{r}^{\,B}_{3o})] \\
\vec{B}_4 &= \frac{1}{\sqrt{2}}(\vec{r}^{\,B}_{1o} - \vec{r}^{\,B}_{2o}) \\
\vec{B}_5 &= \frac{1}{\sqrt{6}}(\vec{r}^{\,B}_{1o} + \vec{r}^{\,B}_{2o} - 2\vec{r}^{\,B}_{3o}) \\
\vec{B}_6 &= \frac{1}{\sqrt{6}}[(\vec{r}^{\,B}_{1o} + \vec{r}^{\,B}_{2o} + \vec{r}^{\,B}_{3o}) - (\vec{r}^{\,A}_{1o} + \vec{r}^{\,A}_{2o} + \vec{r}^{\,A}_{3o})]
\end{aligned} \tag{4.2.45}$$

The vectors $\vec{r}_i$ are then

$$\begin{aligned}
\vec{r}_i &= \frac{\vec{p}_{io}}{m\omega_\alpha}\sin\omega_\alpha t + \vec{r}_{io}\cos\omega_\alpha t \qquad i = 1,2 \\
\vec{r}_3 &= \frac{\vec{p}_{3o}}{m}t + \vec{r}_{3o} \\
\vec{r}_i &= \frac{\vec{p}_{io}}{m\omega_\gamma}\sin\omega_\gamma t + \vec{r}_{io}\cos\omega_\gamma t \qquad i = 4,5 \\
\vec{r}_6 &= \frac{\vec{p}_{6o}}{m\omega}\sin\omega t + \vec{r}_{6o}\cos\omega t
\end{aligned} \tag{4.2.46}$$

Substituting Eq.(4.2.46) into Eq.(4.2.43) we obtain

$$\vec{r}^{\,A}_i \quad and \quad \vec{r}^{\,B}_i \qquad\qquad i = 1,2,3$$

For example the the position vector of the first particle of species A and species B

$$\begin{aligned}
\vec{r}^{\,A}_j(t) &= \frac{1}{6}[\frac{1}{m\omega_\alpha}(4\vec{p}^{\,A}_{jo} - \sum_{i\neq j}\vec{p}^{\,A}_{io})\sin\omega_\alpha t + (4\vec{r}^{\,A}_{jo} - \sum_{i\neq j}\vec{r}^{\,A}_{io})\cos\omega_\alpha t \\
&- [\frac{1}{m\omega}\sum_{i=1,2,3}(\vec{p}^{\,B}_{io} - \vec{p}^{\,A}_{io})\sin\omega t + \sum_{i=1,2,3}(\vec{r}^{\,B}_{io} - \vec{r}^{\,A}_{io})\cos\omega t \\
&- \frac{1}{m}\sum_{i=1,2,3}(\vec{p}^{\,B}_{io} + \vec{p}^{\,A}_{io})t - \sum_{i=1,2,3}(\vec{r}^{\,B}_{io} + \vec{r}^{\,A}_{io})]] \\
\vec{r}^{\,B}_j(t) &= \frac{1}{6}[\frac{1}{m\omega_\gamma}(4\vec{p}^{\,B}_{jo} - \sum_{i\neq j}\vec{p}^{\,B}_{io})\sin\omega_\gamma t + (4\vec{r}^{\,B}_{jo} - \sum_{i\neq j}\vec{r}^{\,B}_{io})\cos\omega_\gamma t \\
&+ [\frac{1}{m\omega}\sum_{i=1,2,3}(\vec{p}^{\,B}_{io} - \vec{p}^{\,A}_{io})\sin\omega t + \sum_{i=1,2,3}(\vec{r}^{\,B}_{io} - \vec{r}^{\,A}_{io})\cos\omega t \\
&- \frac{1}{m}\sum_{i=1,2,3}(\vec{p}^{\,B}_{io} + \vec{p}^{\,A}_{io})t - \sum_{i=1,2,3}(\vec{r}^{\,B}_{io} + \vec{r}^{\,A}_{io})]]
\end{aligned} \tag{4.2.47}$$

The position vector $\vec{r}_j^{\,A}(t), \vec{r}_j^{\,B}(t)$ display a *Beat*. To visualize the motion, we plot $\vec{r}_1^{\,A}$ as a function of time, for $N = 6$ and $\alpha = 0.95$.

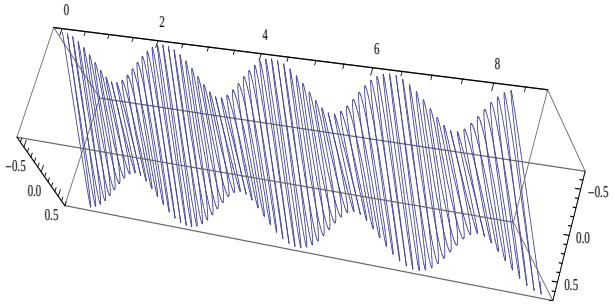

Figure 4.1: Position vector for particle of species A versus time

Motion of each particle is superposition of two frequencies: one associated with oscillation of two particle of same species and the other corresponding to oscillation of the position vector connecting the center of mass of each species.

The classical motion is described as follows: Particles belonging to the same species execute simple harmonic motion with the same frequency about a center which moves with uniform velocity. The position vector connecting center of mass of particles of species A and those of species B oscillates with frequency ω. This amplitude of oscillation depends on the particle initial position and momentum.

We consider the limit $\alpha \to 1$ and $\gamma \to 1$. In this limit the frequency ω_α and ω_γ vanishes i.e. $\omega_\alpha \to 0$ and $\omega_\gamma \to 0$.
Using

$$\lim_{(\omega_\alpha t)\to 0} \frac{\sin \omega_\alpha t}{\omega_\alpha t} = 1 \qquad \lim_{(\omega_\gamma t)\to 0} \frac{\sin \omega_\gamma t}{\omega_\gamma t} = 1$$

we find that the vectors $\vec{r}_i$ given in Eq.(4.2.46) become

$$\begin{aligned} \vec{r}_i &= \frac{\vec{A}_i}{m} t + \vec{B}_i \qquad i = 1, .., 5 \\ \vec{r}_6 &= \frac{\vec{A}_6}{m\omega} \sin \omega t + \vec{B}_6 \cos \omega t \end{aligned} \tag{4.2.48}$$

Using Eqs.(4.2.45), (4.2.46) with Eq.(4.2.44) we obtain

$$\begin{aligned} \vec{r}_i &= \frac{\vec{p}_{io}}{m} t + \vec{r}_{io} \qquad i = 1, 2, \cdots 5 \\ \vec{r}_6 &= \frac{\vec{p}_{6o}}{m\omega} \sin \omega t + \vec{r}_{6o} \cos \omega t \end{aligned} \tag{4.2.49}$$

then we have five free modes in addition to one oscillator mode with frequency ω. The position vectors $\vec{r}_i^A, \vec{r}_i^B$ are obtained by combining Eqs.(4.2.44) and (4.2.47) we obtain

$$\begin{aligned}
\vec{r}_j^A(t) &= \frac{1}{6}[(5\vec{r}_{jo}^A - \sum_{i\neq j}\vec{r}_{io}^A + \sum_{i=1,2,3}\vec{r}_{io}^B) + \frac{1}{m}(5\vec{p}_{jo}^A - \sum_{i\neq j}\vec{p}_{io}^A + \sum_{i=1,2,3}\vec{p}_{io}^B)t \\
&+ \sum_{i=1,2,3}[\frac{1}{m\omega}(\vec{p}_{io}^A - \vec{p}_{io}^B)\sin\omega t + (\vec{r}_{io}^A - \vec{r}_{io}^B)\cos\omega t]] \\
\vec{r}_j^B(t) &= \frac{1}{6}[(5\vec{r}_{jo}^B - \sum_{i\neq j}\vec{r}_{io}^B + \sum_{i=1,2,3}\vec{r}_{io}^A) + \frac{1}{m}(5\vec{p}_{jo}^B - \sum_{i\neq j}\vec{p}_{io}^B + \sum_{i=1,2,3}\vec{p}_{io}^A)t \\
&- \sum_{i=1,2,3}[\frac{1}{m\omega}(\vec{p}_{io}^A - \vec{p}_{io}^B)\sin\omega t + (\vec{r}_{io}^A - \vec{r}_{io}^B)\cos\omega t]] \qquad i = 1,2,3 \quad (4.2.50)
\end{aligned}$$

Comparing Eqs.(4.2.50),(4.2.51) with Eqs.(3.2.39),(3.2.40) we see that in the limit $\alpha \to 1$ and $\gamma \to 1$ the original model is recovered.

4.3 Exact solution of the quantum system

The quantum behavior of the system is determined by the Hamiltonian operator $\hat{H}$ which is obtained from the classical Hamiltonian by replacing the dynamical variables by operators. In the coordinate representation we have:

$$\begin{aligned} \vec{r}_i^A &\rightarrow \vec{r}_i^A \qquad \vec{r}_i^B \rightarrow \vec{r}_i^B \\ \vec{p}_i^A &\rightarrow \frac{\hbar}{i}\vec{\nabla}_i^A \qquad \vec{p}_i^B \rightarrow \frac{\hbar}{i}\vec{\nabla}_i^B \qquad i = 1, 2, \cdots N \end{aligned}$$

Substituting into Eq.(4.1.5) we get

$$\begin{aligned} \hat{H} &= \sum_{i=1}^{N} \frac{1}{2m}[(\vec{\nabla}_i^A)^2 + (\vec{\nabla}_i^B)^2] + \frac{1}{2}Ng_{AB}(1-\alpha)\sum_{i=1}^{N}(\vec{r}_i^A)^2 \\ &+ \frac{1}{2}Ng_{AB}(1-\gamma)\sum_{j=1}^{N}(\vec{r}_j^B)^2 + \frac{1}{2}g_{AB}\sum_{i=1}^{N}\sum_{j=1}^{N}(\alpha\vec{r}_i^A.\vec{r}_j^A - 2\vec{r}_i^A.\vec{r}_j^B + \gamma\vec{r}_i^B.\vec{r}_j^B)] \end{aligned}$$

The wave function of the system

$$\psi = \psi(t, \vec{r}_i^A, \vec{r}_i^B)$$

is a solution of the time dependent Schroedinger equation

$$i\hbar\frac{\partial\psi(t, \vec{r}_i^A, \vec{r}_i^B)}{\partial t} = \hat{H}\psi(t, \vec{r}_i^A, \vec{r}_i^B)$$

the energy eigenfunctions $\psi_E(\vec{r}_i, \vec{r}_j)$ are solutions of the time independent Schroedinger equation

$$\hat{H}\psi_E(\vec{r}_i, \vec{r}_j) = E\psi_E(\vec{r}_i, \vec{r}_j)$$

Under the transformation of coordinates given by Eq.(4.2.17) the Hamiltonian operator takes the simple form:

$$\hat{H} = \sum_{i=1}^{2N}\frac{-\hbar^2}{2m}(\vec{\nabla}_i)^2 + \frac{1}{2}Ng_{AB}(1-\alpha)\sum_{i=1}^{N-1}\vec{r}_i^2 + \frac{1}{2}Ng_{AB}(1-\gamma)\sum_{i=1}^{N-1}\vec{r}_{i+N}^2 + Ng_{AB}\vec{r}_{2N}^2 \qquad (4.3.1)$$

The Hamiltonian operator splits up into the single particle Hamiltonians:

$$\begin{aligned} \hat{h}_i &= \frac{-\hbar^2}{2m}\vec{\nabla}_i^2 + Ng_{AB}(1-\alpha)\vec{r}_i^2 \qquad i = 1, 2, \cdots (N-1) \\ \hat{h}_N &= \frac{-\hbar^2}{2m}\vec{\nabla}_N^2 \\ \hat{h}_{i+N} &= \frac{-\hbar^2}{2m}\vec{\nabla}_{i+N}^2 + Ng_{AB}(1-\gamma)\vec{r}_{i+N}^2 \qquad i = 1, 2, \cdots (N-1) \\ \hat{h}_{2N} &= \frac{-\hbar^2}{2m}\vec{\nabla}_{2N}^2 + Ng_{AB}\vec{r}_{2N}^2 \end{aligned} \qquad (4.3.2)$$

so that the total Hamiltonian is:

$$\hat{H} = \sum_{i=1}^{N-1}(\hat{h}_i + \hat{h}_{i+N}) + \hat{h}_N + \hat{h}_{2N} \tag{4.3.3}$$

Inserting the Hamiltonian $\hat{H}$ into the Schroedinger equation, we obtain

$$\left(\sum_{i=1}^{N-1}(\hat{h}_i + \hat{h}_{i+N}) + \hat{h}_N + \hat{h}_{2N}\right)\psi_E(\vec{r}_1, \cdots \vec{r}_{2N}) = E\psi_E(\vec{r}_1, \cdots \vec{r}_{2N})$$

The wave function ψ_E of the total system can be expressed as a product of wave functions each of which depends on the variables of a single particle

$$\psi_E(\vec{r}_1, \cdots \vec{r}_{2N}) = \Phi(\vec{r}_N)\varphi(\vec{r}_{2N}) \prod_{i=1}^{N-1} \phi(\vec{r}_i) \prod_{j=1}^{N-1} \phi(\vec{r}_{j+N}) \tag{4.3.4}$$

where

$$\begin{aligned}
\hat{h}_N\Phi(\vec{r}) &= \varepsilon_N\Phi(\vec{r}_N) \\
\hat{h}_{2N}\varphi(\vec{r}_{2N}) &= \varepsilon_{2N}\varphi(\vec{r}_{2N}) \\
\hat{h}_i\phi(\vec{r}_i) &= \varepsilon_i\phi(\vec{r}_i) \qquad i = 1, \cdots N-1 \\
\hat{h}_{i+N}\phi(\vec{r}_{i+N}) &= \varepsilon_{i+N}\phi(\vec{r}_{i+N}) \qquad i = 1, \cdots N-1
\end{aligned} \tag{4.3.5}$$

The total energy of the system is the sum of energies ε_i

$$E = \sum_{i=1}^{2N} \varepsilon_i \tag{4.3.6}$$

Substituting Eq.(4.3.2) into Eq.(4.3.5) we get

$$\frac{-\hbar^2}{2m}\vec{\nabla}_N^2\Phi(\vec{r}_N) = \varepsilon_N\Phi(\vec{r}_N) \tag{4.3.7}$$

$$\left(\frac{-\hbar^2}{2m}\vec{\nabla}_{2N}^2 + g_{AB}N\vec{r}_{2N}^2\right)\varphi(\vec{r}_{2N}) = \varepsilon_{2N}\varphi(\vec{r}_{2N}) \tag{4.3.8}$$

$$\left(\frac{-\hbar^2}{2m}\vec{\nabla}_i^2 + g_{AB}N(1-\alpha)\vec{r}_i^2\right)\phi(\vec{r}_i) = \varepsilon_i\phi(\vec{r}_i) \qquad i = 1, \cdots N-1 \tag{4.3.9}$$

$$\left(\frac{-\hbar^2}{2m}\vec{\nabla}_{i+N}^2 + g_{AB}N(1-\gamma)\vec{r}_{i+N}^2\right)\phi(\vec{r}_{i+N}) = \varepsilon_{i+N}\phi(\vec{r}_{i+N}) \quad i = 1, \cdots N-1 \tag{4.3.10}$$

Eq.(4.3.7) is the Schroedinger equation for a free particle of energy ε_N.
To solve the equation, we again imagine the system to be in a very large cubic box of volume

$$V = L^3$$

and impose periodic boundary conditions:

$$\begin{aligned}
\psi(x_N + L, y_N, z_N) &= \psi(x_N, y_N, z_N) \\
\psi(x_N, y_N + L, z_N) &= \psi(x_N, y_N, z_N) \\
\psi(x_N, y_N, z_N + L) &= \psi(x_N, y_N, z_N),
\end{aligned} \tag{4.3.11}$$

to obtain the free particle solution:

$$\varphi(\vec{r}_N) = \frac{1}{\sqrt{V}} e^{ik.\vec{r}_N} \tag{4.3.12}$$

Using the periodic boundary conditions we obtain

$$k_N = \frac{2\pi}{L}(n_x, n_y, n_z) \qquad\qquad n_x, n_y, n_z = 0, \pm 1, \pm 2, \cdots \tag{4.3.13}$$

The energy of the free particle is

$$\varepsilon_N = \frac{\hbar^2 \vec{k}_N^2}{2m} \tag{4.3.14}$$

We next consider Eqs(4.3.8), (4.3.9) and (4.3.10). Each of these equations is the Schroedinger equation for a three dimensional harmonic oscillator of frequency $\omega = N g_{AB}, \omega_\alpha = N(1-\alpha) g_{AB}$ and $\omega_\gamma = N(1-\gamma) g_{AB}$ respectively.
The corresponding wave functions

$$\phi(\vec{r}_i), \quad \phi(\vec{r}_{i+N}) \qquad i = 1, \cdots, (N-1) \quad and \quad \varphi(\vec{r}_{2N})$$

are given by:

$$\begin{aligned}
\phi_{n_{i,u}} &= \prod_{u=x,y,z} \left[(\sqrt{2^{n_{i,u}} (n_{i,u})!})^{-1/2} \left[\frac{m\omega_\alpha}{\pi\hbar} \right]^{3/4} H_{n_{\alpha,u}}(\sqrt{\frac{m\omega_\alpha}{\pi\hbar}} u) e^{-m\omega_\alpha u^2/2\hbar} \right] \\
\phi_{n_{i+N,u}} &= \prod_{u=x,y,z} \left[(\sqrt{2^{n_{i+N,u}} (n_{i+N,u})!})^{-1/2} \left[\frac{m\omega_\gamma}{\pi\hbar} \right]^{3/4} H_{n_{i+N,u}}(\sqrt{\frac{m\omega_\gamma}{\pi\hbar}} u) e^{-m\omega_\gamma u^2/2\hbar} \right] \\
\varphi_{n_{2N,u}} &= \prod_{u=x,y,z} \left[(\sqrt{2^{n_{2N,u}} (n_{2N,u})!})^{-1/2} \left[\frac{m\omega}{\pi\hbar} \right]^{3/4} H_{n_{2N,u}}(\sqrt{\frac{m\omega}{\pi\hbar}} u) e^{-m\omega u^2/2\hbar} \right]
\end{aligned} \tag{4.3.15}$$

