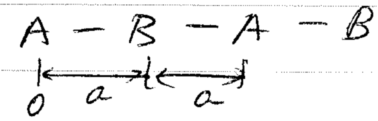
PHY 521 Solutions Problem Set 7

1) Because atoms A and B are different we must regard this as a BL with 2-point basis



primitive vector of BL: $\vec{a}_1 = 2a\hat{x}$

BL vectors: $\vec{R} = 2an\hat{x}$, n integer

basis vectors: $\vec{0}$, $\vec{d} = a\hat{x}$ atom A at origin, B at $\vec{d}$

primitive vector of RL: $\vec{b}_1 = \frac{\pi}{a}\hat{x}$

RL vectors: $\vec{K} = \frac{n\pi}{a}\hat{x}$, n integer

1^{st} BZ: $\vec{k} = k\hat{x}$ with $k \in \left(-\frac{\pi}{2a}, \frac{\pi}{2a}\right]$

We can write the Hamiltonian H as:

$$H = H_{at\,A} + \Delta U_A(\vec{r}) = H_{at\,B} + \Delta U_B(\vec{r} - a\hat{x})$$

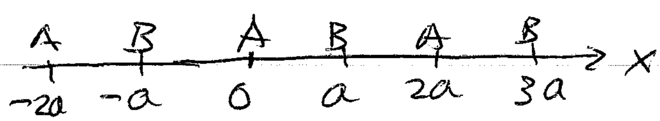
where $H_{at\,A}$ and $H_{at\,B}$ are atomic Hamiltonians of isolated atoms A and B respectively.

$$\Delta U_A(\vec{r}) = U(\vec{r}) - v_A(\vec{r})$$

$U(\vec{r})$: total ionic potential; $v_A(\vec{r})$: potential of atom A at origin

$$\Delta U_B(\vec{r} - a\hat{x}) = U(\vec{r}) - v_B(\vec{r} - a\hat{x})$$

$U(\vec{r})$: total ionic potential; $v_B(\vec{r} - a\hat{x})$: potential of atom B located at $a\hat{x}$



The Bloch wavefunction is assumed to be well approx by

$$\psi_k(\vec{r}) = \sum_R e^{ikR}\left[b_A \varphi_A(\vec{r}-\vec{R}) + b_B \varphi_B(\vec{r}-a\hat{x}-\vec{R})\right)$$

$\varphi_A(\vec{r})$ is atomic orbital of electron on atom A at origin
$\varphi_B(\vec{r}-a\hat{x})$ is atomic orbital of electron on atom B at $a\hat{x}$

We will assume φ_A and φ_B are real functions and are spherically symmetric, ie they depend only on $|\vec{r}|$.

Then:

$$\langle \varphi_A(\vec{r}) | \mathcal{H} - \mathcal{H}_{at\,A} - \Delta U_A(\vec{r}) | \psi_k(\vec{r}) \rangle = 0$$

① $$\Rightarrow \boxed{(\varepsilon - E_A)\langle \varphi_A(\vec{r}) | \psi_k(\vec{r})\rangle - \langle \varphi_A(\vec{r}) | \Delta U_A(\vec{r}) | \psi_k(\vec{r})\rangle = 0}$$

and $$\langle \varphi_B(\vec{r}-a\hat{x}) | \mathcal{H} - \mathcal{H}_{at\,B} - \Delta U_B(\vec{r}-a\hat{x}) | \psi_k(\vec{r}) \rangle = 0$$

② $$\Rightarrow \boxed{(\varepsilon - E_B)\langle \varphi_B(\vec{r}-a\hat{x}) | \psi_k(\vec{r})\rangle - \langle \varphi_B(\vec{r}-a\hat{x}) | \Delta U_B(\vec{r}-a\hat{x}) | \psi_k(\vec{r})\rangle = 0}$$

Where E_A and E_B are atomic energy levels of orbitals φ_A and φ_B
Now we need to compute the matrix elements

$$\langle \varphi_A(\vec{r}) | \psi_k(\vec{r})\rangle = \sum_R e^{ikR}\Big[b_A \int d^3r\, \varphi_A^*(\vec{r})\, \varphi_A(\vec{r}-\vec{R})$$

$$+ b_B \int d^3r\, \varphi_A^*(\vec{r})\, \varphi_B(\vec{r}-a\hat{x}-\vec{R}) \Big]$$

