1. Band Structure of Aluminum

(a) First I will clarify my notations here.

- I denote kinetic energy as $\varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$, and the bands $E^{(1)}(\vec{k})$, $E^{(2)}(\vec{k})$ ...
- Let $\varepsilon_0 = \frac{2\pi^2\hbar^2}{ma^2}$ be the scale of energy
- Suppose U has inversion symmetry so that its Fourier components are real. Let $U_1 = U_{\vec{G}_{111}} = \cdots = U_{\vec{G}_{\bar{1}\bar{1}\bar{1}}}$, and $U_2 = U_{\vec{G}_{200}} = \cdots = U_{\vec{G}_{00\bar{2}}}$

(1) $\Gamma \to X$

Let $\vec{k} = \frac{2\pi}{a}(\alpha, 0, 0)$. Going from Γ to X is equivalent to increasing α from 0 to 1.

(1.1) α is in the neighborhood of 0

i.e. $\vec{k}$ is very close to Γ. The lowest band has no degeneracy and is just a parabola:

$$E^{(1)}(\vec{k}) = \frac{\hbar^2 k^2}{2m} = \varepsilon_0 \alpha^2$$

The second-to-lowest band, however, is more complicated. There are 8 G-points that are closest to Γ and have the same energy: $\vec{G}_{111} \cdots \vec{G}_{\bar{1}\bar{1}\bar{1}}$. So $E^{(2)}(\vec{k})$ must be calculated by diagonalizing the subspace spanned by $|\psi_{\vec{k}-\vec{G}_{111}}\rangle \cdots |\psi_{\vec{k}-\vec{G}_{\bar{1}\bar{1}\bar{1}}}\rangle$.

However, $E^{(2)}(\Gamma) \approx \varepsilon_{\vec{G}_{111}} = 3\varepsilon_0$ is very high. As a comparison, $E^{(2)}(X) \approx \varepsilon_0$ (I have ignored the shift due to avoided crossing). This means that, in the neighborhood of Γ, $E^{(2)}(\vec{k})$ is way above E_F and is thus not of interest. It is not shown in the pset figure.

Therefore, I will not do the calculation of $E^{(2)}(\vec{k})$ in this case.

(1.2) α is far away from 0.
i.e. $\vec{k}$ is sufficiently far away from Γ, such that $|\psi_{\vec{k}-\vec{G}_{1\bar{1}1}}\rangle \cdots |\psi_{\vec{k}-\vec{G}_{\bar{1}\bar{1}\bar{1}}}\rangle$ do not mix into $E^{(2)}(\vec{k})$

Since at X, we have a double degeneracy of $|\psi_X\rangle$ and $|\psi_{X-\vec{G}_{200}}\rangle$, we should diagonalize the subspace spanned by $|\psi_{\vec{k}}\rangle$ and $|\psi_{\vec{k}-\vec{G}_{200}}\rangle$.

Before that, we already know that

(1.2.1) when $1-\alpha \gg \frac{U_2}{\varepsilon_0}$, to the lowest order,

$$E^{(1)}(\vec{k}) = \frac{\hbar^2 k^2}{2m} = \varepsilon_0 \alpha^2$$
$$E^{(2)}(\vec{k}) = \frac{\hbar^2 |\vec{k}-\vec{G}_{200}|^2}{2m} = \varepsilon_0 (2-\alpha)^2$$

we expect $E^{(2)}(\vec{k})$ to be off more than $E^{(1)}(\vec{k})$ due to the coupling with other plane waves, say, $|\psi_{\vec{k}-\vec{G}_{111}}\rangle$.

(1.2.2) when $1-\alpha \ll \frac{U_2}{\varepsilon_0}$, to the lowest order.

$$E^{(1)}(\vec{k}) = \varepsilon_X - U_2 = \varepsilon_0 - U_2$$
$$E^{(2)}(\vec{k}) = \varepsilon_X + U_2 = \varepsilon_0 + U_2.$$

Now let us diagonalize the truncated Hamiltonian for general α.

$$H = \begin{bmatrix} \varepsilon_{\vec{k}} & U_2 \\ U_2 & \varepsilon_{\vec{k}-\vec{G}_{200}} \end{bmatrix}$$

We get

$$E^{(1)}(\vec{k}) = \frac{1}{2}\left[\left(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}-\vec{G}_{200}}\right) - \sqrt{\left(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}-\vec{G}_{200}}\right)^2 + 4U_2^2}\right]$$
$$= \left[1+(1-\alpha)^2\right]\varepsilon_0 - \sqrt{4(1-\alpha)^2\varepsilon_0^2 + U_2^2}$$
$$E^{(2)}(\vec{k}) = \frac{1}{2}\left[\left(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}-\vec{G}_{200}}\right) + \sqrt{\left(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}-\vec{G}_{200}}\right)^2 + 4U_2^2}\right]$$
$$= \left[1+(1-\alpha)^2\right]\varepsilon_0 + \sqrt{4(1-\alpha)^2\varepsilon_0^2 + U_2^2}$$

From this, we can refine (1.2.1) and (1.2.2) to the next order, as well as obtaining band structure of intermediate region.