The energy of the oscillators are given by

$$\begin{aligned} E_{n_{i,x},n_{i,y},n_{i,z}} &= \sum_{i=1}^{N-1} \hbar\omega_\alpha(n_{i,x}+n_{i,y}+n_{i,z}+3/2) \\ E_{n_{i+N,x},n_{i+N,y},n_{i+N,z}} &= \sum_{i=1}^{N-1} \hbar\omega_\gamma(n_{i+N,x}+n_{i+N,y}+n_{i+N,z}+3/2) \\ E_{n_{2N,x},n_{2N,y},n_{2N,z}} &= \hbar\omega(n_{2N,x}+n_{2N,y}+n_{2N,z}+3/2) \end{aligned} \tag{4.3.16}$$

To construct the wave function of the system we need to determine the maximal number of the commuting operators which commute with the Hamiltonian of the system. These are the exchange operators

$$\hat{P}_{ij}, \hat{P}_{i+N,j+N}, \qquad\qquad i,j = 1,2,\cdots N-1$$

The wave function

$$\psi(\vec{r}_1 \cdots \vec{r}_{2N})$$

should be an eigenfunction of the operator $\hat{P}_{ij}, \hat{P}_{i+N,j+N}$. Since we have a system of bosons

$$\begin{aligned} \hat{P}_{ij}\phi(\vec{r}_1,..\vec{r}_i,..\vec{r}_j,..\vec{r}_{\alpha(N-1)}) &= \phi(\vec{r}_1,..\vec{r}_j,..\vec{r}_i,..\vec{r}_{(N-1)}) \\ \hat{P}_{i+N,j+N}\phi(\vec{r}_{N+1},..\vec{r}_{N+i},..\vec{r}_{N+j},..\vec{r}_{2N-1}) &= \phi(\vec{r}_{N+1},..\vec{r}_{N+j},..\vec{r}_{N+i},..\vec{r}_{2N-1}) \end{aligned}$$

with $i,j = 1,2,\cdots N-1$. The wave function should be symmetric with respect to an exchange of coordinates and momenta of each of the $(N-1)$ modes. This gives

$$\begin{aligned} \psi(r_1..r_{2N}) &= \frac{1}{\sqrt{(N-1)S!}} \sum_P \hat{P}[\phi_{k_1}(r_1)\phi_{k_2}(r_2)...\phi_{k_{N-1}}(r_{N-1})] \\ &\times \frac{1}{\sqrt{(N-1)S'!}} \sum_P \hat{P}[\phi_{k_{N+1}}(r_{N+1})\phi_{k_{N+2}}(r_{N+2})...\phi_{k_{2N-1}}(r_{2N-1})] \\ &\times \varphi_{2N,x;2N,y;2N,z} \times \Phi(\vec{r}_N) \end{aligned} \tag{4.3.17}$$

where S, S' are additional normalization constant, and the sum is over all permutations

$$\hat{P}_1, \hat{P}_2, \cdots \hat{P}_{N-1},$$

of

$$1,2,\cdots(N-1),$$

in the argument of the one particle wave function

$$\phi_{n_i}(\vec{r}_i) \quad and \quad \phi_{n_{i+N}}(\vec{r}_{i+N})$$

The total energy of the system is given according to Eq.(4.3.6) by

$$\begin{aligned} E &= \frac{\hbar^2}{2m}\vec{k}_N + \sum_{k}^{2N-1} \hbar\omega_k(n_k + \frac{3}{2}) \\ &= \frac{\hbar^2}{2m}\vec{k}_N + \hbar\omega(n_{\omega,x} + n_{\omega,y} + n_{\omega,z} + 3/2) \\ &+ \sum_{i=1}^{(N-1)} [\hbar\omega_\alpha(n_{(i,x)} + n_{(i,y)} + n_{(i,z)} + 3/2)] \\ &+ \sum_{i=1}^{(N-1)} [\hbar\omega_\gamma(n_{(i+N,x)} + n_{(i+N,y)} + n_{(i+N,z)} + 3/2)] \end{aligned} \tag{4.3.18}$$

The energy E is the sum of the translational energy of one translational mode plus the energy of the $2N-1$ three dimensional harmonic oscillators.

4.4 Exact solution of the statistical mechanical system

As the previous chapter, we assume that the number of particles N of each species as well as volume V occupied by the system is very large, such that

$$N \to \infty, \qquad V \to \infty, \qquad \frac{N}{V} \to \text{finite number}$$

4.4.1 Determination of the grand canonical partition function

Again we study the quantum statistical behaviour of the system within the frame work of the grand canonical ensemble.

As in Chapter 3 the grand canonical partition function is given by:

$$Z(T, V, \mu) = Tr\left\{e^{-\beta(\hat{H}-\mu\hat{N})}\right\} \tag{4.4.1}$$

On the right hand side we have the Hamiltonian of the system $\hat{H}$ given by (4.3.1) and the particle number operator $\hat{N}$. From the grand canonical partition function, we obtain the grand canonical potential via the relation

$$\Phi(T, V, \mu) \;\; = \;\; -kT \ln Z(T, V, \mu),$$

To calculate the trace of the operator on the right hand side of Eq.(4.4.1) we have to choose a basis for the Hilbert space of the system. A suitable basis is given by:

$$\left\{\mid n_{(1,u)}, \cdots, n_{(N-1,u)}\rangle^s \otimes \mid \vec{k}_N\rangle \otimes \mid n_{(N+1,u)}, \cdots, n_{(2N-1,u)}\rangle^s \otimes \mid n_{2N,u}\rangle\right\} \tag{4.4.2}$$

where the subscript $u = x, y, z$. Again the wave function in Eq.(4.3.4) is a coordinate representation of the state vectors. Thus

$$\begin{aligned}\psi(\vec{r}_i; \vec{r}_N; \vec{r}_{i+N}; \vec{r}_{2N}) \;\; = \;\; & (\langle \vec{r}_{2N} \mid \otimes^s \langle \vec{r}_{N+1}, \cdots \vec{r}_{(2N-1)} \mid \otimes \langle \vec{r}_N \mid \otimes^s \langle \vec{r}_1, \cdots \vec{r}_{(N-1)} \mid) \\ & (\mid n_{(1,u)}, \cdots, n_{(N-1,u)}\rangle^s \otimes \mid \vec{k}_N\rangle \otimes \mid n_{(N+1,u)}, \cdots, n_{(2N-1,u)}\rangle^s \otimes \mid n_{2N,u}\rangle)\end{aligned}$$

we get

$$\begin{aligned}\psi(\vec{r}_i; \vec{r}_N; \vec{r}_{i+N}; \vec{r}_{2N}) = \qquad & {}^s\langle \vec{r}_1, \cdots \vec{r}_{N-1} \mid n_{(1,u)}, \cdots, n_{(N-1,u)}\rangle^s \langle \vec{r}_N \mid \vec{k}_N\rangle \\ & {}^s\langle \vec{r}_{N+1}, \cdots \vec{r}_{2N-1} \mid n_{(N+1,u)}, \cdots, n_{(2N-1,u)}\rangle^s \langle \vec{r}_{2N} \mid n_{2N,u}\rangle\end{aligned}$$

From Eq.(4.3.17) we see that

$$
\begin{aligned}
{}^s\langle \vec{r}_1, \cdots \vec{r}_{N-1} \mid n_{(1,u)}, \cdots, n_{(N-1,u)} \rangle^s &= \frac{1}{\sqrt{(N-1)S!}} \sum_P \hat{P} \\
&\quad \Big[\phi_{n_{(1,u)}}(\vec{r}_1), \cdots, \phi_{n_{(N-1,u)}}(\vec{r}_{N-1}) \Big] \\
{}^s\langle \vec{r}_{N+1}, \cdots \vec{r}_{2N-1} \mid n_{(1,u)}, .., n_{(2N-1,u)} \rangle^s &= \frac{1}{\sqrt{(N-1)S'!}} \sum_P \hat{P} \\
&\quad \Big[\phi_{n_{(1,u)}}(\vec{r}_{N+1}), .., \phi_{n_{(2N-1,u)}}(\vec{r}_{2N-1}) \Big]
\end{aligned}
$$

and

$$
\langle \vec{r}_{2N} \mid n_{2N,x}, n_{2N,y}, n_{2N,z} \rangle = \varphi_{n_{2N,x}, n_{2N,y}, n_{2N,z}}(\vec{r}_{2N})
$$

while

$$
\langle \vec{r}_N \mid \vec{k}_N \rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}.\vec{r}_N}
$$

Again the state vectors

$$
\begin{aligned}
&\mid n_{(1,u)}, \cdots n_{(N-1,u)} \rangle^s \\
&\mid n_{(N+1,u)}, \cdots n_{(2N-1,u)} \rangle^s
\end{aligned} \tag{4.4.3}
$$

can also be characterized by the occupation numbers instead the quantum number of the occupied state

$$
\begin{aligned}
\mid m_{\alpha 1}, m_{\alpha 2}, \cdots \rangle^s &\equiv \mid n_{(1,u)}, \cdots n_{(N-1,u)} \rangle^s \\
\mid m_{\gamma 1}, m_{\gamma 2}, \cdots \rangle^s &\equiv \mid n_{(1,u)}, \cdots n_{(2N-1,u)} \rangle^s
\end{aligned} \tag{4.4.4}
$$

These state vectors satisfy orthogonality property

$$
{}^s\langle m'_{j1}, m'_{j2}, \cdots \mid m_{j1}, m_{j2}, \cdots \rangle^s = \delta_{m_{j1}, m'_{j1}} \delta_{m_{j2}, m'_{j2}} \cdots \tag{4.4.5}
$$

with $j = \alpha, \gamma$. The basis vectors (4.4.2) now take the form:

$$
\Big\{ \mid m_{\alpha 1}, m_{\alpha 2}, \cdots \rangle^s \otimes \mid \vec{k}_N \rangle \otimes \mid m_{\gamma 1}, m_{\gamma 2}, \cdots \rangle^s \otimes \mid n_{2N,u} \rangle \Big\} \tag{4.4.6}
$$

We will use these basis vectors to calculate the trace in the equation for the partition function.

$$
\begin{aligned}
Z(T,V,\mu) &= \sum_{m_{n\alpha}} \sum_{m_{n\gamma}} \sum_{n_{2N}} \sum_k \langle n_{2N,u} \mid^s \langle m_{\gamma 1}, m_{\gamma 2}, \cdots \mid \otimes \langle \vec{k}_N \mid \\
&\otimes \ {}^s\langle m_{\alpha 1}, m_{\alpha 2}, \cdots \mid e^{-\beta(\hat{H} - \mu \hat{N})} \mid m_{\alpha 1}, m_{\alpha 2}, \cdots \rangle^s \\
&\otimes \ \mid \vec{k}_N \rangle \otimes \mid m_{\gamma 1}, m_{\gamma 2}, \cdots \rangle^s \otimes \mid n_{2N,u} \rangle
\end{aligned} \tag{4.4.7}
$$

We split the Hamiltonian into four parts

$$\hat{H} = \hat{h}_N + \hat{h}_{2N} + \hat{H}_\alpha + \hat{H}_\gamma \tag{4.4.8}$$

where

$$\begin{aligned} \hat{H}_\alpha &= \sum_{i=1}^{N-1} \hat{h}_i \\ \hat{H}_\gamma &= \sum_{i=1}^{N-1} \hat{h}_{i+N} \end{aligned} \tag{4.4.9}$$

We let

$$\mu = \mu_N + \mu_{2N} + \mu_\alpha + \mu_\gamma \tag{4.4.10}$$

Since

$$\begin{aligned} \left[\hat{h}_i, \hat{h}_{2N}\right] &= 0 \qquad \left[\hat{h}_{i+N}, \hat{h}_{2N}\right] = 0 \\ \left[\hat{h}_i, \hat{h}_{i+N}\right] &= 0 \qquad \left[\hat{h}_N, \hat{h}_{2N}\right] = 0 \end{aligned} \tag{4.4.11}$$

and[1]

$$\begin{aligned} \left[\hat{N}, \hat{h}_i\right] &= 0 \qquad \left[\hat{N}, \hat{h}_{i+N}\right] = 0 \\ \left[\hat{N}, \hat{h}_{2N}\right] &= 0 \qquad \left[\hat{N}, \hat{h}_N\right] = 0 \end{aligned} \tag{4.4.12}$$

we can write

$$e^{-\beta(\hat{H}-\mu\hat{N})} = e^{-\beta(\hat{h}_N-\mu_N\hat{N})} e^{-\beta(\hat{h}_{2N}-\mu_{2N}\hat{N})} e^{-\beta(\hat{H}_\alpha-\mu_\alpha\hat{N})} e^{-\beta(\hat{H}_\gamma-\mu_\gamma\hat{N})} \tag{4.4.13}$$

The matrix element on the right hand side of Eq.(4.4.7) can now be very easily evaluated

$$\begin{aligned} &\langle n_{2N,u} \mid \otimes^s\langle m_{\gamma 1}, m_{\gamma 2}, \cdots \mid \otimes\langle \vec{k}_N \mid \otimes^s\langle m_{\alpha 1}, m_{\alpha 2}, \cdots \mid e^{-\beta(\hat{H}-\mu\hat{N})} \\ &\qquad \mid m_{\alpha 1}, m_{\alpha 2}, \cdots\rangle^s\otimes \mid \vec{k}_N\rangle\otimes \mid m_{\gamma 1}, m_{\gamma 2}, \cdots\rangle^s\otimes \mid n_{2N,u}\rangle \\ &= e^{-\beta[\frac{\hbar^2}{2m}k^2-\mu_N]} e^{-\beta[\hbar\omega(n_{2N}+\frac{3}{2})-\mu_{2N}]} e^{-\beta\sum_{n_i=1}^{\infty} m_{\alpha i}(\epsilon_{n_i}-\mu_\alpha)} e^{-\beta\sum_{n_{i+N}=1}^{\infty} m_{\gamma i}(\epsilon_{n_{i+N}}-\mu_\gamma)} \end{aligned} \tag{4.4.14}$$

[1]We have not constructed the particle number operator $\hat{N}$ since the actual framework for the occupation number representation is the second quantization formalism. Using the technique we can construct $\hat{N}$ and prove Eq.(4.4.12)

We set

$$\mu_N = 0 \qquad and \qquad \mu_{2N} = 0 \tag{4.4.15}$$

$$\begin{aligned} Z(T,V,\mu) = & \left(\sum_{m_{\alpha i}} e^{-\beta\sum_{n_i=1}^{\infty} m_{\alpha i}(\epsilon_{n_i}-\mu_\alpha)}\right) \times \left(\sum_{m_{\gamma i}} e^{-\beta\sum_{n_{i+N}=1}^{\infty} m_{\gamma i}(\epsilon_{n_{i+N}}-\mu_\gamma)}\right) \\ & \times \left(\sum_k e^{-\beta\frac{\hbar^2k^2}{2m}}\right) \times \left(^{-\frac{3}{2}\beta\hbar\omega}\left(\sum_{n_{2N}} e^{-n_{2N}\beta\hbar\omega}\right)^3\right) \end{aligned} \tag{4.4.16}$$

The grand canonical partition function splits into four parts, one which is associated with the $(N-1)$ vibrational modes with chemical potential μ_α and the other which is associated with the $(N-1)$ vibrational modes with μ_γ, the third part is the canonical partition function for the free particle, while the fourth part is associated with the vibrational mode with frequency ω .

$$Z(T,V,\mu) = Z_\alpha(T,V,\mu_\alpha)Z_\gamma(T,V,\mu_\gamma)Z_\omega(T,V)Z_{tr}(T,V) \tag{4.4.17}$$

where

$$Z_\alpha(T,V,\mu_\alpha) = \sum_{m_\alpha} e^{-\beta[\sum_{n_i=1}^{\infty} m_\alpha(\epsilon_{n_i}-\mu_\alpha)]}, \tag{4.4.18}$$

$$Z_\gamma(T,V,\mu_\gamma) = \sum_{m_\gamma} e^{-\beta[\sum_{n_{i+N}=1}^{\infty} m_\gamma(\epsilon_{n_{i+N}}-\mu_\gamma)]}, \tag{4.4.19}$$

$$Z_\omega(T,V) = e^{-\frac{3}{2}\beta\hbar\omega}\left(\sum_{n_{2N}=0}^{\infty} e^{-n_{2N}\beta\hbar\omega}\right)^3 \tag{4.4.20}$$

and

$$Z_{tr}(T,V) = \left(\sum_k e^{-\beta\frac{\hbar^2k^2}{2m}}\right) \tag{4.4.21}$$

