CHAPTER III

ANSATZ INTERACTION AND ITS INTERESTING PROPERTIES

3.1 INTERACTION POTENTIAL

In this chapter, interaction between particles in the system is considered. However, it should be keep in mind that the Lennard-Jones potential is unsolvable, because the Lennard-Jones potential contains two vital characteristics: strongly repulsive behaviour in the short-range limit and weakly attractive behaviour in the long-range limit. These characteristics give more information about the behaviour of the condensation. The long-range attractive potential is the main reason particles go together in the same state and then build up a state which contains a larger number of particles. Discussion about the long-range attractive interaction and the area of bound state condition follows, since both are aim points in this research.

From the above discussion, some problems were experienced when the original Lennard-Jones potential was used or when the problem was attacked with this type of interaction. Unfortunately, the problem came from the $\frac{1}{r^{12}}-\frac{1}{r^{6}}$ terms, as both terms are very complicated for several operations. Introducing the interaction that contains both characteristics of the above discussion, short-range strongly repulsive interaction and long-range weakly attractive interaction, the function.

$$U(\vec{r}) = CU_0\left(\frac{e^{-\alpha r}}{(\beta r)^2} - \frac{e^{-\alpha r}}{(\beta r)}\right) \tag{3.1}$$

is formulated.

Figure 3.1 shows a comparison graph of behaviours between the function formulated for this research and the original Lennard-Jones function. What is seen in figure 3.1 are the corresponding characteristics the two functions, allowing the use of this function instead of the original Lennard-Jones interaction for this research

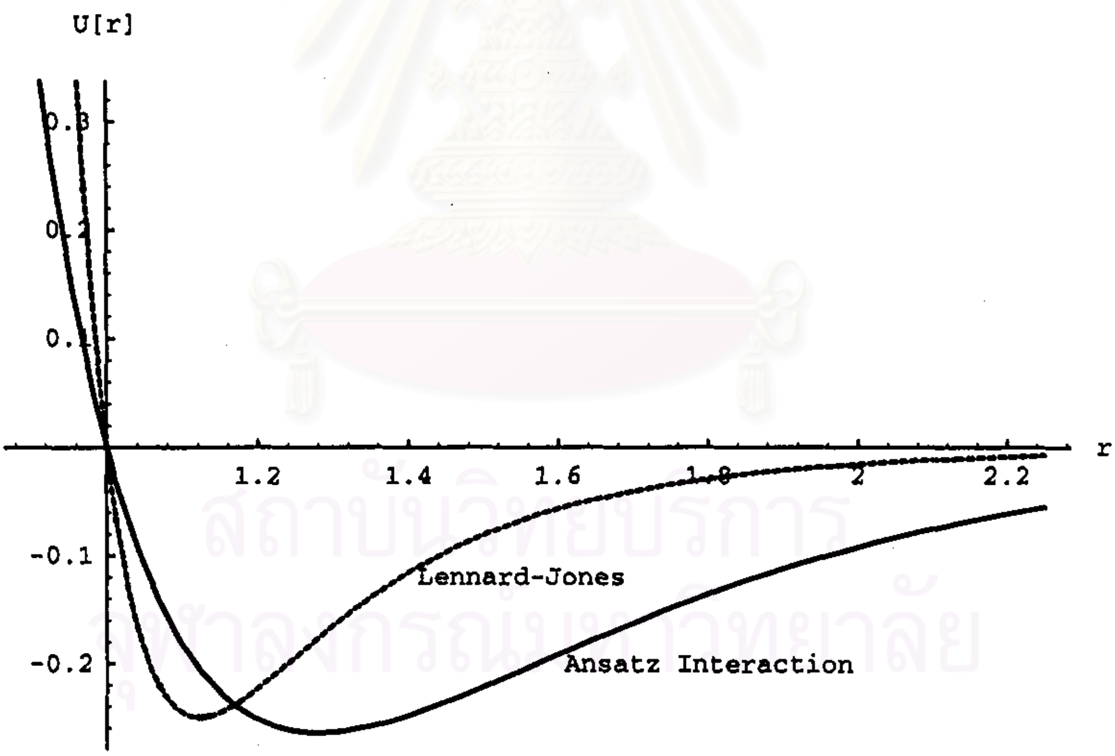


Figure 3.1 An comparison graph of the behaviour of the research function and the Lennard-Jones function

In the next step, an attempt was made to transform an interaction, which is a co-ordinate representation, into momentum representation by the method of Fourier transformation.

