CHAPTER V

CALCULATION OF "β"

In the previous chapter we mentioned a quantity " β ", which plays an important role in the formalism. In eq.(4.47) we see that the state with the smallest β will have the lowest free energy and will be the state which is observed in nature. In this chapter we will determine the lowest possible value of β for flux lattices with one flux line per unit cell. First, we will write the linearized equation of motion as follows :

$$\left(-i\nabla + A\right)^2\Psi = \Psi \tag{5.1}$$

where Ψ is complex, and choose the gauge $A = -Hy\,\hat{\mathbf{x}}$. This equation is equivalent to eq.(4.11) in chapter IV or the original equation

$$\frac{1}{2m^*}\left(-i\hbar\nabla + \frac{e^*}{c}A\right)^2\Psi + a\Psi \approx 0$$

The standard, general solution of this equation (Abrikosov, 1988) can be written as

$$\Psi = e^{ik_z z}\sum_k c(k)e^{ikx}\exp\left\{-\frac{1}{2}H\left(y-\frac{k}{H}\right)^2\right\} \tag{5.2}$$

where $k^2_z = 1 - H$, and $H_{C2} = 1$.

Our purpose is to find the array of the flux lines as shown in fig. 5.1, which gives the minimum free energy. Let ℓ be the lattice constant, and b_1 and b_2 are components of **b** so that

$$\mathbf{a} = \hat{\mathbf{x}}\,\ell$$

$$\mathbf{b} = (b_1\hat{\mathbf{x}} + b_2\hat{\mathbf{y}})\ell \tag{5.3}$$

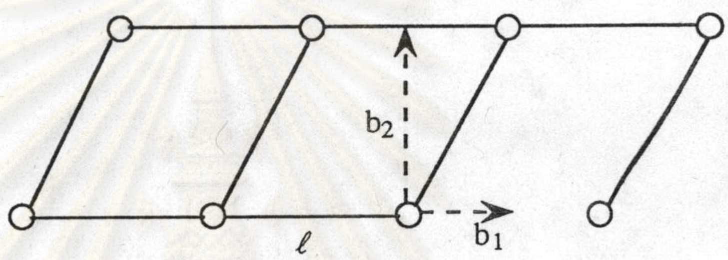

Fig 5.1 Array of flux lines, where ℓ is the lattice constant and the circles denote flux lines.

For a square lattice

$$\mathbf{a} = \hat{\mathbf{x}}\,\ell$$

$$\mathbf{b} = \hat{\mathbf{y}}\,\ell$$

For an equilateral triangular lattice

$$\mathbf{a} = \hat{\mathbf{x}}\,\ell$$

$$\mathbf{b} = \frac{1}{2}(\hat{\mathbf{x}} + \sqrt{3}\,\hat{\mathbf{y}})\ell$$

We let

$$x \rightarrow \ell x,\ \ y \rightarrow \ell y,\ \text{and}\ \ k \rightarrow \frac{2\pi}{\ell}k$$

so that, from eq.(5.2), we have

$$\Psi = \sum_{k} c(k)e^{2\pi ikx} \exp\left\{-\frac{1}{2} H\ell^2\left(y - \frac{2\pi k}{H\ell^2}\right)^2\right\} \tag{5.4}$$

But

$$\Psi(\mathbf{r}) = \Psi(\mathbf{r} + \mathbf{a})$$

so that,

$$\Psi = \sum_{n} c_n e^{2\pi inx} \exp\left\{-\frac{1}{2} H\ell^2\left(y - \frac{2\pi n}{H\ell^2}\right)^2\right\} \tag{5.5}$$

where n is summed over integers.

Now, $\Phi = BA$, where Φ is the magnetic flux in a unit cell, B is the internal magnetic field intensity and A is the total area of a unit cell. Since flux is quantized (Kittel, 1986) and as we mentioned above that there is only one flux quantum per unit cell in reduced units, $\Phi = 2\pi$, and we have that

$$H\ell^2 = \frac{2\pi}{b_2} \tag{5.6}$$

We use H instead of B here because the external magnetic field H is very close to H_{c2} and the induction B differs from H by only a very small quantity.