Assume that only nearest neighbor overlap is significant

$\Rightarrow \begin{cases} \text{in first term only } \vec{R}=0 \text{ contributes} \\ \text{in second term only } \vec{R}=0 \text{ and } \vec{R}=-2a\hat{x} \text{ contribute} \end{cases}$

$$\langle \varphi_A(\vec r)|\psi_k(\vec r)\rangle = b_A \underbrace{\int d^3r\, \varphi_A^*(\vec r)\varphi_A(\vec r)}_{=1 \text{ by normalization}}$$

$$+ b_B \int d^3r\, \varphi_A^*(\vec r)\varphi_B(\vec r - a\hat x)$$

$$+ b_B \int d^3r\, \varphi_A^*(\vec r)\varphi_B(\vec r + a\hat x)\, e^{-2ika}$$

Consider $\int d^3r\, \varphi_A^*(\vec r)\varphi_B(\vec r + a\hat x)$ change integration variable $\vec r \to -\vec r$

$= \int d^3r\, \varphi_A^*(-\vec r)\varphi_B(-\vec r + a\hat x)$ spherical symmetry of orbitals $\varphi_A(-\vec r) = \varphi(\vec r)$

$= \int d^3r\, \varphi_A^*(\vec r)\varphi_B(\vec r - a\hat x)$ same as second term

Define $\boxed{\alpha \equiv \int d^3r\, \varphi_A^*(\vec r)\varphi_B(\vec r - a\hat x)}$

Then $\boxed{\langle \varphi_A(\vec r)|\psi_k(\vec r)\rangle = b_A + b_B\alpha(1 + e^{-2ika})}$

<u>Next</u>:

$$\langle \varphi_B(\vec r - a\hat x)|\psi_k(\vec r)\rangle = \sum_R e^{ikR}\Big[b_A \int d^3r\, \varphi_B^*(\vec r - a\hat x)\varphi_A(\vec r - \vec R)$$

$$+ b_B \int d^3r\, \varphi_B^*(\vec r - a\hat x)\varphi_B(\vec r - a\hat x - \vec R)\Big]$$

only keep nearest neighbor overlaps

$$\Rightarrow \begin{cases} \text{only } \vec R = 0 \text{ in } 2^{\text{nd}} \text{ term} \\ \text{only } \vec R = 0 \text{ and } \vec R = 2a\hat x \text{ in } 1^{\text{st}} \text{ term} \end{cases}$$

$$\langle \varphi_B(\vec r - a\hat x)|\psi_k(\vec r)\rangle = b_B + b_A \int d^3r\, \varphi_B^*(\vec r - a\hat x)\varphi_A(\vec r)$$

$$+ b_A \int d^3r\, \varphi_B^*(\vec r - a\hat x)\varphi_A(\vec r - 2a\hat x)\, e^{2ika}$$

Consider $\int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\, \varphi_A(\vec{r}-2a\hat{x})$ change integration variable $\vec{r}\to-\vec{r}$

$$= \int d^3r\, \varphi_B^*(-\vec{r}-a\hat{x})\,\varphi_A(-\vec{r}-2a\hat{x})$$ use $\varphi(\vec{r})=\varphi(-\vec{r})$

$$= \int d^3r\, \varphi_B^*(\vec{r}+a\hat{x})\,\varphi_A(\vec{r}+2a\hat{x})$$ change integration variable $\vec{r}\to\vec{r}-2a\hat{x}$

$$= \int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\,\varphi_A(\vec{r})$$ same as second term

$$= \alpha^*$$

So $$\boxed{\langle \varphi_B(\vec{r}-a\hat{x})|\psi_k(\vec{r})\rangle = b_B + b_A\alpha^*\left(1+e^{2ika}\right)}$$

Next:

$$\langle\varphi_A(\vec{r})|\Delta U_A(\vec{r})|\psi_k(\vec{r})\rangle = \sum_R e^{ikR}\Big[b_A\int d^3r\, \varphi_A^*(\vec{r})\Delta U_A(\vec{r})\varphi_A(\vec{r}-\vec{R})$$
$$+ b_B\int d^3r\, \varphi_A^*(\vec{r})\Delta U_A(\vec{r})\,\varphi_B(\vec{r}-a\hat{x}-\vec{R})\Big]$$