From a work of Merzbacher [24] it was found that a simple way of transformation starts with the original Fourier transformation

$$U(\bar{k}) = \frac{1}{(2\pi)^{3/2}} \int U(\bar{r}) e^{i\bar{k}\cdot r} d\bar{r} \tag{3.2}$$

$$= \frac{1}{(2\pi)^{3/2}} \int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} U(r) e^{-ikr\cos\theta} r^2 \sin\theta \, d\phi \, d\theta \, dr$$

$$U(\bar{k}) = \frac{\sqrt{2/\pi}}{k} \int_0^{\infty} U(r) r \sin kr \, dr \tag{3.3}$$

Finally, this gives a relationship of interaction between momentum space and co-ordinated space. Transforming the research interaction into momentum space by the above method $U(\bar{r})$ was replaced by the function,

$$U(\bar{r}) = CU_0 \left(\frac{e^{-\alpha r}}{(\beta r)^2} - \frac{e^{-\alpha r}}{(\beta r)} \right)$$

then

$$U(\bar{k}) = \frac{CU_0\sqrt{2/\pi}}{k} \int_0^{\infty} \left(\frac{e^{-\alpha r}}{(\beta r)^2} - \frac{e^{-\alpha r}}{(\beta r)} \right) r \sin kr \, dr. \tag{3.4}$$

The above equation was calculated thus :

$$U(\bar{k}) = \frac{CU_0\sqrt{2/\pi}}{|\bar{k}|} \left[\int_0^{\infty} \frac{e^{-\alpha r}}{(\beta r)^2} r \sin kr \, dr - \int_0^{\infty} \frac{e^{-\alpha r}}{(\beta r)} r \sin kr \, dr \right]. \tag{3.5}$$

Let
$$U_1(\bar{k}) = \frac{CU_0\sqrt{2/\pi}}{k}\int_0^\infty \frac{e^{-\alpha r}}{(\beta r)^2} r \sin kr dr \tag{3.6}$$

and
$$U(\bar{k}) = \frac{CU_0\sqrt{2/\pi}}{k}\int_0^\infty \frac{e^{-\alpha r}}{(\beta r)} r \sin kr dr . \tag{3.7}$$

For a simplest case, $\alpha = 2$ and $\beta = 1$, therefore,

$$U_1(\bar{k}) = \frac{CU_0\sqrt{2/\pi}}{k}\int_0^\infty \frac{e^{-2r}}{r} \sin kr dr$$

Let $U_1'(\bar{k}) = \int_0^\infty \frac{e^{-2r}}{r} \sin kr dr$ then

$$\begin{aligned}
\mathcal{L}\{U_1'(\bar{k})\} &= \mathcal{L}\left\{\int_0^\infty \frac{e^{-2r}}{r} \sin kr dr\right\} \\
&= \int_0^\infty \frac{e^{-2r}}{r} \mathcal{L}\{\sin kr\} dr \\
&= \int_0^\infty \frac{e^{-2r}}{r} \frac{r}{s^2 + r^2} dr \\
&= \int_0^\infty \frac{e^{-2ys}}{1+y^2} dy \\
&= \int_0^\infty e^{-2ys} d(\arctan y) \\
\mathcal{L}\{U_1'(\bar{k})\} &= \mathcal{L}\left\{\arctan\left(\frac{k}{2}\right)\right\} \\
U_1'(\bar{k}) &= \arctan\left(\frac{k}{2}\right)
\end{aligned}$$

Replacing $U_k'(\bar{k})$ then

$$U_1(\bar{k}) = \frac{CU_0\sqrt{2/\pi}}{k}\arctan\left(\frac{k}{2}\right) \tag{3.8}$$