The partition function $Z_\omega(T,V)$ is the canonical partition function for the three dimensional harmonic oscillator. The sum of the geometric series in Eq.(4.4.20) is

$$\sum_{n_{2N}=0}^{\infty} e^{n_{2N}\beta\hbar\omega} = \frac{1}{(1-e^{-\beta\hbar\omega})} \tag{4.4.22}$$

Therefore

$$Z_\omega(T,V) = \frac{e^{-\frac{3}{2}\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^3} \tag{4.4.23}$$

The canonical partition function for the free mode is

$$Z_{tr}(T,V) = V\left(\frac{2\pi m}{\beta h^2}\right)^{3/2} \tag{4.4.24}$$

The partition functions Z_α, Z_γ can be rearranged in the form

$$\begin{aligned} Z_\alpha(T,V,\mu_\alpha) &= \prod_{n_i=1}^{\infty}\sum_{m_\alpha}\left(e^{-\beta(\epsilon_{n_i}-\mu_\alpha)}\right)^{m_\alpha} \\ Z_\gamma(T,V,\mu_\gamma) &= \prod_{n_{i+N}=1}^{\infty}\sum_{m_\gamma}\left(e^{-\beta(\epsilon_{n_{i+N}}-\mu_\gamma)}\right)^{m_\gamma} \end{aligned} \tag{4.4.25}$$

Since we have a system of bosons, any quantum state can be occupied by any number of bosons i.e.

$$m_\alpha, m_\gamma = 0, 1, 2...$$

Therefore

$$\sum_{m_\alpha}\left[e^{-\beta(\epsilon_{n_i}-\mu_\alpha)}\right]^{m_\alpha} = \frac{1}{1-z_\alpha e^{-\beta\epsilon_{n_i}}} \tag{4.4.26}$$

where

$$z_\alpha = e^{\beta(\mu_\alpha-\epsilon_o^\alpha)}, \qquad \epsilon_o^\alpha = \frac{3}{2}\hbar\omega_\alpha \tag{4.4.27}$$

The chemical potential of the $\alpha-$subsystem is measured from the oscillator ground state energy Similarly

$$\sum_{m_\gamma}\left[e^{-\beta(\epsilon_{n_{i+N}}-\mu_\gamma)}\right]^{m_\gamma} = \frac{1}{1-z_\gamma e^{-\beta\epsilon_{n_{i+N}}}} \tag{4.4.28}$$

where

$$z_\gamma = e^{\beta(\mu_\gamma-\epsilon_o^\gamma)}, \qquad \epsilon_o^\gamma = \frac{3}{2}\hbar\omega_\gamma \tag{4.4.29}$$

where z_α, z_γ are the fugicities of the subsystem. Inserting Eqs.(4.4.26),(4.4.28) into Eq.(4.4.25) we obtain

$$\begin{aligned} Z_\alpha(T,V,\mu_\alpha) &= \prod_{n_i=1}^{\infty}\frac{1}{1-z_\alpha e^{-\beta\epsilon_{n_i}^\alpha}} \\ Z_\gamma(T,V,\mu_\gamma) &= \prod_{n_{i+N}=1}^{\infty}\frac{1}{1-z_\gamma e^{-\beta\epsilon_{n_{i+N}}^\gamma}} \end{aligned} \tag{4.4.30}$$

Collecting the different terms we obtain the total partition function of the system,

$$Z(T,V,\mu) = V\left(\frac{2\pi m}{\beta h^2}\right)^{3/2}\left[\frac{e^{-\frac{3}{2}\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^3}\right]\left[\prod_{n_i=1}^{\infty}\frac{1}{1-z_\alpha e^{-\beta\epsilon^\alpha_{n_i}}}\right]\left[\prod_{n_{i+N}=1}^{\infty}\frac{1}{1-z_\gamma e^{-\beta\epsilon^\gamma_{n_{i+N}}}}\right] \quad (4.4.31)$$

We can now obtain the grand canonical potential:

$$\begin{aligned}\Phi(T,V,\mu) &= kT[\sum_{n_i=0}^{\infty}\ln(1-z_\alpha e^{-\beta\epsilon^\alpha_{n_i}}) + \sum_{n_{i+N}=0}^{\infty}\ln(1-z_\gamma e^{-\beta\epsilon^\gamma_{n_{i+N}}})] \\ &+ \frac{3}{2}kT\left(2\ln(1-e^{-\beta\hbar\omega}) + \beta\hbar\omega - \ln(\frac{2\pi m}{\beta h^2}) - \frac{2}{3}\ln V\right) \quad (4.4.32)\end{aligned}$$

We measure the oscillator energy state from the lowest oscillator states so that

$$\epsilon^\alpha_o = 0, \qquad \epsilon^\gamma_o = 0$$

4.4.2 Thermodynamical parameters of the system

The number of the particles of each subsystem is given by:

$$N - 1 = \sum_{n_i=0}^{\infty}\frac{1}{z_\alpha^{-1}e^{\beta\epsilon_{n_i}} - 1} \quad (4.4.33)$$

Since $N \gg 1$ we have

$$N = \sum_{n_i=0}^{\infty}\frac{1}{z_\alpha^{-1}e^{\beta\epsilon_{n_i}} - 1} \quad (4.4.34)$$

Similarly

$$N = \sum_{n_{i+N}=0}^{\infty}\frac{1}{z_\gamma^{-1}e^{\beta\epsilon_{n_{i+N}}} - 1} \quad (4.4.35)$$

Again we split the sum over n_i, n_{i+N} into two parts, the $n_i, n_{i+N} = 0$ and $n_i, n_{i+N} \neq 0$ parts. Since

$$n_i = 0 \Longrightarrow \varepsilon_{n_i} = 0$$
$$n_{i+N} = 0 \Longrightarrow \varepsilon_{n_{i+N}} = 0$$

We have

$$\begin{aligned}N &= N^o_\alpha + N^e_\alpha \\ N &= N^o_\gamma + N^e_\gamma \quad (4.4.36)\end{aligned}$$

The first term gives the contribution of the ground state energy to the total particle number

$$\begin{aligned} N_\alpha^o &= \frac{z_\alpha}{1-z_\alpha} \\ N_\gamma^o &= \frac{z_\gamma}{1-z_\gamma} \end{aligned} \tag{4.4.37}$$

while the second term gives the number of the particle N_e in the excited state

$$\begin{aligned} N_\alpha^e &= \sum_{n_i \neq 0}^{\infty} \frac{1}{z_\alpha^{-1} e^{\beta \epsilon_{n_i}} - 1} \\ N_\gamma^e &= \sum_{n_{i+N} \neq 0}^{\infty} \frac{1}{z_\gamma^{-1} e^{\beta \epsilon_{n_{i+N}}} - 1} \end{aligned} \tag{4.4.38}$$

It is clear that the system condenses into two channels since we have two independent subsystems.

We consider the case where the temperature T is of the order a few micro kelvin and $\omega_\alpha, \omega_\gamma$ are of the order a few hundred Hz, then we have

$$\beta\omega_\alpha \ll 1, \qquad \beta\omega_\gamma \ll 1$$

This enable us to approximate the sums over discrete energy levels in expressions such as (4.4.38) by integrals.

$$\sum_{n \neq 0} f(n) \longrightarrow \int d\varepsilon \rho(\varepsilon) f(\varepsilon) \tag{4.4.39}$$

Using the density of states given in Appendix C to evaluate the above sums,

$$\rho(\epsilon) = \frac{1}{2} \frac{\epsilon^2}{(\hbar\Omega)^3}, \tag{4.4.40}$$

where $\Omega = \omega_\alpha$ or ω_γ. Then we can express the number of particles in the excited state in terms of an integral over the energy ε of the single particle state

$$N_\alpha^e = \frac{1}{2} \frac{1}{(\hbar\omega_\alpha)^3} \int_0^\infty \frac{\varepsilon_{n_i}^2}{z_\alpha^{-1} e^{\beta \varepsilon_{n_i}} - 1} d\varepsilon_{n_i}$$

and

$$N_\alpha^e = \frac{1}{2} \frac{1}{(\hbar\omega_\gamma)^3} \int_0^\infty \frac{\varepsilon_{n_{i+N}}^2}{z_\gamma^{-1} e^{\beta \varepsilon_{n_{i+N}}} - 1} d\varepsilon_{n_{i+N}}$$

we obtain

$$\begin{aligned} N_\alpha^e &= \frac{1}{(\beta\hbar\omega_\alpha)^3} g_3(z_\alpha) \\ N_\gamma^e &= \frac{1}{(\beta\hbar\omega_\gamma})^3 g_3(z_\gamma) \end{aligned} \tag{4.4.41}$$

Substituting using Eq.(4.4.37) and Eq.(4.4.41) into Eq.(4.4.36) we have the number of particles in each subsystem

$$\begin{aligned} N &= N_\alpha^o + (\frac{kT}{\hbar\omega_\alpha})^3 g_3(z_\alpha) \\ N &= N_\gamma^o + (\frac{kT}{\hbar\omega_\gamma})^3 g_3(z_\gamma) \end{aligned} \tag{4.4.42}$$

where N_α^o, N_γ^o are the ground state occupation numbers for each subsystem.

From Eq.(4.4.33), we have $0 \leq z_\nu < 1$, so that $g_3(z_\nu)$, $\nu = \alpha, \gamma$ is bounded by $\zeta(3) \approx 1.202$. Therefore, according to (4.4.36) the particles must condense in the ground state of the trap when the temperature becomes sufficiently low. At the onset of condensation we have $N_\alpha^o, N_\gamma^o = 0$ and $z_\alpha, z_\gamma = 1$ ($\mu = \mu_c = 3/2\hbar\omega_\nu$);

$$N = \left(\frac{kT_c^\alpha}{\hbar\omega_\alpha}\right)^3 \zeta(3) \tag{4.4.43}$$

$$N = \left(\frac{kT_c^\gamma}{\hbar\omega_\gamma}\right)^3 \zeta(3) \tag{4.4.44}$$

from which we can find the condensation temperatures T_c^α, T_c^γ for each subsystem as

$$\begin{aligned} kT_c^\alpha &= \hbar\omega_\alpha \left(\frac{N}{\zeta(3)}\right)^{1/3} \\ kT_c^\gamma &= \hbar\omega_\gamma \left(\frac{N}{\zeta(3)}\right)^{1/3} \end{aligned} \tag{4.4.45}$$

at a given particle density. From these equations we see that

$$\frac{T_c^\alpha}{T_c^\gamma} = \frac{\omega_\alpha}{\omega_\gamma} = \sqrt{\frac{1-\alpha}{1-\gamma}} = \sqrt{\frac{g_{AB} - g_{AA}}{g_{AB} - g_{BB}}}$$

The ratio of the critical temperatures depends on the difference between the coupling constants. When

$$g_{AA} = g_{BB} \neq g_{AB}$$

the two subsystem merge into a single subsystem. The condensation fraction in the ground state is given as a function of temperature by:

$$\begin{aligned} \frac{N_\alpha^o}{N} &= 1 - \left(\frac{T}{T_c^\alpha}\right)^3 \qquad T < {T_c}^\alpha \\ \frac{N_\gamma^o}{N} &= 1 - \left(\frac{T}{T_c^\gamma}\right)^3 \qquad T < T_c^\gamma \end{aligned} \tag{4.4.46}$$

and vanishes above the critical points T_c^α, T_c^γ, while the fraction of particles in the excited states of each subsystem is

$$\begin{aligned} \frac{N_\alpha^e}{N} &= \left(\frac{T}{T_c^\alpha}\right)^3 \qquad T \geq T_c^\alpha \\ \frac{N_\gamma^e}{N} &= \left(\frac{T}{T_c^\gamma}\right)^3 \qquad T \geq T_c^\gamma \end{aligned} \tag{4.4.47}$$

and is equal to unity below the critical points.

Using the boson function $g_n(z)$, we can express the grand canonical potential in the form:

$$\begin{aligned} \Phi(T,V,\mu) &= -\frac{1}{\beta(\beta\hbar)^3}\left[\frac{g_4(z_\alpha)}{\omega_\alpha^3} + \frac{g_4(z_\gamma)}{\omega_\gamma^3}\right] \\ &+ \frac{3}{2}kT\left(2\ln(1-e^{-\beta\hbar\omega}) + \beta\hbar\omega - \ln(\frac{2\pi m}{\beta h^2}) - \frac{2}{3}\ln V\right) \end{aligned} \tag{4.4.48}$$

The internal energy of the system given by

$$\begin{aligned} U &= -\frac{\partial}{\partial\beta}\ln Z(T,V,\mu)\mid_{z,V} \\ &= -\frac{\partial}{\partial\beta}\left(\frac{\Phi}{-kT}\right)\mid_{z,V} \end{aligned} \tag{4.4.49}$$

Using Eq.(4.4.48) we obtain for $T > T_c^\alpha, T > T_c^\gamma$,

$$U = \frac{3}{\beta(\beta\hbar)^3}\left[\frac{g_4(z_\alpha)}{\omega_\alpha^3} + \frac{g_4(z_\gamma)}{\omega_\gamma^3}\right] + \frac{3}{2}\left(\hbar\omega + \frac{2\hbar\omega}{e^{\beta\hbar\omega}-1} + kT\right) \tag{4.4.50}$$

For $T < T_c^\alpha, T < T_c^\gamma$,

$$U = \frac{3}{\beta(\beta\hbar)^3}\left[\frac{1}{\omega_\alpha^3} + \frac{1}{\omega_\gamma^3}\right]\zeta(4) + \frac{3}{2}\left(\hbar\omega + \frac{2\hbar\omega}{e^{\beta\hbar\omega}-1} + kT\right) \tag{4.4.51}$$

The internal energy is the sum of four parts. The first two parts are typically the internal energy for a relatively large numbers of oscillator modes, the third part is

associated with the 3-dimensional harmonic oscillator with frequency ω. The last part gives the contribution of the translational mode.

$$U = U_\alpha + U_\gamma + \frac{3}{2}\left(\hbar\omega + \frac{2\hbar\omega}{e^{\beta\hbar\omega}-1} + kT\right) \tag{4.4.52}$$

where

$$U_\alpha = \begin{cases} \frac{3}{\beta(\beta\hbar\omega_\alpha)^3} g_4(z_\alpha) & T > T_c^\alpha \\ \frac{3}{\beta(\beta\hbar\omega_\alpha)^3}\zeta(4) & T < T_c^\alpha \end{cases} \tag{4.4.53}$$

and

$$U_\gamma = \begin{cases} \frac{3}{\beta(\beta\hbar\omega_\gamma)^3} g_4(z_\gamma) & T > T_c^\gamma \\ \frac{3}{\beta(\beta\hbar\omega_\gamma)^3}\zeta(4) & T < T_c^\gamma \end{cases} \tag{4.4.54}$$

are the internal energy of each subsystem above and below the critical temperature.

The system behaves mainly as two independent subsystems of uncoupled oscillators (quasi-particles). Each of the subsystem is $(N-1)$-fold degenerate. In addition there is a single mode which is associated with the vibrational motion of the position vector connecting the center of mass of each species and another mode corresponding to the translational motion of the center of mass of the system.
Fig.(4.2[a]) shows that for small N, the total internal energy of the system increases linearly with N but for large N it falls to zero. The total energy has a peak at a certain value of particle number. The value of N at which the total energy has its maximum depends on the parameter α.
This may be interpreted as follows: The condensate term is roughly speaking proportional to $N^{-2/3}$ while the oscillator term is proportional to $N^{-1/2}$. Therefore for small number of particle (which satisfies $N \gg 1$) the first term dominates i.e. the major contribution to the energy comes from the condensation term while for large number of particles the major energy contribution comes from the oscillator term. Therefore above T_c, the whole system behaves as two sets of degenerate uncoupled oscillators.

The variation of the total energy with α is shown in Fig.(4.2[b]). We can see that the dependence on α no longer exists above a certain value of α which depends on

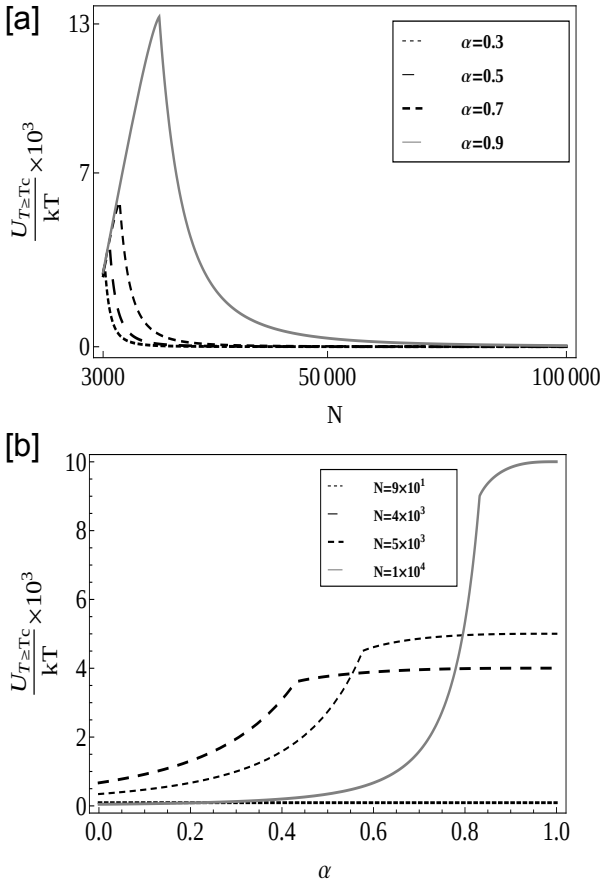

Figure 4.2: Total energy of the system above T_c in unit of kT, [a]variation of total energy above T_c with particle number. [b]variation of total energy above T_c with α.