Now eq.(5.5) becomes

$$\Psi = \sum_{n} c_n e^{2\pi i n x} \exp\left\{ -\frac{\pi}{b_2}(y - nb_2)^2 \right\} \tag{5.7}$$

and, after scaling,

$$\mathbf{a} = \hat{\mathbf{x}} \tag{5.8}$$

$$\mathbf{b} = \left(b_1\hat{\mathbf{x}} + b_2\hat{\mathbf{y}} \right) \tag{5.9}$$

We can obtain unit vectors in reciprocal space by the relations

$$\mathbf{a}^* = 2\pi \frac{\mathbf{b} \times \hat{\mathbf{z}}}{\hat{\mathbf{x}} \cdot \mathbf{b} \times \hat{\mathbf{z}}}$$

$$\mathbf{b}^* = 2\pi \frac{\hat{\mathbf{z}} \times \hat{\mathbf{x}}}{\hat{\mathbf{x}} \cdot \mathbf{b} \times \hat{\mathbf{z}}} \tag{5.10}$$

Now

$$\mathbf{b} \times \hat{\mathbf{z}} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ b_1 & b_2 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

$$= \left(b_2\hat{\mathbf{x}} - b_1\hat{\mathbf{y}} \right)$$

and

$$\hat{\mathbf{z}} \times \hat{\mathbf{x}} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{vmatrix} = \hat{\mathbf{y}}$$

so that

$$\mathbf{a}^* = \frac{2\pi}{b_2}\left(b_2\hat{\mathbf{x}} - b_1\hat{\mathbf{y}}\right) \tag{5.11}$$

$$\mathbf{b}^* = \frac{2\pi}{b_2}\hat{\mathbf{y}} \tag{5.12}$$

as shown in fig.5.2

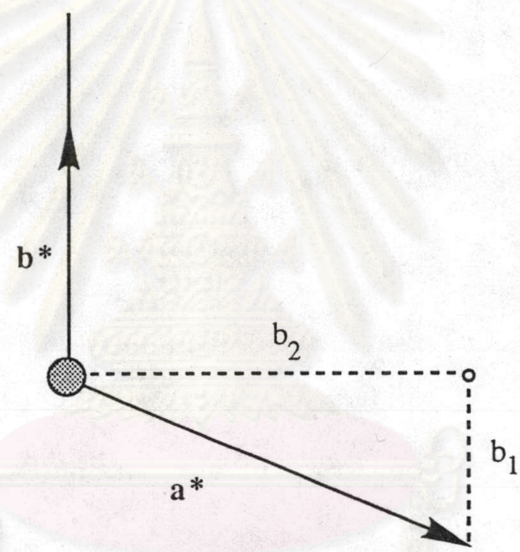

Fig 5.2 Vectors in reciprocal space

Now we can write

$$\mathbf{G} = \frac{2\pi}{b_2}\left(pb_2\hat{\mathbf{x}} - pb_1\hat{\mathbf{y}} + q\hat{\mathbf{y}}\right)$$

$$= \frac{2\pi}{b_2}\left(pb_2\hat{\mathbf{x}} - (pb_1 - q)\hat{\mathbf{y}}\right) \tag{5.13}$$

Note that it is not necessarily true that $\Psi(\mathbf{r+b}) = \Psi(\mathbf{r})$; Ψ is not gauge invariant. The gauge invariant quantity of physical significance is ω.