(1.2.1)' when $1-\alpha \gg \frac{U_2}{\varepsilon_0}$

$$E^{(1)}(\vec{k}) = \varepsilon_0 \alpha^2 - \frac{U_2^2}{4(1-\alpha)\varepsilon_0}$$
$$E^{(2)}(\vec{k}) = \varepsilon_0 (2-\alpha)^2 + \frac{U_2^2}{4(1-\alpha)\varepsilon_0}$$

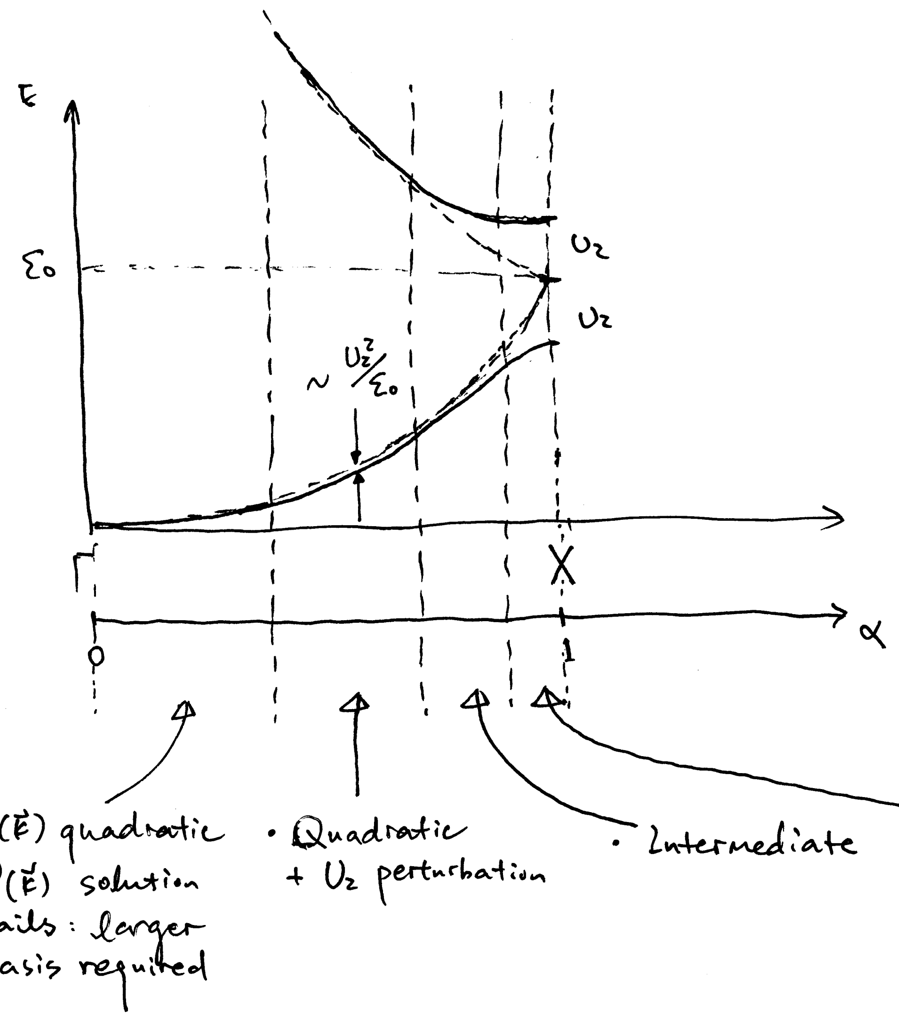
(1.2.2)' when $1-\alpha \ll \frac{U_2}{\varepsilon_0}$

$$E^{(1)}(\vec{k}) = \varepsilon_0(1+(1-\alpha)^2) - U_2 - \frac{2(1-\alpha)^2\varepsilon_0^2}{U_2}$$

$$E^{(2)}(\vec{k}) = \varepsilon_0(1+(1-\alpha)^2) + U_2 + \frac{2(1-\alpha)^2\varepsilon_0^2}{U_2}$$

Specifically, when $\alpha=1$, $E^{(1)}(X) = \varepsilon_0 - U_2$, $E^{(2)}(X) = \varepsilon_0 + U_2$

In conclusion



(2) $X \longrightarrow W$

The entire path is on (200) face. Double degeneracy everywhere. Let $\vec{k} = \frac{2\pi}{a}(1,\beta,0)$ Going from X to W is equivalent to increasing β from 0 to $\frac{1}{2}$.

Degeneracy:

$$\varepsilon_{\vec{k}} = \varepsilon_{\vec{k}-\vec{G}_{200}} = \varepsilon_0(1+\beta^2)$$

$$\varepsilon_{\vec{k}-\vec{G}_{111}} = \varepsilon_{\vec{k}-\vec{G}_{11\bar{1}}} = \varepsilon_0(1+(1-\beta)^2)$$

When $\beta = \frac{1}{2}$, i.e. at W, we have a four-fold degeneracy

$\varepsilon_W = \frac{5}{4}\varepsilon_0$.

(2.1) Start from $\beta = 0$ and keep β far away from $\frac{1}{2}$.

Avoided crossing happens in subspace $\{|\psi_{\vec{k}}\rangle, |\psi_{\vec{k}-\vec{G}_{200}}\rangle\}$ and $\{|\psi_{\vec{k}-\vec{G}_{111}}\rangle, |\psi_{\vec{k}-\vec{G}_{11\bar{1}}}\rangle\}$. But the coupling across subspace is negligible.

Within each subspace, avoided crossing:

$$E^{(1)}(\vec{k}) = \varepsilon_0(1+\beta^2) - U_2 = E_1^-$$
$$E^{(2)}(\vec{k}) = \varepsilon_0(1+\beta^2) + U_2 = E_1^+$$

$$E^{(3)}(\vec{k}) = \varepsilon_0(1+(1-\beta)^2) - U_2 = E_2^-$$
$$E^{(4)}(\vec{k}) = \varepsilon_0(1+(1-\beta)^2) + U_2 = E_2^+$$

The good basis is

$$|\psi_1^\pm\rangle = \frac{1}{\sqrt{2}}\left(|\psi_{\vec{k}}\rangle \pm |\psi_{\vec{k}-\vec{G}_{200}}\rangle\right)$$
$$|\psi_2^\pm\rangle = \frac{1}{\sqrt{2}}\left(|\psi_{\vec{k}-\vec{G}_{111}}\rangle \pm |\psi_{\vec{k}-\vec{G}_{11\bar{1}}}\rangle\right)$$

(2.2) Now add inter-subspace coupling. In this basis,

$$H = \begin{bmatrix} E_1^- & 0 & 0 & 0 \\ 0 & E_1^+ & 0 & 2U_1 \\ 0 & 0 & E_2^- & 0 \\ 0 & 2U_1 & 0 & E_2^+ \end{bmatrix}$$

When U_1 is not negligible, $|\psi_1^\pm\rangle$ will couple to $|\psi_2^\pm\rangle$. However, notice that $|\psi_1^-\rangle$ and $|\psi_2^-\rangle$ are still eigenstates of H. Coupling only happens between $|\psi_1^+\rangle$ and $|\psi_2^+\rangle$.