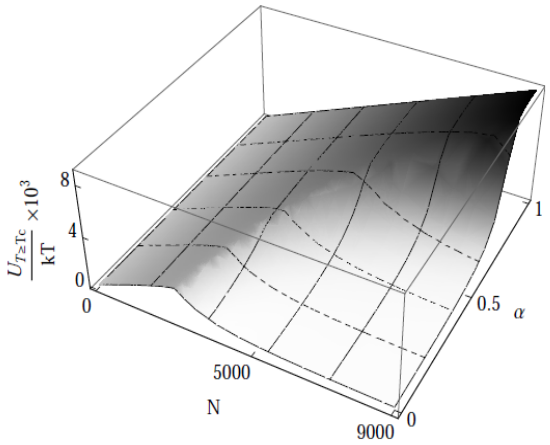

Figure 4.3: Total energy of the system above T_c in unit of kT

the particle number (≈ 0.6 for $N = 5 \times 10^3, \approx 0.8$ for $N = 10^4$).

For very large number of particle and as $\alpha \to 1$, the peak disappears and the total energy of the system results from the non degenerate vibrational mode associated with the relative motion of the center of mass as shown in Fig.(4.4).

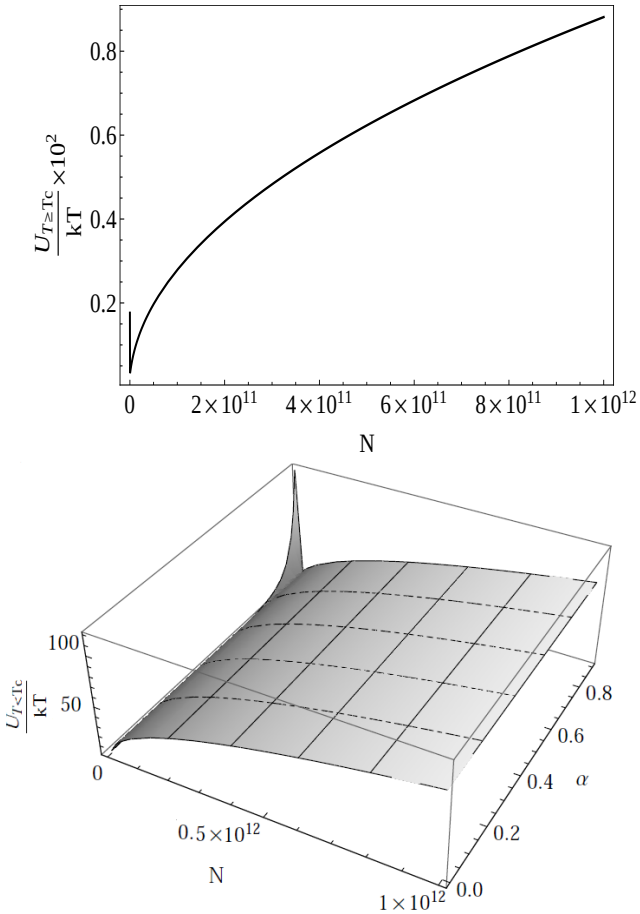

Figure 4.4: Total energy of the system above T_c^{α} in units of kT for very large number of particle, $\alpha = 0.3$

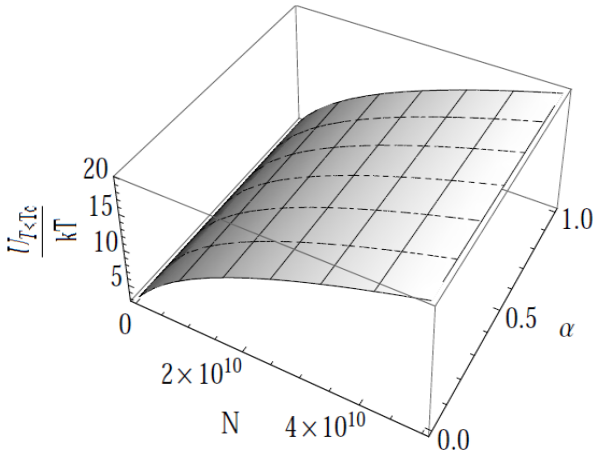

Figure 4.5: Total internal energy of the system below T_c^{α} in units of kT

Below the transition temperature of each subsystem the contribution of each degenerate subsystem becomes negligible due to condensation, and the dominant mode is the oscillator mode associated with the vibrational motion of the position vector connecting the center of mass of each cloud, Fig.(4.5). Now the system behaves as two oscillating clouds of bosons, and the dependence of the total energy on α disappears.

An important physical quantity is the specific heat C_V which can be obtained by differentiating the total energy with respect to temperature.
For $T < T_c^\alpha, \quad T < T_c^\gamma$, using (4.4.51)

$$\begin{aligned} C_{V<} &= \frac{\partial U}{\partial T} \mid_{V,N} \\ &= \frac{(C_{V<})_\alpha}{N_\alpha k} + \frac{(C_{V<})_\gamma}{N_\gamma k} + 3(\beta\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} + \frac{3}{2}k \end{aligned} \tag{4.4.55}$$

where the first and second terms give the contribution of each subsystem to the specific heat of the system. For $T < T_c^\alpha$ and $T < T_c^\gamma$ we have,

$$\begin{aligned} \frac{(C_{V<})_\alpha}{N_\alpha k} &= 12\left(\frac{T}{T_c^\alpha}\right)^3 \frac{\zeta(4)}{\zeta(3)} \qquad T < T_c^\alpha \\ \frac{(C_{V<})_\gamma}{N_\gamma k} &= 12\left(\frac{T}{T_c^\gamma}\right)^3 \frac{\zeta(4)}{\zeta(3)} \qquad T < T_c^\gamma \end{aligned} \tag{4.4.56}$$

Those are typically the specific heats of harmonically trapped bosons below critical temperatures.
At the transition temperature.

$$\left(\frac{(C_{V<})_\alpha}{N_\alpha k}\right)_{T_c^\alpha - 0} = \left(\frac{(C_{V<})_\gamma}{N_\gamma k}\right)_{T_c^\gamma - 0} = 12\frac{\zeta(4)}{\zeta(3)} = 10.805 \qquad for \quad T = T_c^\alpha = T_c^\gamma \tag{4.4.57}$$

Then the total specific heat of the system below the critical temperatures T_c^α, T_c^γ

$$\begin{aligned} C_{v<} &= 12k\left[N_\alpha\left(\frac{T}{T_c^\alpha}\right)^3 + N_\gamma\left(\frac{T}{T_c^\gamma}\right)^3\right]\frac{\zeta(4)}{\zeta(3)} \\ &+ 3(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} + \frac{3}{2}k \end{aligned}$$

For $T > T_c^\alpha, T > T_c^\gamma$ we use the expression for U given in (4.4.50), this gives

$$C_{V>} = \frac{(C_{V>})_\alpha}{Nk} + \frac{(C_{V>})_\gamma}{Nk} + 3(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} + \frac{3}{2}k$$

$$\frac{(C_{V>})_\alpha}{k} = 12\frac{1}{(\beta\hbar\omega_\alpha)^3}g_4(z_\alpha) + 3\frac{1}{(\beta\hbar\omega_\alpha)^3}\frac{\partial z_\alpha}{\partial T}|_{N,v}\frac{\partial g_4(z_\alpha)}{\partial z_\alpha} \quad T > T_c^\alpha$$

To obtain the derivative of the fugacity we use Eq.(4.4.42)

$$3\frac{k}{\beta^2(\hbar\omega_\alpha)^3}g_3(z_\alpha) + \frac{g_2(z_\alpha)}{(\beta\hbar\omega_\alpha)^3}\frac{\partial z_\alpha}{\partial T}|_{N,v} = 0$$

This give

$$\frac{\partial z_\alpha}{\partial T}|_{N,v} = -3k\beta\frac{g_3(z_\alpha)}{g_2(z_\alpha)}$$

Using

$$\frac{\partial g_n(z_\alpha)}{\partial z_\alpha} = \frac{1}{z_\alpha}g_{n-1}(z_\alpha)$$

and Eq.(4.4.42) we have

$$\frac{(C_{V>})_\alpha}{Nk} = 12\frac{g_4(z_\alpha)}{g_3(z_\alpha)} - 9\frac{g_3(z_\alpha)}{g_2(z_\alpha)} \quad T > T_c^\alpha$$

Similarly we obtain for the specific heat of the oscillator mode of frequancy ω_γ

$$\frac{(C_{V>})_\gamma}{Nk} = 12\frac{g_4(z_\gamma)}{g_3(z_\gamma)} - 9\frac{g_3(z_\gamma)}{g_2(z_\gamma)} \quad T > T_c^\gamma \tag{4.4.58}$$

At the critical point

$$\left(\frac{(C_{V>})_\alpha}{N_\alpha k}\right)_{T_c^\alpha+0} = \left(\frac{(C_{V>})_\gamma}{N_\gamma k}\right)_{T_c^\gamma+0} = 12\frac{\zeta(4)}{\zeta(3)} - 9\frac{\zeta(3)}{\zeta(2)} = 4.228 \quad T = T_c^\alpha = T_c^\gamma \tag{4.4.59}$$

Hence, from Eqs.(4.4.57) and (4.4.59), the heat capacity of each subsystem shows a discontinuity at the critical point of each subsystem. The height of the spike is given as

$$\left(\frac{(C_V)_\alpha}{N_\alpha k}\right)_{T_c^\alpha-0} - \left(\frac{(C_V)_\alpha}{N_\alpha k}\right)_{T_c^\alpha+0} = \left(\frac{(C_V)_\gamma}{N_\gamma k}\right)_{T_c^\gamma-0} - \left(\frac{(C_V)_\gamma}{N_\gamma k}\right)_{T_c^\gamma+0} = 6.577 \tag{4.4.60}$$

and the total specific heat of the system above the critical temperatures T_c^α, T_c^γ is

$$\begin{aligned} C_{V>} &= 3k\left[N_\alpha\left(4\frac{g_4(z_\alpha)}{g_3(z_\alpha)} + 3\frac{g_3(z_\alpha)}{g_2(z_\alpha)}\right) + N_\gamma\left(4\frac{g_4(z_\gamma)}{g_3(z_\gamma)} + 3\frac{g_3(z_\gamma)}{g_2(z_\gamma)}\right)\right] \\ &+ 3(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} + \frac{3}{2}k \end{aligned} \tag{4.4.61}$$

The system behaves mainly as two independent subsystems of harmonically trapped bosons. The specific heat of the system has two spikes depending on the critical temperature of each subsystem which shows that the system condenses in two channels.

The free energy of the system is defined by

$$F = \Phi + \mu N$$

Since

$$z_\alpha = e^{\beta(\mu_\alpha - \varepsilon_o^\alpha)}$$

we have

$$\begin{aligned} \mu_\alpha &= kT \ln z_\alpha + \varepsilon_o^\alpha \\ &= kT \ln z_\alpha + \frac{3}{2}\hbar\omega_\alpha \end{aligned}$$

The free energy is therefore

$$F_\alpha = -\frac{1}{(\beta\hbar\omega_\alpha)^3} g_4(z_\alpha) + kT \ln(1 - z_\alpha) + NkT \ln z_\alpha + \frac{3}{2}\hbar\omega_\alpha$$

The second term is negligible in compression with the third term hence

$$F_\alpha = -\frac{1}{(\beta\hbar\omega_\alpha)^3} g_4(z_\alpha) + NkT \ln z_\alpha + \frac{3}{2}\hbar\omega_\alpha$$

Hence the total free energy of the system

$$F = F_\alpha + F_\gamma + \frac{3}{2}kT \left[2\ln(1 - e^{-\beta\hbar\omega}) + \beta\hbar\omega - \ln(\frac{2\pi m}{\beta h^2}) - \frac{2}{3} lnV \right] \quad (4.4.62)$$

where

$$\begin{aligned} F_\alpha &= -\frac{1}{(\beta\hbar\omega_\alpha)^3} g_4(z_\alpha) + kT \ln(1 - z_\alpha) + NkT \ln z_\alpha + \frac{3}{2}\hbar\omega_\alpha \\ F_\gamma &= -\frac{1}{(\beta\hbar\omega_\gamma)^3} g_4(z_\gamma) + kT \ln(1 - z_\gamma) + NkT \ln z_\gamma + \frac{3}{2}\hbar\omega_\gamma \end{aligned}$$

are the free energies of each subsystem.

The free energy versus particle number shows that the system has a well defined minimum at $N \approx 0.7 \times 10^4$. Fig.(4.6[b]) shows that free energy of the system is nearly constant with respect to α, but for $\alpha \approx 0.7$ and $N = 10^4$ free energy falls to zero.

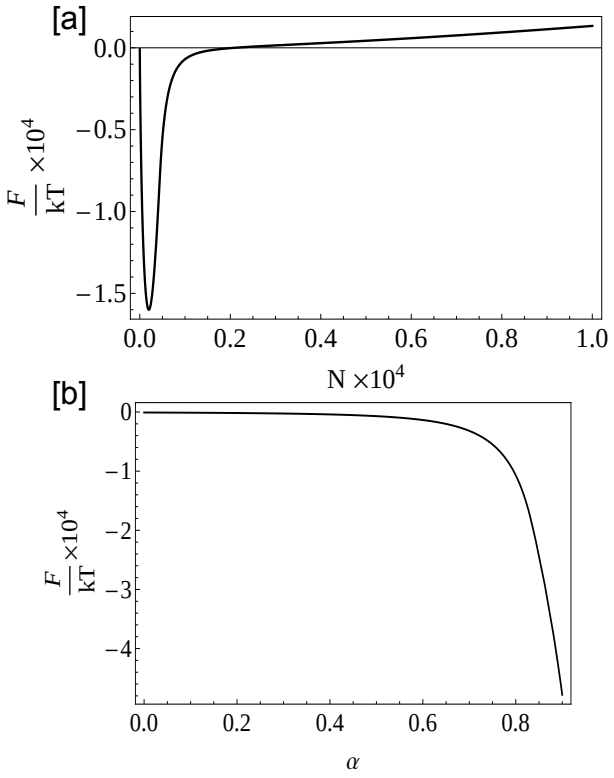

Figure 4.6: Free energy of the system [a] variation of free energy with particle number [b] variation of free energy with α in unit of k, $N = 10^4$.

Chapter 5

Conclusion and future work

In this thesis we have studied a system containing equal numbers of bosons belonging to two different species. The bosons are assumed to move in three dimensions and interact via a two body harmonic oscillator potential.
This model appeared in the work of Le Yaouanc [88] on confinement and chiral symmetry breaking. Another version of the model containing fermion instead of bosons appeared in the work of [89]. We showed that the model is exactly solvable on the classical and quantum levels. We also obtained the grand canonical partition function in the thermodynamic limit and studied its thermodynamic properties. The system is exactly solvable due to the dynamical symmetry of the harmonic oscillator interaction potential.

In Chapter 3, when we assumed that the coupling constant is independent of the particle species, it is found that the interacting system is described by $(N-1)$ translational modes in three dimensions in addition to a three-dimensional harmonic oscillator.
On the classical level these oscillations represent the motion of the position vector connecting the center of masses of the two clouds.

In the thermodynamics limit, the system behaves as a system of free particles above T_c, while below T_c the system behaves as two oscillating clouds of bosons about the position vector connecting their center of mass. Our study shows that the system

under consideration displays a phase transition, in which a macroscopic fraction of particles occupy the ground state of the system below the critical temperature T_c. Below T_c the relation between the entropy of the system and the particle number shows a constant relation, because the contribution of the oscillator mode to the system entropy is negligible. The Gibbs free energy of the system shows a stable minima at $N \approx 2.5 \times 10^5$

In Chapter 4, we considered the case where the coupling strength depends on the particle species. By diagonalizing the Hamiltonian of the system, we found that the system is composed of two degenerate subsystems of quasi-particles, each has $(N-1)$ degree of degeneracy. In addition to two simple eigenmodes; one describing the translational motion of the center of mass and the other the vibrational motion of the position vector connecting the center of mass of each cloud.
It is realized that the system has two transition temperatures T_c^{α} and T_c^{γ}, which depend on the particle number of each subsystem. Each subsystem looks like a set of bosons in external harmonic trap with the same frequency. For a relatively small particle number and above its transition temperature, the system behaves as two subsystems of free oscillators. The total energy above T_c^{α} with particle number display a maximum at certain value of N. By increasing the particle numbers the system behaves as two oscillating clouds of bosons. In other words for large particle numbers, the non degenerate vibrational mode associated with the position vector connecting the center of mass of each cloud is the dominant.
Below the transition temperature the free oscillators no longer contribute to the thermodynamics of the system. The system behaviour is mainly due to the relative vibrational motion of the center of mass of each species. This is an evidence that the system displays BEC below the transition temperature.
In brief, the system behaves as two oscillating clouds of bosons below its transition temperature and for large particle number, whether the coupling strengths are equal or not. On the other hand it behaves as a system of free particles (quasi-particles) for $T > T_c$ and for a relatively small particle number.

In Chapter 4, we did not take into account the fact that the system occupies a finite volume V. Including this effect will change the density of states [90] given in Eq.(4.4.40) by a factor proportional to

$$\frac{\epsilon}{\hbar\Omega}$$

where again, $\Omega = \omega_\alpha$ or ω_β. This will affect the expression for the critical temperature but will not change the behaviour of the system described above.

