CHAPTER V

PARTITION FUNCTION AND EXCITATION SPECTRUM

5.1 PARTITION FUNCTION

The main work in statistical mechanicial problems is finding a partition function of a system. From a discussion in the chapter II the partition function was defined as

$$Q = Tr\left[e^{-\beta H}\right] = Tr_{\{a^+,a\}} Tr_{\{b^+,b\}} e^{-\beta H} \tag{5.1}$$

with another form of the partition function in path integral formalism as a functional integral of action,

$$Q = \int \prod_q Da_q^* Da_q \int \prod_k Db_k^+ Db_k e^{S/\hbar}. \tag{5.2}$$

Adding the constraint of conservation of the number of particles into the above equation, the partition function for a system of N interacting bosons becomes,

$$Q = \int \prod_q Da_q^* Da_q \int \prod_k Db_k^+ Db_k \frac{1}{\sqrt{2\pi}} \int dy Exp\left[iy(n-N) + \frac{\tilde{S}}{\hbar}\right] \tag{5.3}$$

where, $\frac{1}{\sqrt{2\pi}} \int dy e^{iy(n-N)}$ is a Fourier integral form of $\delta(n-N)$.

Substituting $\tilde{S}$ from the last chapter and separate n into two parts, a new form of Q is derived,

$$Q=\frac{1}{\sqrt{2\pi}}\int\prod_{q}Da_q^{*}Da_q\int\prod_{k}Db_k^{+}Db_k\int dyExp\left[iy\left(|a|^2-N\right)+\frac{\tilde{S}}{\hbar}\right] \tag{5.4}$$

where,

$$\begin{aligned}\tilde{S}=&\frac{1}{\beta V}\int_0^{\beta}\left\{\sum_q\left[a_q^{*}\partial_t a_q+\left(i\omega-\frac{\hbar^2q^2}{2m}\right)a_q^{*}a_q\right]+\sum_k\left[b_k^{+}\partial_t b_k+\left(i\omega-\frac{\hbar^2k^2}{2m}\right)b_k^{+}b_k\right]\right\}dt\\&-\frac{1/2}{(\beta V)^2}\int dt\left\{\sum_q a_q^{*}a_q a_q^{*}a_q g(\bar{q},\bar{q})+2\sum_{k,q}\left[b_k^{+}a_q a_q^{*}a_q g(\bar{k},\bar{q})+h.c.\right]\right\}\\&-\frac{1/2}{(\beta V)^2}\int dt\left\{\sum_{k,q}\left[a_q^{*}a_{-q}^{*}b_k b_{-k}g(\bar{k},\bar{q})+h.c.\right]+2\sum_{k,q}b_k^{+}a_q^{*}b_k a_q g(\bar{k},\bar{k})\right\}\\&-\frac{1/2}{(\beta V)^2}\int dt\left\{2\sum_{k,q}b_k^{+}a_q^{*}b_k a_q g(\bar{q},\bar{q})\right\}\end{aligned} \tag{5.5}$$

From the above equation, it was found the functional Q, is also $\tilde{S}$. Returning to a consideration of the functional $\tilde{S}$, it was found that $\tilde{S}$ consists of some integrals of pure a_q terms and a mixture of a_q and b_k terms.

In the first step, an attempt was made to arrange a number of terms of a_q and b_k to a matrix form. Two new matrix parameters were established:

$$B_k=\begin{bmatrix}-\frac{d}{dt}-\omega_k+\nu & -\gamma_k\\ -\gamma_k^{*} & -\frac{d}{dt}-\omega_k+\nu\end{bmatrix} \tag{5.6}$$

and,

$$f_k = \sum_q \begin{bmatrix} a_q \\ a^*_{-q} \end{bmatrix} \rho(q) g(\vec{k}, \vec{q}) \tag{5.7}$$

where,

$$\omega_k = \frac{\hbar^2 k^2}{2m} + \left(g(\vec{q},\vec{q}) + g(\vec{k},\vec{k})\right)\rho(q), \tag{5.8}$$

$$\gamma_k = \frac{1}{2V}\sum_q a_q a_q g(\vec{k},\vec{q}), \tag{5.9}$$

and

$$\rho(q) = \frac{1}{V}\sum_q a^*_q a_q. \tag{5.10}$$

Then,

$$\begin{aligned} \tilde{S} = &-\frac{1}{2}\int_0^\beta \sum_q \rho^2(q) g(\vec{q},\vec{q}) dt + \frac{1}{V}\int_0^\beta \sum_q \left(a^*_q \frac{\partial a_q}{\partial t} - \frac{\hbar^2 q^2}{2m} a^*_q a_q \right) dt \\ &+ \frac{1}{V}\int_0^\beta \left\{ \sum_k [b^+_k \quad b_{-k}][B_k] \begin{bmatrix} b_k \\ b^+_k \end{bmatrix} \right\} dt + \frac{1}{2V}\int_0^\beta \sum_k \left\{ [b^+_k \quad b_{-k}] f_k + f^*_k \begin{bmatrix} b_k \\ b^+_k \end{bmatrix} \right\} dt \end{aligned} \tag{5.11}$$