In the subspace spanned by $\{|\psi_1^+\rangle, |\psi_2^+\rangle\}$,

$$H = \begin{bmatrix} E_1^+ & 2U_1 \\ 2U_1 & E_2^+ \end{bmatrix}$$

$$E^\pm = \frac{1}{2}\left[(E_1^+ + E_2^+) \pm \sqrt{(E_1^+ - E_2^+)^2 + 16U_1^2}\right] + U_2$$
$$= \left\{1 + \frac{1}{2}\left(\beta^2 + (1-\beta)^2\right)\right\}\varepsilon_0 \pm \sqrt{\tfrac{1}{4}(1-2\beta)^2\varepsilon_0^2 + 4U_1^2} + U_2$$

(2.2.1) When $1-2\beta \gg \frac{U_1}{\varepsilon_0}$.

$$E^+ = \varepsilon_0(1+(1-\beta)^2) + U_2 + \frac{4U_1^2}{(1-2\beta)\varepsilon_0}$$
$$E^- = \varepsilon_0(1+\beta^2) + U_2 - \frac{4U_1^2}{(1-2\beta)\varepsilon_0}$$

Ordering of levels is

$$E^{(1)}(\vec{k}) = E_1^-$$
$$E^{(2)}(\vec{k}) = E^-$$
$$E^{(3)}(\vec{k}) = E_2^-$$
$$E^{(4)}(\vec{k}) = E^+$$

(2.2.2) when $1-2\beta \ll \frac{U_1}{\varepsilon_0}$

$$E^+ = \left(1+\tfrac{1}{2}(\beta^2+(1-\beta)^2)\right)\varepsilon_0 + 2U_1 + U_2$$
$$E^- = \left(1+\tfrac{1}{2}(\beta^2+(1-\beta)^2)\right)\varepsilon_0 - 2U_1 + U_2$$

Ordering of levels is

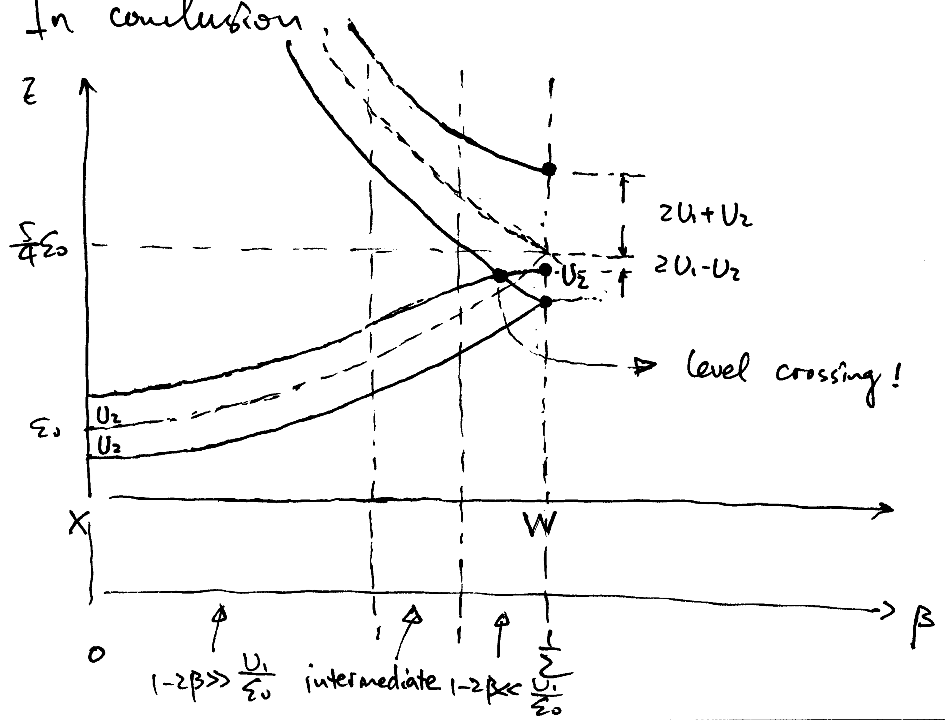
$$E^{(1)}(\vec{k}) = E_1^-$$
$$E^{(2)}(\vec{k}) = E_2^-$$
$$E^{(3)}(\vec{k}) = E^-$$
$$E^{(4)}(\vec{k}) = E^+$$

Comparing (2.2.1) and (2.2.2), we notice a level crossing between $E^{(2)}(\vec{k})$ and $E^{(3)}(\vec{k})$. This does not turn into an avoided crossing, since $|\psi_2^-\rangle$ does not couple with $\{|\psi_1^+\rangle, |\psi_2^+\rangle\}$ subspace.

At X, $E_1^- = E_2^- = \frac{5}{4}\varepsilon_0 - U_2$

$$E^\pm = \tfrac{5}{4}\varepsilon_0 \pm 2U_1 + U_2 .$$

In conclusion,



(3) $W \to L$

The entire path is on (111) face. Double degeneracy everywhere.
Let $\vec{k} = \frac{2\pi}{a}(1-\gamma, \frac{1}{2}, \gamma)$ Going from W to L is equivalent to increasing γ from 0 to $\frac{1}{2}$.