We expand ω as follows

$$\omega = \sum_{\mathbf{G}} \omega_{\mathbf{G}} e^{i\,\mathbf{G}\cdot\mathbf{r}} \tag{5.18}$$

where $\omega_{\mathbf{G}}$ is the Fourier coefficient , given by

$$\omega_{\mathbf{G}} = \left\langle \omega e^{-i\,\mathbf{G}\cdot\mathbf{r}} \right\rangle \tag{5.19}$$

$$= \frac{1}{L_x L_y} \int d\mathbf{r}\, \omega(\mathbf{r})\, e^{-i\,\mathbf{G}\cdot\mathbf{r}} \tag{5.20}$$

The average of ω is

$$\langle\omega\rangle = \sum_{\mathbf{G}} \omega_{\mathbf{G}} \left\langle e^{i\,\mathbf{G}\cdot\mathbf{r}} \right\rangle$$

$$= \sum_{\mathbf{G}} \omega_{\mathbf{G}}\, \delta_{\mathbf{G},0}$$

$$= \omega_{\mathbf{G}=0}$$

$$= \left\langle |\Psi|^2 \right\rangle \tag{5.21}$$

Note that it is not necessarily true that $\Psi(\mathbf{r}+\mathbf{b}) = \Psi(\mathbf{r})$; Ψ is not gauge invariant. The gauge invariant quantity of physical significance is ω.

We expand ω as follows

$$\omega = \sum_{G} \omega_G e^{i\,G\cdot r} \tag{5.18}$$

where ω_G is the Fourier coefficient, given by

$$\omega_G = \left\langle \omega e^{-i\,G\cdot r} \right\rangle \tag{5.19}$$

$$= \frac{1}{L_x L_y} \int dr\, \omega(r)\, e^{-i\,G\cdot r} \tag{5.20}$$

The average of ω is

$$\langle\omega\rangle = \sum_{G} \omega_G \left\langle e^{i\,G\cdot r}\right\rangle$$

$$= \sum_{G} \omega_G\, \delta_{G,0}$$

$$= \omega_{G=0}$$

$$= \left\langle |\Psi|^2 \right\rangle \tag{5.21}$$

Also

$$
\begin{aligned}
\langle \omega^2 \rangle &= \langle |\Psi|^4 \rangle \\
&= \sum_{GG'} \omega_G \, \omega_{G'} \left\langle e^{i(G+G')\cdot r} \right\rangle \\
&= \sum_{GG'} \omega_G \, \omega_{G'} \, \delta_{G+G',0} \\
&= \sum_{G} \omega_G \, \omega_{-G} \\
&= \sum_{G} |\omega_G|^2
\end{aligned}
\tag{5.22}
$$

For $\mathbf{G} = 0$,

$$\omega_{G=0} = \langle \omega \rangle$$

$$
\begin{aligned}
&= \frac{1}{L_y L_x} \sum_{nm} c_n c_m^* \int dx \int dy \; e^{2\pi i(n-m)x} \exp\left\{ -\frac{2\pi}{b_2}(y - nb_2)^2 - \frac{2\pi}{b_2}(y - mb_2)^2 \right\} \\
&= \frac{1}{L_y} \sum_{n} \int dy \exp\left\{ -\frac{2\pi}{b_2} y^2 \right\} |c_n|^2 \\
&= \frac{1}{L_y} \sqrt{\frac{b_2}{2}} \sum_{n} |c_n|^2
\end{aligned}
\tag{5.23}
$$

Since

$$\frac{1}{L_x} \int dx \; e^{2\pi i(n-m)x} = \delta_{m,n} \tag{5.24}$$

eq.(5.19) now becomes,

$$\omega_G = \sum_n c_n c^*_{n-p} \frac{1}{L_y} \int dy \;\; e^{-iG_y \cdot y} \; \exp\left[-\frac{\pi}{b_2}\left\{(y - nb_2)^2 + (y - (n-p)b_2)^2\right\}\right] \tag{5.25}$$