and,

$$\begin{aligned} Q = &\int \prod_q D|a_q|^2 Exp\left[-\frac{1}{2\hbar}\int \left(\sum_q \rho(q)^2 g(\vec{q},\vec{q}) + \frac{1}{V}\sum_q a^*_q \frac{\partial a_q}{\partial t} \right) \right] \\ &\times \int \prod_k Db^+_k Db_k Exp\left[\frac{1}{\hbar}\int \frac{dt}{V} \sum_k \left\{ [b^+_k \quad b_{-k}][B_k] \begin{bmatrix} b_k \\ b^+_{-k} \end{bmatrix} + \frac{1}{2}\left([b^+_k \quad b_{-k}] f_k + f^*_k \begin{bmatrix} b_k \\ b^+_{-k} \end{bmatrix} \right) \right\} \right] \end{aligned} \tag{5.12}$$

From here the value of q will be zero while k corresponds to every momentum larger than zero. Using a Guassian integration method [26] the partition function becomes

$$\begin{aligned} Q = &\int D|a_0|^2 Exp\left[-\frac{1}{2\hbar}\int \left(\sum_q \rho_0^2 g(0,0) + \frac{1}{V}\sum_q a^*_0 \frac{\partial a_0}{\partial t} \right) \right] \\ &\times \prod_k [Det[B_k]]^{-1} Exp\left[\frac{1}{\hbar}\int dt \left(f^*_k [-B_k]^{-1} f_k \right) \right] \end{aligned} \tag{5.13}$$

The problem is how to calculate both terms inside the product $\prod_k$ of the above result.

Yarunin [18, 19] has shown the determinant of the matrix M_k

$$\text{where,}\qquad M_k = \begin{bmatrix} -\frac{d}{dt} - x_k & -\frac{z_k}{2} \\ -\frac{z_k^*}{2} & \frac{d}{dt} - x_k \end{bmatrix}$$

$$\text{is}\qquad Det[-M_k]^{-1} = \frac{1}{4}\frac{Exp\left[\frac{\beta}{2}x_k\right]}{Sinh^2\left(\frac{\beta}{4}\left(x_k^2 - |z_k|^2\right)\right)}.$$

Then, the determinant of the research matrix is $\frac{1}{4}\frac{Exp\left[\frac{\beta}{2}(\omega_k - \nu)\right]}{Sinh^2\left(\frac{\beta}{4}\left((\omega_k - \nu)_k^2 - 4|\gamma_k|^2\right)\right)}$

$$\left[Det(-B_k)\right]^{-1} = \frac{1}{4}\frac{Exp\left[\frac{\beta}{2}(\omega_k - \nu)\right]}{Sinh^2\left(\frac{\beta}{4}\left[\left(T_k + \rho(0)\left(g(\vec{k},\vec{k}) + g(0,0)\right) - \nu\right)^2 - \left(\rho(0)\left(\frac{g(\vec{k},\vec{k}) + g(0,0)}{2}\right)\right)^2\right]^{1/2}\right)}$$

$$= \frac{1}{4}\frac{Exp\left[\frac{\beta}{2}(\omega_k - \nu)\right]}{Sinh^2\left(\frac{\beta}{4}\left[\left(T_k + \rho(0)g(0,0) - \nu\right)^2 + 2\rho(0)g(\vec{k},\vec{k})\left(T_k + \rho(0)g(0,0) - \nu\right) + \rho^2(0)\left(g^2(\vec{k},\vec{k}) - g^2(\vec{k},0)\right)\right]^{1/2}\right)} \tag{5.14}$$

where, $T_k = \frac{\hbar^2 k^2}{2m}$.

In the next step, the idea to calculate the last integral in equation (5.13) is evaluated. Consider the matrix B_k which has differentiation operators in diagonal parts. The research system is, surely, closed to thermal equilibrium. Therefore, all terms which depend on time or temperature can be neglected. Thus. it is necessary to replace B_k by C_k

$$C_k = \begin{bmatrix} \omega_k - v & \gamma_k \\ -\gamma_k & -\omega_k + v \end{bmatrix} \tag{5.15}$$

Then,

$$Q = \int \prod_q D|a_0|^2 Exp\left[-\frac{1}{2\hbar}\int\left(\sum_q \rho_0^2 g(0,0) + \frac{1}{V}\sum_q a_0^* \frac{\partial a_0}{\partial t}\right)\right] \\ \times \prod_k \left[Det[B_k]\right]^{-1} Exp\left[\frac{1}{\hbar}\int dt\left(f_k^*[C_k]^{-1} c f_k\right)\right] \tag{5.16}$$

where,

$$c = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Finally, the partition function becomes

$$Q = -i\beta V \int d\rho(0) \int dv Exp\left[\frac{V}{\hbar}\int_0^\beta (\rho(0) - R) v dt - \frac{1}{2\hbar}\int_0^\beta \left(\sum_q (\rho(0))^2 g(0,0)\right) dt\right] \prod_k \Im_k \tag{5.17}$$

where[(1)],

[(1)] E_k is evaluated in section 5.2 by definition of singularities of partition function.

