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Theoretical Study of Phase Transitions in Dilute Bose-Einstein Condensates

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Abstract
In this work, we study phase transitions in dilute Bose-Einstein Condensates theoretically. The Gross-Pitaevskii equation (GPE) is applied to describe the properties of dilute Bose gases near zero temperature for various confining geometries. Then, using the harmonic trap, the Thomas Fermi equation has been investigated. The Bose-Hubbard Model has been also investigated using the mean field approach. It is indicated that Bose-Einstein condensation is a second order phase transition. We also presented an exactly solvable phase transition model in which the phase transition is purely statistically derived. It is found out that the mean field theory can be applied to a number of physical systems so as to study the phenomena of Berezinsky-Kosterlitz- Thouless (BKT) phase transitions.
Keywords: Phase Transition, BEC, GPE, Bose-Hubbard Model, Berezinsky-Kosterlitz-Thouless (BKT), Mean Field equation

1. Introduction

Phase transitions and existence of long-range order are core areas of contemporary statistical mechanics. This general concept can be utilized to predict properties of various materials of scientific and technological interest as well as to gain understanding of a myriads of phenomena ranging from the origin of the universe to the behavior of water at different temperatures. One of the most interesting phase transitions is the formation of Bose-Einstein condensation (BEC) [1]. Phase transitions are ubiquitous in nature, and can be arranged into universality classes such that systems having unrelated microscopic physics show identical scaling behavior near the critical point [2, 3]. BEC was originally conceived by S. Bose and Albert Einstein, who concluded that if a gas of atoms could be cooled below a transition temperature, it should suddenly condense into a remarkable state in which all the atoms have exactly the same location and energy. The wave-function of each atom in a BEC should extend across the entire sample of gas. For a dilute gas, the requisite transition temperature is so low as to be un-achievable by the technology of Einstein's day [2, 4].

In nature, particles can be divided into two categories: bosons which are particles with integer spin (e.g. photons) and fermions which have half-integer spin (e.g. electrons). A key difference between the two is that fermions are limited to only one particle per state as per the Pauli- exclusion principle, while bosons can occupy the same state in any number. In the Bose- Einstein statistics, the occupation of the ground state of the system diverges in the limit of zero temperature, leading to macroscopic population of this single state [11]. All of these aspects are well described by a non-linear Schrödinger equation, in which the non-linearity arises from repulsive potentials between the Bo-sonic atoms that make up the condensate [12].

BEC is a state of matter of bosons confined in an external potential and cooled to temperatures very near to absolute zero. Under such super-cooled conditions, a large fraction of the atoms collapse into the lowest quantum state of the external potential, at which point quantum effects become apparent on a macroscopic scale. When a Bo-sonic system is cooled below the critical temperature of BEC, the behavior of the system will change dramatically, because the condensed particles behave like a single quantum entity [14, 15].

The Gross-Pitaevskii (GP) theory was developed by Pitaevskii [19] and Gross [20] independently in 1960s. For a long time, the validity of this mean field approximation lacks of rigorous mathematical justification. Mean field theories, for instance the Gross-Pitaevskii theory successfully describe a broad variety of interesting phenomena observable for the spatial distribution of the gas in a harmonic trap, for recent reviews of numerous successful applications of the mean field theories in BEC in atomic gases [21]. This work provides the theory of phase transitions in dilute BEC. Applying the mean field theory it is also attempted to study the consequences of phase transitions in dilute BEC and investigate the Gross-Pitaevskii mean-field ground state properties in interacting and non-interacting limits.

2. Methodology

2.1. The Mean-Field Theory

The mean field theory the many-body Hamiltonian is given by the same as the basis of field operators the total Hamiltonian can be written in the form. We consider the general case of N spineless bosons that are interacting with a potential$U\ (r - r')$. Thus using again the basis of field operators the total Hamiltonian can be written in the form

$$\hat{H} = \int d^3 r \hat{\psi}^{\dagger}(r)\left[-\frac{\psi\hbar^2\ \dagger}{2m}\nabla^2 + \mathrm{V_{trap}(r)}\right]\hat{\psi}\ (r) + \frac{1}{2}\iint d^3 r d^3 r' \hat{\psi}^{\dagger}(r)\hat{\psi}^{\dagger}(r')U(r-r')\hat{\psi}\ (r')\hat{\psi}(r)\ \ (1)$$

In the case of weak interactions BEC occurs when a macroscopic number of atoms N_o occupies the same single-particle wave function and the ratio (N − N0) /N << 1 in the thermodynamic limit $N \to \infty$. In this case, $N_o + 1 \cong 1$ and the operators $\widehat{a_0}$ and $\widehat{a_0}^{\dagger}$ and can be treated as real numbers: $\widehat{a_0} = \widehat{a_0}^{\dagger} = \sqrt{N_0}$ and the field operator can be decomposed in

$$\hat{\psi}\ (r) = \psi_0 + \hat{\psi}'(r) = \sqrt{\frac{N_0}{V}} + \hat{\psi}'(r') \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.\ (2)$$

Where $\hat{\psi}'(r) \ll \sqrt{\frac{N_0}{V}}$ is called quantum depletion. Treating the depletion as a small perturbation, Bogoliubov built the first-order theory of uniform Bose gases.