Considering that,

$$(y - nb_2)^2 + (y - (n-p)b_2)^2$$

$$= y^2 - 2nb_2y + n^2b_2 + y^2 - 2(n-p)b_2y + (n-p)^2{b_2}^2$$

$$= 2y^2 - 2(2n-p)b_2y + n^2b_2 + {b_2}^2\left(n^2 + (n-p)^2\right)$$

we see that

$$\omega_G = \sum_n c_n c^*_{n-p} \frac{1}{L_y} \int dy \;\; \exp\left[-\, iG_y \cdot y - \frac{\pi}{b_2}\left\{2y^2 - 2(2n-p)b_2y + n^2b_2 + {b_2}^2\left(n^2 + (n-p)^2\right)\right\}\right]$$

$$= \sum_n c_n c^*_{n-p} \frac{1}{L_y} \int dy \;\; \exp\left[-\left\{\frac{2\pi}{b_2} y^2 - (2\pi(2n-p) - iG_y)y + \pi b_2\left(n^2 + (n-p)^2\right)\right\}\right] \tag{5.26}$$

From

$$\int_{-\infty}^{\infty} dx \, e^{-(ax^2 + bx + c)} = \sqrt{\frac{\pi}{a}} \; \exp\left\{\frac{b^2}{4a} - c\right\}$$

so that, using the expression (5.13) for **G**, we have

$$\omega_G = \sum_n c_n c^*_{n-p} \frac{1}{L_y}\sqrt{\frac{b_2}{2}} \exp\left[\frac{b_2}{8\pi}(2\pi(2n-p) - iG_y)^2 - \pi b_2\left(n^2 + (n-p)^2\right)\right]$$

$$= \frac{1}{L_y}\sqrt{\frac{b_2}{2}} \exp\left[-\frac{b_2}{8\pi} G^2\right]$$

$$\times \sum_n c_n c^*_{n-p} \exp\left[\frac{b_2}{8\pi}\left\{4\pi^2(2n-p)^2 - 4\pi(2n-p)iG_y + G^2{}_x\right\} - \pi b_2\left(n^2 + (n-p)^2\right)\right]$$

$$= \sqrt{\frac{b_2}{2}} \frac{1}{L_y} \exp\left[-\frac{b_2}{8\pi} G^2\right] \sum_n c_n c^*_{n-p} \exp\left[-\frac{b_2}{2}(2n-p)iG_y\right]$$

Next, substituting for G_y

$$\omega_G = \sqrt{\frac{b_2}{2}} \frac{1}{L_y} \exp\left[-\frac{b_2}{8\pi} G^2\right] \sum_n c_n c^*_{n-p} \exp\left[2\pi i\left(n - \frac{p}{2}\right)(pb_1 - q)\right] \tag{5.27}$$

so that

$$\sum_G |\omega_G|^2 = \frac{1}{L_y^2}\frac{b_2}{2} \sum_{pq} \exp\left[-\frac{b_2}{4\pi} G^2\right] \sum_{nm} c_n c^*_{n-p} c^*_m c_{m-p} \exp\left[2\pi i(n-m)(pb_1)\right]$$

Since from eq.(5.17)

$$c^*_{n-p} c_{m-p} = c^*_n c_m \exp\left[-2\pi i(n-m)\, pb_1\right]$$

and we find that

$$\sum_{G} |\omega_G|^2 = \frac{1}{L_y^2}\frac{b_2}{2}\sum_{pq} \exp\left[-\frac{b_2}{4\pi}G^2\right]\left(\sum_{n}|c_n|^2\right)^2 \tag{5.28}$$

Now β is defined according to

$$\beta = \frac{\left\langle |\Psi|^4 \right\rangle}{\left\langle |\Psi|^2 \right\rangle^2}$$

$$= \frac{\left\langle \omega^2 \right\rangle}{\left\langle \omega \right\rangle^2}$$

$$= \frac{\sum_{G} |\omega_G|^2}{\left(\omega_{G=0}\right)^2} \tag{5.29}$$

From eqs.(5.23) and (5.28) we obtain

$$\beta = \sum_{G} \exp\left[-\frac{b_2}{4\pi}G^2\right] \tag{5.30}$$

Here

$$G^2 = \frac{4\pi^2}{b_2^{\,2}}\left[\, p^2 b_2 + (pb_1 - q)^2\right]$$

$$= \frac{4\pi^2}{b_2^{\,2}}\left[\left(b_1^{\,2} + b_2^{\,2}\right)p^2 - 2b_1pq + q^2\right] \tag{5.31}$$