$$\Im_k = \frac{e^{-\frac{\beta}{2}(\omega_k - \nu)}}{4Sinh^2\left\{\frac{\beta}{4}E_k^{(1)}\right\}} Exp\left\{\int_0^\beta \frac{dt}{4}(\rho(0))^2 g(\vec{k},0)\left[\frac{(\omega_k - \nu)\left(\omega_k - \frac{\hbar^2 k^2}{2m}\right) - 2|\gamma_k|^2}{E_k^2 + 3|\gamma_k|^2}\right]\right\} \quad (5.18)$$

Replacing the magnetude of $g(\vec{k},0)$ by $\frac{g(\vec{k},\vec{k}) + g(0,0)}{2}$, the partition function depends on the interaction between condensate particles and the interaction between over condensate particles.

5.2 EXCITATION SPECTRUM

From the partition function of our system we know that its poles shown that excitation spectrum has two poles at

$$Sinh^2\left(\frac{\beta}{4}\left[(T_k + \rho(0)g(0,0) - \nu)^2 + 2\rho(0)g(\vec{k},\vec{k})(T_k + \rho(0)g(0,0) - \nu) + \rho^2(0)\left(g^2(\vec{k},\vec{k}) - g^2(\vec{k},0)\right)\right]^{1/2}\right) = 0 \quad (5.19)$$

Defining E_k as excitation spectrums, then,

$$E_k = \left[(T_k + \rho(0)g(0,0) - \nu)^2 + 2\rho(0)g(\vec{k},\vec{k})(T_k + \rho(0)g(0,0) - \nu) + \rho^2(0)\left(g^2(\vec{k},\vec{k}) - g^2(\vec{k},0)\right)\right]^{1/2} \quad (5.20)$$

and, from the gapless characteristic of the excitation spectrums, it is possible to separate the spectrum into two branches. By the gapless condition it is possible to set the value of E_k when $k=o$ is zero, then

$$E_{k=0} = \left(E_{k=0}\right)^2 = \left[\left(\rho(0)g(0,0)-\nu\right)^2 + 2\rho(0)g(0,0)\left(\rho(0)g(0,0)-\nu\right)\right] \tag{5.21}$$

$$\left(E_{k=0}\right)^2 = \left(\rho(0)g(0,0)-\nu\right)\left(3\rho(0)g(0,0)-\nu\right) \tag{5.22}$$

The parameter ν which satisfies the above condition are $\nu = \rho(0)g(0,0)$ and $\nu = 3\rho(0)g(0,0)$. Substituting ν into equation (5.20), two branches of the excitation spectrum of the research system corresponding to ν are established:

$$E_{k,1} = \left[\left(T_k + \rho(0)g(\vec{k},\vec{k})\right)^2 - \left(\rho(0)g(\vec{k},0)\right)^2\right]^{\frac{1}{2}} \;,\;\; \nu = \rho(0)g(0,0) \tag{5.23}$$

$$E_{k,2} = \left[\left(T_k - 2\rho(0)g(0,0)\right)\left(T_k - 2\rho(0)\left(g(0,0) - g(\vec{k},\vec{k})\right)\right) + \rho^2(0)\left(g^2(\vec{k},\vec{k}) - g^2(\vec{k},0)\right)\right]^{\frac{1}{2}}, \quad \nu = 3\rho(0)g(0,0)$$

Both spectrums are dependent of the interaction between intercondensate particles, $g(0,0)$, and the interaction between the over condensate particles, $g(\vec{k},\vec{k})$. If $g(0,0)$, and $g(\vec{k},\vec{k})$ from chapter 3 are replaced, the final form of $E_{k,1}$ and $E_{k,2}$ becomes

$$E_{k,1} = \left\{\left(\left(\frac{\hbar^2 k^2}{2m}\right) + \frac{2}{(2\pi)^2} CU_0\,\rho(0)\left(\frac{\arctan\left(\frac{k}{2}\right)}{k} - \frac{1}{4+k^2}\right)\right)^2 - \left(\frac{2}{(2\pi)^2} CU_0 \frac{\rho(0)}{4}\left(\frac{\arctan\left(\frac{k}{2}\right)}{k} - \frac{1}{4+k^2} + \frac{1}{4}\right)\right)^2\right\}^{1/2} \tag{5.25}$$

and,

$$E_{k,2}=\left[\left(T_k-2\rho(0)g(0,0)\right)^2+2\rho(0)g(\vec{k},\vec{k})\left(T_k-2\rho(0)g(0,0)\right)+\rho^2(0)\left(g^2(\vec{k},\vec{k})-g^2(\vec{k},0)\right)\right]^{\frac{1}{2}}$$

$$=\left\{\left(\frac{\hbar^2k^2}{2m}\right)^2+\frac{\rho(0)CU_0}{\pi^2}\left(\frac{\arctan\left(\frac{k}{2}\right)}{k}-\frac{1}{4+k^2}-\frac{1}{2}\right)\left(\frac{\hbar^2k^2}{2m}\right)\right.$$

$$-\left(\frac{2\rho(0)CU_0}{(2\pi)^2}\right)^2\left(\frac{\arctan\left(\frac{k}{2}\right)}{k}-\frac{1}{4+k^2}-\frac{1}{16}\right)$$

$$\left.+\left(\frac{\rho(0)CU_0}{(2\pi)^2}\right)^2\left(\left(\frac{\arctan\left(\frac{k}{2}\right)}{k}-\frac{1}{4+k^2}\right)^2-\left(\frac{1}{4}\right)^2\right)\right\}^{\frac{1}{2}} \qquad (5.26)$$

