Chapter 3
Ground State Energy

3.1 Introduction

Since the first observations of the Bose-Einstein condensation in trapped gas in 1995 [1,2,3] many theoretical studies of the system have been done [13]. The literature concerning this topic is abundant so it is redundant to repeat it here. The reader is referred to some good reviews [14,15]. Among all theoretical approaches to Bose-Einstein condensation in trapped gas, the most successful one is the Gross-Pitaevskii mean field theory [16] since it is applicable for both statical and dynamical aspects. However, this method is suitable for some forms of the interaction between particles such as the contact potential which can be described by a Dirac-delta function and the strength of the interaction is in the form of s-wave scattering length. Some works have been done in the case of finite range interaction [17,18,19]. The remarkable work is the one by Brosens et al. [7,8] in which the authors successfully use the many-body path integrals developed by Feynman [6] to study thermodynamic properties of the system. However the calculations are long and tedious. In this chapter we show that the density matrix of the distinguishable particles in a harmonic potential with interactions can be derived by using the cumulant expansion. The upper bound of the ground state energy of the system can be estimated variationally by using the Feynman-Jensen inequality. This upper bound is equivalent to the ground energy of the Bose-Einstein condensation of atomic gas in a harmonic trap. The result is in agreement with the variational ground state energy of the same system obtained by Baym and Pethick [20] using the Gross-Pitaevskii equation.

3.2 Approximate Density Matrix

In order to compare our result to the aforementioned work we use the model Lagrangian of the N-particle system in an anisotropic trap. According to the many-body theory the two-body interaction between particles should be represented by the T-matrix in which the effects of other particles in the system are taken into account. However, because of the diluteness of the system and the fact that the system is at a very low temperature, we can approximate the interaction by a contact potential which is in the form of the Dirac-delta function. The strength of the interaction is characterized by a, the s-wave scattering length. We then write the Lagrangian,

$$\mathcal{L} = \sum_{i=1}^{N} \frac{1}{2} \dot{\vec{r}}_i^{\,2} + \frac{1}{2} \sum_{i=1}^{N} \left[\omega_\perp^2 \left(x_i^2 + y_i^2 \right) + \omega_z^2 z_i^2 \right] + 4\pi a \sum_{i=1}^{N} \sum_{j=1}^{N} \delta^3 \left(\vec{r}_i - \vec{r}_j \right) \tag{3.1}$$

where we have used the natural unit $\hbar = 1$ and the atomic mass m has been set to unity. Above, $\vec{r}_i$ and $\vec{r}_j$ are respectively the coordinates of the i^{th} and j^{th} particle; and $\omega_\perp$ and ω_z are the trap frequency in the radial and axial direction respectively. This is effectively the form of the potential used in the first observation by Cornell and Wieman group [1,2,3].

The imaginary-time path integral relevant to this Lagrangian cannot be solved exactly. So we use the variational path integral technique [21] which is normally used for estimation of the ground state energy [22]. Introduce the trial action to be that of the harmonic oscillator with radial and axial frequency $\Omega_\perp$,

Ω_z serving as variational parameters,

$$\mathcal{L}_\circ = \sum_{i=1}^{N} \frac{1}{2}\dot{\vec{r}}_i^{\,2} + \frac{1}{2}\sum_{i=1}^{N}\left[\Omega_\perp^2\left(x_i^2+y_i^2\right)+\Omega_z^2 z_i^2\right]. \tag{3.2}$$