2.2 The Gross-Pitaevskii Equation (GPE)

The Gross-Pitaevskii Equation (GPE) is a form of Non-Linear Schr¨odinger Equation (NLSE) that has been successfully used to describe the static and dynamic properties of BEC at very low temperatures. The condition for BEC phase-transition does not depend on interaction between atoms, the product (the condensate) is strongly affected by the interaction between atoms. The dilute-gas condensate can be well described by a macroscopic wave function or order parameter

$\hat{\psi}\ (r)$, which satisfies the Gross-Pitaevskii equation [11]. The field operator can be decomposed as

$$\hat{\psi}(r,t) = \psi(r,t) + \hat{\psi}'(r,t) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.\ (3)$$

Where $\psi(r,t)$ is a classical field defined as the expectation value of the field operator, $\psi(r,t) = \langle\hat{\psi}'(r,t)\rangle$. It has a well-defined phase and its modulus gives the density of the condensate $n_0 = |\psi(r,t)|^2$. It is often called the wave function of the condensate and it characterizes the off-diagonal behavior of the one-particle density matrix:

$$\rho(r',r,t) = \langle\psi^*(r',t)\psi(r,t)\rangle \qquad (4)$$

Which is different from zero for macroscopic distances |r – r'| of the order of the size of the sample (long-range order). In order to derive the equation of the condensate wave function $\psi(r,t)$ we use the time evolution for the field operator $\hat{\psi}(r,t)$ in the Heisenberg equation with the many-body Hamiltonian, Eq. (1). These yields

$$i\hbar\frac{d}{dt}\hat{\psi}(r',t) = [\hat{\psi}(r',t),\hat{H}], \qquad (5)$$

Where

$$\hat{H} = \int d^3 r\left[\hat{\psi}\ (r',t)\hat{\psi}^{\dagger}(r,t)(-\frac{\psi\hbar^2\ \dagger}{2m}\nabla^2(\mathrm{r}) + \mathrm{V_{trap}(r)})\right]\hat{\psi}\ (r,t) + \frac{g}{2}\int d^3 r[\hat{\psi}\ (r',t),\hat{\psi}^{\dagger}(r,t)\hat{\psi}^{\dagger}(r,t)\hat{\psi}\ (r,t)\hat{\psi}\ (r,t)\ ]. \qquad (6)$$

Where using the properties of commutation relation we have $[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} - \hat{B}[\hat{A},\hat{C}]$.

From commutation relations we assume set the values of $\hat{A}, \hat{B}\ and\ \hat{C}$ are

$$\hat{A} = \hat{\psi}\ (r',t), \hat{B} = \hat{\psi}^{\dagger}(r,t)\hat{\psi}^{\dagger}(r,t), and\ \hat{C} = \hat{\psi}\ (r,t)\hat{\psi}\ (r,t) \qquad (7)$$

For the interaction (non-linear) part of the Hamiltonian in Eq. (7) and similarly let us consider the following for the linear part of the Hamiltonians,

$$\hat{A} = \hat{\psi}\ (r',t), \hat{B} = \hat{\psi}^{\dagger}(r,t), and\ \hat{C} = \hat{\psi}\ (r,t) \qquad (8)$$

The application of the relation of commutation and the substitution of Eq. (7) and Eq. (8) Followed by replacement of r' by r gives us the time dependant GPE in the operator form

$$i\hbar\frac{d}{dt}\hat{\psi}(r',t) = \left(-\frac{\psi\hbar^2\dagger}{2m}\nabla^2(\mathrm{r}) + \mathrm{V_{trap}}(\mathrm{r})\right)\hat{\psi}(r,t) + g\hat{\psi}^\dagger(r,t)\hat{\psi}(r,t)\hat{\psi}(r,t) \quad (9)$$

To solve the GPE in non-operator form, let us split the Bose field operator in Eq. (9) into the

$$\hat{\psi}(r,t) = \hat{\phi}(r,t) + \delta\hat{\psi}(r,t) \quad (10)$$

Where, $\phi(r,t) = \langle\hat{\psi}(r,t)\rangle$ (11)

is the ground state expectation values of the bose field that describes a non-uniform condensate, and $\delta\hat{\psi}(r,t)$ and $\hat{\psi}^\dagger(r,t)$ annihilates and creates non-condensate particles density. By using the decomposition in Eq. (11) and setting

$\hat{\phi}(r,t) = \phi, \phi^*(r,t) = \phi^*, \delta\hat{\psi}(r,t) = \delta\psi(r,t), \delta\hat{\psi}^\dagger(r,t) = \delta\hat{\phi}$ and express the cubic non-linearity of the Bose operator in Eq. (9) in terms of the following expression as

$$\hat{\psi}^\dagger\hat{\psi}\hat{\psi} = (\phi^* + \delta\hat{\psi}^\dagger)(\phi + \delta\psi)(\phi + \delta\psi)$$
$$= |\phi|^2 + 2|\phi|^2\delta\hat{\psi} + \phi^2\delta\hat{\psi}^\dagger + \phi^*\delta\hat{\psi}\delta\hat{\psi} + 2\phi\delta\hat{\psi}^\dagger\delta\hat{\psi} + \delta\hat{\psi}^\dagger\delta\hat{\psi}\delta\hat{\psi} \quad (12)$$

The self consistent mean-field approximation given as

$$\delta\hat{\psi}^\dagger\delta\hat{\psi}\delta\hat{\psi} = 2\langle\delta\hat{\psi}^\dagger\delta\hat{\psi}\rangle\delta\hat{\psi} + \langle\delta\hat{\psi}\delta\hat{\psi}\rangle\delta\hat{\psi}^\dagger + \langle\delta\hat{\psi}\delta\hat{\psi}\rangle\delta\hat{\psi}^\dagger \quad (13)$$