From a mathematical point of view, we can look at the model as a transformation from a system of bosons trapped in a harmonic oscillator potential to the two species bosons system. This may shed light on some of the properties of the harmonically trapped boson system.
The model can easily be extended to system of two species of fermions or one-species of fermions and one-species of bosons interacting via harmonic oscillator potential. In the fermion-Fermion case we will not have Bose-Einstein condensation due to the pauli exclusion principle.

We can also consider more realistic two-body potentials. But the dynamical symmetries of the harmonic oscillator potential, which is the reason that the system is exactly solvable, will disappear totally or partially, depending on the form of the potential, and the system may or may not be exactly solvable.

Appendix A

A.1 Computation of the characteristic equation for the potential energy matrix

In this appendix we compute the characteristic equation for the potential energy matrices given in Chapter 3 and Chapter 4.

We express the potential energy matrix in the block diagonal form

$$V = \left(\begin{array}{c|c} V_{11} & V_{12} \\ \hline V_{21} & V_{22} \end{array}\right) \tag{A.1.1}$$

where each submatrix is an $(N \times N)$ square matrix.

The characteristic polynomial $D(\lambda)$ for the matrix is defined by:

$$D(\lambda) = \det(V - \lambda I_{2N}) \tag{A.1.2}$$

The characteristic equation is obtained by equating the characteristic polynomial to zero

$$D(\lambda) = 0 \tag{A.1.3}$$

We begin with the computing the characteristic polynomial for the potential energy matrix V_1given in Chapter 3. In this case the submatrices are given by:

$$(V_1)_{11} = (V_1)_{22} = -(V_1)_{12} = -(V_1)_{21} = C \tag{A.1.4}$$

where

$$C = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \tag{A.1.5}$$

Using Eq.(A.1.2) we obtain the explicit form of the characteristic polynomial

$$D(\lambda) = \left|\begin{array}{ccccc:ccccc} 1-\lambda & 1 & \cdots & 1 & 1 & -1 & -1 & \cdots & -1 & -1 \\ 1 & 1-\lambda & \cdots & 1 & 1 & -1 & -1 & \cdots & -1 & -1 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & 1-\lambda & -1 & -1 & \cdots & -1 & -1 \\ \hdashline -1 & -1 & \cdots & -1 & -1 & 1-\lambda & 1 & \cdots & 1 & 1 \\ -1 & -1 & \cdots & -1 & -1 & 1 & 1-\lambda & \cdots & 1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & \cdots & -1 & -1 & 1 & 1 & \cdots & 1 & 1-\lambda \end{array}\right| \tag{A.1.6}$$

We subtract row number N from each of the rows numbered $1, 2 \cdots, N-1$. Similary we subtract row number $2N$ from each of rows numbered $N{+}1, N{+}2 \cdots, 2N{-}1$.

This gives:

$$D(\lambda) = \left|\begin{array}{ccccc:ccccc} -\lambda & 0 & 0 & \cdots & 0 & \lambda & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\lambda & 0 & \cdots & 0 & \lambda & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -\lambda & \lambda & 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 1 & \cdots & 1 & 1-\lambda & -1 & -1 & -1 & \cdots & -1 & -1 \\ \hdashline 0 & 0 & 0 & \cdots & 0 & 0 & -\lambda & 0 & 0 & \cdots & 0 & \lambda \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -\lambda & 0 & \cdots & 0 & \lambda \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & -\lambda & \lambda \\ -1 & -1 & -1 & \cdots & -1 & -1 & 1 & 1 & 1 & \cdots & 1 & 1-\lambda \end{array}\right| \tag{A.1.7}$$

Collecting the common factors, we obtain

$$D(\lambda) = \lambda^{2N-2} M(\lambda) \tag{A.1.8}$$

where

$$M(\lambda) = \left|\begin{array}{cccccc:cccccc} -1 & 0 & 0 & \cdots & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 1 & \cdots & 1 & 1-\lambda & -1 & -1 & -1 & \cdots & -1 & -1 \\ \hdashline 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & -1 & 1 \\ -1 & -1 & -1 & \cdots & -1 & -1 & 1 & 1 & 1 & \cdots & 1 & 1-\lambda \end{array}\right| \tag{A.1.9}$$

Adding the first coulmn to column number N, the second column to column number $N, \cdots$, the $(N-1)^{th}$ column to the column number N, we obtain:

$$M(\lambda) = \left|\begin{array}{cccccc:cccccc} -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 1 & \cdots & 1 & N-\lambda & -1 & -1 & -1 & \cdots & -1 & -1 \\ \hdashline 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & -1 & 1 \\ -1 & -1 & -1 & \cdots & -1 & -N & 1 & 1 & 1 & \cdots & 1 & 1-\lambda \end{array}\right| \tag{A.1.10}$$

Expanding the determinant using the first row we obtain

$$M(\lambda) = (-1)^{N-1} \left| \begin{array}{c|cccccc} N-\lambda & -1 & -1 & -1 & \cdots & -1 & -1 \\ \hline 0 & -1 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & -1 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 1 \\ -N & 1 & 1 & 1 & \cdots & 1 & 1-\lambda \end{array} \right| \tag{A.1.11}$$

On the right hand-side of Eq.(A.1.11) we have a determinant of an $(N+1)\times(N+1)$ matrix. To calculate this determinant we add row number $N+1$ to the first row and collect a common factor of $(-\lambda)$. This gives

$$M(\lambda) = (-1)^{N}\lambda \left| \begin{array}{c|cccccc} 1 & 0 & 0 & 0 & \cdots & 0 & 1 \\ \hline 0 & -1 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & -1 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 1 \\ -N & 1 & 1 & 1 & \cdots & 1 & 1-\lambda \end{array} \right| \tag{A.1.12}$$

Subtracting the first column from coulmn number $(N+1)$ and expanding the determinant using the first row we obtain

$$M(\lambda) = (-1)^{N}\lambda \left| \begin{array}{ccccccc} -1 & 0 & 0 & \cdots & 0 & 1 \\ 0 & -1 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 \\ 1 & 1 & 1 & \cdots & 1 & N+1-\lambda \end{array} \right| \tag{A.1.13}$$

Adding the first column to column number N, the second column to number N we

obtain

$$M(\lambda) = (-1)^N\lambda \begin{vmatrix} -1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 \\ 1 & 1 & 1 & \cdots & 1 & 2N-\lambda \end{vmatrix} \tag{A.1.14}$$

We have reduced the determinant to a lower trianglar form. Therefore its value is equal to the product of the elements on the main diagonal

$$M(\lambda) = (-1)^{2N-1}\lambda(2N-\lambda) \tag{A.1.15}$$

Substituting Eq.(A.1.8) into Eq.(A.1.15), we obtain

$$D(\lambda) = \lambda^{2N-1}(2N-\lambda) \tag{A.1.16}$$

The characteristic equation for the potential energy matrix is therefore,

$$\lambda^{2N-1}(2N-\lambda) = 0 \tag{A.1.17}$$

We next consider the potential energy matrix V_2 given in chapter 4.
In this case, the submatrices

$$(V_2)_{ij} \qquad\qquad i,j = 1,2$$

have the form

$$\begin{aligned} (V_2)_{11} &= N(1-\alpha)I_N + \alpha C \\ (V_2)_{12} &= (V_2)_{21} = -C \\ (V_2)_{22} &= N(1-\gamma)I_N + \gamma C \end{aligned} \tag{A.1.18}$$

Using Eq.(A.1.13) we obtain the explicit form of the characteristic polynomial:

$$D(\lambda) = \left|\begin{array}{ccccc:ccccc} \alpha-\lambda_\alpha & \alpha & \cdots & \alpha & \alpha & -1 & -1 & \cdots & -1 & -1 \\ \alpha & \alpha-\lambda_\alpha & \cdots & \alpha & \alpha & -1 & -1 & \cdots & -1 & -1 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \alpha & \alpha & \cdots & \alpha-\lambda_\alpha & \alpha & -1 & -1 & \cdots & -1 & -1 \\ \alpha & \alpha & \cdots & \alpha & \alpha-\lambda_\alpha & -1 & -1 & \cdots & -1 & -1 \\ \hdashline -1 & -1 & \cdots & -1 & -1 & \gamma-\lambda_\gamma & \gamma & \cdots & \gamma & \gamma \\ -1 & -1 & \cdots & -1 & -1 & \gamma & \gamma-\lambda_\gamma & \cdots & \gamma & \gamma \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & \cdots & -1 & -1 & \gamma & \gamma & \cdots & \gamma-\lambda_\gamma & \gamma \\ -1 & -1 & \cdots & -1 & -1 & \gamma & \gamma & \cdots & \gamma & \gamma-\lambda_\gamma \end{array}\right| \tag{A.1.19}$$

where

$$\begin{aligned} \lambda_\alpha &= \lambda - N(1-\alpha) \\ \lambda_\gamma &= \lambda - N(1-\gamma) \end{aligned} \tag{A.1.20}$$

We proceed as before. We subtract row number N from each of the row numbered $1, 2, \cdots, N-1$. Similarly row number $2N$ from each of the rows numbered $N+1, N+2, \cdots, 2N-1$. This gives

$$D(\lambda) = \left|\begin{array}{ccccc:ccccc} -\lambda_\alpha & 0 & \cdots & 0 & \lambda_\alpha & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\lambda_\alpha & \cdots & 0 & \lambda_\alpha & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -\lambda_\alpha & \lambda_\alpha & 0 & 0 & \cdots & 0 & 0 \\ \alpha & \alpha & \cdots & \alpha & \alpha-\lambda_\alpha & -1 & -1 & \cdots & -1 & -1 \\ \hdashline 0 & 0 & \cdots & 0 & 0 & -\lambda_\gamma & 0 & \cdots & 0 & \lambda_\gamma \\ 0 & 0 & \cdots & 0 & 0 & 0 & -\lambda_\gamma & \cdots & 0 & \lambda_\gamma \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & -\lambda_\gamma & \lambda_\gamma \\ -1 & -1 & \cdots & -1 & -1 & \gamma & \gamma & \cdots & \gamma & \gamma-\lambda_\gamma \end{array}\right| \tag{A.1.21}$$

Collecting the common factors, we obtain

$$D(\lambda) = \lambda_\alpha^{N-1}\lambda_\gamma^{N-1}M(\lambda_\alpha,\lambda_\gamma) \tag{A.1.22}$$

where

$$M(\lambda_\alpha,\lambda_\gamma) = \left|\begin{array}{ccccc:ccccc} -1 & 0 & \cdots & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & -1 & \cdots & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & 1 & 0 & 0 & \cdots & 0 & 0 \\ \alpha & \alpha & \cdots & \alpha & \alpha-\lambda_\alpha & -1 & -1 & \cdots & -1 & -1 \\ \hdashline 0 & 0 & \cdots & 0 & 0 & -1 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 0 & 0 & -1 & \cdots & 0 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & -1 & 1 \\ -1 & -1 & \cdots & -1 & -1 & \gamma & \gamma & \cdots & \gamma & \gamma-\lambda_\gamma \end{array}\right| \tag{A.1.23}$$

Comparing the determinant in Eq.(A.1.23) with the determinant in Eq.(A.1.10) we see that, by expanding the determinant using the first row, we obtain

$$M(\lambda_\alpha,\lambda_\gamma) = (-1)^{N-1}\left|\begin{array}{c:cccccc} N-\lambda_\alpha & -1 & -1 & -1 & \cdots & -1 & -1 \\ \hdashline 0 & -1 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & -1 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 1 \\ -N & \gamma & \gamma & \gamma & \cdots & \gamma & \gamma-\lambda_\gamma \end{array}\right| \tag{A.1.24}$$

where we have used Eq.(A.1.20).

We add column number 2 to the column number $N+1$, column number 3 to the column number $N+1$,$\cdots$, column number N to the column number $N+1$, we

obtain after using Eq.(A.1.20):

$$M(\lambda_\alpha,\lambda_\gamma) = (-1)^{N-1}\left|\begin{array}{c|cccccc} N-\lambda_\alpha & -1 & -1 & -1 & \cdots & -1 & -N \\ \hline 0 & -1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 0 \\ -N & \gamma & \gamma & \gamma & \cdots & \gamma & N-\lambda_\gamma \end{array}\right| \tag{A.1.25}$$

We next subtract row number 2 from row number 1, row number 3 from row number 1,$\cdots$, row number N from row number 1, we obtain

$$M(\lambda_\alpha,\lambda_\gamma) = (-1)^{N-1}\left|\begin{array}{c|cccccc} N-\lambda & 0 & 0 & 0 & \cdots & 0 & -N \\ \hline 0 & -1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 0 \\ -N & \gamma & \gamma & \gamma & \cdots & \gamma & N-\lambda \end{array}\right| \tag{A.1.26}$$

Rearranging the determinant

$$M(\lambda_\alpha,\lambda_\gamma) = (-1)^{N-1}(-1)^{N+N-1}\left|\begin{array}{ccccc|cc} -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 & 0 \\ \hline 0 & 0 & 0 & \cdots & 0 & -N & N-\lambda \\ \gamma & \gamma & \gamma & \cdots & \gamma & N-\lambda & -N \end{array}\right| \tag{A.1.27}$$

Expanding the determinant, we get

$$\begin{aligned} M(\lambda_\alpha,\lambda_\gamma) &= -(-1)^{N-1}(-1)^{N-1}\left|\begin{array}{cc} -N & N-\lambda \\ N-\lambda & -N \end{array}\right| \\ &= \lambda(\lambda-2N) \end{aligned} \tag{A.1.28}$$

Substituting Eq.(A.1.28) into Eq.(A.1.22) we obtain the characteristic polynomial

$$D(\lambda) = \lambda(\lambda-2N)[\lambda-N(1-\alpha)]^{N-1}[\lambda-N(1-\gamma)]^{N-1} \tag{A.1.29}$$

The characteristic equation is therefore,

$$\lambda(\lambda - 2N)[\lambda - N(1-\alpha)]^{N-1}[\lambda - N(1-\gamma)]^{N-1} = 0 \tag{A.1.30}$$

Appendix B

Diagonalization of the potential energy matrix

In this appendix we diagonalize the potential energy matrices given in Chapter 3 and Chapter 4.

B.1 Diagonalization of the potential energy matrix V_1

The potential energy matrix V_1 introduced in Chapter 3 is given by:

$$V_1 = \left(\begin{array}{c|c} (V_1)_{11} & (V_1)_{12} \\ \hline (V_1)_{21} & (V_1)_{22} \end{array}\right) \tag{B.1.1}$$

where,

$$(V_1)_{11} = (V_1)_{22} = -(V_1)_{12} = -(V_1)_{21} = C \tag{B.1.2}$$

The matrix C is an $(N \times N)$ matrix

$$C = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix}$$

whose elements are the (3×3) unit matrix

$$I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

We have shown in Appendix A that the characteristic equation for the matrix V_1 is

$$\lambda^{2N} - 2N\lambda^{2N-1} = 0 \tag{B.1.3}$$

Eq.(B.1.3) has two real roots

$$\lambda = 2N \qquad and \qquad \lambda = 0 \tag{B.1.4}$$

If we consider our vector space to be the configuration space of the system, then $\lambda = 2N$ is a simple eigenvalue while $\lambda = 0$ is a $2N-1$ degenerate eigenvalue. On the other hand if we take our vector space to be R^{3N} then the $\lambda = 2N$ is 3-fold degenerate eigenvalue while $\lambda = 0$ is $3(2N-1)$ degenerate eigenvalue. To simplify the calculations we choose the first vector space.