Since the path integral for this Lagrangian can be solved analytically [21], the density matrix of the N-particle system is conveniently expressed as

$$\rho\left(\bar{r}',\beta|\bar{r},0\right) = \int_{\bar{r}}^{\bar{r}'} \mathcal{D}[\bar{r}]\, e^{-S} = \rho_\circ\left(\bar{r}',\beta|\bar{r},0\right)\left\langle e^{-(S-S_\circ)}\right\rangle \tag{3.3}$$

where $\bar{r}$ represents the set of coordinates of N particles, namely $\bar{r} = \{\vec{r}_1, \vec{r}_2, ..., \vec{r}_N\}$. The trial density matrix derived from Eq.(3.2) is

$$\rho_\circ\left(\bar{r}',\beta|\bar{r},0\right) = \prod_{i=1}^{N}\rho_\circ\left(\vec{r}_i',\beta|\vec{r}_i,0\right) \tag{3.4}$$

with the one-dimensional harmonic osciallator with frequency Ω is

$$\rho_\circ\left(x',\beta|x,0\right) = \left(\frac{\Omega}{2\pi\sinh\Omega\beta}\right)^{\frac{1}{2}} \exp\left[-\frac{\Omega}{2}\frac{\left(x'^2+x^2\right)\cosh\Omega\beta - 2x'x}{\sinh\Omega\beta}\right]. \tag{3.5}$$

Above, the Euclidean action is defined as $S = \int_0^\beta \mathcal{L}\, d\tau$ with τ being the imaginary time and $\beta = 1/(k_B T)$; the bracket represents an average of the quantity inside with respect to $S_\circ$, that is $\langle A\rangle = \int \mathcal{D}[\bar{r}] A \exp(-S_\circ) / \int \mathcal{D}[\bar{r}]\exp(-S_\circ)$. Using the cumulant expansion [23] of the $\left\langle e^{-(S-S_\circ)}\right\rangle$ term, the density matrix now takes the form

$$\rho\left(\bar{r}',\beta|\bar{r},0\right) \approx \rho_\circ\left(\bar{r}',\beta|\bar{r},0\right) e^{\left(-\langle S-S_\circ\rangle - \frac{1}{2}\left(\left\langle (S-S_\circ)^2\right\rangle - \langle S-S_\circ\rangle^2\right)+\ldots\right)}. \tag{3.6}$$

If we keep only the first term in the exponent which is called the first cumulant, we obtain the approximate density matrix as

$$\begin{aligned}\rho\left(\bar{r}',\beta|\bar{r},0\right) \;\approx\;& \rho_\circ\left(\bar{r}',\beta|\bar{r},0\right)\exp\left[-\int_0^\beta d\tau\left\{\sum_{i=1}^{N}\frac{m}{2}(\omega_\perp^2-\Omega_\perp^2)\left\langle x_i^2+y_i^2\right\rangle\right.\right.\\ &\left.\left.+\frac{m}{2}(\omega_z^2-\Omega_z^2)\left\langle z_i^2\right\rangle + 4\pi a\sum_{i=1}^{N}\sum_{j=1}^{N}\left\langle \delta^3\left(\vec{r}_i-\vec{r}_j\right)\right\rangle\right\}\right].\end{aligned} \tag{3.7}$$

Now we have to calculate the quantities $\langle x_i^2 + y_i^2 \rangle$, $\langle z_i^2 \rangle$ and $\left\langle \delta^3 \left(\vec{r}_i - \vec{r}_j \right) \right\rangle$ which can be done by using the generating functional technique [21]. For the first two quantities, the result is standard, that is,

$$\begin{aligned} \left\langle x_i^2 (\tau) \right\rangle = \left\langle y_i^2 (\tau) \right\rangle &= \left(\frac{\sinh \Omega_\perp (\beta - \tau) \sinh \Omega_\perp \tau}{m\Omega_\perp \sinh \Omega_\perp \beta} \right) - \left[x_i' \frac{\sinh \Omega_\perp \tau}{\sinh \Omega_\perp \beta} \right. \\ &\quad \left. + x_i \frac{\sinh \Omega_\perp (\beta - \tau)}{\sinh \Omega_\perp \beta} \right]^2 \end{aligned} \tag{3.8}$$

and

$$\left\langle z_i^2 (\tau) \right\rangle = \left(\frac{\sinh \Omega_z (\beta - \tau) \sinh \Omega_z \tau}{m\Omega_z \sinh \Omega_z \beta} \right) - \left[x_i' \frac{\sinh \Omega_z \tau}{\sinh \Omega_z \beta} + x_i \frac{\sinh \Omega_z (\beta - \tau)}{\sinh \Omega_z \beta} \right]^2 . \tag{3.9}$$