We can be used to simplify the last term of Eq. (12). Therefore, using this approximation, Eq. (12) can be written as

$$\hat{\psi}^\dagger\hat{\psi}\hat{\psi} = |\phi|^2 + 2\left[|\phi|^2 + \langle\delta\hat{\psi}^\dagger\delta\hat{\psi}\rangle\right]\delta\hat{\psi} + \left[\phi^2 + \langle\delta\hat{\psi}^\dagger\delta\hat{\psi}\rangle\right]\delta\hat{\psi} + 2\phi\delta\hat{\psi}^\dagger\delta\hat{\psi}$$
$$+ \phi^*\delta\hat{\psi}\delta\hat{\psi} \quad (14)$$

Substituting Eqs. (13 and 14) into Eq. (9) gives us

$$i\hbar\left(\frac{\partial\phi}{\partial t} + \frac{\partial\delta\hat{\psi}}{\partial t}\right) = \left(-\frac{h}{2m}\nabla^2 + V_{trap}(r)\right)(\phi + \delta\hat{\psi}) + g|\phi|^2\phi + 2g\left(|\phi|^2 + \langle\delta\hat{\psi}^\dagger\delta\hat{\psi}\rangle\right)\delta\hat{\psi}$$
$$+ g\left(\phi^2 + \langle\delta\hat{\psi}^\dagger\delta\hat{\psi}\rangle\right)\delta\hat{\psi} + 2g\phi\hat{\psi}^\dagger\delta\hat{\psi} + g\phi^*\delta\hat{\psi}\delta\hat{\psi} \quad (15)$$

Assuming that all sorts of fluctuations can be ignored, the variation terms in the above equation can be canceled. Thus, we are left with

$$i\hbar\frac{\partial\phi(r,t)}{\partial t} = \left(-\frac{\hbar}{2m}\nabla^2 + V_{trap}(r)\right)\phi(r,t) + g|\phi(r,t)|^2\phi(r,t) \quad (16)$$

where m is the atomic mass, g is the self-interaction constant and $V_{trap}(r)$ is the total confining potential which shows the variation of condensate wave function with respect to time [5]. We also make some additional approximations such as for T = 0 and for weakly interacting systems we can replace $\hat{\psi}(r,t)$ with the classical field $\psi(r,t)$. With the approximation we can replace

$$U(r - r') = g\sigma(r - r'), \quad (17)$$

Where g is coupling constant given by the equation

$$g = \frac{4\pi\hbar^2 a_s}{m} \quad (18)$$

This characterizes the strength of inter-particle interactions. The value of g can be either zero, positive or negative according to the sign of the scattering length a. For s = 0 we recover the ideal, non-interacting limit. Positive (negative) values of correspond a to effective repulsive (attractive) interactions respectively. In the most common case of a three dimensional magnetic trap $V_{trap}(r)$ has the form,

$$V_{trap}(r) = \frac{1}{2}m((\omega^2{}_\perp)(x^2 + y^2) + \omega^2{}_\parallel Z^2 \quad (19$$

where $\omega_\perp$ and $\omega_\parallel$ are the transverse and the social trap frequencies respectively and $\lambda = \frac{\omega_\parallel}{\omega_\perp}$is called the asymmetry parameter. If $\lambda = 1$ the trap is spherical, whereas if $\lambda < 1$ the trap is cigar-shaped and for $\lambda > 1$

the trap is pancake-like. The condensate wave function is normalized to unity that is

$$\int_{-\infty}^{\infty} |\psi(r,t)|^2 \, d^3r = 1 \qquad (20)$$

Eq. (16) is called the Gross-Pitaevskii equation (GPE). It has the form of a non-linear Schr¨odinger equation [23].

3. Discussion

3.1. A Bose Gas in a Harmonic Trap

The BEC of ideal Bose gases is a special case of the generalized BEC phase transition. By studying this exactly solvable model, we can also obtain a deeper insight into the BEC of ideal Bose gases. The conservative traps used to confine the ultra cold atoms in this work create potentials U(r) that can be approximated as harmonic trap potential

$$U(r) = \frac{1}{2} m\left(\omega^2{}_x x^2 + \omega^2{}_y y^2 + \omega^2{}_z Z^2\right) \qquad (21)$$

The total number of atoms N in the grand-canonical ensemble and using Bose statistics is given by the sum over the eigen-states of single-particle Hamiltonians ($\hat{h}i$)

$$N = \sum_{n_x,n_y,n_z} \frac{1}{\exp\left(\beta\left(\mathcal{E}_{n_x,n_y,n_z} - \mu\right)\right) - 1}$$

Where μ is the chemical potential and $\beta = (\mathrm{KBT})^{-1}$ KB is the Boltzmann constant and T is the temperature. The confining potential for alkali atoms at low energies is given by

$$V_{trap}(r) = \frac{m}{2}\left(\omega^2{}_x + \omega^2{}_y + \omega^2{}_z\right) \qquad (23)$$