Figures 5.1-5.6, below, show the behaviour patterns of $E_{k,1}$ and $E_{k,2}$ with replacing $\rho(0)$ in equation (5.25) and equation (5.26) by $(2\pi)^{3/2}\,\rho_0$.

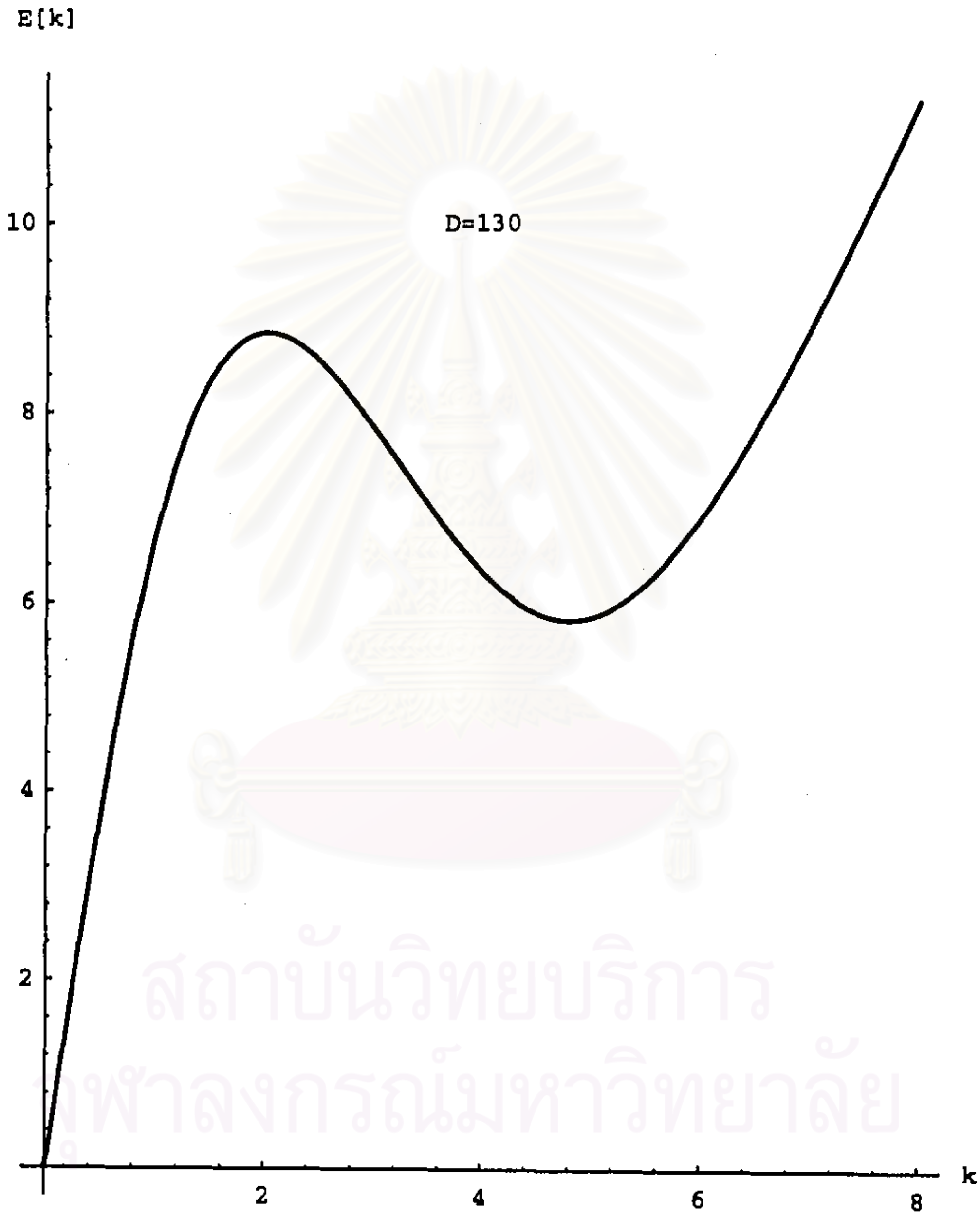