As for the average of the interaction potential, we need to show the calculation in more detail. We first express the delta function as a Fourier transform,

$$\left\langle \delta^3 \left(\vec{r}_i (\tau) - \vec{r}_j (\tau) \right) \right\rangle = \int \frac{d^3 k}{(2\pi)^3} \left\langle \exp i\vec{k} \cdot \left(\vec{r}_i (\tau) - \vec{r}_j (\tau) \right) \right\rangle . \tag{3.10}$$

Since $\mathcal{L}_\circ$ is simply the sum of x_i, y_i and z_i terms each having the form of the one-dimensional harmonic oscillator, the integrand in Eq. (3.10) can be expressed as a product of terms like

$$\begin{aligned} \langle \exp ik_x (x_i - x_j) \rangle &= \frac{1}{\int D[\bar{x}] \exp(-S_{\circ x})} \int D[\bar{x}] \exp(-S_{\circ x} + ik_x (x_i - x_j)) \\ &\equiv K_i^- (\Omega)\, K_j^+ (\Omega) \end{aligned} \tag{3.11}$$

where, for simplicity, we have used Ω for both $\Omega_\perp$ and Ω_z depending on which coordinate we are interested in. We denote $\bar{x}$ for the set of coordinates x of N particles and $S_{\circ x}$ is the part of the action involving only the x-coordinate. In Eq. (3.11) we have defined $K_i^\pm (\Omega) = \int D[x_i] \exp(-(S_{\circ x_i} (\Omega) \pm ik_x x_i)) / \int D[x_i] \exp(-S_{\circ x_i} (\Omega))$ which can be evaluated easily if we notice that the exponent of the denominator is just the action of the forced harmonic oscillator with the force defined by

$f^{\pm}(s) = \pm ik\delta\left(\tau - s\right)$. The result is

$$K_{xi}^{\pm}(\Omega) = \exp\left[\pm ik_x\left(\frac{x_i' \sinh\Omega\tau + x_i \sinh\Omega(\beta-\tau)}{\sinh\Omega\beta}\right) - \frac{k_x^2}{m\Omega}\frac{\sinh\Omega(\beta-\tau)\sinh\Omega\tau}{\sinh\Omega\beta}\right]. \tag{3.12}$$

We thus find

$$\begin{aligned}\left\langle\delta^3\left(\vec{r}_i\left(\tau\right) - \vec{r}_j\left(\tau\right)\right)\right\rangle \ = \ & \int\frac{dk_x}{2\pi}K_{xi}^{-}\left(\Omega_\perp\right)K_{xj}^{+}\left(\Omega_\perp\right)\int\frac{dk_y}{2\pi}K_{yi}^{-}\left(\Omega_\perp\right)K_{yj}^{+}\left(\Omega_\perp\right) \\ & \int\frac{dk_z}{2\pi}K_{zi}^{-}\left(\Omega_z\right)K_{zj}^{+}\left(\Omega_z\right),\end{aligned} \tag{3.13}$$

where the k-integrals are simply Gaussian and simple to evaluate, for example,

$$\begin{aligned}\int\frac{dk_x}{2\pi}K_{xi}^{-}\left(\Omega_\perp\right)K_{xj}^{+}\left(\Omega_\perp\right) = \left(\frac{m\Omega_\perp\sinh\Omega_\perp\beta}{4\pi\sinh\Omega_\perp(\beta-\tau)\sinh\Omega_\perp\tau}\right)^{\frac{1}{2}} \\ \times\exp\left[\frac{m\Omega_\perp\sinh\Omega_\perp\beta}{8\sinh\Omega_\perp(\beta-\tau)\sinh\Omega_\perp\tau}\left(\left(x_i'-x_j'\right)\frac{\sinh\Omega_\perp\tau}{\sinh\Omega_\perp\beta} + \left(x_i - x_j\right)\frac{\sinh\Omega_\perp(\beta-\tau)}{\sinh\Omega_\perp\beta}\right)^2\right].\end{aligned} \tag{3.14}$$

