Phys 617 - P.S. 4 Solns.

(1) we have $\overleftrightarrow{\sigma} = \mathbb{R}\cdot\overleftrightarrow{\sigma}\cdot\mathbb{R}^{-1}$ for symmetry operators,

and $\mathbb{R} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$ for example, a rotation about $\hat{z}$.

60° about z is symmetry $\left(\cos\theta = \frac{1}{2}, \ \sin\theta = \frac{\sqrt{3}}{2}\right)$
also 180° about x or y.

Start with 180° about x: $\mathbb{R} = \begin{pmatrix} 1 & & \\ & -1 & \\ & & -1 \end{pmatrix} = \mathbb{R}^{-1}$

$$\mathbb{R}\cdot\sigma\cdot\mathbb{R}^{-1} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ -\sigma_{yx} & -\sigma_{yy} & -\sigma_{yz} \\ -\sigma_{zx} & -\sigma_{zy} & -\sigma_{zz} \end{pmatrix}\begin{pmatrix} 1 & & \\ & -1 & \\ & & -1 \end{pmatrix}$$

$$= \begin{pmatrix} \sigma_{xx} & -\sigma_{xy} & -\sigma_{xz} \\ -\sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ -\sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

Compare with original $\overleftrightarrow{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$,

we see that $\boxed{\sigma_{yx} = \sigma_{zx} = \sigma_{xy} = \sigma_{xz} = 0}$

Similarly, a $180°$ rotation about y, $\mathbb{R} = \begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix}$

shows that $\boxed{\sigma_{zy} = \sigma_{yz} = 0}$.

So far, $\overleftrightarrow{\sigma}$ must be of form, $\begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$.

Now apply $60°$ about x: $\mathbb{R} = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} & \\ \sqrt{3} & 1 & \\ & & 2 \end{pmatrix}$

$$\mathbb{R}\cdot\sigma\cdot\mathbb{R}^{-1} = \frac{1}{2}\begin{pmatrix} \sigma_{xx} & -\sqrt{3}\,\sigma_{yy} & 0 \\ \sqrt{3}\,\sigma_{xx} & \sigma_{yy} & 0 \\ 0 & 0 & 2\sigma_{zz} \end{pmatrix}\cdot\mathbb{R}^{-1}$$

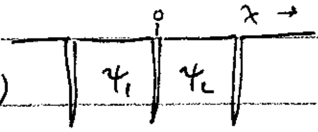
$$= \frac{1}{4}\begin{pmatrix} \sigma_{xx} + 3\sigma_{yy} & \sqrt{3}\,\sigma_{xx} - \sqrt{3}\,\sigma_{yy} & 0 \\ \sqrt{3}\,\sigma_{xx} - \sqrt{3}\,\sigma_{yy} & 3\sigma_{xx} + \sigma_{yy} & 0 \\ 0 & 0 & 4\sigma_{zz} \end{pmatrix}$$

comparing term by term, $\sigma_{xx} - \sigma_{yy} = 0 \Rightarrow \boxed{\sigma_{xx} = \sigma_{yy}}$

Finally we get $\sigma = \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_1 & 0 \\ 0 & 0 & \sigma_2 \end{pmatrix}$

(symmetric with respect to <u>arbitrary</u> rotations about $\hat{z}$, but only $180°$ about $\hat{x}$ or $\hat{y}$.)

(2) Kronig - Penney model

(a) 

between δ-fns, $\psi = Ae^{Kx} + Be^{-Kx}$,
where $K = \sqrt{\frac{-2mE}{\hbar^2}}$ (for $E<0$)

for $x \approx 0$, identify regions 1 & 2:

(i) $\psi_2(0^+) = \psi_1(0^-) \rightarrow A_1 + B_1 = A_2 + B_2$

(ii) $\left[\psi_2'\big|_{0^+} - \psi_1'\big|_{0^-}\right] = \frac{2m}{\hbar^2} aV\psi(0)$ by

integrating Schrödinger eqn.