Let

$$\vec{u} = \left(\begin{array}{c} \vec{x} \\ \hline \vec{y} \end{array}\right) \tag{B.1.5}$$

where

$$\vec{x} = \begin{pmatrix} \vec{x}_1 \\ \vec{x}_2 \\ \vdots \\ \vec{x}_N \end{pmatrix} \qquad and \qquad \vec{y} = \begin{pmatrix} \vec{y}_1 \\ \vec{y}_2 \\ \vdots \\ \vec{y}_N \end{pmatrix} \tag{B.1.6}$$

be an eigenvector of V_1. Then

$$V_1\vec{u} = \lambda\vec{u} \tag{B.1.7}$$

The matrix form of this equation is

$$\left(\begin{array}{c:c} C & -C \\ \hdashline -C & C \end{array}\right) \left(\begin{array}{c} \vec{x} \\ \hline \vec{y} \end{array}\right) = \lambda \left(\begin{array}{c} \vec{x} \\ \hline \vec{y} \end{array}\right) \tag{B.1.8}$$

Expanding we obtain the two equations

$$\begin{aligned} C\vec{x} - C\vec{y} &= \lambda\vec{x} \\ -C\vec{x} + C\vec{y} &= \lambda\vec{y} \end{aligned} \tag{B.1.9}$$

Now

$$C\vec{x} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \begin{pmatrix} \vec{x}_1 \\ \vec{x}_2 \\ \vdots \\ \vec{x}_N \end{pmatrix} = (\sum_{k=1}^{N} x_k) \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \tag{B.1.10}$$

Using Eq.(B.1.10) we can rewrite Eqs.(B.1.9) in the system form

$$\begin{aligned} \sum_{k=1}^{N} x_k - \sum_{k=1}^{N} y_k &= \lambda x_i \qquad i = 1, 2, \cdots, N \\ \sum_{k=1}^{N} x_k - \sum_{k=1}^{N} y_k &= -\lambda y_i \qquad i = 1, 2, \cdots, N \end{aligned} \tag{B.1.11}$$

Consider the eigenvalue

$$\lambda = 0$$

The system of Eq.(B.1.11) reduces to

$$\sum_{k=1}^{N} (x_k - y_k) = 0 \tag{B.1.12}$$

Since the eigenvectors of a real symmetric matrix are linearly independent, we can choose the $2N-1$ eigenvectors belonging to the eigenvalue $\lambda = 0$ to be orthogonal. We choose the first vector as follows:

$$\begin{aligned} x_2 &= x_3 = \cdots = x_N = 0 \\ y_2 &= y_3 = \cdots = y_N = 0 \end{aligned}$$

Then Eq.(B.1.12) gives

$$x_1 = y_1$$

Hence

$$\vec{u}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \hline 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{B.1.13}$$

In the same manner we choose:

$$\vec{u}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ \hline 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad \vec{u}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ \hline 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \cdots, u_N = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \hline 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \tag{B.1.14}$$

Next let

$$\vec{w} = \begin{pmatrix} x_1 \\ \vdots \\ \hline x_N \\ y_1 \\ \vdots \\ y_N \end{pmatrix}$$

be another eigenvector belonging to $\lambda = 0$ and orthogonal to

$$\vec{u}_1, \vec{u}_2, \cdots, \vec{u}_N$$

Then in addition to Eq.(B.1.12), the components of $\vec{w}$ should satisfy:

$$x_1 + y_1 = 0 \qquad x_2 + y_2 = 0 \quad \cdots \quad x_N + y_N = 0$$

Thus

$$y_1 = -x_1 \qquad y_2 = -x_2 \quad \cdots \quad y_N = -x_N \tag{B.1.15}$$

Substituting Eq.(B.1.15) into Eq.(B.1.12) we obtain

$$\sum_{i=1}^{N} x_i = 0 \tag{B.1.16}$$

So that

$$\vec{w} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ \hline x_N \\ -x_1 \\ -x_2 \\ \vdots \\ -x_N \end{pmatrix}$$

where $x_1, x_2, \cdots, x_N$ satisfy Eq.(B.1.16).

We choose

$$x_1 \neq 0 \quad x_2 \neq 0 \quad and \quad x_3 = x_4 = \cdots = x_N = 0 \tag{B.1.17}$$

then Eq.(B.1.16) gives

$$x_2 = -x_1$$

and we obtain the eigenvector

$$\vec{u}_{N+1} = \frac{1}{\sqrt{4}} \begin{pmatrix} 1 \\ -1 \\ 0 \\ \vdots \\ 0 \\ \hline -1 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{B.1.18}$$

We choose the eigenvector $\vec{w}_1$ to be orthogonal to $\vec{u}_{N+1}$. This imposes the condition

$$x_1 - x_2 + x_1 - x_2 = 0$$

Or

$$x_2 = x_1$$

Hence

$$\vec{w}_1 = \begin{pmatrix} x_1 \\ x_1 \\ x_2 \\ \vdots \\ x_N \\ \hline -x_1 \\ -x_1 \\ -x_2 \\ \vdots \\ -x_N \end{pmatrix}$$

The component of $\vec{w}_1$ should satisfy (B.1.12) so that

$$2x_1 + 2x_3 + x_4 + \cdots + x_N = 0$$

we choose

$$x_1 \neq 0 \quad x_3 \neq 0 \quad and \quad x_4 = x_5 = \cdots = x_N = 0$$

Then

$$x_3 = -x_1$$

and we obtain the eigenvector

$$\vec{u}_{N+2} = \frac{1}{\sqrt{12}} \begin{pmatrix} 1 \\ 1 \\ -2 \\ 0 \\ \vdots \\ 0 \\ \hline -1 \\ -1 \\ 2 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{B.1.19}$$

Next we choose the eigenvector $\vec{w}_2$ to be orthogonal to $\vec{u}_{N+2}$. This gives:

$$2x_1 - 2x_3 + 2x_1 - 2x_3 = 0$$

Or

$$x_3 = x_1$$

Hence

$$\vec{w}_2 = \begin{pmatrix} x_1 \\ x_1 \\ x_1 \\ x_4 \\ x_5 \\ \vdots \\ \hline x_N \\ -x_1 \\ -x_1 \\ -x_1 \\ -x_4 \\ -x_5 \\ \vdots \\ -x_N \end{pmatrix}$$

Substituting the component of $\vec{w}_2$ into Eq.(B.1.12), we get

$$3x_1 + x_4 + x_5 + \cdots + x_N = 0$$

We choose

$$x_1 \neq 0 \qquad x_4 \neq 0 \qquad x_5 = x_6 = \cdots = x_N = 0$$

This gives

$$x_4 = -3x_1$$

and we obtain the eigenvector

$$\vec{u}_{N+3} = \frac{1}{\sqrt{24}} \begin{pmatrix} 1 \\ 1 \\ 1 \\ -3 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \hline -1 \\ -1 \\ -1 \\ 3 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{B.1.20}$$

Continuing this process we obtain:

$$\vec{u}_{N+k} = \frac{1}{\sqrt{2k(k+1)}} \begin{pmatrix} \left.\begin{matrix} 1 \\ 1 \\ \vdots \\ 1 \end{matrix}\right\} k \\ -k \\ 0 \\ \vdots \\ 0 \\ \hline \left.\begin{matrix} -1 \\ -1 \\ \vdots \\ -1 \end{matrix}\right\} k \\ k \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad k = 1, 2, \cdots N-1 \tag{B.1.21}$$

Next we consider the eigenvalue $\lambda = 2N$. The system (B.1.11) takes the form

$$\sum_{i=1}^{N}(x_i - y_i) = 2Nx_k \qquad k = 1, 2 \cdots N \tag{B.1.22}$$

$$\sum_{i=1}^{N}(x_i - y_i) = -2Ny_k \qquad k = 1, 2 \cdots N \tag{B.1.23}$$

Adding k^{th} equation in (B.1.22) to the k^{th} equation in (B.1.23)

$$2N(x_k - y_k) = 0$$

or

$$y_k = -x_k \qquad k = 1, 2 \cdots N \tag{B.1.24}$$

Inserting Eq.(B.1.24) into Eq.(B.1.23) we get

$$\sum_{i=1}^{N} x_i = N x_k,$$

so that

$$x_k = \frac{1}{N} \sum_{i=1}^{N} x_i \qquad k = 1, 2 \cdots N \tag{B.1.25}$$

Usin Eq.(B.1.24) we get

$$y_1 = y_2 = \cdots = y_N = -x_1 = -x_2 = \cdots = -x_N \tag{B.1.26}$$

Hence

$$\vec{u} = x_1 \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ \hline -1 \\ -1 \\ \vdots \\ -1 \end{pmatrix}$$

We choose x_1 so that $\vec{u}$ is a unit vector. Then

$$x_1 = \frac{1}{\sqrt{2N}}$$

We obtain the eigenvector

$$\vec{u}_{2N} = \frac{1}{\sqrt{2N}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ \hline -1 \\ -1 \\ \vdots \\ -1 \end{pmatrix} \tag{B.1.27}$$

Since eigenvector of a symmetric matrix belonging to different eigenvectors are orthogonal. The eigenvector $\vec{u}_{2N}$ is orthogonal to the eigenvectors

$$\vec{u}_1, \vec{u}_2, \cdots \vec{u}_{2N}$$

The diagonalizing matrix O_1 is obtained by grouping the orthonormal eigenvectors together in the matrix

$$O_1 \;=\; \left(\vec{u}_1 \;\vdots\; \vec{u}_2 \;\vdots\; \cdots \;\vdots\; \vec{u}_{2N-1} \;\vdots\; \vec{u}_{2N} \right)$$

O_1 is an orthogonal matrix since the vectors $\vec{u}_i$ $i = 1, \cdots, N$ are orthonormal

$$\vec{u}_i . \vec{u}_j = \delta_{ij}$$

Substituting for

$$\vec{u}_1, \vec{u}_2, \cdots \vec{u}_{2N}$$

we obtain the explicit form of the matrix O_1

$$O_1 = \left(\begin{array}{ccccccc:ccccc}
\frac{1}{\sqrt{2}} & 0 & 0 & 0 & \cdots & 0 & 0 & \frac{1}{\sqrt{4}} & \frac{1}{\sqrt{12}} & \cdots & \frac{1}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}} \\
0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{\sqrt{4}} & \frac{1}{\sqrt{12}} & \cdots & \frac{1}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}} \\
0 & 0 & \frac{1}{\sqrt{2}} & 0 & \cdots & 0 & 0 & 0 & -\frac{2}{\sqrt{12}} & \cdots & \frac{1}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \cdots & \frac{1}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}} \\
0 & 0 & 0 & 0 & \cdots & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & -\frac{(N-1)}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}} \\
\hdashline
\frac{1}{\sqrt{2}} & 0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{\sqrt{4}} & -\frac{1}{\sqrt{12}} & \cdots & -\frac{1}{\sqrt{2N(N-1)}} & -\frac{1}{\sqrt{2N}} \\
0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 & 0 & \frac{1}{\sqrt{4}} & -\frac{1}{\sqrt{12}} & \cdots & -\frac{1}{\sqrt{2N(N-1)}} & -\frac{1}{\sqrt{2N}} \\
0 & 0 & \frac{1}{\sqrt{2}} & 0 & \cdots & 0 & 0 & 0 & \frac{2}{\sqrt{12}} & \cdots & -\frac{1}{\sqrt{2N(N-1)}} & -\frac{1}{\sqrt{2N}} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{2N(N-1)}} & -\frac{1}{\sqrt{2N}} \\
0 & 0 & 0 & 0 & \cdots & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & -\frac{(N-1)}{\sqrt{2N(N-1)}} & -\frac{1}{\sqrt{2N}}
\end{array}\right) \tag{B.1.28}$$

We define the $(N \times N)$ matrix T by

$$T = \left(\begin{array}{ccccc}
\frac{1}{\sqrt{4}} & \frac{1}{\sqrt{12}} & \cdots & \frac{1}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}} \\
-\frac{1}{\sqrt{4}} & \frac{1}{\sqrt{12}} & \cdots & \frac{1}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}} \\
0 & -\frac{2}{\sqrt{12}} & \cdots & \frac{1}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & \frac{1}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}} \\
0 & 0 & \cdots & -\frac{(N-1)}{\sqrt{2N(N-1)}} & \frac{1}{\sqrt{2N}}
\end{array}\right) \tag{B.1.29}$$

Eq.(B.1.29) shows that the $T_{ij}-$ element is given by:

$$T_{ij} = \frac{1}{\sqrt{2j(j+1-j\delta_{jN})}} \begin{cases} 1 & i \leq j \\ -j(1-\delta_{jN}) & i = j+1 \\ 0 & i > j+1 \end{cases} \tag{B.1.30}$$

The transformation matrix can be expressed in the block form:

$$O_1 \;=\; \left(\begin{array}{c:c} \frac{1}{\sqrt{2}} I_N & T \\ \hdashline \frac{1}{\sqrt{2}} I_N & -T \end{array}\right) \tag{B.1.31}$$

where I_N is the $(N \times N)$ unit matrix.

We can easily see that

$$T^2 \;=\; \frac{1}{2} I_N \tag{B.1.32}$$

The orthogonality of the matrix O_1 can also be checked directly using Eq.(B.1.31)

$$O_1 O_1^T = \left(\begin{array}{c|c} \frac{1}{\sqrt{2}} I_N & T \\ \hline \frac{1}{\sqrt{2}} I_N & -T \end{array}\right) \left(\begin{array}{c|c} \frac{1}{\sqrt{2}} I_N & \frac{1}{\sqrt{2}} I_N \\ \hline T & -T \end{array}\right) = \left(\begin{array}{c|c} I_N & 0 \\ \hline 0 & I_N \end{array}\right) = I_{2N} \tag{B.1.33}$$

The new coordinates vectors

$$\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{2N}$$

are related to the old coordinate vectors

$$\vec{r}_1^{\,A}, \cdots, \vec{r}_N^{\,A}, \vec{r}_1^{\,B}, \cdots, \vec{r}_N^{\,B}$$

by

$$\begin{pmatrix} \vec{r}_1 \\ \vec{r}_2 \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} = O_1^T \begin{pmatrix} \vec{r}_1^{\,A} \\ \vdots \\ \vec{r}_N^{\,A} \\ \vec{r}_1^{\,B} \\ \vdots \\ \vec{r}_N^{\,B} \end{pmatrix} \tag{B.1.34}$$

Substituting for O_1 we obtain

$$\left(\begin{array}{c} \vec{r}_1 \\ \vdots \\ \vec{r}_N \\ \hline \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{array}\right) = \left(\begin{array}{c|c} \frac{1}{\sqrt{2}} I_N & \frac{1}{\sqrt{2}} I_N \\ \hline T^T & -T^T \end{array}\right) \left(\begin{array}{c} \vec{r}_1^{\,A} \\ \vdots \\ \vec{r}_N^{\,A} \\ \hline \vec{r}_1^{\,B} \\ \vdots \\ \vec{r}_N^{\,B} \end{array}\right) \tag{B.1.35}$$

Expanding this product we obtain

$$\begin{pmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_N \end{pmatrix} = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} \vec{r}_1^{\,A} \\ \vdots \\ \vec{r}_N^{\,A} \end{pmatrix} + \begin{pmatrix} \vec{r}_1^{\,B} \\ \vdots \\ \vec{r}_N^{\,B} \end{pmatrix} \right] \tag{B.1.36}$$

$$\begin{pmatrix} \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} = T^T \left[\begin{pmatrix} \vec{r}_1^A \\ \vdots \\ \vec{r}_N^A \end{pmatrix} - \begin{pmatrix} \vec{r}_1^B \\ \vdots \\ \vec{r}_N^B \end{pmatrix} \right] \tag{B.1.37}$$

Now

$$\begin{aligned} (T^T \vec{r}^A)_k &= \sum_{j=1}^{N} (T^T)_{kj} \vec{r}_j^A \\ &= \sum_{j=1}^{N} T_{jk} \vec{r}_j^A \\ &= \sum_{j=1}^{k} T_{jk} \vec{r}_j^A + T_{k+1,k} \vec{r}_{k+1}^A + \sum_{j=k+2}^{N} T_{j,k} \vec{r}_{k+1}^A \end{aligned}$$

Using Eq.(B.1.32) we obtain for

$$(T^T \vec{r}^A)_k = \frac{1}{\sqrt{2k(k+1-k\delta_{kN})}} \left(\sum_{j=1}^{k} \vec{r}_j^A - k(1-\delta_{kN}) \vec{r}_k^A \right) \tag{B.1.38}$$

Hence

$$\begin{aligned} \vec{r}_k &= \frac{1}{\sqrt{2}} (\vec{r}_k^A + \vec{r}_k^B) \\ \vec{r}_{N+k} &= \frac{1}{\sqrt{2k(k+1-k\delta_{kN})}} \left[\sum_{j=1}^{k} (\vec{r}_j^A - \vec{r}_j^B) - k(1-\delta_{kN})(\vec{r}_{k+1}^A + \vec{r}_{k+1}^B) \right] \end{aligned} \tag{B.1.39}$$

The inverse transformation is given by:

$$\begin{pmatrix} \vec{r}^A \\ \hline \vec{r}^B \end{pmatrix} = O_1 \begin{pmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_N \\ \hline \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} \tag{B.1.40}$$

Substituting for O_1 we obtain

$$\begin{pmatrix} \vec{r}_1^A \\ \vdots \\ \vec{r}_N^A \end{pmatrix} = \frac{1}{\sqrt{N}} \begin{pmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_N \end{pmatrix} + T \begin{pmatrix} \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} \tag{B.1.41}$$

$$\begin{pmatrix} \vec{r}_1^B \\ \vdots \\ \vec{r}_N^B \end{pmatrix} = \frac{1}{\sqrt{N}} \begin{pmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_N \end{pmatrix} - T \begin{pmatrix} \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} \tag{B.1.42}$$

Thus

$$\begin{aligned} (T^T \begin{pmatrix} \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix})_k &= \sum_{j=1}^{N} T_{kj} \vec{r}_{N+j} \\ &= \sum_{j=1}^{k-2} T_{kj} \vec{r}_{N+j} + T_{k,k-1} \vec{r}_{N+k-1} + \sum_{j=k}^{N} T_{kj} \vec{r}_{N+j} \\ &= \frac{-(k-1)}{\sqrt{2k(k-1)}} \vec{r}_{N+k-1} + \sum_{j=k}^{N} \frac{1}{\sqrt{2j(j+1-j\delta_{jN})}} \vec{r}_{N+j} \end{aligned} \tag{B.1.43}$$

Hence

$$\begin{aligned} \vec{r}_k^A &= \frac{1}{\sqrt{N}} \vec{r}_k - \frac{(k-1)}{\sqrt{2k(k-1)}} \vec{r}_{N+k-1} + \sum_{j=k}^{N} \frac{1}{\sqrt{2j(j+1+j\delta_{jN})}} \vec{r}_{N+j} \\ \vec{r}_k^B &= \frac{1}{\sqrt{N}} \vec{r}_k + \frac{(k-1)}{\sqrt{2k(k-1)}} \vec{r}_{N+k-1} - \sum_{j=k}^{N} \frac{1}{\sqrt{2j(j+1+j\delta_{jN})}} \vec{r}_{N+j}, \quad k = 1, \cdots N \end{aligned} \tag{B.1.44}$$

B.2 Diagonalization of the potential energy matrix V_2

The potential energy matrix V_2 given in chapter 4 has the block form

$$V_2 = \left(\begin{array}{c:c} (V_2)_{11} & (V_2)_{12} \\ \hdashline (V_2)_{21} & (V_2)_{22} \end{array}\right) \tag{B.2.1}$$

$$\begin{aligned} (V_2)_{11} &= N(1-\alpha) I_N + \alpha C \\ (V_2)_{12} &= (V_2)_{21} = -C \\ (V_2)_{22} &= N(1-\gamma) I_N + \gamma C \end{aligned} \tag{B.2.2}$$

According to Eq.(A.1.30) the characteristic equation for the matrix V_2 is given by:

$$\lambda(\lambda - 2N)[\lambda - N(1-\alpha)]^{N-1}[\lambda - N(1-\gamma)]^{N-1} = 0 \tag{B.2.3}$$

We have two simple eigenvalues

$$\lambda = 0 \qquad and \qquad \lambda = 2N \tag{B.2.4}$$

and two eigenvalues

$$\lambda = N(1-\alpha) \qquad and \qquad \lambda = N(1-\gamma) \tag{B.2.5}$$

of multiplicity $(N-1)$.