The thermodynamic limit in the case of harmonic trapping is defined by setting $N \to \infty$ and$\omega_0 \to 0$, with the combination $N\omega^3{}_0$ kept fixed where $\omega_0 = (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric average of trap frequencies. The eigenvalues of this single-particle of Hamiltonian of the form

$$\mathcal{E}_{n_x,n_y,n_z} = \mathcal{E}_{nx} + \mathcal{E}_{ny} + \mathcal{E}_{nz} = \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y + \left(n_z + \frac{1}{2}\right)\hbar\omega_z \qquad (24)$$

With the quantum numbersn_x, n_y, n_z the population of the ground state N_0 becomes microscopic of the order N, when the chemical potential μ becomes equal to the energy of the lowest state $\mathcal{E}_{000} = \frac{3}{2}\hbar\overline{\omega}$ where $\overline{\omega} = (\omega^2{}_x + \omega^2{}_y + \omega^2{}_z)/3$ is the arithmetic average of the trapping frequencies. Using the condition that the excitation energies are much larger than the level spacing of the trapping potential one can replace the sum by an integral over Eigen states of the single-particle Hamiltonian. This semi-classical approximation is valid when$KBT \gg \hbar\omega_0$. If we separate the number of particles in the ground state N0 from the rest of the integral one can find the number of particles in the excited states,

$$N - N_0 = \int_0^\infty dn_x \int_0^\infty dn_y \int_0^\infty dn_z \frac{1}{\exp(\omega_x n_x + \omega_y n_y + \omega_z n_z) - 1} \qquad (25)$$

The above integral can be evaluated if we make a change of variables$\beta\hbar\omega_x n_x = x$, etc, giving

$$N - N_0 = \xi(3)\left(\frac{K_B T}{\hbar\omega h_0}\right)^3 \qquad 26$$

Where $\xi(x) = 1 + 2^{-x} + 4^{-x} + \cdots$, ξ is the Riemann zeta function yielding results such as $\xi(3) = 1.202, \xi(3/2) = 2.612$, etc. We can also calculate the transition temperature T^0 c for non-interacting bosons, by setting $N_0 \to \infty$ at the transition. One finds that

$$K_B T_c{}^0 = \hbar\omega_0\left(\frac{N}{\xi(3)}\right)^{1/3}$$

$$K_B = \frac{\hbar\omega_0}{T_c{}^0}\left(\frac{N}{\xi(3)}\right)^{1/3} \qquad (27)$$

Inserting the above expression for the transition temperature into Eq. (26) one finds the T dependence of the condensate fraction for $T < T^0$

$$N - N_0 = \xi(3)\left(\frac{T\hbar\omega_0 \left(\frac{N}{\xi(3)}\right)^{1/3}}{\hbar\omega_0 T_c{}^0} \right)^3$$

$$= N\left(\frac{T}{T_c{}^0}\right)^3 \qquad (28)$$

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c{}^0}\right)^3$$

For the transition temperature and the condensate fraction can be compared with those for an ideal i.e.

$$\mathrm{K_B T_c{}^0} = \frac{2\pi\hbar^2}{\mathrm{m}}\left(\frac{\mathrm{N}}{\mathrm{V}\xi(3/2)}\right)^{3/2} = 3.313\frac{\hbar^2}{\mathrm{m}}\left(\frac{\mathrm{N}}{\mathrm{V}}\right)^{\frac{2}{3}} \qquad (29)$$

For the transition temperature and

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c{}^0}\right)^{\frac{3}{2}} \qquad (30)$$

For the condensate fraction compare Eqs. (25) And Eq. (28) we note that the trapping potential affects the transition temperature and the number of particles in the condensate. For the same total number of atoms, the number of atoms in the ground state is larger in the case of a confined system than a free system [5, 13]. In such harmonic trapping potentials the conditions for Bose-Einstein condensation can be calculated. For a gas trapped in 3D the critical temperature is given by

$$T_c = \frac{T\hbar\omega_0}{K_B}\left(\frac{N}{1.202}\right)^{\frac{1}{3}}, \qquad (31)$$

With N the number of atoms [13]. For large number of particles and when the chemical potential μ greatly exceeds the level spacing of the trap the quantum pressure, i.e. the kinetic energy term for many properties of BECs it is useful to examine the possible approximations of the GP- equation. To do so, one has to look at the different parts of the total energy of the system. It can be distinguished in three parts. These are the kinetic, the potential and the interaction energy respectively which are $E_c + E_p + E_i$. From Eq. (16) for the GPE to obtain the equilibrium properties of a Bose-Einstein condensate it is useful to look for the stationary solutions of the GP-Equation. Those can be found by separating the time-dependant solutions in a time-independent part and a time evolution term:

$$\psi(r,t) = \psi(r)e^{\frac{-i\mu t}{\hbar}}, \qquad (32)$$

Where the temporal evolution is fixed by the chemical potential and the stationary GP-Equation
For the wave function (r) then reads:

$$\frac{-\hbar\nabla^2}{2m} + U(r) + g|\psi(r)|^2]\psi(r) = \mu\psi(r) \qquad 33$$

Then neglecting $E_c = \frac{-\hbar\nabla^2}{2m}$ this regime is called Tomas-Fermi (TF) regime within the TF [1] regime the stationary GPE becomes

$$|\psi(r)|^2 = \frac{\mu - U(r)}{g} \qquad 34$$

$$|\psi(r)|^2 = \begin{cases} \frac{\mu - U(r)}{g} & ,if\ \mu - U(r) > 0 \\ zero, & Otherwise \end{cases}$$

The condensate density $|\psi|^2$ assumes a parabolic density profile, or more generally its shape is an inverted potential U(r). In this notation also the role of μ controlling the number of particles becomes immediately clear. Both densities represent the same number of atoms, enabling us to see the influence of the interactions. In the case of the Gross-Pitaevskii equation, the non-linear $|\psi(r)|^2$ term allows the term between square brackets individually to become small, canceling the need for highly oscillatory terms [5].