so, $K[A_2 - B_2 - A_1 + B_1] = \frac{2m}{\hbar^2} aV(A_1 + B_1)$

(iii) Bloch theorem: $A_2e^{Ka} + B_2e^{-Ka} = e^{ika}(A_1 + B_1)$

(iv) Differentiate Bloch theorem:

$$\left(\psi'\big|_{a^-}\right) = e^{ika}\left(\psi'\big|_{0^-}\right)$$

$$\cancel{K}\left(A_2e^{Ka} - B_2e^{-Ka}\right) = e^{ika}\cancel{K}(A_1 - B_1)$$

~~Given~~ i into iii $\Rightarrow$ $A_2(e^{Ka} - e^{ika}) = B_2(e^{ika} - e^{-Ka})$ (I)

i & ii $\rightarrow$ $A_1 - B_1 = A_2 - B_2 - \frac{2maV}{\hbar^2K}(A_2 + B_2)$

into (iv) $\rightarrow$ $A_2\left(e^{Ka} - e^{ika} + e^{ika}\left[\frac{2maV}{\hbar^2K}\right]\right) = B_2\left(e^{-Ka} - e^{ika} - e^{ika}\left[\frac{2maV}{\hbar^2K}\right]\right)$,

(II)

divide I & II $\Rightarrow$

$$1 + \frac{2maV}{\hbar^2K}\left(\frac{e^{ika}}{e^{Ka} - e^{ika}}\right) = -1 - \frac{2maV}{\hbar^2K}\left(\frac{e^{ika}}{e^{ika} - e^{-Ka}}\right)$$

$$1 = \frac{maV}{\hbar^2K}\left(\frac{-e^{ika}}{e^{Ka} - e^{ika}} + \frac{e^{ika}}{e^{-Ka} - e^{ika}}\right)$$

$$e^{-ika} - e^{Ka} - e^{-Ka} + e^{ika} = \left(\frac{maV}{\hbar^2K}\right)\left(e^{Ka} + e^{-Ka}\right)$$

$$\cos ka - \cosh Ka = \frac{Vma}{\hbar^2K}\sinh Ka$$

so $\rightarrow$ desired form $\left(\phi \equiv Ka = \sqrt{\frac{-2mEa^2}{\hbar^2}}\right)$

(b) large V $\to$ large $(|\mathcal{E}|)$, so $\Phi \gg 1$.

so eliminate $e^{-\phi}$ terms:

$$\cos ka \simeq \left(1 + \frac{Vma^2}{\hbar^2 \phi}\right) \frac{e^{\phi}}{2}$$

must have $\phi \simeq \frac{-Vma^2}{\hbar^2}$, so try:

$$\phi = \frac{-Vma^2}{\hbar^2}(1 + x + \dots)$$

$$\cos ka \simeq \frac{1}{2} e^{-\frac{Vma^2}{\hbar^2}}\left(1 - \frac{Vma^2 x}{\hbar^2} + \dots\right)\left(1 + \frac{-1}{1+x} + \dots\right)$$

$$\simeq \frac{1}{2} e^{-\frac{Vma^2}{\hbar^2}}\left(1 - \cancel{\frac{Vma^2}{\hbar^2} x}^{\text{small}}\right)\left(\frac{x}{1+\cancel{x}}\right) \text{ neglect.}$$

$$x \simeq 2\cos ka \, e^{+\frac{Vma^2}{\hbar^2}}$$

and $$\phi \simeq \frac{-Vma^2}{\hbar^2}\left(1 + 2\cos ka \, e^{+\frac{Vma^2}{\hbar^2}} + \dots\right)$$

$$\mathcal{E} \simeq \frac{-\hbar^2}{2ma^2}\phi^2 = \underbrace{\frac{-V^2 ma^2}{2\hbar^2}}_{A}\left[1 + \underbrace{4e^{+\frac{Vma^2}{\hbar^2}}}_{B} \cos ka\right]$$

(3) [Note: M is the (1,1) direction, not (111) since it is 2D, sorry about that.]