Figure 5.1 The first branch the excitation spectrum of m=4 and $\rho_0 = 130$

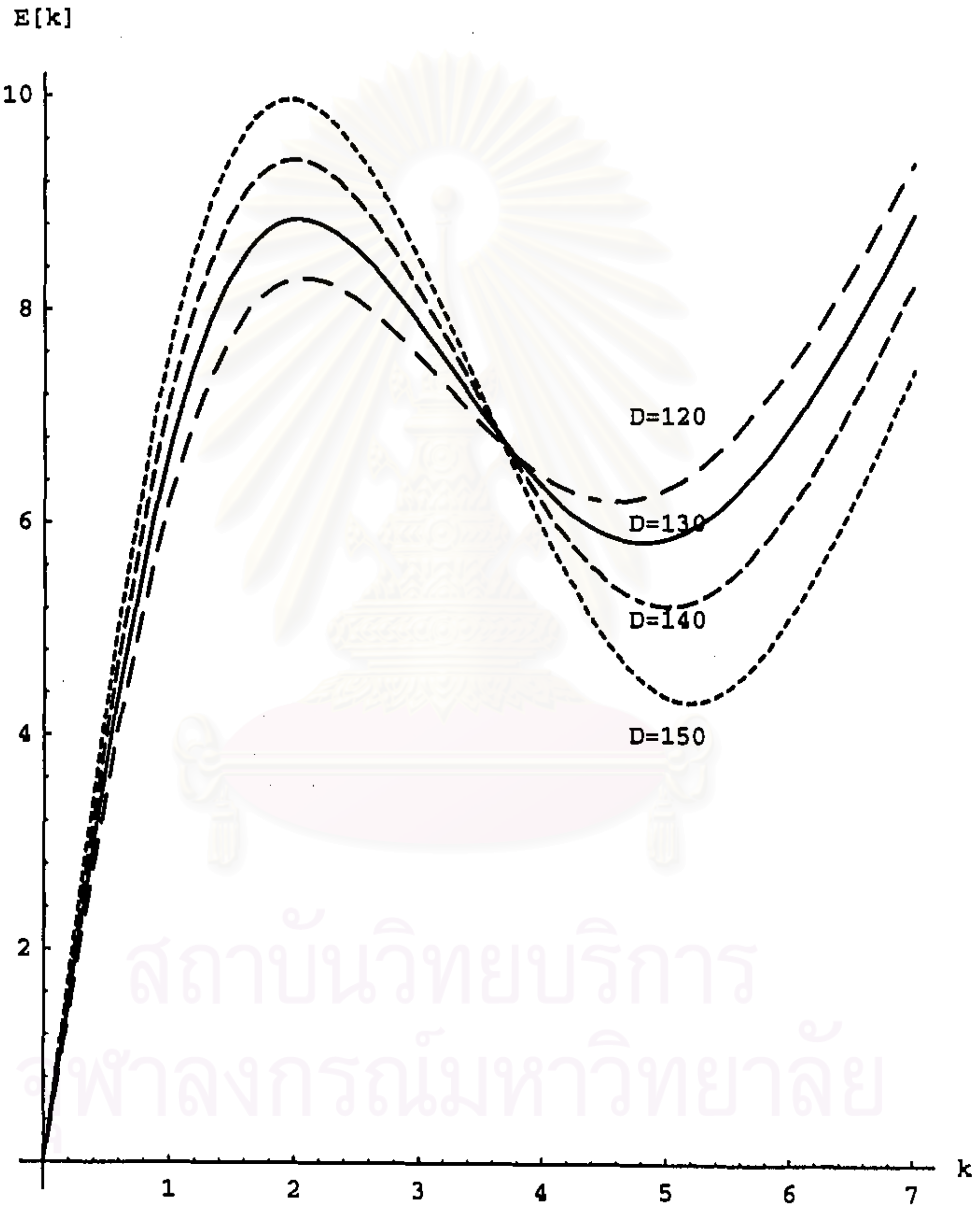

Figure 5.2 The first branch of excitation spectrum of m=4 and $\rho_0 = 120,130,140,150$