The eigenvalue equation now takes the form

$$\left(\begin{array}{c:c} N(1-\alpha)I_N + \alpha C & -C \\ \hdashline -C & N(1-\gamma)I_N + \gamma C \end{array}\right) \left(\begin{array}{c} \vec{x} \\ \vec{y} \end{array}\right) = \lambda \left(\begin{array}{c} \vec{x} \\ \vec{y} \end{array}\right) \tag{B.2.6}$$

Carrying out the matrix multiplication we get

$$\begin{aligned} [N(1-\alpha) - \lambda]\vec{x} + \alpha C\vec{x} - C\vec{y} &= 0 \\ -C\vec{x} + [N(1-\gamma) - \lambda]\vec{y} + \gamma C\vec{y} &= 0 \end{aligned} \tag{B.2.7}$$

Using Eq.(B.1.10) the above system can be written as

$$\begin{aligned} [N(1-\alpha) - \lambda]x_i + \alpha \sum_{k=1}^{N} x_k - \sum_{k=1}^{N} y_k &= 0 \\ -\sum_{k=1}^{N} x_k + [N(1-\gamma) - \lambda]y_i + \gamma \sum_{k=1}^{N} y_k &= 0 \end{aligned} \tag{B.2.8}$$

We first consider the eigenvalue

$$\lambda = N(1-\alpha) \tag{B.2.9}$$

Inserting this back into the system (B.2.8), we get

$$\alpha \sum_{k=1}^{N} x_k - \sum_{k=1}^{N} y_k = 0 \tag{B.2.10}$$

$$-\sum_{k=1}^{N} x_k + N(\alpha - \gamma)y_i + \gamma \sum_{k=1}^{N} y_k = 0 \tag{B.2.11}$$

Multiplying Eq.(B.2.11) by α and adding the result to (B.2.10)

$$N\alpha(\alpha-\gamma)y_i \;=\; (1-\alpha\gamma)\sum_{k=1}^{N} y_k \qquad i=1,2,\cdots,N \tag{B.2.12}$$

summing from i from 1 to N we obtain,

$$(1-\alpha^2)\sum_{k=1}^{N} y_k \;=\; 0 \tag{B.2.13}$$

If

$$1-\alpha^2 \;\neq\; 0 \qquad i.e \quad \alpha \neq \pm 1 \tag{B.2.14}$$

then

$$\sum_{k=1}^{N} y_k \;=\; 0 \tag{B.2.15}$$

Substituting the equation back into Eqs.(B.2.10) and (B.2.11) we obtain

$$\sum_{k=1}^{N} x_k \;=\; 0 \tag{B.2.16}$$

$$-\sum_{k=1}^{N} x_k + N(\alpha-\gamma)y_i \;=\; 0 \qquad i=1,2,\cdots,N \tag{B.2.17}$$

The last equation reduces to

$$(\alpha-\gamma)y_i \;=\; 0 \qquad i=1,2,\cdots,N \tag{B.2.18}$$

If

$$\alpha \;\neq\; \gamma \tag{B.2.19}$$

then

$$y_i \;=\; 0 \qquad i=1,2,\cdots,N \tag{B.2.20}$$

Thus an eigenvectors belonging to the eigenvalue

$$\lambda = N(1-\alpha)$$

where $\alpha \neq 1$ and $\alpha \neq \gamma$ has the form

$$\vec{u}_1 = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{B.2.21}$$

where

$$x_1, x_2, \cdots, x_N$$

satisfy Eq.(B.2.16)

We construct $(N-1)$ orthogonal eigenvectors following the same procedure used above. We first choose

$$x_3 = x_4 = \cdots = x_N = 0$$

Then Eq.(B.2.10) gives

$$x_1 + x_2 = 0$$

and we obtain the eigenvectors belonging to $\lambda = N(1-\alpha)$ namely

$$\vec{u}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{B.2.22}$$

The eigenvectors $\vec{u}_2$ is orthogonal to $\vec{u}_1$ and therefore satisfy

$$x_1 - x_2 = 0 \Rightarrow x_1 = x_2$$

The condition given in Eq.(B.2.16) now reads

$$2x_1 + x_3 + x_4 + \cdots + x_N = 0$$

we choose

$$x_4 = x_5 = \cdots = x_N = 0$$

This gives

$$x_3 = -2x_1$$

Thus $\vec{u}_2$ has the form

$$\vec{u}_2 = \begin{pmatrix} x_1 \\ x_1 \\ -2x_1 \\ 0 \\ \vdots \\ 0 \\ \hline 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

We choose x_1 so that $\vec{u}_2$ is a unit vector

$$\vec{u}_2 = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 1 \\ -2 \\ 0 \\ \vdots \\ 0 \\ \hline 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{B.2.23}$$

Continuing this process we obtain the $(N-1)$ eigenvectors belonging to eigenvalue

$$\lambda = N(1-\alpha)$$

given by

$$\vec{u}_k = \frac{1}{\sqrt{k(k+1)}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ -k \\ 0 \\ \vdots \\ 0 \\ \hline 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \begin{matrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{matrix} \left.\begin{matrix} \\ \\ \\ \\ \end{matrix}\right\}\text{k} \qquad k = 1, 2, \cdots, N-1 \tag{B.2.24}$$

We next consider the eigenvalue

$$\lambda = 0 \tag{B.2.25}$$

Substituting this value of λ into the system (B.2.8) we obtain

$$\begin{aligned} N(1-\alpha)x_i + \alpha\sum_{k=1}^{N} x_k - \sum_{k=1}^{N} y_k &= 0 \\ -\sum_{k=1}^{N} x_k + N(1-\gamma)y_i + \gamma\sum_{k=1}^{N} y_k &= 0 \end{aligned} \tag{B.2.26}$$

summing both equations from i to N we obtain the equation:

$$\sum_{i=1}^{N} x_i = \sum_{k=1}^{N} y_k \tag{B.2.27}$$

Inserting Eq.(B.2.27) into Eq.(B.2.26) we get

$$\begin{aligned} N(1-\alpha)x_i &= (1-\alpha)\sum_{k=1}^{N} x_k \\ N(1-\gamma)y_i &= (1-\gamma)\sum_{k=1}^{N} y_k \qquad k = 1, 2, \cdots, N \end{aligned}$$

Assuming that

$$\alpha \neq 1 \qquad and \qquad \gamma \neq 1 \tag{B.2.28}$$

we obtain

$$\begin{aligned} x_i &= \frac{1}{N}\sum_{k=1}^{N} x_k \\ y_i &= \frac{1}{N}\sum_{k=1}^{N} y_k \qquad k = 1, 2, \cdots, N \end{aligned} \tag{B.2.29}$$

Using Eq(B.2.27) we get

$$x_i = y_i \qquad k = 1, 2, \cdots, N \tag{B.2.30}$$

Hence the eigenvector belongs to the eigenvalue $\lambda = 0$ is

$$\vec{u}_N = x_1 \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

We normalize the vector

$$\vec{u}_N = \frac{1}{\sqrt{2N}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ -1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \tag{B.2.31}$$

We next consider the eigenvalues

$$\lambda = N(1-\gamma) \tag{B.2.32}$$

the system of Eq.(B.2.8) now reads:

$$N(\gamma-\alpha)x_i + \alpha\sum_{k=1}^{N} x_k - \sum_{k=1}^{N} y_k = 0 \tag{B.2.33}$$

$$-\sum_{k=1}^{N} x_k + \gamma\sum_{k=1}^{N} y_k = 0 \tag{B.2.34}$$

If we make the transformation

$$\alpha \to \gamma \qquad\qquad x_i \to y_i$$

Then Eq.(B.2.33) is transformed into Eq.(B.2.11) and Eq.(B.2.34) goes to Eq.(B.2.10). So if we assume that

$$\alpha \neq \gamma$$

then eigenvectors belonging to eigenvalue

$$\lambda = N(1-\gamma)$$

are

$$\vec{u}_{N+k} = \frac{1}{\sqrt{k(k+1)}} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \hline 1 \\ 1 \\ \vdots \\ 1 \\ -k \\ 0 \\ 0 \end{pmatrix} \Bigg\}_{\text{k}} \qquad k = 1, 2, \cdots, N-1 \tag{B.2.35}$$

We finally consider the eigenvalue

$$\lambda = 2N \tag{B.2.36}$$

In this case the system of equation given by Eq.(B.2.8) takes the form

$$-N(1+\alpha)x_i + \alpha\sum_{k=1}^{N} x_k - \sum_{k=1}^{N} y_k = 0 \tag{B.2.37}$$

$$-\sum_{k=1}^{N} x_k - N(1+\gamma)y_i + \gamma\sum_{k=1}^{N} y_k = 0 \tag{B.2.38}$$

Summing both equations from i to N we obtain the single equation

$$\sum_{i=1}^{N} x_i + \sum_{k=1}^{N} y_k = 0 \tag{B.2.39}$$

Inserting Eq.(B.2.39) into Eq.(B.2.37) and Eq.(B.2.38) we get

$$\begin{aligned} x_i &= \frac{1}{N}\sum_{k=1}^{N} x_k \\ y_i &= \frac{1}{N}\sum_{k=1}^{N} x_k \qquad i = 1, 2, \cdots, N \end{aligned} \tag{B.2.40}$$

substituting Eq.(B.2.40) into Eq.(B.2.39) we obtain

$$y_i = -x_i \qquad\qquad i = 1, 2, \cdots, N \tag{B.2.41}$$

Then the eigenvector belongs to the eigenvalue $\lambda = 2N$ is given by

$$\vec{u}_{2N} = \frac{1}{\sqrt{2N}} \begin{pmatrix} -1 \\ -1 \\ \vdots \\ -1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \tag{B.2.42}$$

The diagonalizing matrix is obtained by grouping the eigenvectors together

$$O_2 = \left(\vec{u}_1 \;\vdots\; \vec{u}_2 \;\vdots\; \cdots \;\vdots\; \vec{u}_{2N-1} \;\vdots\; \vec{u}_{2N} \right) \tag{B.2.43}$$

We introduce the matrices D and S :

$$D = \begin{pmatrix} 0 & 0 & \cdots & 1 \\ 0 & 0 & \cdots & 1 \\ 0 & 0 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} \tag{B.2.44}$$

with matrix elements

$$D_{ij} = \delta_{jN} \qquad\qquad i,j = 1,2,\cdots,N \tag{B.2.45}$$

and

$$S = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \cdots & \frac{1}{\sqrt{N(N-1)}} & \frac{1}{\sqrt{2N}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \cdots & \frac{1}{\sqrt{N(N-1)}} & \frac{1}{\sqrt{2N}} \\ 0 & -\frac{2}{\sqrt{6}} & \cdots & \frac{1}{\sqrt{N(N-1)}} & \frac{1}{\sqrt{2N}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{N(N-1)}} & \frac{1}{\sqrt{2N}} \\ 0 & 0 & \cdots & -\frac{(N-1)}{\sqrt{N(N-1)}} & \frac{1}{\sqrt{2N}} \end{pmatrix} \tag{B.2.46}$$

The element S_{ij} of S is given by:

$$S_{ij} = \frac{1}{\sqrt{j[j+1+(1-j)\delta_{jN}]}} \begin{cases} 1 & i \leq j \\ -j(1-\delta_{jN}) & i = j+1 \\ 0 & i > j+1 \end{cases} \tag{B.2.47}$$

The matrix S is not orthogonal since its last column represents a vector which is not normalized. We have

$$S^T S = I_N - \frac{1}{2} E_{NN} \tag{B.2.48}$$

where

$$E_{ij} = \begin{pmatrix} 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix} \qquad \begin{matrix} \leftarrow_{i^{th}-row} \\ \\ \\ \\ \\ \\ \\ \uparrow_{j^{th}col} \end{matrix} \qquad i,j = 1,2,\cdots,N$$

The matrix D satisfies

$$\begin{aligned} D^2 &= D \\ DD^T &= C \\ D^T D &= NE_{NN} \\ CD &= ND \end{aligned} \tag{B.2.49}$$

Direct computation shows that

$$\begin{aligned} S^T D &= D^T S = \sqrt{\frac{N}{2}} E_{NN} \\ SD^T &= DS^T = \frac{1}{\sqrt{2N}} C \\ CS &= \frac{N}{\sqrt{2N}} D \end{aligned} \tag{B.2.50}$$

Using the matrices D and S we represent the diagonalizing matrix O_2 in the form

$$O_2 = \left(\begin{array}{c|c} S & -\frac{1}{\sqrt{2N}} D \\ \hline \frac{1}{\sqrt{2N}} D & S \end{array}\right) \tag{B.2.51}$$

We can verify the orthogonality of the matrix O_2 directly using Eq.(B.2.49) and (B.2.50) we have

$$\begin{aligned} O_2^T O_2 &= \left(\begin{array}{c|c} S^T & \frac{1}{\sqrt{2N}} D^T \\ \hline -\frac{1}{\sqrt{2N}} D^T & S^T \end{array}\right) \left(\begin{array}{c|c} S & -\frac{1}{\sqrt{2N}} D \\ \hline \frac{1}{\sqrt{2N}} D & S \end{array}\right) \\ &= \left(\begin{array}{c|c} S^T S + \frac{1}{2N} D^T D & \frac{1}{\sqrt{2N}} (D^T S - S^T D) \\ \hline -\frac{1}{\sqrt{2N}} (D^T S - S^T D) & S^T S + \frac{1}{2N} D^T D \end{array}\right) \\ &= \left(\begin{array}{c|c} I_N & 0 \\ \hline 0 & I_N \end{array}\right) = I_{2N} \end{aligned} \tag{B.2.52}$$

The diagonal form of the potential matrix V_D is given

$$O_2^T V O_2 = V_D \tag{B.2.53}$$

Substituting for V and V_D we obtain

$$O_2^T \begin{pmatrix} N(1-\alpha)+\alpha & \alpha & \cdots & \alpha & -1 & -1 & \cdots & -1 \\ \alpha & N(1-\alpha)+\alpha & \cdots & \alpha & -1 & -1 & \cdots & -1 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \alpha & \alpha & \cdots & N(1-\alpha)+\alpha & -1 & -1 & \cdots & -1 \\ -1 & \cdots & -1 & -1 & N(1-\gamma)+\gamma & \gamma & \cdots & \gamma \\ -1 & \cdots & -1 & -1 & \gamma & N(1-\gamma)+\gamma & \cdots & \gamma \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & \cdots & -1 & -1 & \gamma & \gamma & \cdots & N(1-\gamma)+\gamma \end{pmatrix} O_2 =$$

$$\begin{pmatrix} N(1-\alpha) & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & N(1-\alpha) & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & N(1-\alpha) & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & N(1-\gamma) & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & N(1-\gamma) & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & N(1-\gamma) & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 2N \end{pmatrix} \quad \text{(B.2.54)}$$

(N-1)-col. 1-col. (N-1)-col. 1-col.