(a) $\mathcal{E}(k) = \frac{\hbar^2}{2m}\left[\vec{k} + m_1 \frac{2\pi}{a}\hat{\imath} + m_2 \frac{2\pi}{a}\hat{\jmath}\right]^2$

along (10), Γ to X, $\vec{k} = (k, 0)$ gives

$$\mathcal{E}_{10}(k) = \frac{\hbar^2}{2m}\left[\left(k + \frac{2\pi m_1}{a}\right)^2 + \left(\frac{2\pi m_2}{a}\right)^2\right]$$

along (11), Γ to M, $\vec{k} = \frac{1}{\sqrt{2}}(k, k)$,

$$\mathcal{E}_{11}(k) = \frac{\hbar^2}{2m}\left[\left(\frac{k}{\sqrt{2}} + \frac{2\pi m_1}{a}\right)^2 + \left(\frac{k}{\sqrt{2}} + \frac{2\pi m_2}{a}\right)^2\right]$$

(b) at Γ, $\mathcal{E} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left[m_1^2 + m_2^2\right] = 4\frac{\hbar^2\pi^2}{2ma^2}\left(m_1^2 + m_2^2\right)$,

lowest $\mathcal{E} \neq 0$ is $\boxed{\mathcal{E} = 4\frac{\hbar^2\pi^2}{2ma^2}}$ for $(m_1, m_2) = (\pm 1, 0)$ or $(0, \pm 1)$

next is $\boxed{\mathcal{E} = 8\frac{\hbar^2\pi^2}{2ma^2}}$ for $(m_1, m_2) = (\pm 1, \pm 1)$

at X, $\mathcal{E} = \frac{\hbar^2\pi^2}{2ma^2}\left[(2m_1+1)^2 + (2m_2)^2\right]$

lowest $(m_1, m_2) = (0,0)$, $\boxed{\mathcal{E} = \frac{\hbar^2\pi^2}{2ma^2}}$ (also $(-1,0)$)

next $(m_1, m_2) = (0, \pm 1)$, $\boxed{\mathcal{E} = 5\frac{\hbar^2\pi^2}{2ma^2}}$

at M, $\mathcal{E} = \frac{\hbar^2\pi^2}{2ma^2}\left[(2m_1+1)^2 + (2m_2+1)^2\right]$

lowest (0,0), (-1,0) & (0,-1) & (-1,-1) $\Rightarrow$ $\boxed{\mathcal{E} = 2\frac{\hbar^2\pi^2}{2ma^2}}$

next (1,0) & 3 others $\boxed{\mathcal{E} = 10\frac{\hbar^2\pi^2}{2ma^2}}$

(c) 4 degenerate $\vec{k}$ points are $\left(\pm\frac{\pi}{a}, \pm\frac{\pi}{a}\right)$, so that $\left(\frac{\pi}{a}, \frac{\pi}{a}\right)$ is joined to $\left(\frac{\pi}{a}, -\frac{\pi}{a}\right)$ by $G = \left(0, -\frac{2\pi}{a}\right)$, to $\left(-\frac{\pi}{a}, \frac{\pi}{a}\right)$ by $G = \left(-\frac{2\pi}{a}, 0\right)$ and to $\left(-\frac{\pi}{a}, -\frac{\pi}{a}\right)$ by $G = \left(-\frac{2\pi}{a}, -\frac{2\pi}{a}\right)$

④ (a) $|\psi_{\vec{k}}\rangle = \sum_{m,n} |m,n\rangle e^{i\vec{k}\cdot\vec{r}_{mn}}$

or writing $\vec{r}_{mn} = (ma, nb)$,

so that $\vec{k}\cdot\vec{r}_{mn} = (mak_x + nbk_y)$,

$$|\psi_{\vec{k}}\rangle = \sum_{m,n}' |m,n\rangle e^{ik_x am} e^{ik_y bn}$$

(b) Looking for $H|\psi_{\vec{k}}\rangle = \mathcal{E}|\psi_{\vec{k}}\rangle$, which is:

$$\sum_{mn} \Big(\mathcal{E}_0 |m,n\rangle e^{i\vec{k}\cdot\vec{r}_{mn}} - t_1 |m,n\rangle e^{i\vec{k}\cdot\vec{r}_{mn}} \times \left[e^{ik_y b} + e^{-ik_y b} \right]$$

$$- t_2 |m,n\rangle e^{i\vec{k}\cdot\vec{r}_{mn}} \times \left[e^{ik_x a} + e^{-ik_x a} \right] = \mathcal{E}|\psi_{\vec{k}}\rangle$$