Only keep nearest neighbor overlaps

$$\Rightarrow \begin{cases} \text{only } R=0 \text{ in } 1^{st} \text{ term} \\ \text{only } \vec{R}=0 \text{ and } \vec{R}=-2a\hat{x} \text{ in } 2^{nd} \text{ term}\end{cases}$$

$$\langle\varphi_A(\vec{r})|\Delta U_A(\vec{r})|\psi_k(\vec{r})\rangle = b_A\int d^3r\, \varphi_A^*(\vec{r})\,\Delta U_A(\vec{r})\,\varphi_A(\vec{r})$$
$$+ b_B\int d^3r\, \varphi_A^*(\vec{r})\Delta U_A(\vec{r})\,\varphi_B(\vec{r}-a\hat{x})$$
$$+ b_B\int d^3r\, \varphi_A^*(\vec{r})\,\Delta U_A(\vec{r})\,\varphi_B(\vec{r}+a\hat{x})\,e^{-2ika}$$

Define $$\boxed{\beta_A \equiv -\int d^3r\, \varphi_A^*(\vec{r})\,\Delta U_A(\vec{r})\,\varphi_A(\vec{r})}$$

Consider $\int d^3r\, \varphi_A^*(\vec{r})\, \Delta U_A(\vec{r})\, \varphi_B(\vec{r}+a\hat{x})$ change integration variable $\vec{r} \to -\vec{r}$

$$= \int d^3r\, \varphi_A^*(-\vec{r})\, \Delta U_A(-\vec{r})\, \varphi_B(-\vec{r}+a\hat{x})$$ use $\varphi(\vec{r}) = \varphi(-\vec{r})$ also $\Delta U_A(\vec{r}) = \Delta U_A(-\vec{r})$

$$= \int d^3r\, \varphi_A^*(\vec{r})\, \Delta U_A(\vec{r})\, \varphi_B(\vec{r}-a\hat{x})$$ same as 2nd term

Define $\boxed{\gamma_A \equiv -\int d^3r\, \varphi_A^*(\vec{r})\, \Delta U_A(\vec{r})\varphi_B(\vec{r}-a\hat{x})}$

Then $\boxed{\langle \varphi_A(\vec{r}) | \Delta U_A(\vec{r}) | \psi_k(\vec{r}) \rangle = -b_A \beta_A - b_B \gamma_A (1+e^{-2ika})}$

Finally:

$\langle \varphi_B(\vec{r}-a\hat{x}) | \Delta U_B(\vec{r}-a\hat{x}) | \psi_k(\vec{r}) \rangle$

$$= \sum_R e^{ikR} \Big[b_A \int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\, \Delta U_B(\vec{r}-a\hat{x})\, \varphi_A(\vec{r}-\vec{R})$$

$$+ b_B \int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\, \Delta U_B(\vec{r}-a\hat{x})\, \varphi_B(\vec{r}-a\hat{x}-\vec{R}) \Big]$$

Only keep nearest neighbor overlaps

$\Rightarrow \begin{cases} \text{only } \vec{R}=0 \text{ and } \vec{R}=2a\hat{x} \text{ in 1st term} \\ \text{only } \vec{R}=0 \text{ in 2nd term} \end{cases}$

$$\langle \varphi_B(\vec{r}-a\hat{x}) | \Delta U_B(\vec{r}-a\hat{x}) | \psi_k(\vec{r}) \rangle = b_B \int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\, \Delta U_B(\vec{r}-a\hat{x})\varphi_B(\vec{r}-a\hat{x})$$

$$+ b_A \int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\, \Delta U_B(\vec{r}-a\hat{x})\, \varphi_A(\vec{r})$$

$$+ b_A \int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\, \Delta U_B(\vec{r}-a\hat{x})\, \varphi_A(\vec{r}-2a\hat{x})\, e^{2ika}$$

Define $\boxed{\beta_B \equiv -\int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\, \Delta U_B(\vec{r}-a\hat{x})\varphi_B(\vec{r}-a\hat{x})}$