3.2. Bose-Einstein Condensates as Phase Transitions

An ideal gas consisting of non-interacting Bose particles is a fictitious system since every realistic Bose gas shows some level of particle-particle interaction. Nevertheless, such a mathematical model provides the simplest example for the realization of Bose-Einstein condensation.

This simple model, first studied by A. Einstein [14], correctly describes important basic properties of actual non-ideal (interacting) Bose gas. In particular, such basic concepts as BEC critical temperature T_c (or critical particle density n_c), condensate fraction $N_0 = N$ and the dimensionality issue will be obtained. By neglecting atom-atom interactions the BEC behaves as an ideal gas with all atoms occupying the ground state of the harmonic potential U(r). This case is accurately described by the ground state wavefunction of a three dimensional harmonic trap and the ground state of the system is obtained when setting all non-interacting bosons occupy the lowest single-particle state; there, ψ_0 has the Gaussian profile

$$\phi_0(r) = (\frac{m\omega h_0}{\pi\hbar})^{\frac{3}{4}} \exp\left(\frac{-m}{2\hbar}\left(\omega^2{}_x x^2 + \omega^2{}_y y^2 + \omega^2{}_z Z^2\right)\right) \qquad (35)$$

The ground state of the ideal gas of harmonic trap is then substituting in to the equation of the time independent of GPE. The density distribution of the ground state $|\psi_0(r)|^2$ has a Gaussian profile and grows linearly with N. In contrast, the size of the condensed cloud is independent of N and is determined by the harmonic oscillator length

$$ah_0 = \sqrt{\frac{\hbar}{m\omega h_0}}, \qquad (36)$$

Which is the average width, the individual condensate widths $\sigma_i = ah_0, i = \sqrt{\frac{\hbar}{m\omega i}}$, where i = x, y, z can then be used to determine the momentum spread using the Heisenberg uncertainty principle

$$\sigma_{P,i} = \frac{\hbar}{\sigma i} = \frac{\hbar}{ah_0} = \sqrt{\hbar m\omega i} \qquad (37)$$

By using $E_{rel} = \frac{P^2}{2m}$ the average release energy for a non-interacting condensate can be calculated and is independent of N

$$E_{rel} = \frac{1}{2}\hbar\left(\omega_x{}^2 + \omega_y{}^2 + \omega_z{}^2\right) \qquad (38)$$

The theoretical description of Bose-Einstein condensation does not need a special trapping geometry. It was in fact formulated first for uniform systems. For dilute atomic gases in practice however some kind of trap is needed, to keep the atoms thermally isolated from their environment. In this case, the trapping scheme generally relies on the magnetic interaction of the atom's magnetic moment with an external magnetic field. Most of these traps provide harmonic confinement with axial symmetry [29].

3.3. Excited State Population in Harmonic Traps

The Bose-Einstein statistic gives the probability that in a system of temperature T a particle populates a state of energy ϵ,

$$n(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)-1}} \qquad (39)$$

As we treat the ground state separately, it is adequate to compute the maximum number of thermal particles at a given temperature in the continuum approximation

$$N_T^{max} = \int d\epsilon \frac{1}{e^{\beta\epsilon-1}} \qquad (40)$$

The critical particle number at a given temperature is defined by

$$N_c = N_T^{max}(T) \qquad (41)$$

In a harmonic trap one can write explicitly the energy dependence of the density of states, which for any dimensional system with axial symmetry is

$$\rho_{(\varepsilon)}^{(d)} = \Omega_d\left(\frac{L}{2\pi}\right)^d \frac{1}{2}(\frac{2m}{\hbar^2})^{\frac{d}{2}}\varepsilon^{\frac{d}{2}-1}, \qquad (42)$$

Where $$\Omega_d = \begin{cases} 4\pi, (d = 3); \\ 2\pi, (d = 2); \\ 1, (d = 1). \end{cases}$$

For temperatures K_BT one can replace the sum over the excited states by an integral (this approximation is called the semi-classical approximation), and as $(\epsilon) = 0 for\ \epsilon = 0,$, one can take this integral from $0\ to\ \infty$. The population of the excited states for 3D system is

$$\rho_{(\varepsilon)}^{(3)} = \frac{V}{4\pi^2}(\frac{2m}{\hbar^2})^{\frac{3}{2}}\varepsilon^{\frac{1}{2}}\ Then\ we\ have$$

$$N_{exc} = \int_0^\infty \rho(\epsilon)n(\varepsilon)d\epsilon \quad (43)$$

$$N_{exc} = \frac{V}{4\pi^2}(\frac{2m}{\hbar^2})^{\frac{3}{2}}\int_0^\infty \sqrt{\varepsilon}\frac{d\epsilon}{e^{\beta\epsilon-1}}$$