Finally,

$$\beta(b_1,b_2) = \sum_{pq} \exp\left[-\frac{\pi}{b_2}\left\{(b_1{}^2 + b_2{}^2)p^2 - 2b_1pq + q^2\right\}\right] \tag{5.32}$$

By minimizing eq.(5.32) numerically we found that there are two lattice structures which have the same lowest value of β. These are for $(b_1, b_2) = (1/2, \sqrt{3}/2)$ and $(1/2, 1/2\sqrt{3})$, as shown analytically below.

In the case of $b_1 = 1/2$ and $b_2 = \sqrt{3}/2$ (triangular lattice, $\theta = 60°$), we have

$$\beta\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) = \sum_{pq} \exp\left[-\frac{2\pi}{\sqrt{3}}\left\{(p^2 - pq + q^2)\right\}\right] \tag{5.33}$$

For $b_1 = 1/2$ and $b_2 = 1/2\sqrt{3}$ ($\theta = 30°$, where θ is the angle between b_1 and b_2), we obtain

$$\begin{aligned}
\beta\left(\frac{1}{2}, \frac{1}{2\sqrt{3}}\right) &= \sum_{pq} \exp\left[-2\pi\sqrt{3}\left\{\left(\frac{1}{3}p^2 - pq + q^2\right)\right\}\right] \\
&= \sum_{pq} \exp\left[-\frac{2\pi}{\sqrt{3}}\left\{(p^2 - 3pq + 3q^2)\right\}\right] \\
&= \sum_{pq} \exp\left[-\frac{2\pi}{\sqrt{3}}\left\{((p-q)^2 - pq + 2q^2)\right\}\right] \\
&= \sum_{pq} \exp\left[-\frac{2\pi}{\sqrt{3}}\left\{((p-q)^2 - (p-q)q + q^2)\right\}\right] \\
&= \sum_{pq} \exp\left[-\frac{2\pi}{\sqrt{3}}\left\{(p^2 - pq + q^2)\right\}\right] \\
&= \beta\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)
\end{aligned} \tag{5.34}$$

Numerical Minimization of β

Return now to the optimization of β problem. Numerical calculations show that for the square lattice of Abrikosov, $\beta = 1.18$ (Abrikosov, 1957), while for the equilateral triangular lattice, $\beta = 1.16$ (Kleiner *et al.*, 1964). Considering this small difference, it is understandable that a numerical error could have led Abrikosov originally to conclude that the square array was more stable. Later work by Kleiner *et al.* rectified this error, and showed that the triangular array has in fact the most favorable value of β.

According to eq.(5.32), we now try to seek the appropriate values of b_1 and b_2 which make the value of β a minimum. By numerical work, we found two lattices which have the same value of $\beta = 1.15959526$ (the results are shown in figs. 5.3 - 5.6). However in fig.5.3 we will see that these two triangles are the same equilateral triangles (60°). Where

a). $b_1 = 0.49999997$ and $b_2 = 0.86602546$ ($\theta = 60°$)

and

b). $b_1 = 0.49999999$ and $b_2 = 0.28867520$ ($\theta = 30°$)

Note that the size of the equilateral triangle is irrelevant since we have used an arbitrary scaling factor.

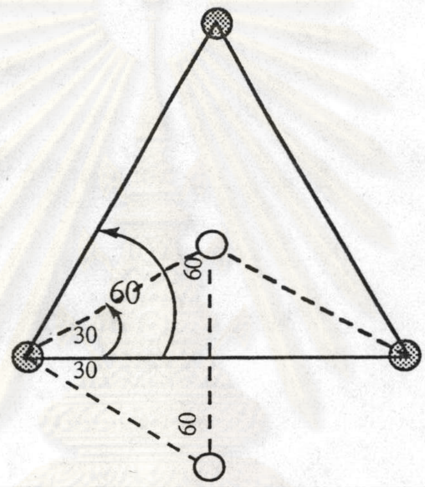

Fig. 5.3 Numerical results of two lattice structures of flux lines with the same value of β. The smaller triangular lattice has the same structure as the bigger one.