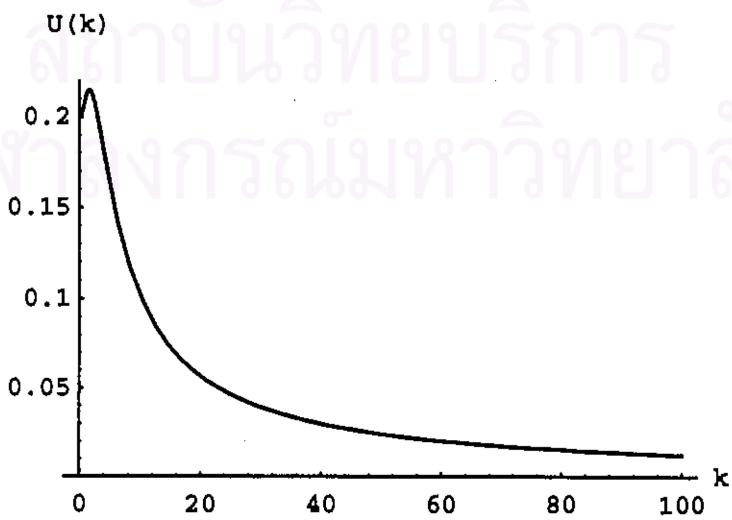
and,

$$U_2(\bar{k}) = -\frac{CU_0\sqrt{2/\pi}}{k}\int_0^{\infty} e^{-2r}\sin krdr$$
$$= -\frac{CU_0\sqrt{2/\pi}}{k}\left(\frac{k}{4+k^2}\right)$$
$$U_2(\bar{k}) = -CU_0\sqrt{2/\pi}\left(\frac{1}{4+k^2}\right) \tag{3.9}$$

Therefore,

$$U(\bar{k}) = CU_0\sqrt{2/\pi}\left(\frac{\arctan\left(\frac{k}{2}\right)}{k} - \frac{1}{4+k^2}\right) \tag{3.10}$$

The behaviour of $U(\bar{k}), U_1(\bar{k})$ and $U_2(\bar{k})$ are illustrated by a set of graphs in figure 3.2, where it can be seen that interaction is always positive in momentum space, and corresponds to the Bogoliubov postulate [15].



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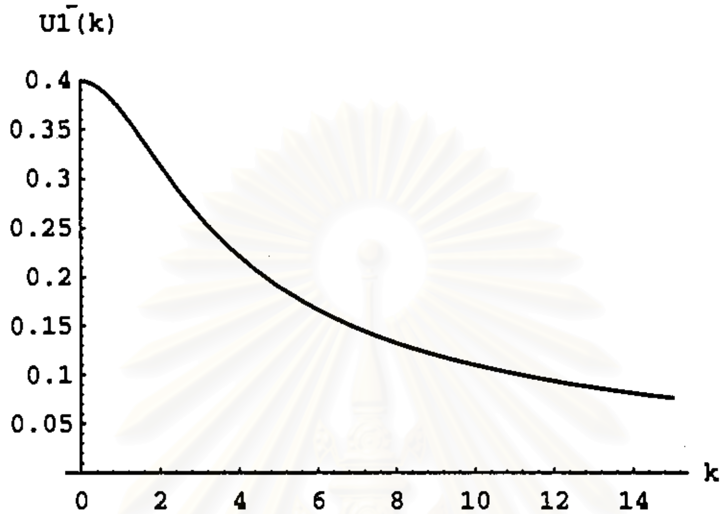

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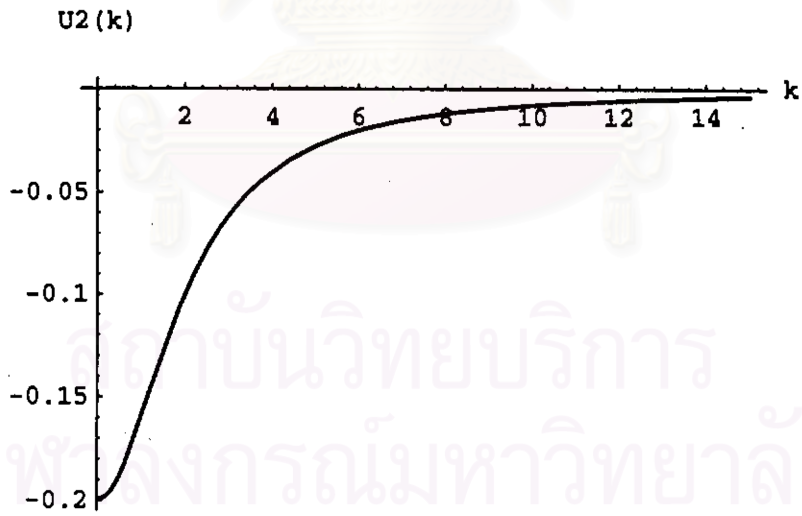

c

Figure 3.2 The transformation interaction in k space

(a) shows the behaviour of $U(\bar{k})$ (b) $U_1(\bar{k})$ and (c) $U_2(\bar{k})$.