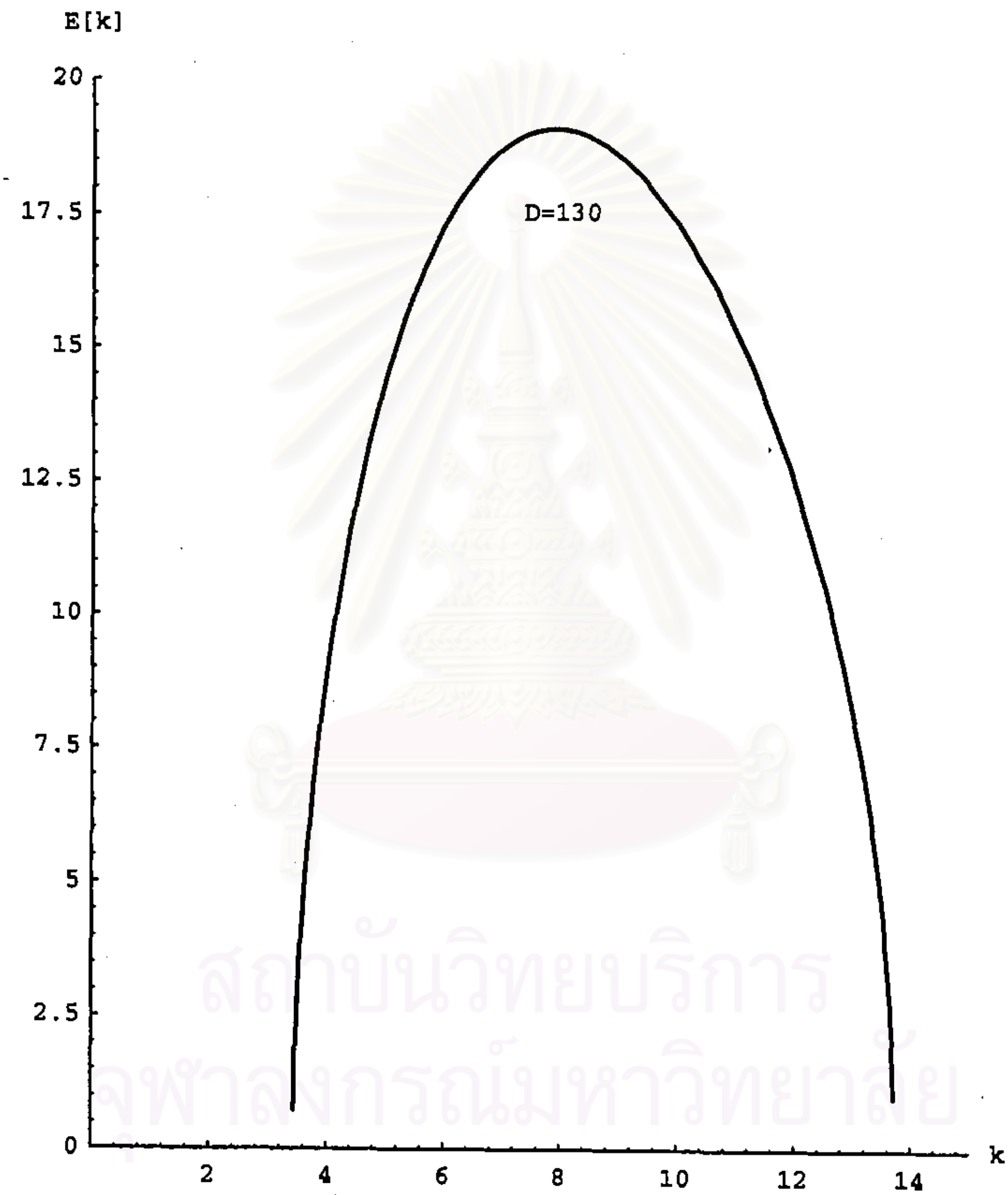

Figure 5.3 The second branch of excitation spectrum of m=4 and $\rho_0 = 130$

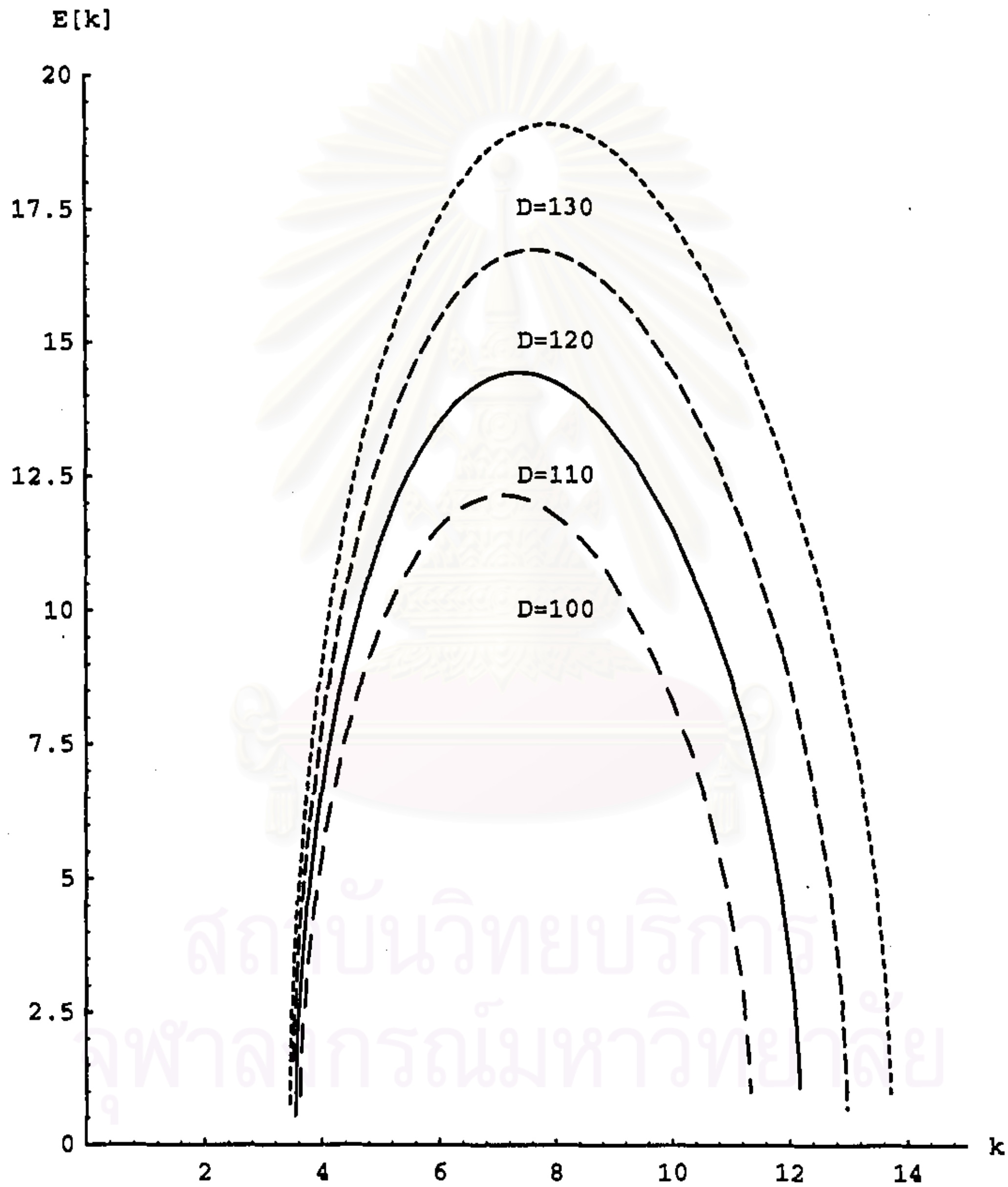