(2^{ND} and third term can be rewritten this way by suitable substitution, e.g. $n \pm 1 \to n'$, etc.)

taking out common factors:

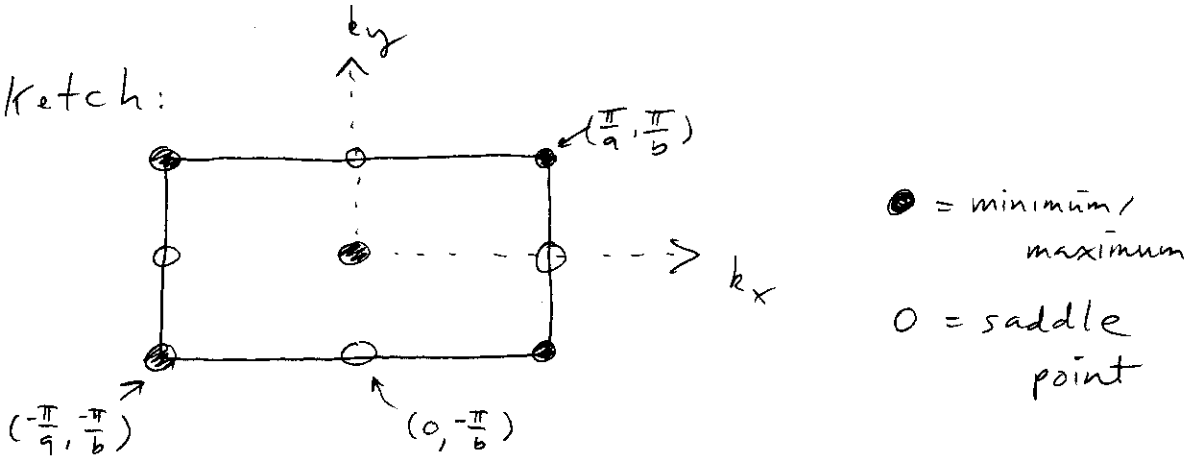
$$\underbrace{\sum_{mn}' |m,n\rangle e^{i\vec{k}\cdot\vec{r}_{mn}}}_{|\psi\rangle} \cdot \left(\mathcal{E}_0 - t_1 \times 2\cos k_y b - t_2 \times 2\cos k_x a \right) = \mathcal{E}|\psi\rangle$$

So eigenvalue equation works with $\mathcal{E} = \mathcal{E}_0 - 2(t_1 \cos k_y b + t_2 \cos k_x a)$

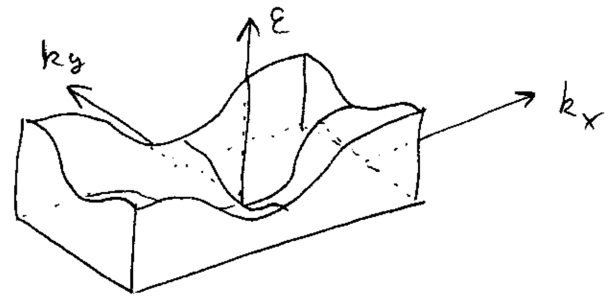
$\mathcal{E}_{min} = \mathcal{E}_0 - 2t_1 - 2t_2$ at $(0,0)$; $\mathcal{E}_{max} = \mathcal{E}_0 + 2t_1 + 2t_2$ at $\left(\pm\frac{\pi}{a}, \pm\frac{\pi}{b}\right)$

also $\vec{\nabla}_k \mathcal{E} = 0$ at $k_x = 0, \pm\frac{\pi}{a}$ and $k_y = 0, \pm\frac{\pi}{b}$. So saddle points at $\left(0, \pm\frac{\pi}{b}\right)$ and $\left(\pm\frac{\pi}{a}, 0\right)$

sketch:



here (assuming $a < b$) the 1st B.Z. is a rectangle as shown, with 4 maxima & 4 saddle points.



(rough sketch of $\mathcal{E}(k)$)