3.2 UNIFORM AND NON-UNIFORM MEDIA

If this system is considered in uniform media condition, $\bar{r}$ can be replaced by $(\bar{x}-\bar{y})$. However, the research sytem is in a non-uniform media. Therefore, a method with non-uniform parameters are parametized by uniform parameters.

Defining[(1)] the uniform representation of non-uniform parameters by

$$U(\bar{x},\bar{y})=\frac{1}{2}U(\bar{x}-\bar{y})\left[e^{i\varphi(\bar{x},t)}+e^{i\varphi(\bar{y},t)}\right], \tag{3.11}$$

where $\varphi(\bar{x},t)$ is the configuration function of transformation.

From equationm (3.2), replacing $\bar{r}$ by $(\bar{x}-\bar{y})$, then,

$$U(\bar{k})=\frac{1}{(2\pi)^{3/2}}\int U(\bar{x}-\bar{y})e^{-i\bar{k}\cdot(\bar{x}-\bar{y})}d(\bar{x}-\bar{y}) \tag{3.12}$$

$$U(\bar{k},\bar{s})=\frac{1}{(2\pi)^{3}}\int U(\bar{x}-\bar{y})e^{i\bar{k}\cdot\bar{x}-i\bar{s}\cdot\bar{y}}d\bar{x}d\bar{y}. \tag{3.13}$$

Substituting $U(\bar{x},\bar{y})$ from equation (3.11), gives

$$U(\bar{k},\bar{h})=\frac{1}{(2\pi)^{3}}\frac{1}{2}\int U(\bar{x}-\bar{y})\left[e^{i\varphi(\bar{x},t)}+e^{i\varphi(\bar{y},t)}\right]\left[e^{i\bar{k}\cdot\bar{x}-i\bar{h}\cdot\bar{y}}\right]d\bar{x}d\bar{y} \tag{3.14}$$

$$=\frac{1/2}{(2\pi)^{3}}\int U(\bar{x}-\bar{y})e^{i\varphi(\bar{x},t)}e^{i\bar{k}\cdot\bar{x}-i\bar{h}\cdot\bar{y}}d\bar{x}d\bar{y}+\frac{1/2}{(2\pi)^{3}}\int U(\bar{x}-\bar{y})e^{i\varphi(\bar{y},t)}e^{i\bar{k}\cdot\bar{x}-i\bar{h}\cdot\bar{y}}d\bar{x}d\bar{y} \tag{3.15}$$

Considering the first term of equation (3.15)

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(1) by Yarunin V. S.(1996) from private communication and Yarunin, V. S., Sa-yakanit V. and Nisamaneephong P. to be published

$$U_1(\bar{k},\bar{h}) = \frac{1/2}{(2\pi)^3}\frac{1}{(2\pi)^{3/2}}\int_{-\infty}^{\infty} U(\bar{m})e^{-i\bar{m}\cdot(\bar{x}-\bar{y})}d\bar{m}\int_{-\infty}^{\infty} e^{i\varphi(\bar{x},t)+i\bar{k}\cdot\bar{x}}d\bar{x}\int_{-\infty}^{\infty} e^{-i\bar{h}\cdot\bar{y}}d\bar{y}$$

$$= \frac{1/2}{(2\pi)^3}\int_{-\infty}^{\infty} U(\bar{m})d\bar{m}\int_{-\infty}^{\infty} e^{i\varphi(\bar{x},t)+i(\bar{k}-\bar{m})\cdot\bar{x}}d\bar{x}\frac{1}{(2\pi)^{\frac{3}{2}}}\int_{-\infty}^{\infty} e^{i(\bar{m}-\bar{h})\cdot\bar{y}}d\bar{y}$$

$$= \frac{1/2}{(2\pi)^3}\int_{-\infty}^{\infty} U(\bar{m})\delta(\bar{m}-\bar{h})d\bar{m}\int_{-\infty}^{\infty} e^{i\varphi(\bar{x},t)+i(\bar{k}-\bar{m})\cdot\bar{x}}d\bar{x}$$

$$= \frac{1/2}{(2\pi)^3}U(\bar{h})\int_{-\infty}^{\infty} e^{i\varphi(\bar{x},t)+i(\bar{k}-\bar{h})\cdot\bar{x}}d\bar{x} \tag{3.16}$$