Consider $\int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\Delta U_B(\vec{r}-a\hat{x})\,\varphi_A(\vec{r}-2a\hat{x})$ change integration variable $\vec{r}\to-\vec{r}$

$$= \int d^3r\, \varphi_B^*(-\vec{r}-a\hat{x})\Delta U_B(-\vec{r}-a\hat{x})\varphi_A(-\vec{r}-2a\hat{x})$$ use $\varphi(\vec{r})=\varphi(-\vec{r})$ and $\Delta U_B(\vec{r})=\Delta U_B(-\vec{r})$

$$= \int d^3r\, \varphi_B^*(\vec{r}+a\hat{x})\Delta U_B(\vec{r}+a\hat{x})\varphi_A(\vec{r}+2a\hat{x})$$ change integration variable $\vec{r}\to\vec{r}-2a\hat{x}$

$$= \int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\Delta U_B(\vec{r}-a\hat{x})\varphi_A(\vec{r})$$ same as 2nd term

Define $\boxed{\gamma_B^* \equiv -\int d^3r\, \varphi_B^*(\vec{r}-a\hat{x})\Delta U_B(\vec{r}-a\hat{x})\varphi_A(\vec{r})}$

Then
$$\boxed{\langle\varphi_B(\vec{r}-a\hat{x})|\Delta U_B(\vec{r}-a\hat{x})|\psi_k(\vec{r})\rangle = -b_B\beta_B - b_A\gamma_B^*(1+e^{2ika})}$$

Substitute all these results into equations ① and ②

① $$(\varepsilon-E_A)[b_A+b_B\alpha(1+e^{-2ika})] + b_A\beta_A + b_B\gamma_A(1+e^{-2ika}) = 0$$

② $$(\varepsilon-E_B)[b_B+b_A\alpha^*(1+e^{2ika})] + b_B\beta_B + b_A\gamma_B^*(1+e^{2ika}) = 0$$

Regrouping

$$(\varepsilon-E_A+\beta_A)\,b_A + [(\varepsilon-E_A)\alpha+\gamma_A](1+e^{-2ika})\,b_B = 0$$
$$[(\varepsilon-E_B)\alpha^*+\gamma_B^*](1+e^{2ika})\,b_A + (\varepsilon-E_B+\beta_B)\,b_B = 0$$

For φ_A and φ_B <u>real</u> functions, $\alpha^*=\alpha$, $\gamma_B^*=\gamma_B$

we use this and rewrite above as matrix equation

$$\begin{pmatrix} \varepsilon - E_A + \beta_A & [(\varepsilon - E_A)\alpha + \gamma_A](1+e^{-2ika}) \\ [(\varepsilon - E_B)\alpha + \gamma_B](1+e^{2ika}) & \varepsilon - E_B + \beta_B \end{pmatrix} \begin{pmatrix} b_A \\ b_B \end{pmatrix} = 0$$

A non trivial solution requires determinant of matrix to vanish

$$0 = (\varepsilon - E_A + \beta_A)(\varepsilon - E_B + \beta_B) - [(\varepsilon - E_B)\alpha + \gamma_B][(\varepsilon - E_A)\alpha + \gamma_A](2 + 2\cos 2ka)$$

Above is quadratic equation in ε. Roots of this equation give the two band energies $\varepsilon_\pm(k)$.

To make things simpler lets assume $\alpha \ll \gamma_A, \gamma_B$

Then above becomes

$$(\varepsilon - E_A + \beta_A)(\varepsilon - E_B + \beta_B) - \gamma_A\gamma_B(2 + 2\cos 2ka) = 0$$

$$\varepsilon^2 + \varepsilon(\beta_B + \beta_A - E_B - E_A) + (\beta_A - E_A)(\beta_B - E_B) - \gamma_A\gamma_B(2 + 2\cos 2ka) = 0$$

$$\varepsilon_\pm = \frac{E_A + E_B - \beta_A - \beta_B}{2} \pm \sqrt{\left(\frac{E_A + E_B - \beta_A - \beta_B}{2}\right)^2 - (\beta_A - E_A)(\beta_B - E_B) + \gamma_A\gamma_B(2 + 2\cos 2ka)}$$

$$\boxed{\varepsilon_\pm(k) = \frac{E_A + E_B - \beta_A - \beta_B}{2} \pm \sqrt{\left(\frac{E_A - E_B - \beta_A + \beta_B}{2}\right)^2 + \gamma_A\gamma_B(2 + 2\cos 2ka)}}$$