The full density matrix $\rho\left(\bar{r}', \beta|\bar{r}, 0\right)$ is obtained by simply substituting Eqs. (3.8), (3.9), (3.13) and (3.14) into Eq. (3.7) and we obtain

$$\begin{aligned}\rho\left(\bar{r}',\beta|\bar{r},0\right) = & \left(\frac{\Omega_\perp}{2\pi\sinh\Omega_\perp\beta}\right)^N\left(\frac{\Omega_z}{2\pi\sinh\Omega_z\beta}\right)^{\frac{N}{2}}\times\exp\left[-\frac{N\Omega_z}{2}\frac{(z'^2+z^2)\cosh\Omega_z\beta - 2z'z}{\sinh\Omega_z\beta}\right] \\ & \times\exp\left[-\frac{N\Omega_\perp}{2}\frac{(x'^2+x^2+y'^2+y^2)\cosh\Omega_\perp\beta - 2x'x - 2yy'}{\sinh\Omega_\perp\beta}\right] \\ & \times\exp\left[-\int_0^\beta d\tau\left\{\sum_{i=1}^N\frac{m}{2}(\omega_\perp^2-\Omega_\perp^2)\left\{2\left(\frac{\sinh\Omega_\perp(\beta-\tau)\sinh\Omega_\perp\tau}{m\Omega_\perp\sinh\Omega_\perp\beta}\right)\right.\right.\right. \\ & -\left(x_i'\frac{\sinh\Omega_\perp\tau}{\sinh\Omega_\perp\beta} + x_i\frac{\sinh\Omega_\perp(\beta-\tau)}{\sinh\Omega_\perp\beta}\right)^2 - \left.\left(y_i'\frac{\sinh\Omega_\perp\tau}{\sinh\Omega_\perp\beta} + y_i\frac{\sinh\Omega_\perp(\beta-\tau)}{\sinh\Omega_\perp\beta}\right)^2\right\} \\ & +\frac{m}{2}(\omega_z^2-\Omega_z^2)\left\{\left(\frac{\sinh\Omega_z(\beta-\tau)\sinh\Omega_z\tau}{m\Omega_z\sinh\Omega_z\beta}\right) - \left(x_i'\frac{\sinh\Omega_z\tau}{\sinh\Omega_z\beta} + x_i\frac{\sinh\Omega_z(\beta-\tau)}{\sinh\Omega_z\beta}\right)^2\right\} \\ & +4\pi a\sum_{i=1}^N\sum_{j=1}^N\left(\frac{m\Omega_\perp\sinh\Omega_\perp\beta}{4\pi\sinh\Omega_\perp(\beta-\tau)\sinh\Omega_\perp\tau}\right)\left(\frac{m\Omega_\perp\sinh\Omega_\perp\beta}{4\pi\sinh\Omega_\perp(\beta-\tau)\sinh\Omega_\perp\tau}\right)^{\frac{1}{2}}\end{aligned}$$

$$\times \exp\left[\frac{m\Omega_\perp \sinh\Omega_\perp\beta}{8\sinh\Omega_\perp(\beta-\tau)\sinh\Omega_\perp\tau}\left((x_i'-x_j')\frac{\sinh\Omega_\perp\tau}{\sinh\Omega_\perp\beta}+(x_i-x_j)\frac{\sinh\Omega_\perp(\beta-\tau)}{\sinh\Omega_\perp\beta}\right)^2\right]$$
$$\times \exp\left[\frac{m\Omega_\perp \sinh\Omega_\perp\beta}{8\sinh\Omega_\perp(\beta-\tau)\sinh\Omega_\perp\tau}\left((y_i'-y_j')\frac{\sinh\Omega_\perp\tau}{\sinh\Omega_\perp\beta}+(y_i-y_j)\frac{\sinh\Omega_\perp(\beta-\tau)}{\sinh\Omega_\perp\beta}\right)^2\right]$$
$$\times \exp\left[\frac{m\Omega_z \sinh\Omega_z\beta}{8\sinh\Omega_z(\beta-\tau)\sinh\Omega_z\tau}\left((y_i'-y_j')\frac{\sinh\Omega_z\tau}{\sinh\Omega_z\beta}+(y_i-y_j)\frac{\sinh\Omega_z(\beta-\tau)}{\sinh\Omega_z\beta}\right)^2\right]\Bigg\}\Bigg] \tag{3.15}$$