Degeneracy: $\varepsilon_{\vec{k}} = \varepsilon_{\vec{k}-\vec{G}_{111}} = \varepsilon_0(\frac{1}{4}+\gamma^2+(1-\gamma)^2)$

$$\varepsilon_{\vec{k}-\vec{G}_{200}} = \varepsilon_{\vec{k}-\vec{G}_{11\bar{1}}} = \varepsilon_0(\tfrac{1}{4}+\gamma^2+(1+\gamma)^2)$$

When $\gamma=0$ i.e. at W, we have four-fold degeneracy.
Use basis $\{ |\psi_1^\pm\rangle = \frac{1}{\sqrt{2}}(|\psi_{\vec{k}}\rangle \pm |\psi_{\vec{k}-\vec{G}_{111}}\rangle),\ |\psi_2^\pm\rangle = \frac{1}{\sqrt{2}}(|\psi_{\vec{k}-\vec{G}_{200}}\rangle \pm |\psi_{\vec{k}-\vec{G}_{11\bar{1}}}\rangle) \}$

$$H = \begin{pmatrix} \varepsilon_{\vec{k}}-U_1 & 0 & U_2-U_1 & 0 \\ 0 & \varepsilon_{\vec{k}}+U_1 & 0 & U_2+U_1 \\ U_2-U_1 & 0 & \varepsilon_{\vec{k}-\vec{G}_{200}}-U_1 & 0 \\ 0 & U_2+U_1 & 0 & \varepsilon_{\vec{k}-\vec{G}_{200}}+U_1 \end{pmatrix}$$

Different from $X \to W$, none of $|\psi_1^\pm\rangle, |\psi_2^\pm\rangle$ is an eigenstate of H. I don't want to diagonalize a 4×4 matrix. So I use perturbation theory.

(3.1) When $\gamma \ll \frac{|U_2-U_1|}{\varepsilon_0}$. Treat $\varepsilon_{\vec{k}-\vec{G}_{200}} - \varepsilon_{\vec{k}} = 4\gamma\varepsilon_0$ as a perturbation.

$$H_0 = \frac{1}{2}(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}-\vec{G}_{200}})I + \begin{pmatrix} -U_1 & 0 & U_2-U_1 & 0 \\ 0 & U_1 & 0 & U_2+U_1 \\ U_2-U_1 & 0 & -U_1 & 0 \\ 0 & U_2+U_1 & 0 & U_1 \end{pmatrix}$$

$$\delta H = 2\gamma\varepsilon_0 \begin{pmatrix} -1 & & & \\ & -1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$$

Diagonalizing H_0:

$E_1 = (\frac{5}{4}+2\gamma^2)\varepsilon_0 - U_2$ $\quad |\phi_1\rangle = \frac{1}{\sqrt{2}}(1, 0, -1, 0)^T$

$E_2 = (\frac{5}{4}+2\gamma^2)\varepsilon_0 - U_2$ $\quad |\phi_2\rangle = \frac{1}{\sqrt{2}}(0, 1, 0, -1)^T$

$E_3 = (\frac{5}{4}+2\gamma^2)\varepsilon_0 + U_2 - 2U_1$ $\quad |\phi_3\rangle = \frac{1}{\sqrt{2}}(1, 0, 1, 0)^T$

$E_4 = (\frac{5}{4}+2\gamma^2)\varepsilon_0 + U_2 + 2U_1$ $\quad |\phi_4\rangle = \frac{1}{\sqrt{2}}(0, 1, 0, 1)^T$

In the eigenbasis:

$$\delta H = 2\gamma\varepsilon_0 \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}.$$

Second order perturbation:

$$\delta E_1 = \frac{(2\gamma\varepsilon_0)^2}{(-U_2)-(U_2-2U_1)} = -\frac{2\gamma^2\varepsilon_0^2}{U_2-U_1} = -\delta E_3$$

$$\delta E_2 = \frac{(2\gamma\varepsilon_0)^2}{(-U_2)-(U_2+2U_1)} = -\frac{2\gamma^2\varepsilon_0^2}{U_2+U_1} = -\delta E_4$$

Therefore,

$$E^{(1)}(\vec{k}) = \frac{5}{4}\varepsilon_0 - 2\gamma^2\varepsilon_0\left(\frac{\varepsilon_0}{U_2-U_1}-1\right) - U_2$$

$$E^{(2)}(\vec{k}) = \frac{5}{4}\varepsilon_0 - 2\gamma^2\varepsilon_0\left(\frac{\varepsilon_0}{U_2+U_1}-1\right) - U_2$$

$$E^{(3)}(\vec{k}) = \frac{5}{4}\varepsilon_0 + 2\gamma^2\varepsilon_0\left(\frac{\varepsilon_0}{U_2-U_1}+1\right) + U_2-2U_1$$

$$E^{(4)}(\vec{k}) = \frac{5}{4}\varepsilon_0 + 2\gamma^2\varepsilon_0\left(\frac{\varepsilon_0}{U_2+U_1}+1\right) + U_2+2U_1$$

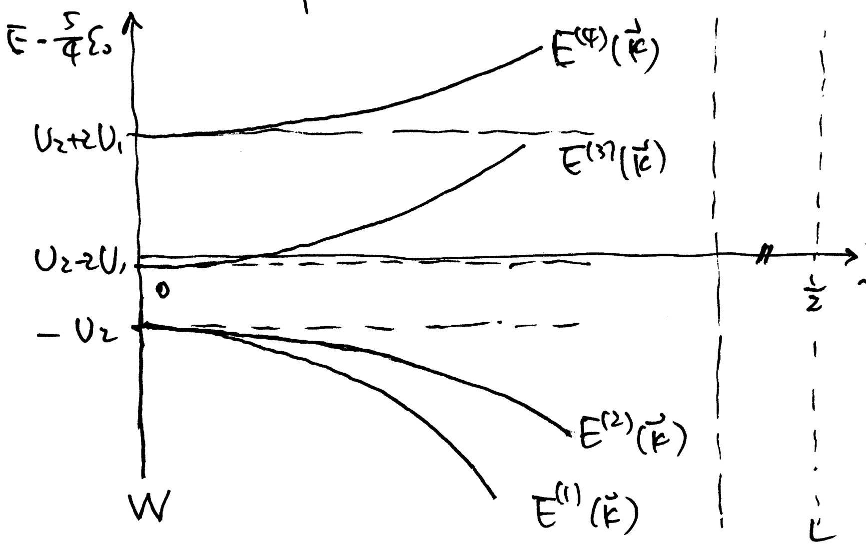
$$\frac{\partial^2 E^{(1)}(\vec{k})}{\partial\gamma^2} = -4\varepsilon_0\left(\frac{\varepsilon_0}{U_2-U_1}-1\right) < 0$$