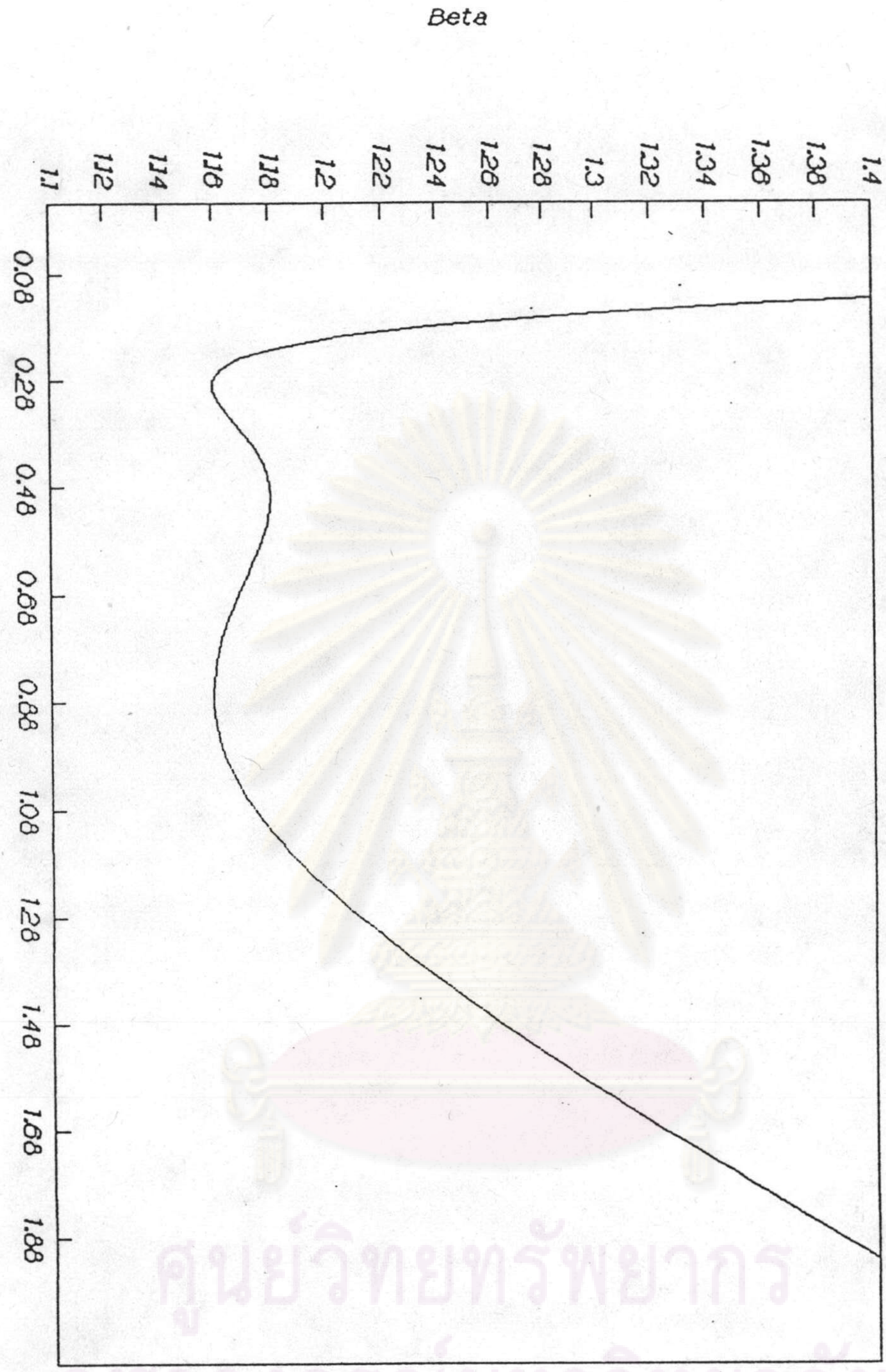

Fig. 5.4 β vs. b_2 where b_1 is fixed at 0.5

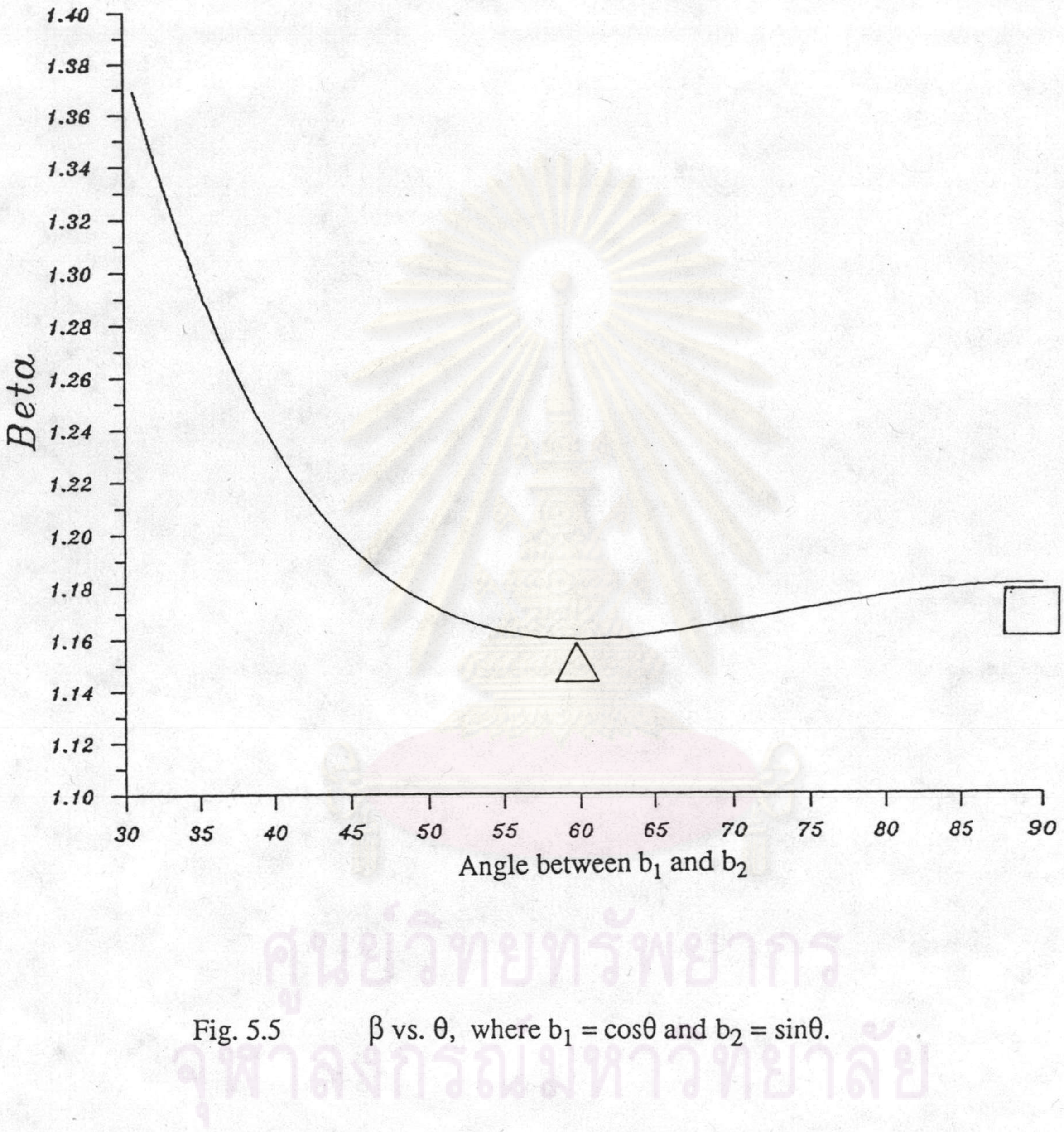