3.3 Ground State Energy of BEC

In the limit $\beta \rightarrow \infty$ or temperature goes to zero, the density matrix can be written in the form

$$\rho\left(\bar{r}', \beta | \bar{r}, 0\right) \underset{\beta\rightarrow\infty}{\sim} \phi\left(\bar{r}'\right)\phi^*\left(\bar{r}\right)e^{-E_{gs}\beta}. \tag{3.16}$$

where $\phi\left(\bar{r}\right)$ and E_{gs} are the ground state wave function and energy respectively. The partition function in the zero temperature limit is

$$Z\left(N, \beta\right) \underset{\beta\rightarrow\infty}{\sim} e^{-E_{gs}\beta}. \tag{3.17}$$

We can see from Eq. (3.16) that the coordinate-dependent terms in Eq. (3.5) contribute to the wave functions and the rest contributes to the energy. We now obtain the ground state energy as follows. We first note that we can roughly write

$$e^{-\langle S-S_\circ\rangle} \sim \exp\left[\int_0^\beta d\tau\left(A\left(\tau\right)+B\left(\tau\right)\bar{r}^2\right)\right]. \tag{3.18}$$

In Eq. (3.14) if we expand the exponential terms we see that, the leading terms contribute to $A\left(\tau\right)$ and the rest goes to $B\left(\tau\right)$. To obtain the ground state energy, we use the Feynman-Jensen inequality [20] so that we can estimate an upper bound of the ground state energy as

$$E_{gs} \leq E_\circ + \lim_{\beta\rightarrow\infty}\frac{1}{\beta}\left\langle S-S_\circ\right\rangle', \tag{3.19}$$

where $\langle S - S_\circ \rangle'$ denotes the coordinate-independent part, say $\int_0^\beta d\tau\, A(\tau)$ and $E_\circ = N(\Omega_\perp + \Omega_z/2)$ is the ground state energy corresponding to the density matrix $\rho_\circ(\bar{r}', \beta | \bar{r}, 0)$. The explicit form of $\langle S - S_\circ \rangle'$ is found to be

$$\begin{aligned}
\langle S - S_\circ \rangle' &= \frac{N(\omega_\perp^2 - \Omega_\perp^2)}{\Omega_\perp} \int_0^\beta d\tau \left(\frac{\sinh \Omega_\perp(\beta - \tau) \sinh \Omega_\perp \tau}{\sinh \Omega_\perp \beta} \right) \\
&\quad + \frac{N(\omega_z^2 - \Omega_z^2)}{2\Omega_z} \int_0^\beta d\tau \left(\frac{\sinh \Omega_z(\beta - \tau) \sinh \Omega_z \tau}{\sinh \Omega_z \beta} \right) \\
&\quad + \frac{N(N-1)a}{2} \int_0^\beta d\tau \left(\frac{\Omega_\perp \sinh \Omega_\perp \beta}{\sinh \Omega_\perp(\beta - \tau) \sinh \Omega_\perp \tau} \right) \\
&\quad \times \left(\frac{\Omega_z \sinh \Omega_z \beta}{4\pi \sinh \Omega_z(\beta - \tau) \sinh \Omega_z \tau} \right)^{\frac{1}{2}} ,
\end{aligned} \tag{3.20}$$