$$\frac{\partial^2 E^{(2)}(\vec{k})}{\partial\gamma^2} = -4\varepsilon_0\left(\frac{\varepsilon_0}{U_2+U_1}-1\right) < 0$$

$$\frac{\partial^2 E^{(3)}(\vec{k})}{\partial\gamma^2} = 4\varepsilon_0\left(\frac{\varepsilon_0}{U_2-U_1}+1\right) > 0$$

$$\frac{\partial^2 E^{(4)}(\vec{k})}{\partial\gamma^2} = 4\varepsilon_0\left(\frac{\varepsilon_0}{U_2+U_1}+1\right) > 0$$

The dispersion near W look like



No level crossing!

$$\uparrow$$
$$\gamma \ll \frac{|U_2-U_1|}{\varepsilon_0}.$$

(3.2) When $\gamma \gg \frac{U_1}{\varepsilon_0}, \frac{U_2}{\varepsilon_0}$.

Use $\{|\psi_1^\pm\rangle, |\psi_2^\pm\rangle\}$ basis. Treat off-diagonal as perturbation.

$$\delta E_{1^-} = \frac{(U_2-U_1)^2}{-4\gamma\varepsilon_0} = -\delta E_{2^-}$$

$$\delta E_{1^+} = \frac{(U_2+U_1)^2}{-4\gamma\varepsilon_0} = -\delta E_{2^+}$$

Therefore, the lowest two bands are:

$$E^{(1)}(\vec{k}) = \varepsilon_{\vec{k}} - U_1 - \frac{(U_2-U_1)^2}{4\gamma\varepsilon_0}$$

$$E^{(2)}(\vec{k}) = \varepsilon_{\vec{k}} + U_1 - \frac{(U_2+U_1)^2}{4\gamma\varepsilon_0}$$

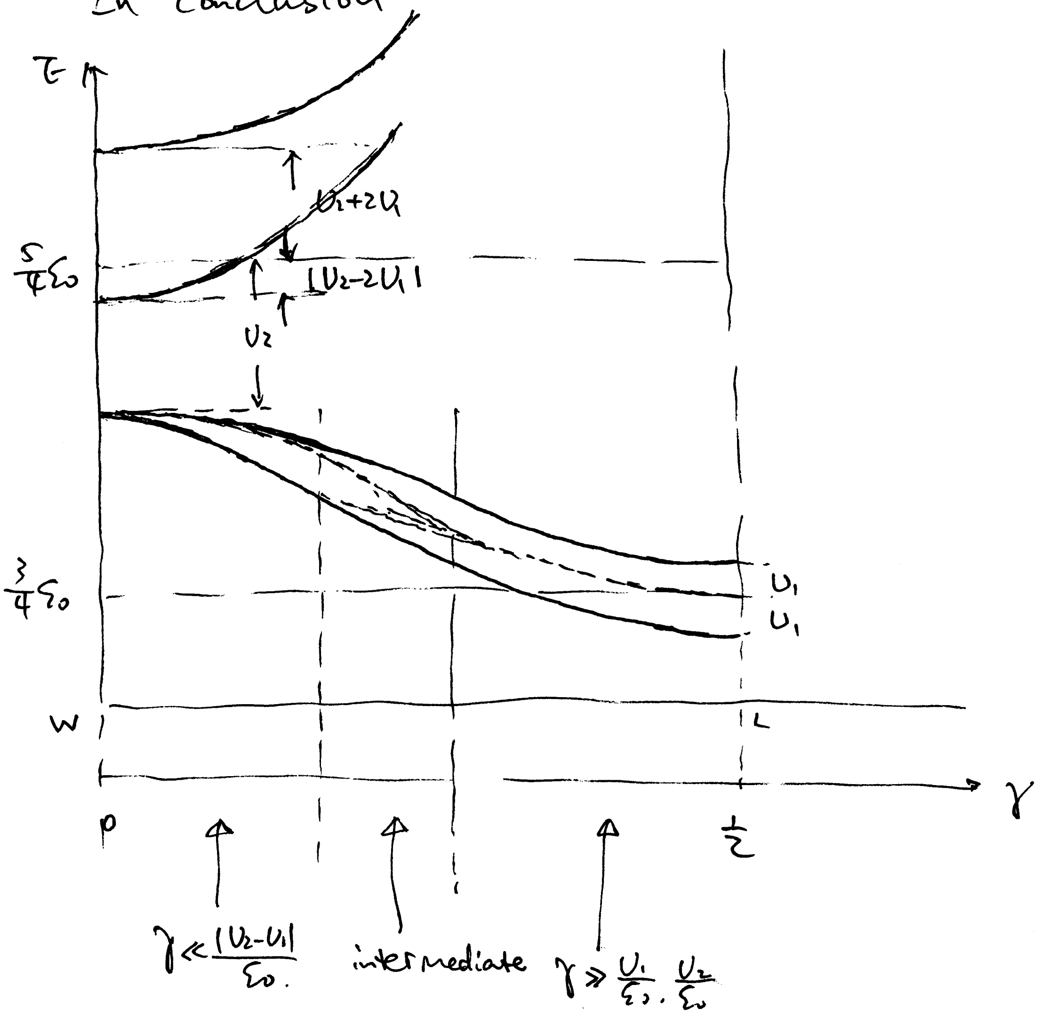
when γ is large enough such that mixing from $\{|\psi_2^\pm\rangle\}$ is negligible. this simplifies (dropping second order)

$$E^{(1)}(\vec{k}) = \varepsilon_{\vec{k}} - U_1 = \varepsilon_0\left(\tfrac{1}{4} + \gamma^2 + (1-\gamma)^2\right) - U_1$$
$$E^{(2)}(\vec{k}) = \varepsilon_{\vec{k}} + U_1 = \varepsilon_0\left(\tfrac{1}{4} + \gamma^2 + (1-\gamma)^2\right) + U_1$$

At L, $\gamma = \frac{1}{2}$

$E^{(1)}(L) = \frac{3}{4}\varepsilon_0 - U_1$ $\qquad$ $E^{(2)}(L) = \frac{3}{4}\varepsilon_0 + U_1$.