At the edge of the 1^{st} BZ, $k = \frac{\pi}{2a}$

so $2 + 2\cos 2ka = 2 + 2\cos\pi = 0$

$$\mathcal{E}_\pm\left(\frac{\pi}{2a}\right) = \frac{E_A + E_B - \beta_A - \beta_B}{2} \pm \frac{E_A - E_B - \beta_A + \beta_B}{2}$$

$$\mathcal{E}_+\left(\frac{\pi}{2a}\right) = E_A - \beta_A$$

$$\mathcal{E}_-\left(\frac{\pi}{2a}\right) = E_B - \beta_B$$

Energy gap $\Delta\mathcal{E} = \mathcal{E}_+\left(\frac{\pi}{2a}\right) - \mathcal{E}_-\left(\frac{\pi}{2a}\right) = E_A - \beta_A - E_B + \beta_B$

Note: If atoms A and B are actually the same, then $E_A = E_B$ and $\beta_A = \beta_B$ and so $\Delta\mathcal{E} = 0$ – the gap at the boundary of 1^{st} BZ vanishes!

But this is as expected since if $A = B$ we really have a BL with primitive vector $a\hat{x}$, and 1^{st} BZ is $k \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$ and there is no Bragg plane at $k = \frac{\pi}{2a}$ and hence no energy gap there.

Note: $2 + 2\cos(2ka) = 4\cos^2 ka$

When $E_A = E_B$, $\beta_A = \beta_B$, $\gamma_A = \gamma_B$ then $\sqrt{\ }$ term becomes

$\sqrt{\ } = \sqrt{0 + 4\gamma^2\cos^2 ka} = 2\gamma\cos ka$

and we recover the s-band we saw when we first started our discussion of tight binding model

In general

$$\boxed{\mathcal{E}_\pm(k) = \frac{E_A + E_B - \beta_A - \beta_B}{2} \pm \sqrt{\left(\frac{E_A - E_B - \beta_A + \beta_B}{2}\right)^2 + 4\gamma_A\gamma_B\cos^2 ka}}$$

To sketch

$$\mathcal{E}_\pm(k) = \frac{E_A+E_B-\beta_A-\beta_B}{2} \pm \sqrt{\left(\frac{E_A-E_B-\beta_A+\beta_B}{2}\right)^2 + 4\gamma_A\gamma_B\cos^2 kx}$$

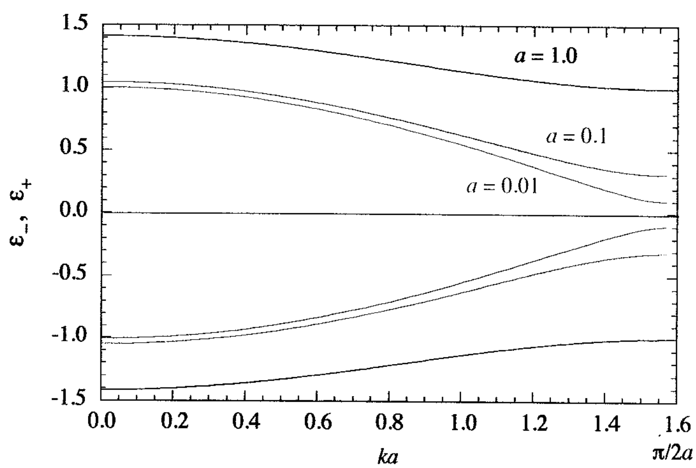
Set overal const of energy so that $\frac{E_A+E_B-\beta_A-\beta_B}{2} = 0$

Set units of energy so that $4\gamma_A\gamma_B = 1$

Denote $\left(\frac{E_A-E_B-\beta_A+\beta_B}{2}\right)^2 \equiv a$

Then $\mathcal{E}_\pm(k) = \pm\sqrt{a+\cos^2 kx}$

Below we plot $\mathcal{E}_\pm(k)$ for values $a = 1,\ 0.1,\ 0.01$



as $a \to 0$ the energy gap $\mathcal{E}_+ - \mathcal{E}_-$ at $k = \frac{\pi}{2a}$ vanishes

Having found eigenvalues, one now can solve for eigenvectors $\begin{pmatrix} b_A \\ b_B \end{pmatrix}$

$$\begin{pmatrix} \mathcal{E}_\pm - E_A + \beta_A & \gamma_A(1+e^{-2ika}) \\ \gamma_B(1+e^{2ika}) & \mathcal{E}_\pm - E_B + \beta_B \end{pmatrix} \begin{pmatrix} b_A \\ b_B \end{pmatrix} = 0$$

when $k = \pi/2a$ at boundary 1st BZ, matrix is diagonal!