In the same way, the last term of equation (3.15) can be moved to

$$U_2(\bar{k},\bar{h}) = \frac{1/2}{(2\pi)^3}\int_{-\infty}^{\infty} U(\bar{x}-\bar{y})e^{i\bar{k}\cdot\bar{x}}d\bar{x}\int_{-\infty}^{\infty} e^{i\varphi(\bar{y},t)-i\bar{h}\cdot\bar{y}}d\bar{y}$$

$$= \frac{1/2}{(2\pi)^3}\frac{1}{(2\pi)^{3/2}}\int_{-\infty}^{\infty} U(\bar{m})e^{-i\bar{m}\cdot(\bar{x}-\bar{y})}d\bar{m}\int_{-\infty}^{\infty} e^{i\bar{k}\cdot\bar{x}}d\bar{x}\int_{-\infty}^{\infty} e^{i\varphi(\bar{y},t)-i\bar{h}\cdot\bar{y}}d\bar{y}$$

$$= \frac{1/2}{(2\pi)^3}\int_{-\infty}^{\infty} U(\bar{m})d\bar{m}\int_{-\infty}^{\infty} e^{i\varphi(\bar{y},t)+i(\bar{m}-\bar{h})\cdot\bar{y}}d\bar{y}\frac{1}{(2\pi)^{\frac{3}{2}}}\int_{-\infty}^{\infty} e^{i(\bar{k}-\bar{m})\cdot\bar{y}}d\bar{x}$$

$$= \frac{1/2}{(2\pi)^3}\int_{-\infty}^{\infty} U(\bar{m})\delta(\bar{k}-\bar{m})d\bar{m}\int_{-\infty}^{\infty} e^{i\varphi(\bar{y},t)+i(\bar{m}-\bar{h})\cdot\bar{y}}d\bar{y}$$

$$= \frac{1/2}{(2\pi)^3}U(\bar{k})\int_{-\infty}^{\infty} e^{i\varphi(\bar{y},t)+i(\bar{k}-\bar{h})\cdot\bar{y}}d\bar{y} \tag{3.17}$$

Defining
$$A_{k-h} = \left|\frac{1}{(2\pi)^{3/2}}\int e^{i\varphi(\bar{x},t)+i(\bar{k}-\bar{h})\cdot\bar{x}}d\bar{x}\right| \tag{3.19}$$

and
$$\varphi_{k-h} = Argument\left[\frac{1}{(2\pi)^{3/2}}\int e^{i\varphi(\bar{x},t)+i(\bar{k}-\bar{h})\cdot\bar{x}}d\bar{x}\right] \tag{3.20}$$

then,

$$U(\vec{k},\vec{h}) = \frac{1/2}{(2\pi)^3}U(\vec{h})\int e^{i\varphi(\bar{x},t)+i\vec{k}\cdot\bar{x}}d\bar{x} + \frac{1/2}{(2\pi)^3}U(\vec{k})\int e^{-i\varphi(\bar{x},t)-i\vec{h}\cdot\bar{x}}d\bar{x}$$

$$= \frac{1/2}{(2\pi)^{3/2}}\left[U(\vec{h})+U(\vec{k})\right]A_{k-h}e^{i\varphi_{k-h}}. \qquad (3.21)$$

The magnitude of $\varphi(\bar{x},t)$ is always smaller than unity.

Then, $$A_k e^{i\varphi_k} \approx \delta(k) + \frac{i}{(2\pi)^{3/2}}\int e^{i\vec{k}\cdot\bar{x}}\varphi(\bar{x},t)d\bar{x}. \qquad (3.22)$$

by the fact of the natural random phase $\varphi(\bar{x},t)$, therefore $\int\varphi(\bar{x},t)d\bar{x} = 0$, then,

$$A_0 = 1 \text{ and } \varphi_0 = 0. \qquad (3.23)$$

Thus these interesting interactions can be reduced to

$$U(\vec{k},\vec{k}) = \frac{1}{(2\pi)^{3/2}}U(\vec{k}), \qquad (3.24)$$

$$U(0,0) = \frac{1}{(2\pi)^{3/2}}U(0), \qquad (3.25)$$

and, $$U(\vec{k},\vec{h}) = \frac{1/2}{(2\pi)^{3/2}}\left[U(\vec{h})+U(\vec{k})\right]A_{k-h}e^{i\varphi_{k-h}}. \qquad (3.26)$$