Figure 5.4 The second branch of excitation spectrum of m=4 and $\rho_0 = 100,110,120,130$

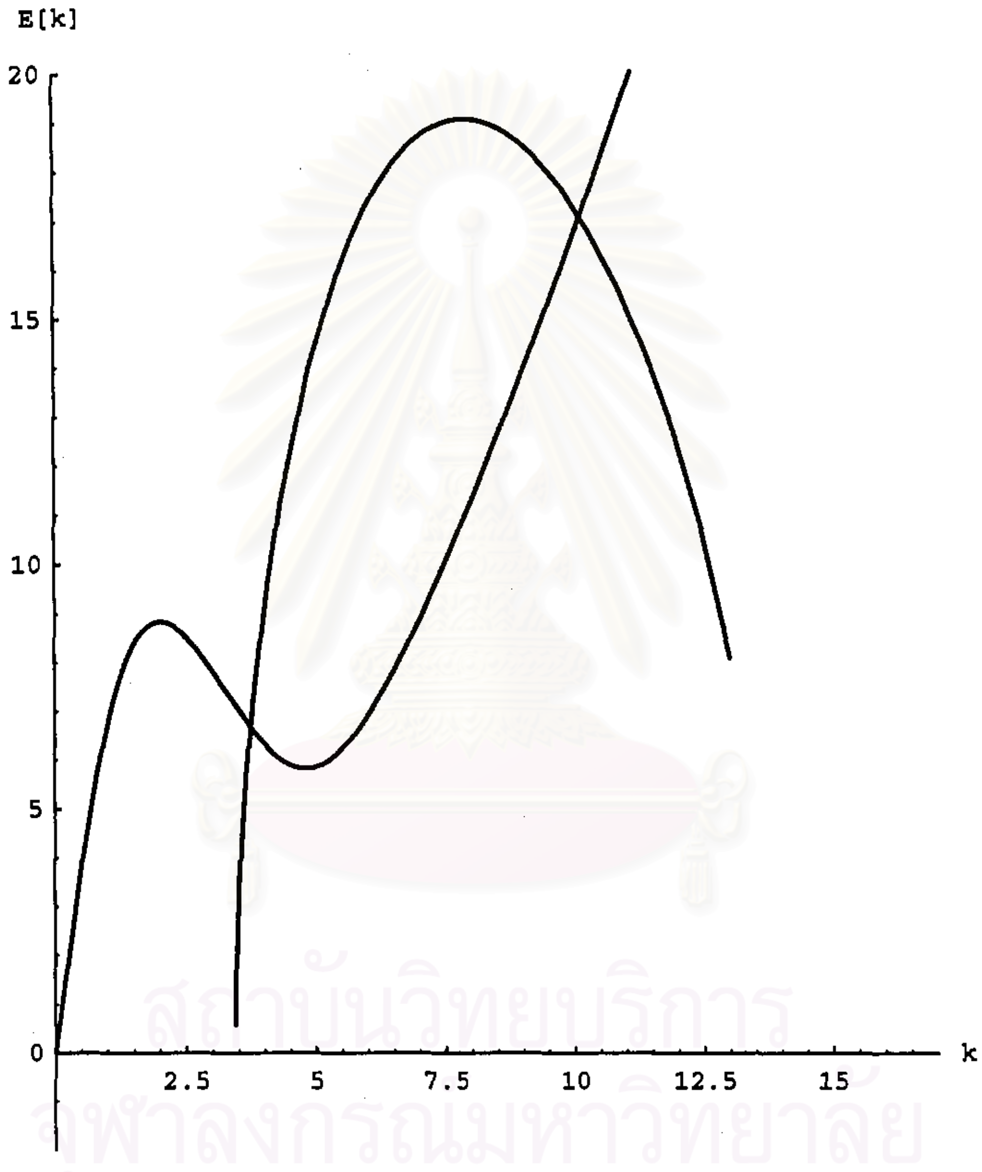

Figure 5.5 The first branch and the second branch of excitation spectrum of m=4 and