We have not displayed the explicit form of the matrix O_2 since it is independent of α and γ. On the left hand side of Eq.(B.2.54) we have polynomials of α and γ. On the right hand side we have monomials of α and γ. These functions are continuous functions so we can take the limit as $\alpha \to 1$ and $\gamma \to 1$. This gives

$$O_2^T \begin{pmatrix} C & -C \\ -C & C \end{pmatrix} O_2 = \begin{pmatrix} 0 & 0 \\ 0 & 2NE_{NN} \end{pmatrix} \quad \text{(B.2.55)}$$

We see that the matrix O_2 diagonalizes also the matrix V_1 encountered in chapter 3. Indeed we can check this directly

$$\begin{aligned} O_2^T \begin{pmatrix} C & -C \\ -C & C \end{pmatrix} O_2 &= \begin{pmatrix} S^T & \frac{1}{\sqrt{2N}} D^T \\ -\frac{1}{\sqrt{2N}} D^T & S^T \end{pmatrix} \begin{pmatrix} C & -C \\ -C & C \end{pmatrix} \begin{pmatrix} S & -\frac{1}{\sqrt{2N}} D \\ \frac{1}{\sqrt{2N}} D & S \end{pmatrix} \\ &= \begin{pmatrix} S^T & \frac{1}{\sqrt{2N}} D^T \\ -\frac{1}{\sqrt{2N}} D^T & S^T \end{pmatrix} \begin{pmatrix} CS - \frac{1}{\sqrt{2N}} CD & -CS - \frac{1}{\sqrt{2N}} CD \\ -CS + \frac{1}{\sqrt{2N}} CD & CS + \frac{1}{\sqrt{2N}} CD \end{pmatrix} \\ &= \begin{pmatrix} (O^T V_1 O_1)_{11} & (O^T V_1 O_1)_{12} \\ (O^T V_1 O_1)_{21} & (O^T V_1 O_1)_{22} \end{pmatrix} \end{aligned}$$

where

$$
\begin{aligned}
(O^T V_1 O_1)_{11} &= S^T CS - \frac{1}{\sqrt{2N}} S^T CD - \frac{1}{\sqrt{2N}} D^T CS + \frac{1}{2N} D^T CD \\
(O^T V_1 O_1)_{12} &= -S^T CS - \frac{1}{\sqrt{2N}} S^T CD + \frac{1}{\sqrt{2N}} D^T CS + \frac{1}{2N} D^T CD \\
(O^T V_1 O_1)_{21} &= -S^T CS + \frac{1}{\sqrt{2N}} S^T CD - \frac{1}{\sqrt{2N}} D^T CS + \frac{1}{2N} D^T CD \\
(O^T V_1 O_1)_{22} &= S^T CS + \frac{1}{\sqrt{2N}} S^T CD + \frac{1}{\sqrt{2N}} D^T CS + \frac{1}{2N} D^T CD
\end{aligned}
$$

Using Eq.(B.2.55) and Eq.(B.2.56) we have

$$
\begin{aligned}
S^T CS &= \frac{N}{\sqrt{2N}} S^T D = \frac{N}{2} E_{NN} \\
S^T CD &= N S^T D = N\sqrt{\frac{N}{2}} E_{NN} = D^T CS \\
D^T CD &= N D^T D = N^2 E_{NN}
\end{aligned}
\tag{B.2.56}
$$

Therefore

$$
\begin{aligned}
(O^T V_1 O_1)_{11} &= \frac{N}{2} E_{NN} - \frac{N}{2} E_{NN} - \frac{N}{2} E_{NN} + \frac{N}{2} E_{NN} = 0 \\
(O^T V_1 O_1)_{12} &= 0 \\
(O^T V_1 O_1)_{21} &= 0 \\
(O^T V_1 O_1)_{22} &= 2N E_{NN}
\end{aligned}
$$

Hence

$$
O_2^T V_1 O_2 = \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & 2NE_{NN} \end{array}\right)
$$

The difference between the diagonalizing matrices O_1 and O_2 is the way by which they cluster the particles. To see that, we consider the new coordinate vectors

$$
\vec{r}_1, \vec{r}_2, \cdots \vec{r}_{2N}
$$

They are related to the old coordinate vectors

$$
\vec{r}_1^{\,A}, \vec{r}_2^{\,A}, \cdots, \vec{r}_N^{\,A}, \vec{r}_1^{\,B}, \vec{r}_2^{\,B}, \cdots \vec{r}_N^{\,B}
$$

by:

$$\begin{pmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_N \\ \hline \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} = O_2^T \begin{pmatrix} \vec{r}_1^A \\ \vdots \\ \vec{r}_N^A \\ \vec{r}_1^B \\ \vdots \\ \vec{r}_N^B \end{pmatrix} = \left(\begin{array}{c|c} S^T & \frac{1}{\sqrt{2N}} D^T \\ \hline -\frac{1}{\sqrt{2N}} D^T & S^T \end{array}\right) \begin{pmatrix} \vec{r}_1^A \\ \vdots \\ \vec{r}_N^A \\ \vec{r}_1^B \\ \vdots \\ \vec{r}_N^B \end{pmatrix} \tag{B.2.57}$$

Or

$$\begin{pmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_N \end{pmatrix} = S^T \begin{pmatrix} \vec{r}_1^A \\ \vdots \\ \vec{r}_N^A \end{pmatrix} + \frac{1}{\sqrt{2N}} D^T \begin{pmatrix} \vec{r}_1^B \\ \vdots \\ \vec{r}_N^B \end{pmatrix} \tag{B.2.58}$$

$$\begin{pmatrix} \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} = S^T \begin{pmatrix} \vec{r}_1^B \\ \vdots \\ \vec{r}_N^B \end{pmatrix} - \frac{1}{\sqrt{2N}} D^T \begin{pmatrix} \vec{r}_1^A \\ \vdots \\ \vec{r}_N^A \end{pmatrix} \tag{B.2.59}$$

Carrying out the multiplication

$$\begin{aligned} \vec{r}_k &= \sum_{j=1}^{N} S_{jk} \vec{r}_j^A + \frac{1}{\sqrt{2N}} \sum_{j=1}^{N} D_{jk} \vec{r}_j^B \\ \vec{r}_{N+k} &= \sum_{j=1}^{N} S_{jk} \vec{r}_j^B - \frac{1}{\sqrt{2N}} \sum_{j=1}^{N} D_{jk} \vec{r}_j^A \qquad k = 1, \cdots, N \end{aligned} \tag{B.2.60}$$

Now

$$\begin{aligned} \sum_{j=1}^{N} S_{jk} \vec{r}_j^A &= \sum_{j=1}^{k} S_{jk} \vec{r}_j^A + S_{k+1,k} \vec{r}_{k+1}^A + \sum_{j=k+2}^{N} S_{jk} \vec{r}_j^A \\ &= \frac{1}{\sqrt{k(k+1+(1-k)\delta_{kN})}} \left[\sum_{j=1}^{k} \vec{r}_j^A - k(1-\delta_{kN}) \vec{r}_{k+1}^A \right] \end{aligned} \tag{B.2.61}$$

Also

$$\sum_{j=1}^{N} D_{jk} \vec{r}_j^B = \sum_{j=1}^{N} \delta_{kN} \vec{r}_j^B = \delta_{kN} \sum_{j=1}^{N} \vec{r}_j^B \tag{B.2.62}$$

Hence

$$\begin{aligned}
\vec{r}_k &= \frac{1}{\sqrt{k(k+1+(1-k)\delta_{kN})}}\left[\sum_{j=1}^{k}\vec{r}_j^{\,A} - k(1-\delta_{kN})\vec{r}_{k+1}^{\,A}\right] \\
&+ \frac{1}{\sqrt{N}}\delta_{kN}\sum_{j=1}^{N}\vec{r}_j^{\,B} \\
\vec{r}_{N+k} &= \frac{1}{\sqrt{k(k+1+(1-k)\delta_{kN})}}\left[\sum_{j=1}^{k}\vec{r}_j^{\,B} - k(1-\delta_{kN})\vec{r}_{k+1}^{\,B}\right] \\
&- \frac{1}{\sqrt{N}}\delta_{kN}\sum_{j=1}^{N}\vec{r}_j^{\,A} \qquad k=1,\cdots,N
\end{aligned} \tag{B.2.63}$$

The inverse transformation is given by

$$\begin{pmatrix} \vec{r}_1^{\,A} \\ \vdots \\ \vec{r}_N^{\,A} \\ \hline \vec{r}_1^{\,B} \\ \vdots \\ \vec{r}_N^{\,B} \end{pmatrix} = \left(\begin{array}{c|c} S & -\frac{1}{\sqrt{2N}}D \\ \hline \frac{1}{\sqrt{2N}}D & S \end{array}\right) \begin{pmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_N \\ \hline \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} \tag{B.2.64}$$

Or

$$\begin{pmatrix} \vec{r}_1^{\,A} \\ \vdots \\ \vec{r}_N^{\,A} \end{pmatrix} = S\begin{pmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_N \end{pmatrix} - \frac{1}{\sqrt{2N}}D\begin{pmatrix} \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} \tag{B.2.65}$$

$$\begin{pmatrix} \vec{r}_1^{\,B} \\ \vdots \\ \vec{r}_N^{\,B} \end{pmatrix} = S\begin{pmatrix} \vec{r}_{N+1} \\ \vdots \\ \vec{r}_{2N} \end{pmatrix} + \frac{1}{\sqrt{2N}}D\begin{pmatrix} \vec{r}_1 \\ \vdots \\ \vec{r}_N \end{pmatrix} \tag{B.2.66}$$

Carrying out the multiplication

$$\begin{aligned}
\vec{r}_k^{\,A} &= \sum_{j=1}^{N} S_{kj}\vec{r}_j - \frac{1}{\sqrt{2N}}\sum_{j=1}^{N} D_{kj}\vec{r}_{N+j} \\
\vec{r}_N^{\,B} &= \sum_{j=1}^{N} S_{kj}\vec{r}_{N+j} + \frac{1}{\sqrt{2N}}\sum_{j=1}^{N} D_{kj}\vec{r}_j
\end{aligned} \tag{B.2.67}$$

Consider the first sum on the right hand side of the first equation

$$\begin{aligned}\sum_{j=1}^{N} S_{kj}\vec{r}_j &= \sum_{j=1}^{k-2} S_{kj}\vec{r}_j + S_{k,k-1}\vec{r}_{k-1} + \sum_{j=k}^{N} S_{kj}\vec{r}_j \\ &= -\frac{(k-1)}{\sqrt{k(k-1)}}\vec{r}_{k-1} + \sum_{j=1}^{N} \frac{1}{\sqrt{j(j+1+(1-j)\delta_{jN})}}\vec{r}_j \quad \text{(B.2.68)}\end{aligned}$$

To evaluate the second term we have

$$\sum_{j=1}^{N} D_{jk}\vec{r}_j = \sum_{j=1}^{N} \delta_{jN}\vec{r}_{j+N} = \vec{r}_{2N} \quad \text{(B.2.69)}$$

Hence

$$\begin{aligned}\vec{r}_k^{A} &= \sum_{k=j}^{N} \frac{1}{\sqrt{j(j+1+(1-j)\delta_{jN})}}\vec{r}_j - \frac{(k-1)}{\sqrt{k(k-1)}}\vec{r}_{k-1} - \frac{1}{\sqrt{2N}}\vec{r}_{2N} \\ \vec{r}_k^{B} &= \sum_{k=j}^{N} \frac{1}{\sqrt{j(j+1+(1-j)\delta_{jN})}}\vec{r}_{N+j} - \frac{(k-1)}{\sqrt{k(k-1)}}\vec{r}_{N+k-1} + \frac{1}{\sqrt{2N}}\vec{r}_{2N} \quad \text{(B.2.70)}\end{aligned}$$

In the term

$$-\frac{(k-1)}{\sqrt{k(k-1)}}\vec{r}_{k-1}$$

the case $k = 1$ is considered as a limiting case which gives zero.

We see the diagonalizing matrix O_2 clusters the particles of each species together while the matrix O_1 clusters equal particles from the two species.

Appendix C

C.1 Density of states for a single particle in a harmonic trap

The density of states for a single particle is given by:

$$g(\epsilon) = \frac{1}{h^3}\int d^3x \int d^3p \delta(\epsilon - \hat{H}) \tag{C.1.1}$$

In our system, the Hamiltonian is given by:

$$\hat{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2$$

Eq.(C.1.1) becomes

$$g(\epsilon) = \frac{1}{(2\pi\hbar)^3}\int d^3x \int d^3p \delta(\epsilon - \frac{p^2}{2m} - \frac{1}{2}m\omega^2 r^2) \tag{C.1.2}$$

We introduce a new variable E

$$E = \frac{p^2}{2m} \tag{C.1.3}$$

$$\begin{aligned} d^3p &= 4\pi p^2 dp \\ 2pdp &= 2mdE \\ d^3p &= 4\pi m^{3/2}(2E)^{1/2}dE \end{aligned}$$

Substituting in Eq.(C.1.2)

$$\begin{aligned} g(\epsilon) &= \frac{1}{(2\pi\hbar)^3}\int_{-\infty}^{\infty} d^3x \int_0^{\infty} 4\pi m^{3/2}(2E)^{1/2}dE\delta(\epsilon - E - \frac{1}{2}m\omega^2 r^2) \\ &= \frac{m^{3/2}}{2\pi^2\hbar^3}\int_{-\infty}^{\infty} d^3x \int_0^{\infty} (2E)^{1/2}dE\delta(E - (\epsilon - \frac{1}{2}m\omega^2 r^2)), \end{aligned} \tag{C.1.4}$$

From Eq.(C.1.3) we have $E > 0$ therefore $\epsilon - \frac{1}{2}m\omega^2 r^2 > 0$, this gives

$$g(\epsilon) = \frac{m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int_{-\infty}^{\infty} d^3x(\epsilon - \frac{1}{2}m\omega^2 r^2)^{1/2}\Theta(\epsilon - \frac{1}{2}m\omega^2 r^2) \qquad \text{(C.1.5)}$$

where Θ is the step function defined as

$$\Theta(x) = \{^{0 \quad x<0}_{1 \quad x>0}$$

Since the Θ function is equal to unity when its argument $(\epsilon - \frac{1}{2}m\omega^2 r^2)$ is greater than zero, we have

$$\epsilon - \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) > 0$$

so that

$$(x^2 + y^2 + z^2) < \frac{2\epsilon}{m\omega^2}$$

We see that the Θ function vanishes outside a 3-D sphere of radius $\frac{2\epsilon}{m\omega^2}$ the integral becomes

$$g(\epsilon) = \frac{m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int\int\int_{(x^2+y^2+z^2)<\frac{2\epsilon}{m\omega}} dxdydz(\epsilon - \frac{1}{2}m\omega^2(x^2 + y^2 + z^2))^{1/2}$$

Introducing spherical coordinates and using the spherical symmetry:

$$\begin{aligned} dxdydz &= 4\pi r^2 dr \qquad 0 < r < \sqrt{\frac{2\epsilon}{m\omega^2}} \\ g(\epsilon) &= \frac{(2m)^{3/2}}{\pi\hbar^3}\int_0^{\sqrt{\frac{2\epsilon}{m\omega^2}}} r^2 dr(\epsilon - \frac{1}{2}m\omega^2 r^2)^{1/2} \end{aligned} \qquad \text{(C.1.6)}$$

To evaluate the integral we introduce variable θ defined as

$$r = \sqrt{\frac{2\epsilon}{m\omega^2}}\sin\theta \qquad \text{(C.1.7)}$$

Then we have,

$$\begin{aligned} g(\epsilon) &= \frac{(2m)^{3/2}}{\pi\hbar^3}\int_0^{\pi/2}(\frac{2\epsilon}{m\omega^2})^{3/2}\epsilon^{1/2}d\theta\sin^2\theta\cos^2\theta \\ &= \frac{(2m)^{3/2}}{\pi\hbar^3}(\frac{2\epsilon}{m\omega^2})^{3/2}\epsilon^{1/2}\int_0^{\pi/2} d\theta\sin^2\theta\cos^2\theta \\ &= \frac{8\epsilon^2}{\pi(\hbar\omega)^3}\int_0^{\pi/2} d\theta\sin^2\theta\cos^2\theta \\ &= \frac{8\epsilon^2}{\pi(\hbar\omega)^3}\frac{1}{2}B(\frac{3}{2},\frac{3}{2}), \end{aligned} \qquad \text{(C.1.8)}$$

where $B(m,n)$ is the beta function. Then using the equation

$$B(m,n) = \frac{\Gamma[m]\Gamma[n]}{\Gamma[m+n]}$$

hence,

$$\begin{aligned} g(\epsilon) &= \frac{8\epsilon^2}{\pi(\hbar\omega)^3}\frac{1}{2}\frac{\Gamma[\frac{3}{2}]\Gamma[\frac{3}{2}]}{\Gamma[3]} \\ &= \frac{\epsilon^2}{2(\hbar\omega)^3} \end{aligned} \tag{C.1.9}$$

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الملخص

هذه الرسالة تدرس نظام يحتوى على اعداد متساوية من البوزونات تنتمى لفئتين مختلفتين وتتفاعل بوساطة جهد متذبذب توافقى. نحن نفترض ان البوزونات تتحرك فى ثلاثة ابعاد و الجسيمات التى تنتمى لنفس الفئة تتنافر بينما التى تنتمى لفئات مختلفة تتجاذب. تم دراسة الحالتين حيث شدة الاقتران متماثلة وشدة الازدواج تعتمد على فئة الجسيم. بحل مسائلة الحالة الذاتية، اعدنا صياغة الهاملتونيان للنظام بدلالة الاحداثيات الطبيعية للنظام بدلا من احداثيات الجسيم الفردى.

اولا، تم حل مشكلة القيمة الاولية الكلاسيكية عند شروط اولية اختيارية لمواضع وكمية تحرك الجسيمات, عن طريق تقطير الهاملتونيان الكلاسيكى للنظام وحصلنا على مسارات الجسيمات كدالة فى الزمن. النظام يعرض نبضات عندما يكون شدة الاقتران مختلفة. تم فحص النظام الكمى, والحصول على الطيف الكامل للحالات الذاتية عديدة الجزيئ. اخيرا, تم دراسة السلوك الاحصائى الميكانيكى للنظام فى اطار الفرق الكنسى الكبير وحصلنا على الخواص الثيرموديناميكية للنظام ودرجة الحرارة الحرجة. تم توضيح ان النظام يتكثف فى قناة واحدة عندما يكون شدة الاقتران متماثلة وقناتين عندما يكون شدة الاقتران مختلفة.

دراسة نموذج قابل للحل تماما لنوعين من البوزونات المتماثلة تتفاعل بواسطة جهد متذبذب توافقى

اسم الطالب

عباس حسين عباس

كجزء من متطلبات الحصول على درجة الماجستير فى العلوم

قسم الفيزياء

كلية العلوم

جامعة القاهرة

جيزة - مصر