If h is small enough, it is possible to deduce $U(\vec{k},\vec{h})$ in the last equation as

$$U(\vec{k},\vec{h}) \approx \frac{1/2}{(2\pi)^{3/2}}\left[U(\vec{k})+U(\vec{h})\right]A_k e^{i\varphi_k} \qquad (3.27)$$

From here, some quantitative characteristics of this interaction are shown. The first one is an attempt to account for its ground state interaction, $U(0)$.

$$U(0)=\lim_{k\to 0} U(\vec{k})$$

$$=\lim_{k\to 0} CU_0\sqrt{2/\pi}\left(\frac{\arctan\left(\frac{k}{2}\right)}{k}-\frac{1}{4+k^2}\right)$$

$$=CU_0\sqrt{2/\pi}\lim_{k\to 0}\left(\frac{2}{1+\left(\frac{k}{2}\right)^2}-\frac{1}{4+k^2}\right)$$

$$=CU_0\sqrt{\frac{2}{\pi}}\frac{1}{4}$$

$U(\vec{k},\vec{k})$ is going to $U(\vec{k})$ and $|U(\vec{k},0)|$ is going to $\frac{1}{2}(U(\vec{k})+U(0))$ with multiply by $\frac{1}{(2\pi)^{3/2}}$. The behaviour of $U(\vec{k},\vec{k})$, $U(\vec{k},0)$, and $U(0,0)$ are shown in figure 3.3, below.

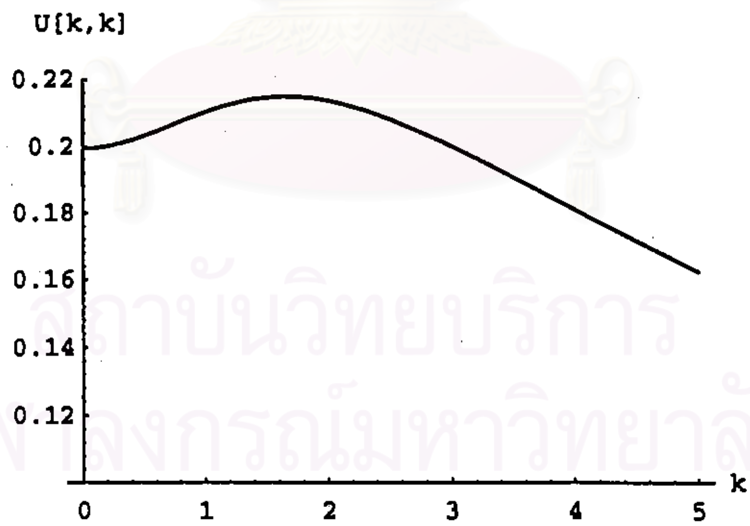
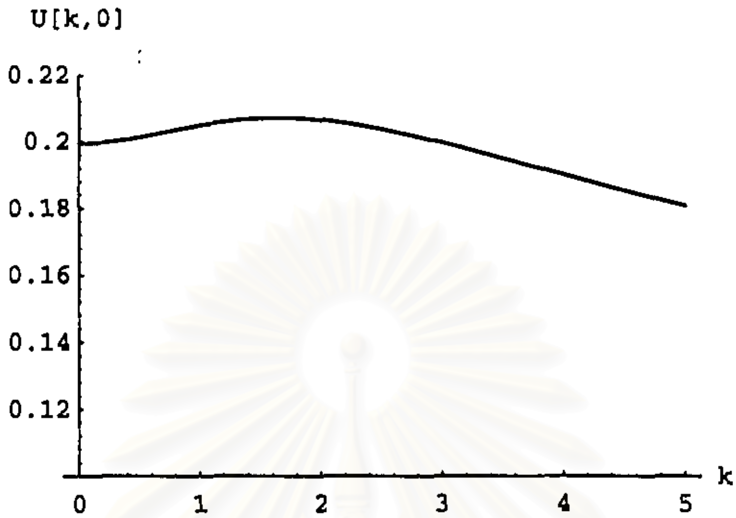


Figure 3.3 The interaction between particles in k space

(a) Interaction between particles in over excited states, $U(\vec{k},\vec{k})$.