where we have used the relations $\sum_{j=1}^N = N$ and $\sum_{j=1}^N \sum_{i=1 \neq j}^N = N(N-1)$ since all the terms are independent of i. In the limit $\beta \to \infty$, Eq. (3.17) becomes

$$\langle S - S_\circ \rangle' \underset{\beta \to \infty}{\approx} N\beta \left(\frac{\omega_\perp^2}{2\Omega_\perp} - \frac{\Omega_\perp}{2} + \frac{\omega_z^2}{4\Omega_z} - \frac{\Omega_z}{4} + \frac{(N-1)\, a \Omega_\perp \Omega_z^{\frac{1}{2}}}{\sqrt{2\pi}} \right) . \tag{3.21}$$

Using Eq. (3.18) together with the contribution from $E_\circ$, we obtained the upper limit of the ground state energy of the system,

$$E_{gs} \leq N \left(\frac{\omega_\perp^2}{2\Omega_\perp} + \frac{\Omega_\perp}{2} + \frac{\omega_z^2}{4\Omega_z} + \frac{\Omega_z}{4} + \frac{N a \Omega_\perp \Omega_z^{\frac{1}{2}}}{\sqrt{2\pi}} \right) , \tag{3.22}$$

which is exactly the same as the result from the mean field method [20]. In fact, in going from Eq. (3.17) to Eq. (3.18) we encounter a mathematical problem. In the last term of Eq. (3.17) the integral diverges at the two ends of the range of integration. However, when $\beta \to \infty$, the integral can be written as (we set $\Omega_\perp = \Omega_z$ for convenience)

$$\lim_{\beta \to \infty} \int_0^\beta d\tau \frac{\sinh \Omega \beta}{(\sinh \Omega(\beta - \tau) \sinh \Omega \tau)^{3/2}} \approx 2\beta + \text{divergent terms.} \tag{3.23}$$

Our experience in mean-field theory suggests that this divergency is corresponding to the quantum correction of the self-energy diagram. This correction is analogue to the correlation energy in the Hatree-Fock approximation. Hence, the result of the ground state energy and its divergency implies that our approximation is equivalent to the mean-field approximation.

Our result shows that the ground state properties of the interacting particles in a harmonic potential can be calculated by using the variational path integral technique. The density matrix can be derived by using the cumulant expansion and the generating functional technique. The upper bound of the ground state energy of the system can be estimated by considering the density matrix at zero temperature and using the Feynman-Jensen inequality. For the contact interaction the ground state energy coincides with the result obtained by using mean field theory [20] for the variational ground state energy of the Bose-Einstein condensation in trapped gas. As our result is obtained by evaluating only the first cumulant in Eq. (3.4), it suggests that the result could be improved by evaluating the second cumulant to give the correction terms which is beyond the mean field approximation. One of the advantages of this method is that it can be applied to various forms of interaction as long as we can calculate the average of the particle coordinates.

However, the application of this method to the system of indistinguishable particles is not valid because to find the partition function we have to do the sum over all permutations,

$$Z = \int d\bar{r}\, \rho\left(\bar{r}, \beta | \bar{r}, 0\right) = \int d\bar{r}\, \frac{1}{N!} \sum_{P} \rho_D\left(P\bar{r}, \beta | \bar{r}, 0\right) \tag{3.24}$$

As discussed in the previous chapter, this can be done only in the case when the density matrix can be expressed as a product of single-particle density matrices.

In our case, however, as pointed out in the previous chapter we cannot write the one particle density matrix explicitly because of the coupling between particles via the interaction terms. Our attempt in obtaining the analytic form of the density matrix for the indistinguishable-particle case thus fails. Nevertheless, the ground state energy we obtained is still correct because at zero temperature the ground state of the distinguishable-particle system coincides with the free energy of the indistinguishable-particle system. The reader is referred to the works by Brosens, Lemmens and Devreese [7,8] for the many-body path integral calculations at finite temperature of both bosons and fermions. The free energy and other thermodynamic properties can also be obtained successfully in those works. However, the calculations are very complicated. Our method thus provides a relatively simple way to study some ground state quantities.