$\Rightarrow$ eigenvectors at $k = \frac{\pi}{2a}$ are $\begin{pmatrix} b_A \\ b_B \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\boxed{b_B = \frac{-\gamma_B(1+e^{2ika})}{\mathcal{E}_\pm - E_B + \beta_B}\, b_A}$$

2) We found the π and π^* band energies were

$$\varepsilon_\pm(\vec{k}) = E - \beta \pm |\gamma| f(k)$$

where $f(\vec{k}) = \left[1 + 4\cos^2\left(\frac{k_x a}{2}\right) + 4\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{\sqrt{3}}{2} k_y a\right)\right]^{1/2}$

a) For small k, expand the cosines to $o(k^2)$

$$\cos\left(\frac{k_x a}{2}\right) \simeq 1 - \frac{1}{8}(k_x a)^2$$

$$\cos\left(\frac{\sqrt{3}}{2} k_y a\right) \simeq 1 - \frac{3}{8}(k_y a)^2$$

$$\cos^2\left(\frac{k_x a}{2}\right) \simeq 1 - \frac{1}{4}(k_x a)^2$$

So

$$f^2 \simeq 1 + 4 - (k_x a)^2 + 4\left(1 - \frac{1}{8}(k_x a)^2\right)\left(1 - \frac{3}{8}(k_y a)^2\right)$$

to $o(k^2)$ $\quad \simeq 1 + 4 - (k_x a)^2 + 4 - \frac{1}{2}(k_x a)^2 - \frac{3}{2}(k_y a)^2$

$$= 9 - \frac{3}{2}(k_x a)^2 - \frac{3}{2}(k_y a)^2$$

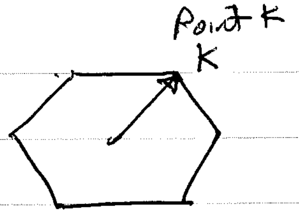
$$= 9 - \frac{3}{2}|\vec{k}a|^2$$

$$f = 3\sqrt{1 - \frac{1}{6}|\vec{k}a|^2} \simeq 3\left(1 - \frac{1}{12}|\vec{k}a|^2\right) = 3 - \frac{1}{4}k^2a^2$$

So $\boxed{\varepsilon_\pm(\vec{k}) \simeq E - \beta \pm 3|\gamma| \mp \frac{1}{4}|\gamma| k^2 a^2}$ $\qquad k = |\vec{k}|$

lower band increases energy as k increases
upper band decreases energy as k increases

since $\varepsilon_\pm(k) \sim \text{const} - ck^2$ depends only on $\vec{k}$ through $|\vec{k}| = k$, the constant energy surfaces of circles centered at the origin.

b) 

$\vec{k}_K = \frac{2\pi}{a}\left(\frac{1}{3}, \frac{1}{\sqrt{3}}\right) \qquad k_{Kx} = \frac{2\pi}{3a}, \; k_{Ky} = \frac{2\pi}{\sqrt{3}a}$

for $\vec{k} = \vec{k}_K + \delta\vec{k}$ expand cosines for small $\delta\vec{k}$.

$$\cos\left(\frac{k_x a}{2}\right) = \cos\left(\frac{\pi}{3} + \frac{\delta k_x a}{2}\right) = \frac{1}{2}\cos\left(\frac{\delta k_x a}{2}\right) - \frac{\sqrt{3}}{2}\sin\left(\frac{\delta k_x a}{2}\right)$$

$$\cos\left(\frac{\sqrt{3}}{2}k_y a\right) = \cos\left(\pi + \frac{\sqrt{3}}{2}\delta k_y a\right) = -\cos\left(\frac{\sqrt{3}}{2}\delta k_y a\right)$$

$$f^2 = 1 + \left[\cos\left(\frac{\delta k_x a}{2}\right) - \sqrt{3}\sin\left(\frac{\delta k_x a}{2}\right)\right]^2$$