In conclusion



(4) $L \to \Gamma$

Let $\vec{k} = \frac{2\pi}{a}\left(\frac{1}{2}-\delta, \frac{1}{2}-\delta, \frac{1}{2}-\delta\right)$. Going from L to Γ is equivalent to increasing δ from 0 to $\frac{1}{2}$.

The calculation is similar to $\Gamma \to X$. So I will skip some steps.

(4.1) δ is in the neighborhood of $\frac{1}{2}$

$E^{(1)}(\vec{k}) = \frac{\hbar^2 k^2}{2m} = 3\varepsilon_0\left(\frac{1}{2}-\delta\right)^2$

$E^{(2)}(\vec{k})$ requires diagonalizing a much larger matrix.

$E^{(2)}(\vec{k})$ high above E_F.

(4.2) δ is far away from $\frac{1}{2}$.

Consider the mixing of $|\varphi_{\vec{k}}\rangle$ and $|\varphi_{\vec{k}-\vec{G}_{111}}\rangle$.

$$H = \begin{bmatrix} \varepsilon_{\vec{k}} & U_1 \\ U_1 & \varepsilon_{\vec{k}-\vec{G}_{111}} \end{bmatrix}$$

$$E^{(1)}(\vec{k}) = \frac{1}{2}\left[(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}-\vec{G}_{111}}) - \sqrt{(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}-\vec{G}_{111}})^2 + 4U_1^2}\right]$$

$$E^{(2)}(\vec{k}) = \frac{1}{2}\left[(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}-\vec{G}_{111}}) + \sqrt{(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}-\vec{G}_{111}})^2 + 4U_1^2}\right]$$

In terms of δ,

$$E^{(1)}(\vec{k}) = 3\left(\delta^2 + \tfrac{1}{4}\right)\varepsilon_0 - \sqrt{(3\delta\varepsilon_0)^2 + U_1^2}$$

$$E^{(2)}(\vec{k}) = 3\left(\delta^2 + \tfrac{1}{4}\right)\varepsilon_0 + \sqrt{(3\delta\varepsilon_0)^2 + U_1^2}$$

(4.2.1) when $\delta \gg \frac{U_1}{\varepsilon_0}$

$$E^{(1)}(\vec{k}) = 3\left(\delta - \tfrac{1}{2}\right)^2\varepsilon_0 - \frac{U_1^2}{6\delta\varepsilon_0} \xrightarrow{\text{lowest order}} 3\left(\delta - \tfrac{1}{2}\right)^2\varepsilon_0$$

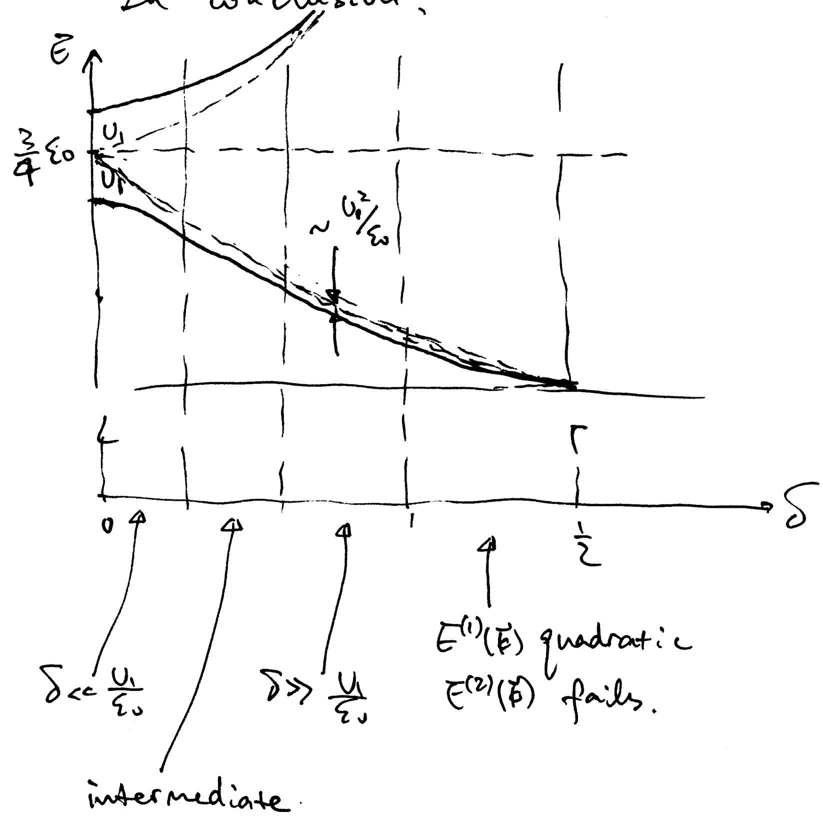
$$E^{(2)}(\vec{k}) = 3\left(\delta + \tfrac{1}{2}\right)^2\varepsilon_0 + \frac{U_1^2}{6\delta\varepsilon_0} \xrightarrow{\text{lowest order}} 3\left(\delta + \tfrac{1}{2}\right)^2\varepsilon_0$$