$\rho_0 = 130$

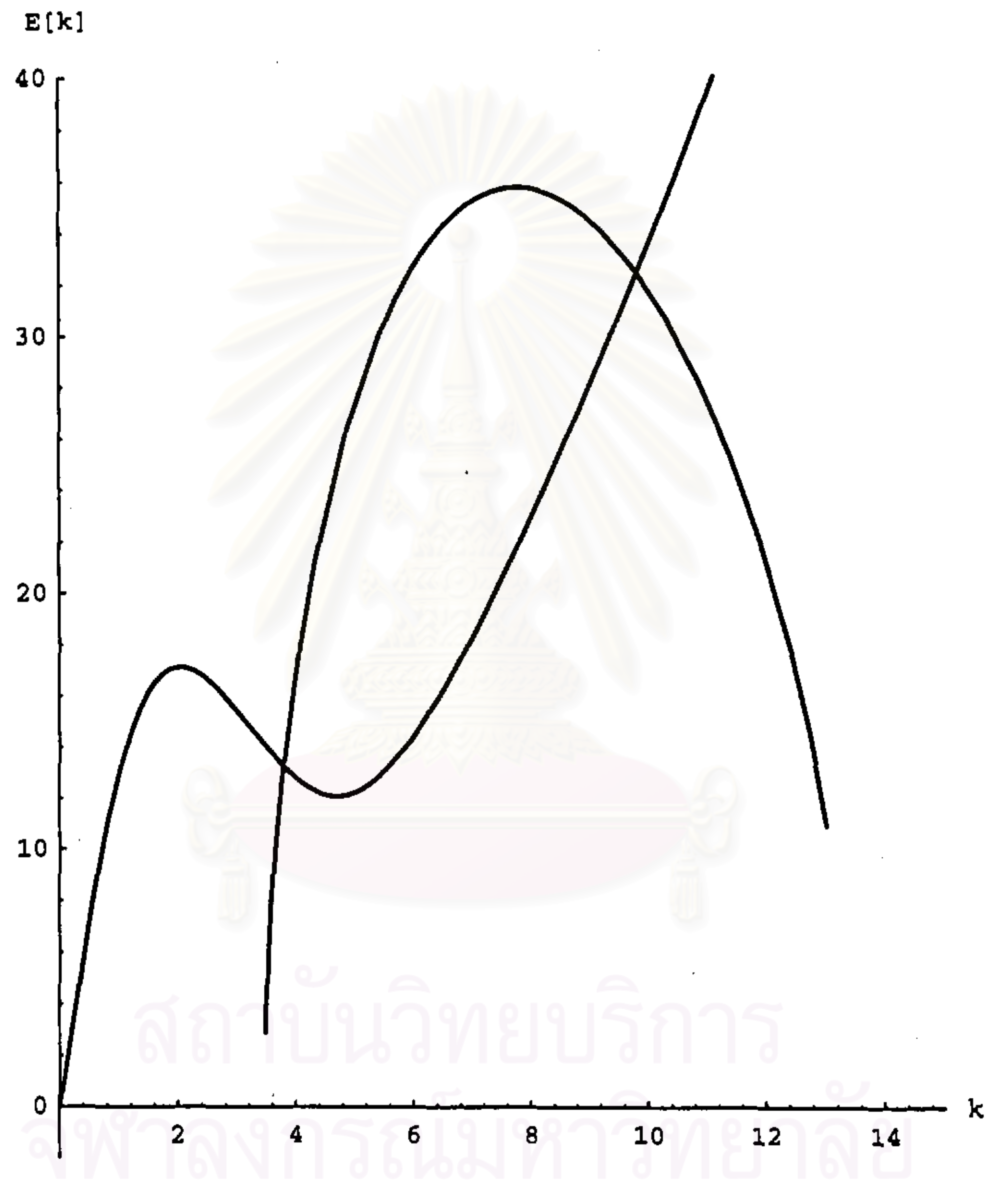

Figure 5.6 The first branch and the second branch of excitation spectrum of m=2 and

$\rho_0 = 250$

It can be seen that $E_{k,l}$ has a similar shape to the excitation spectrums of liquid helium investigated by Landau [9, 10] and Feynman [14, 27]. However, by present research method it is possible to derive the excitation spectrums from the microscopic point of view.

For another branch, it can be seen that it is available at a high momentum regime. The density of ground state particles is the only parameter to characterize the existence of the first and the second branches when we fix the others variables. The first branch requires a large enough density of the ground state particles in the low momentum limit but the second branch exist in any of the density of ground state particles which is lower than the existed density of the first branch.

Finally, the existence of the second in the conditions that the density of the ground state particles is lower than the existed density of the ground state particles of the first branch and the particles occupied high momentum is consistent with the experimental results of Griffin and Glyde [16] and [28, 29].