$$- 2\left[\cos\left(\frac{\delta k_x a}{2}\right) - \sqrt{3}\sin\left(\frac{\delta k_x a}{2}\right)\right]\cos\left(\frac{\sqrt{3}}{2}\delta k_y a\right)$$

$$= 1 + \cos^2\left(\frac{\delta k_x a}{2}\right) - 2\sqrt{3}\cos\left(\frac{\delta k_x a}{2}\right)\sin\left(\frac{\delta k_x a}{2}\right) + 3\sin^2\left(\frac{\delta k_x a}{2}\right)$$

$$- 2\cos\left(\frac{\delta k_x a}{2}\right)\cos\left(\frac{\sqrt{3}}{2}\delta k_y a\right) + 2\sqrt{3}\sin\left(\frac{\delta k_x a}{2}\right)\cos\left(\frac{\sqrt{3}}{2}\delta k_y a\right)$$

expand to $o(\delta k^2)$

$$\simeq 1 + \left(1 - \frac{1}{8}(\delta k_x a)^2\right)^2 - 2\sqrt{3}\left(1 - \frac{1}{8}(\delta k_x a)^2\right)\left(\frac{\delta k_x a}{2}\right) + \frac{3}{4}(\delta k_x a)^2$$

$$- 2\left(1 - \frac{1}{8}(\delta k_x a)^2\right)\left(1 - \frac{3}{8}(\delta k_y a)^2\right) + 2\sqrt{3}\left(\frac{\delta k_x a}{2}\right)\left(1 - \frac{3}{8}(\delta k_y a)^2\right)$$

to $o(\delta k^2)$

$$\simeq 1 + 1 - \frac{1}{4}(\delta k_x a)^2 - \sqrt{3}\,\delta k_x a + \frac{3}{4}(\delta k_x a)^2$$

$$- 2 + \frac{1}{4}(\delta k_x a)^2 + \frac{3}{4}(\delta k_y a)^2 + \sqrt{3}\,\delta k_x a$$

$$= \frac{3}{4}(\delta k_x a)^2 + \frac{3}{4}(\delta k_y a)^2 = \frac{3}{4}|\delta k a|^2$$

$$f = \frac{\sqrt{3}}{2}|\delta\vec{k} a| = \frac{\sqrt{3}}{2}a|\vec{k} - \vec{k}_K|$$

so $\boxed{\varepsilon_\pm(\vec{k}) = E - \beta \pm \frac{\sqrt{3}}{2}|\gamma| a |\vec{k} - \vec{k}_K|}$

c) since $\varepsilon_\pm(\vec{k})$ depends only on the distance of $\vec{k}$ to $\vec{k}_K$, ie on $|\vec{k}-\vec{k}_K|$, the constant energy surfaces are circles centered at $\vec{k}_K$.

d) $f^2 = 1 + 4\cos^2\left(\frac{k_x a}{2}\right) + 4\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{\sqrt{3}}{2} k_y a\right)$

To have a nested constant energy surface, there must be a segment of the surface that is a <u>straight line</u>, say $k_y = c_0 k_x + c_1$
Along this line, $f(k_x, k_y)$ must be constant.

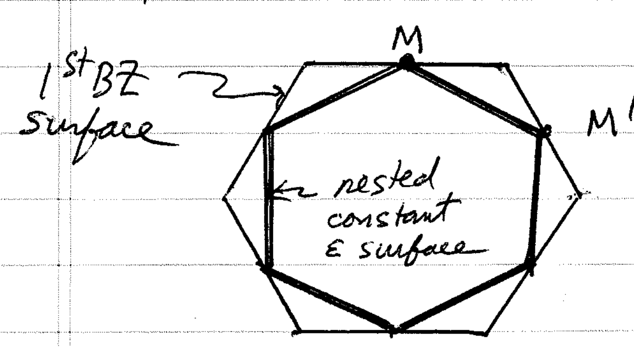
We can keep f constant by choosing k_y such that $\cos\left(\frac{\sqrt{3}}{2} k_y a\right) = -\cos\left(\frac{k_x a}{2}\right)$ so that $f = 1$

$\Rightarrow \boxed{k_y = \frac{2}{\sqrt{3}}\left(\pm \frac{k_x}{2} \pm \frac{\pi}{a}\right)}$ four possible lines