We can evaluate the energy integral using the relation, $\frac{1}{e^{\beta\epsilon-1}} = \sum_{n=1}^{\infty} e^{-nx}, where\ x = \beta\epsilon$:

$$\int_0^\infty \sqrt{\varepsilon}\frac{d\epsilon}{e^{\beta\epsilon-1}} = \beta^{\frac{-3}{2}}\int_0^\infty \sum_{n=1}^{\infty} e^{-nx}x^{\frac{1}{2}}dx = \beta^{\frac{-3}{2}}\sum_{n=1}^{\infty} n^{\frac{-3}{2}}\int_0^\infty e^{-t}\sqrt{t}dt = \beta^{\frac{-3}{2}}\xi(\frac{3}{2})\Gamma(\frac{3}{2}) \quad (44)$$

Where $\xi\left(\frac{3}{2}\right) = \sum_{n=1}^{\infty} n^{\frac{3}{2}}\ and\ \Gamma\left(\frac{3}{2}\right) = \int_0^\infty e^{-t}\sqrt{t}dt$ then substituting this equation in to Eq. (43) it gives as

$$N_{exc} = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\beta^{\frac{-3}{2}}\xi\left(\frac{3}{2}\right)\Gamma\left(\frac{3}{2}\right) \quad or \quad (45)$$

$$N_{exc} = \left(\frac{K_BT}{\hbar\omega h_0}\right)g_3(e^{\beta\mu}),$$

Where $g_3(Z)$ is the BEC critical condition expressed in terms of the Bose function $g_p(Z)$ defined by

$$g_p(Z) = \frac{1}{\Gamma(p)}\int_0^\infty dx x^{p-1}\frac{1}{Z^{-1e^x-1}} = \sum_{l=1}^{\infty}\frac{Z^l}{lp}, \quad (46)$$

$$\text{And } g_3(Z) = \sum_n \frac{Z^3}{n^3},$$

Where $Z = e^{\beta\mu}$ is a fugacity and $\Gamma(p) = (p-1)$. The energy integral for uniform 3D, 2D and 1D system are then reduced to the Bose function of $Z = 1$ and $p = 3/2, p = 1$ and $p = 1/2$ respectively. As μ is negative for all $T \neq 0$ is smaller than 1 and $g_3\left(e^{\beta\mu}\right)$ smaller than $g_3(1) \approx 1.202$. This means that the population of the excited states N_{exc} has an upper bound:

$$N_{Texc}^{max} = 1.202\left(\frac{K_BT}{\hbar\omega h_0}\right)^3 \quad (47)$$

This is the maximal population of the excited states for a given temperature T. To obtain the BEC critical density for 3D system is give as

$$n_c = \frac{N_{exc}}{V} = \frac{1}{4\pi^2}\left(\frac{2m}{\beta\hbar^2}\right)^{\frac{3}{2}}\xi\left(\frac{3}{2}\right)\Gamma\left(\frac{3}{2}\right) \cong 2.612\frac{1}{\lambda_{T_c}^3} \quad (48)$$

From these the simplest way to include repulsive interaction is the mean field. Assuming that all the effects of interaction can be described by all s wave scattering length one can generalized equation

$$n(\epsilon) = \int\frac{d^3k}{2\pi^3}\frac{1}{e^{\beta(\epsilon-\mu)}} = \frac{1}{\lambda^3}g_{\frac{3}{2}}(Z).$$

The simplest way to include repulsive interaction is the mean field. The critical density number

$$n = \frac{1}{\lambda^3}g_{\frac{3}{2}}\left(e^{\beta(\mu-\Delta\mu)}\right),$$

is a simple consequence of the Hartree-Fock approximation using a pseudo potential to a, in which the shift of the single particle energies is give by $\sum H_F = 2g_n$. The factor of two comes from exchange. Since $\sum H_F$ is the independent of momentum we have to increase the chemical potential by $\Delta\mu$ to keep the same particle

density as the ideal gas. Because the Hartree-Fock self energy depends on the density it is more complicated than in the non-interacting case and the equation $\mu - \Delta\mu = 0$ is non linear.
This means that BEC occurs when the inter particle distance becomes comparable to the deBroglie wave length of the particle at a given temperature. For generally the density of the thermal boson in the trap $n_{th}(r) = \frac{g_{\frac{3}{2}}}{\lambda_{dB}^3 Z}$, for the corresponding peak density $n_0 = n_{th}(r=0)$. In free phase space density is $\rho_c = 2.612$. When the temperature is lower than T_c or equivalent the density is larger thann_c, the mixture of the condensate at $\epsilon_0 = 0$ is single particle ground state and the thermal population at $\epsilon > 0$single particle ground state is formed $n = \frac{2.612}{\lambda_T^3} + n_0$.

3.4. Bose-Hubbard Model

While a Bose-Einstein condensate must occur even for a non-interacting system because of the Bose-Einstein statistics, systems with interaction also show Bose-Hubbard Model (BHM) is a kind of phase transition. To study the general concepts of quantum phase transitions is the Bose-Hubbard Model. The Bose-Hubbard Hamiltonian was first studied by Fisher et.al [31] in 1989 and reads:

$$H_B = H_t + H_\varepsilon + H_{u,}$$

$$H_B = \frac{-\omega}{U}\left(\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i\right) - \mu \sum_i \hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \quad (49)$$