(4.2.2) when $\delta \ll \frac{U_1}{\varepsilon_0}$

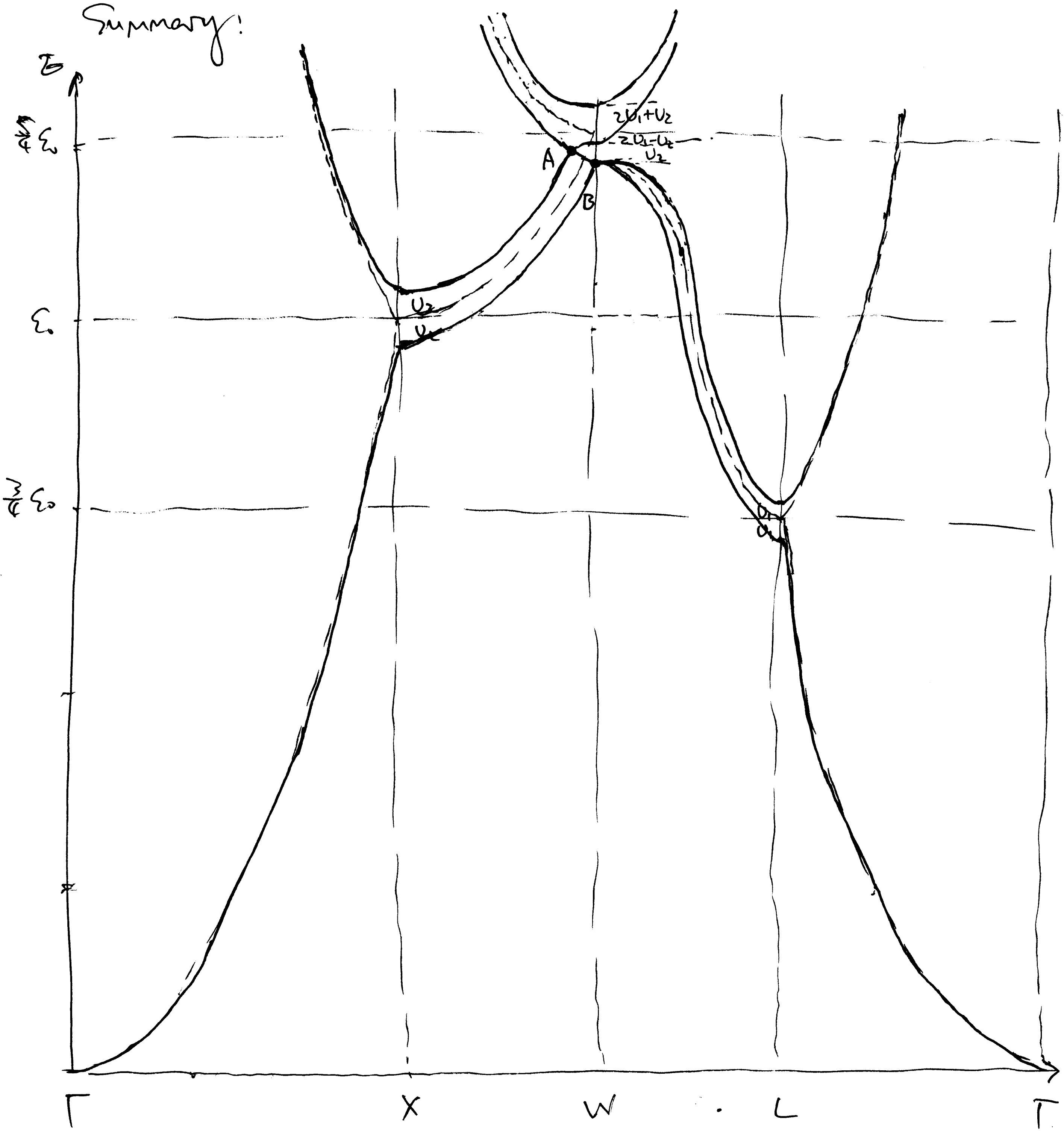
$$E^{(1)}(\vec{k}) = 3\left(\delta^2 + \tfrac{1}{4}\right)\varepsilon_0 - U_1 - \frac{(3\delta\varepsilon_0)^2}{2U_1} \xrightarrow{\text{lowest order}} \tfrac{3}{4}\varepsilon_0 - U_1$$

$$E^{(2)}(\vec{k}) = 3\left(\delta^2 + \tfrac{1}{4}\right)\varepsilon_0 + U_1 + \frac{(3\delta\varepsilon_0)^2}{2U_1} \xrightarrow{\text{lowest order}} \tfrac{3}{4}\varepsilon_0 - U_1$$

In conclusion,



Summary!



points A, B have double degeneracies that are not broken.

(b). $\Omega = \frac{1}{4}a^3$.

$$V(q) = \frac{1}{\Omega}\int_c d^3\vec{r}\; e^{-i\vec{q}\cdot\vec{r}}\; V(\vec{r})$$

$$\approx \frac{1}{\Omega}\int_{R_c}^{\infty} r^2 dr \int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} d\varphi \cdot e^{-iqr\cos\theta} \cdot \left(-\frac{Ze^2}{r}\right)$$

$$= -\frac{2\pi Ze^2}{\Omega}\int_{R_c}^{\infty} r dr \int_0^{\pi} e^{-iqr\cos\theta}\sin\theta d\theta$$

$$= -\frac{2\pi Ze^2}{\Omega}\cdot\int_{R_c}^{\infty} \cancel{r} dr \cdot \frac{1}{-iq\cancel{r}}\left(e^{-iqr} - e^{iqr}\right).$$

$$= -\frac{2\pi Ze^2}{q\Omega}\int_{R_c}^{\infty} 2\sin qr\, dr$$

$$= -\frac{4\pi Ze^2}{q^2\Omega}\left[-\cos qr\right]\Big|_{R_c}^{\infty}$$

$$= -\frac{4\pi Ze^2}{q^2\Omega}\cos(qR_c).$$

$$= -\frac{16\pi Ze^2}{q^2a^3}\cos(qR_c).$$

U_1: $\vec{q} = \frac{2\pi}{a}(1,1,1)$ $\quad q = \frac{2\pi}{a}\sqrt{3}$

$$U_1 = -\frac{16\pi Ze^2}{\frac{4\pi^2\cdot 3}{a^2}\cdot a^3}\cos\left(2\sqrt{3}\pi\frac{R_c}{a}\right)$$

$$= -\frac{4Ze^2}{3\pi a}\cos\left(2\sqrt{3}\pi\frac{R_c}{a}\right)$$

$$\approx 0.188 \text{ eV}.$$

U_2: $\vec{q} = \frac{2\pi}{a}(2,0,0)$ $\quad q = \frac{4\pi}{a}$.