Or, we can choose k_x such that $\cos\left(\frac{k_x a}{2}\right) = 0$

$\rightarrow \boxed{k_x = \pm \frac{\pi}{a}}$ two possible lines

these lines can be sketched in the 1^{st} BZ as below



e) Since $\varepsilon(\vec{k})$ depends on k_x and k_y and not just the magnitude $|\vec{k}|$ (ie depends also on direction of $\vec{k}$) we cannot use the simple result for $g(\varepsilon)$ that we had for free electrons

[Recall, when ε depends only on $|\vec{k}|$ we had

$$g(\varepsilon)d\varepsilon = 2\frac{S_d}{(2\pi)^d}k^{d-1}dk$$

S_d = surface area of unit sphere in d dimensions]

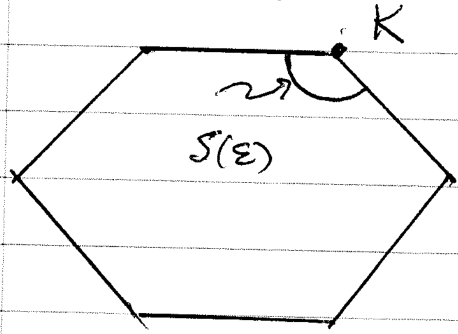
Here we will use the general formula AM (8.63)

$$g(\varepsilon) = 2\int_{S(\varepsilon)}\frac{dS}{(2\pi)^d}\frac{1}{|\vec{\nabla}\varepsilon|}$$

where d is dimension and $S(\varepsilon)$ is surface of constant energy ε in k-space

Here we have near pt K, $\varepsilon(\vec{k}) = E-\beta \pm \frac{\sqrt{3}}{2}|\gamma| a\,|\vec{\delta k}|$ where $\vec{\delta k} = \vec{k}-\vec{k}_K$

$\Rightarrow$ Surface of constant energy is just a circle about point K (part (c)) with radius $\delta k = |\vec{\delta k}|$



Note, since $S(\varepsilon)$ must lie in 1st BZ, we have only 1/3 of a circle. But there are 6 points equivalent to pt K (the vertices of 1st BZ)

So $6\times\frac{1}{3}$ = net factor 2

on this circle, $|\vec{\nabla}\varepsilon| = \left|\frac{\partial \varepsilon}{\partial \delta k}\right| = \frac{\sqrt{3}}{2}|\gamma|a$ constant!

So $g(\varepsilon) = \frac{1}{2\pi^2} \frac{2}{\sqrt{3}|\gamma|a} \int_{S(\varepsilon)} dS$

$$g(\varepsilon) = \frac{1}{2\pi^2} \frac{2}{\sqrt{3}|\gamma|a} \, 2\pi \, \delta k \times 2$$

factor 2 since have $\frac{1}{3}$ of circle at the 6 pts equivalent to K

Now $\delta k = \pm \dfrac{(\varepsilon - E + \beta)}{\frac{\sqrt{3}}{2}|\gamma|a}$

and

$$E - \beta = \varepsilon_K \quad \text{energy at pt } K \text{ - see lecture notes}$$
$$= \varepsilon_F$$

($\varepsilon_K = \varepsilon_F$ since there are 2 electrons per BL site, so π band gets completely filled, and K is point of highest energy in π band - see lecture notes)

$$\delta k = \pm \frac{(\varepsilon - \varepsilon_F)}{\frac{\sqrt{3}}{2}|\gamma|a}$$

+ is for π^* band where $\varepsilon_+ > \varepsilon_F$

− is for π band where $\varepsilon_- < \varepsilon_F$

or $\delta k = \dfrac{|\varepsilon - \varepsilon_F|}{\frac{\sqrt{3}}{2}|\gamma|a}$ works for both π and π^* bands

So

$$g(\varepsilon) = \frac{1}{\pi} \frac{2}{\sqrt{3}|\gamma|a} \times 2 \left[\frac{|\varepsilon - \varepsilon_F|}{\frac{\sqrt{3}}{2}|\gamma|a}\right]$$

$$\boxed{g(\varepsilon) = \frac{1}{\pi} \frac{8}{3|\gamma|^2 a^2} |\varepsilon - \varepsilon_F|}$$

vanishes linearly as $\varepsilon \to \varepsilon_F$ ✓