Here H_t is the kinetic, $H_\varepsilon$is the site population and H_u is appropriate interaction. $\hat{b}_i^\dagger$ and $\hat{b}_i$ are creation and annihilation operators for bosons at site $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ being the occupation number operator at the same site. The creation and annihilation operators act on the eigenstates of the single-site occupation number operator, satisfies the Fock space. To verify the Hamiltonian H_B is invariant under a global U (1) phase transformation under which $\hat{b}_i \to e^{i\phi}$. The first term is called the hopping term and describes the hopping of the particles from one site to its nearest site $\langle i, j \rangle$ denotes that we sum up only over pairs of nearest neighbors. Hence accounting for the delocalization of particles in the lattice this is the kinetic term of the Hamiltonian. The last term is the on-site repulsion denoting the repulsion between two particles at the same site. The chemical potential μ allows controlling the total density of particles in the system. Comparing the hopping and the on-site repulsion we can see that, while the former favors states in which the particles are delocalized throughout the lattice, the latter makes multiple occupied sites energetically expensive and favors states in which the particles are well localized. We can expect that both terms will compete in the intermediate coupling regime, when μ is small enough, and, following the arguments presented in the introduction, we can expect a quantum phase transition. However, before going into a mean-field analysis of H_B, which will allow us to verify that this is indeed the case, it is instructive to analyze the two limits $\frac{\omega}{U} \to \infty$ (where on-site repulsion dominates) and $\frac{\omega}{U} \to 0$ (where hopping dominates).

3.5. Limit at Zero Hopping

In the limit $\frac{\omega}{U} \to 0$the Hamiltonian reduces to

$$H_B = \frac{-\omega}{U}\left(\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i\right) - \mu \sum_i \hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \quad (50)$$

This Hamiltonian is just a sum of single-site Hamiltonian and therefore the ground state is just the tensor product of well defined single-site eigenstates. We can therefore look at a single site by considering a state with n_0 particles at this site; we get an energy contribution of this site like

$$E_{ss}^n = \frac{U}{2} n_0(n_0 - 1) - \mu n_0. \quad (51)$$

This would be minimal for $n_0/2 = \frac{1}{2} + \frac{\mu}{U}$ but casted to an integer value, meaning that the value of n_0 changes only for integer values of $\frac{\mu}{U}$. As this result is independent of the lattice site, we know that we have a commensurate filling of the lattice and the total density would be pinned at an integer value for a whole range of the chemical potential. To introduce the $\hat{b}_q^\dagger$ q and $\hat{b}_q$ as the creation and annihilation operators for particles at momentum q, which are given by the Fourier transform of the corresponding real space operators as

$$\hat{b}_q^\dagger = \frac{1}{\sqrt{M}}\sum_{i=1}^{M}\hat{b}_i^\dagger e^{-iqri}, and\ \hat{b}_q = \frac{1}{\sqrt{M}}\sum_{i=1}^{M}\hat{b}_i e^{iqri} \qquad (52)$$

When M denotes the total number of sites the expectation values of $\hat{n}_q = \hat{b}_i^\dagger\hat{b}_q$

$$\hat{n}_q = \langle \hat{n}_q = \hat{b}_i^\dagger\hat{b}_q\rangle = \frac{1}{\sqrt{M}}\sum_{i=1}^{M}\hat{b}_i^\dagger e^{-iqri}\cdot\frac{1}{\sqrt{M}}\sum_{i=1}^{M}\hat{b}_i e^{iqri}\,(\hat{n}_q = \hat{b}_i^\dagger\hat{b}_q)_{gs} = \frac{1}{M}\langle\sum_{i,j=1}^{M}\hat{b}_i^\dagger\hat{b}_j\, e^{iq(r_i-r_j)}\rangle_{gs}. \qquad (53)$$

The sum and the phase factor can be taken out of the expectation brackets, such that we get the sum over the expectation values $\langle\hat{b}_i^\dagger\hat{b}_q\rangle_{gs}$ but this would be zero for $i \neq j$, as the ground state is product of single-site wave functions, hence it follows

$$\langle\hat{b}_i^\dagger\hat{b}_q\rangle_{gs} = \frac{1}{M}\sum_{i,j=1}^{M} n\delta_{ij}\, e^{iq(r_i-r_j)}, \qquad (54)$$

For $i = j = \delta_{ij} = 1\ and\ e^{iq(r_i-r_j)} = e^0 = 1$

$$\frac{1}{M}\sum_{i,j=1}^{M} n = n, \qquad (55)$$

And n has no index. This expectation value is independent of q and hence every momentum is covered with the same weight which denotes the total delocalization in fourier space and therefore the strict localization in real space.

3.6. Limit at Dominant Hopping

In this case the Hamiltonian of Eq. (49) reduces to

$$H_{hopp} = -\omega\sum_{\langle i,j\rangle}(\hat{b}_i^\dagger\hat{b}_j + \hat{b}_j^\dagger\hat{b}_i) \qquad (56)$$

It means that $\frac{\omega}{U} \to \infty$. We will first rewrite this Hamiltonian in Fourier space. For that we need the Fourier-back-expansion

$$\hat{b}_i^\dagger = \frac{1}{M}\sum_{i=1}^{M}\hat{b}_q^\dagger\, e^{iqri}, \qquad and\ \hat{b}_i = \frac{1}{M}\sum_{i=1}^{M}\hat{b}_q\, e^{-iqri} \qquad (57)$$

Then the expectation value of $\hat{b}_i^\dagger\hat{b}_q$q using the Fourier space this would be given as