b



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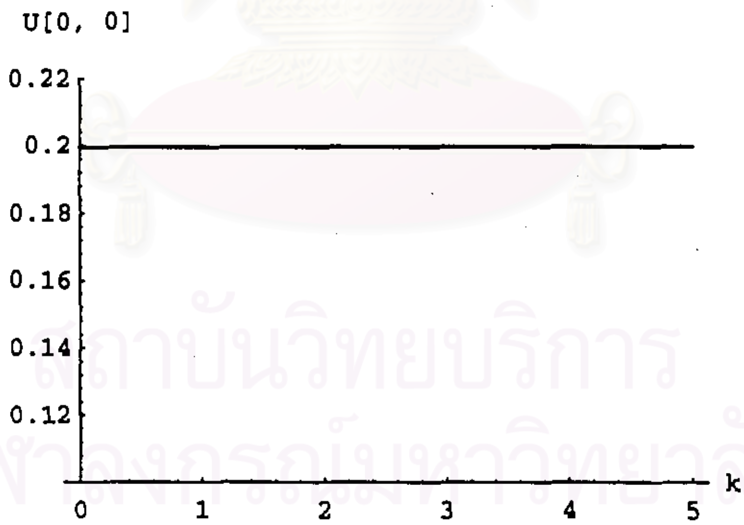

Figure 3.3 The interaction between particles in k space

(b) Interaction between particles in condensate state and over excited states, $U(\vec{k},0)$.

(c) Interaction between particles in condensate state, $U(0,0)$.

Now a new problem about the cut off position, which separates the area of small momentum from the area of large momentum, becomes obvious. Surely, this cut off is crucial for interpretating the new formula. An argument to support the idea of defining the cut off as a point, k_0, is that $k_0 r_0 = 1$, where r_0 is the point where interaction has minimum value. Further, the space where all k are smaller than k_0 is a small (slow) momentum area and, on the other hand, where all k are larger than k_0 is a large (rapid) momentum area. The reason for this argument is the same as the reason for the Heinsenberg uncertainty principle. Next, the second point is to find the value of r_0 and its corresponding k_0,

$$U(\bar{r}) = CU_0\left(\frac{e^{-2\bar{r}}}{(\bar{r})^2} - \frac{e^{-2\bar{r}}}{\bar{r}}\right)$$

$$\frac{dU(\bar{r})}{dr} = CU_0\left(-2\frac{e^{-2\bar{r}}}{(\bar{r})^3} - 2\frac{e^{-2\bar{r}}}{(\bar{r})^2} + \frac{e^{-2\bar{r}}}{(\bar{r})^2} + 2\frac{e^{-2\bar{r}}}{\bar{r}}\right)$$

$$\left.\frac{dU(\bar{r})}{dr}\right|_{r=r_0} = CU_0 e^{-2\bar{r}_0}\left(-\frac{2}{(\bar{r}_0)^3} - \frac{2}{(\bar{r}_0)^2} + \frac{1}{(\bar{r}_0)^2} + \frac{2}{\bar{r}_0}\right) = 0$$

$$e^{-2\bar{r}_0} = 0 \quad \text{or} \quad -\frac{2}{(\bar{r}_0)^3} - \frac{2}{(\bar{r}_0)^2} + \frac{1}{(\bar{r}_0)^2} + \frac{2}{\bar{r}_0} = 0$$

Here, two solutions satisfy: $e^{-2\bar{r}_0} = 0$ and $-2 - \bar{r}_0 + 2(\bar{r}_0)^2 = 0$. The first condition gives a trivial solution, therefore, only the non-trivial solution in the last condition is used.

$$-2 - \bar{r}_0 + 2(\bar{r}_0)^2 = 0$$

$$r_0 = \frac{1 \pm \sqrt{17}}{4} \approx \pm 1.28$$

The value of r_0 is the only positive value, therefore, $r_0 \approx 1.28$ units and then k_0 is 0.78 units by the above definition.

Comparing the research r_0 with r_0 of the original Lennard-Jones interaction,

$$U_{L-J}(r) = C\left(\frac{1}{r^{12}} - \frac{1}{r^6}\right)$$
$$\left(-\frac{12}{r_0^{13}} + \frac{6}{r_0^7}\right) = 0$$
$$r_0 = \sqrt[6]{2} \approx 1.12$$

it can be seen that r_0 is very closed to r_0 from the original interaction.