$$U_2 = -\frac{16\pi Ze^2}{\frac{16\pi^2}{a^2}a^3}\cos\left(4\pi\frac{R_c}{a}\right)$$

$$= -\frac{Ze^2}{\pi a}\cos\left(4\pi\frac{R_c}{a}\right)$$

$$\approx 0.974 \text{ eV}$$

Therefore, splitting at X:

$$E^{(2)}(X) - E^{(1)}(X) = 2U_2 \approx 1.948 \text{ eV}$$

Splitting at W:

$$E^{(2)}(W) - E^{(1)}(W) = 0$$

$$E^{(3)}(W) - E^{(2)}(W) = (U_2 - 2U_1) - (-U_2) = 2U_2 - 2U_1 \approx 1.572 \text{ eV}$$

$$E^{(4)}(W) - E^{(3)}(W) = (U_2 + 2U_1) - (U_2 - 2U_1) = 4U_1 \approx 0.752 \text{ eV}$$

Splitting at L:

$$E^{(2)}(L) - E^{(1)}(L) = 2U_1 \approx 0.376 \text{ eV}.$$

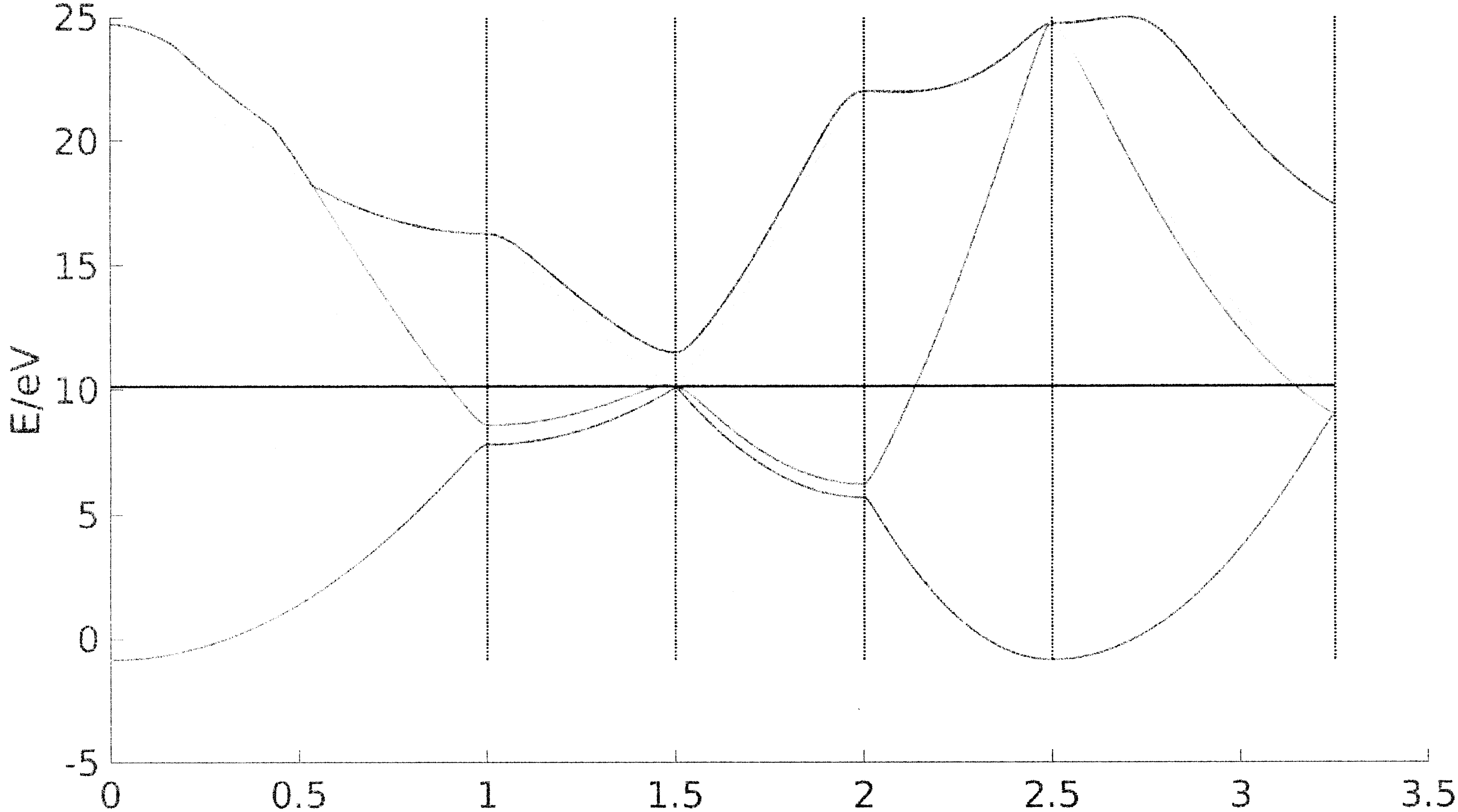
(c) To make the calculation accurate, I use a Hilbert space whose dimension is $d = 559$.

The band structure is shown in Fig. 1 on next page.

(d) The electrons should take up 1.5 bands. Since my bands are discrete points, I just need to sort their energies and cut at 1.5-band level. The estimation is

$$E_F \approx 10.16 \text{ eV}$$

KKR method gives $E_F \approx 0.83 \sim 0.84$ Ry., which is around $11.3 \sim 11.4$ eV. So I am off by 10%. Still OK.


E/eV
25
20
15
10
5
0
-5
0
0.5
1
1.5
2
2.5
3
3.5