As we consider only nearest neighbors, we can write,$r_j = r_i + \hat{a}$, where $\hat{a}$ is a unitary vector connecting nearest-neighbor sites. The summation over i would then give us $M\times\delta_{qk}$ and the left phase factor with $\hat{a}$ just can be expressed as a cosine

$$H_{hopp} = -\omega\sum_{q,k,\hat{a}}(\hat{b}_q^\dagger\hat{b}_q\delta(q-k)(e^{-ik\hat{a}} + e^{ik\hat{a}}) = -2\omega\sum_{q,\hat{a}}\hat{n}_q(q\hat{a}) \qquad (59)$$

A system of free Bosonic particles will, at $T = 0$, form a perfect condensate and hence all particles would occupy the state with lowest available energy. As ω is positive the ground state of this Hamiltonian would be at $q = 0$ and therefore the particles occupying the ground state would have zero momentum $\langle\hat{b}_q^\dagger\hat{b}_q\rangle_{gs} = \delta_{\vec{q},\vec{0}}$, only one momentum contributes and hence they are well localized at one particular point in momentum space. This means, the particles in this state are spread out over the whole lattice in real space and they have a constant phase equal for all i phase coherence.

3.7. Phase Transitions in Bose Gases

Thermodynamics of Phase Transitions A phase diagram is a representation typically in a plane of the regions where some substance is stable in a given phase. The axes represent external control variables (intensive parameters), such as pressure, temperature, chemical potential or an external field, or sometimes one extensive variable (volume, magnetization, etc) density is sometimes used in the case of fluids. The different phases are separated by lines, indicating phase transitions, or regions where the system is unstable.

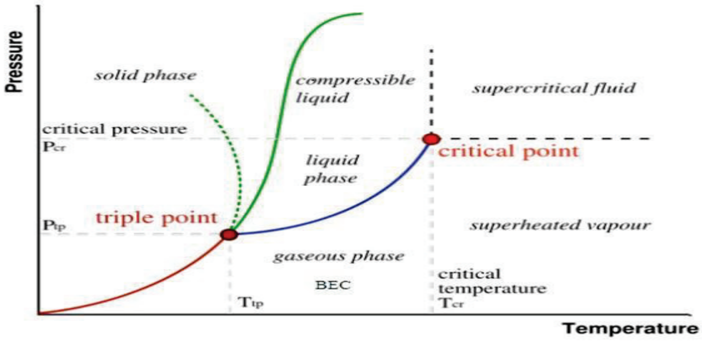

Figure 1: Phase Diagram of State under the $P - T$, the dotted green line gives the anomalous behavior of water, the Clausius-Clapeyron relation can be used to find the relationship between pressure and temperature along phase boundaries.

This graph is the most important features of the phase diagram of a simple substance. The three possible phases (solid, liquid and gas) are separated by first-order phase transition lines (continuous lines in the graph) where two phases coexist at the same time (hence the name coexistence lines). Phases are indicated by their names, and two special points are called T (triple point) and C (critical point). BEC is occurs when the temperature T less than the critical temperature i.e. (T < Tc). In the case of homogenous gas BEC occurs only at$T = 0$. Sublimation line is the solid coexists with the gas. This line exists from zero temperature up to the triple-point temperature, T_{tp}. On lowering the temperature at constant pressure starting from the gas side, the gas would reach the sublimation line, at which crystallites would begin to form until the whole system becomes a crystal [13, 16].

3.8. BKT Phase Transition

The formation of a Bose-Einstein condensate represents the most obvious phase transition in dilute Bose gases, but the internal degrees of freedom can also give rise to other phase transitions. For the spin or Bose gases, the formation of a ferromagnetic or anti ferromagnetic order is an example of a phase transition which shares an important common feature with the onset of a BEC a broken symmetry. The BKT transition is perhaps the most notable example of phase transitions. The transition from the super fluid phase to the normal fluid phase in two dimensions is associated with the unbinding of pairs composed of vortices and anti-vortices. This phase transition is the Berezinskii-Kosterlitz-Thouless (BKT) transition. This is infinite order transition, continuous but no symmetry breaking. At temperatures much below the BKT transition temperature, the phase fluctuations in the quasi-condensate are dominated by the phonons. By the fact that in thermal equilibrium at finite temperature, the free energy $F = E - TS$ must be minimized, it is easy to capture the physical picture of BKT transition.

4. Conclusions

In this paper we have studied different aspects of theoretical study of phase transitions in dilute BEC. BEC, a kind of phase transition is discussed for interacting and non-interacting cases. From the many body Hamiltonian equation neglecting the fluctuation terms, we derived GPE. The mean field approach leads to the GPE which has to be fulfilled by the single-particle wave functions in order to minimize the total energy in the system. In the third chapter we showed BEC of harmonic traps and the Thomas Fermi approximation is calculated by neglecting the kinetic energy term of the GPE. The ground state of an ideal gas in a harmonic trap is then calculated using the time independent of GPE ground state. The BEC of ideal Bose gases is a special case of the generalized BEC phase transition. By studying this exactly solvable model, we can also obtain a deeper insight into the BEC of ideal Bose gases. The Bose-Hubbard Model can be expressed in terms of the mean field approach in the limit at Dominant Hopping and zero Hopping methods. In chapter four, we discussed about phase transition in Bose Gases. A phase transition is the transformation of a thermodynamics system from one phase to the other state of matter. The mean field theory can be applied to a number of physical systems so as to study the phenomena of Berezinskii-Kosterlitz-Thouless transitions.

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