Fig. 5.5 β vs. θ, where $b_1 = \cos\theta$ and $b_2 = \sin\theta$.

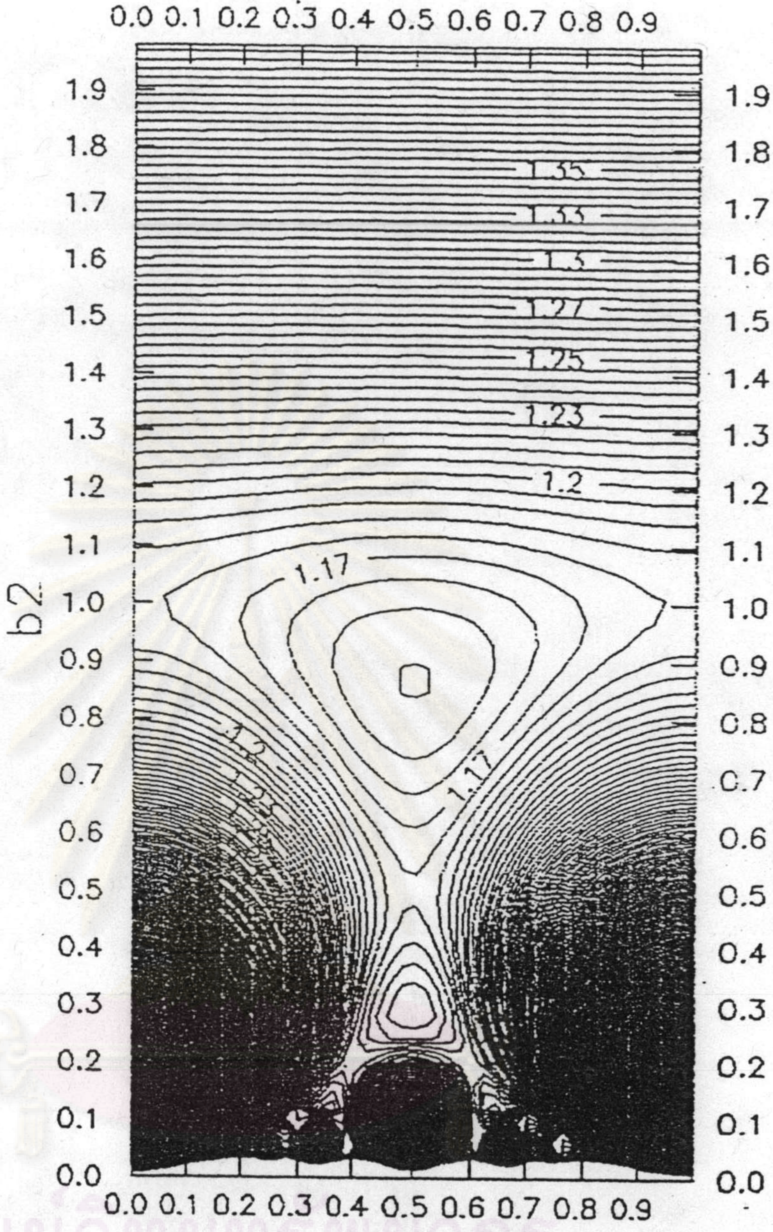

Fig.5.6 Contour plot of β in the b_1-b_2 plane. The two small circles are the lowest values of $\beta = 1.1595$. ($b_1 = 0.5$ while $b_2 = 0.2886$ and 0.8660).