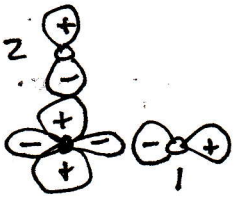
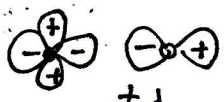
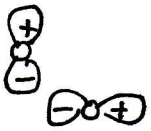
Long problem 2 solution



couplings:





$t_d, t_p > 0$

Bloch functions

$$\Psi_n(\vec{k}) = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot(\vec{R}_i + \vec{d}_n)} \varphi_n(\vec{R}_i)$$

$\varphi_1 = p_x$, $\vec{d}_1 = \frac{a}{2}\hat{x}$

$\varphi_2 = p_y$, $\vec{d}_2 = \frac{a}{2}\hat{y}$

$\varphi_3 = d_{x^2-y^2}$, $\vec{d}_3 = 0$

$$H_{nn'}(\vec{k}) = \langle \Psi_n(\vec{k}) | H | \Psi_{n'}(\vec{k}) \rangle$$

$$H_{nn'}(\vec{k}) = \sum_i \langle \varphi_n(R=0)\, H\, \varphi_{n'}(R_i) \rangle\, e^{i\vec{k}\cdot(\vec{R}_i + \vec{d}_{n'} - \vec{d}_n)}$$

$H_{11}(\vec{k}) = \varepsilon_p = H_{22}(\vec{k})$

$H_{33}(\vec{k}) = \varepsilon_d$

$H_{12}(\vec{k}) = e^{-ik_x a/2 + ik_y a/2}\left[-t_p + t_p e^{ik_x a} + t_p e^{-ik_y a} - t_p e^{i(k_x - k_y)a}\right]$

$\Rightarrow H_{12}(\vec{k}) = -4t_p \sin\frac{k_x a}{2} \sin\frac{k_y a}{2}$

$H_{13}(\vec{k}) = e^{-ik_x a/2}\left(-t_d + t_d e^{ik_x a}\right) = 2it_d \sin\frac{k_x a}{2}$

$H_{23}(\vec{k}) = e^{-ik_y a/2}\left(t_d - t_d e^{ik_y a}\right) = -2it_d \sin\frac{k_y a}{2}$

$$H_{nn'} = \begin{pmatrix} \varepsilon_p & a & b_x \\ a & \varepsilon_p & b_y \\ b_x^* & b_y^* & \varepsilon_d \end{pmatrix}$$

$a = -4t_p \sin\frac{k_x a}{2} \sin\frac{k_y a}{2}$

$b_x = 2it_d \sin\frac{k_x a}{2}$

$b_y = -2it_d \sin\frac{k_y a}{2}$

(c) Find eigenvalues at $\Gamma = (0,0)$, $D = \left(\frac{\pi}{a}, 0\right)$, $X = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$

Γ: $a = b_x = b_y = 0 \Rightarrow$ eigenvalues are $\boxed{\varepsilon_1 = \varepsilon_2 = \varepsilon_p,\ \varepsilon_3 = \varepsilon_d}$

D: $a = 0$, $b_x = 2it + d$, $b_y = 0$

$$H = \begin{array}{c} \begin{matrix} \psi_1 & \psi_2 & \psi_3 \end{matrix} \\ \begin{pmatrix} \varepsilon_p & 0 & b_x \\ 0 & \varepsilon_p & 0 \\ b_x^* & 0 & \varepsilon_d \end{pmatrix} \end{array}$$

so ψ_2 is decoupled, eigenvalue is $\boxed{\varepsilon_2 = \varepsilon_p}$

$$H_{13} = \begin{pmatrix} \varepsilon_p & b_x \\ b_x^* & \varepsilon_d \end{pmatrix}$$

$\Rightarrow$ eigenvalues are

$$\boxed{\varepsilon_{1,3} = \frac{\varepsilon_p + \varepsilon_d}{2} \pm \sqrt{\left(\frac{\varepsilon_p - \varepsilon_d}{2}\right)^2 + |b_x|^2}} \qquad \boxed{b_x = 2it + d}$$

X: $a = -4t_p$, $b_x = 2it + d$, $b_y = -b_x$

$$H = \begin{pmatrix} \varepsilon_p & a & b_x \\ a & \varepsilon_p & -b_x \\ b_x^* & -b_x^* & \varepsilon_d \end{pmatrix}$$

to diagonalize this, change basis.

Note that:

$$H\psi_1 = \varepsilon_p \psi_1 + a\psi_2 + b_x^* \psi_3$$

$$H\psi_2 = a\psi_1 + \varepsilon_p \psi_2 + b_y^* \psi_3$$

$$\Rightarrow H(\psi_1 - \psi_2) = \varepsilon_p(\psi_1 - \psi_2) - a(\psi_1 - \psi_2) + (b_x^* - b_y^*)\psi_3$$

$$H(\psi_1 + \psi_2) = (\varepsilon_p + a)(\psi_1 + \psi_2) + (b_x^* + b_y^*)\psi_3$$

Along the line $b_x = b_y$, $b_y = -b_x \Rightarrow$ $\psi_1 + \psi_2$ does not couple to ψ_3.

So change basis to:

$$\vartheta_1 = \frac{\psi_1 + \psi_2}{\sqrt{2}} \; ; \; \vartheta_2 = \frac{\psi_1 - \psi_2}{\sqrt{2}} \; ; \; \vartheta_3 = \psi_3$$

In this basis, Hamiltonian:

$$H = \begin{array}{c} \begin{matrix} \vartheta_1 & \vartheta_2 & \vartheta_3 \end{matrix} \\ \begin{pmatrix} \varepsilon_p + a & 0 & \frac{b_x + b_y}{\sqrt{2}} \\ 0 & \varepsilon_p - a & \frac{b_x - b_y}{\sqrt{2}} \\ \frac{b_x^* + b_y^*}{\sqrt{2}} & \frac{b_x^* - b_y^*}{\sqrt{2}} & \varepsilon_d \end{pmatrix} \end{array}$$

in particular along the $b_x = b_y$ line, $b_y = -b_x \Rightarrow$

$$H = \begin{pmatrix} \varepsilon_p + a & 0 & 0 \\ 0 & \varepsilon_p - a & \sqrt{2} b_x \\ 0 & \sqrt{2} b_x^* & \varepsilon_d \end{pmatrix}$$

$\Rightarrow$ eigenvalues are:

$$\varepsilon_1 = \varepsilon_p + a$$

$$\varepsilon_{2,3} = \frac{\varepsilon_p - a + \varepsilon_d}{2} \pm \sqrt{\left(\frac{\varepsilon_p - a - \varepsilon_d}{2}\right)^2 + 2|b_x|^2}$$

$$a = -4t_p \sin^2 \frac{b_x a}{2}$$

$$b_x = 2it_d \sin \frac{b_x a}{2}$$

So we have for eigenvalues at Γ, D and X:

Γ: $\varepsilon_1 = \varepsilon_2 = \varepsilon_p$, $\varepsilon_3 = \varepsilon_d$

D: $\varepsilon_{1,3} = \frac{\varepsilon_p + \varepsilon_d}{2} \pm \sqrt{\left(\frac{\varepsilon_p - \varepsilon_d}{2}\right)^2 + 4t_d^2}$; $\varepsilon_2 = \varepsilon_p$

X: $\varepsilon_1 = \varepsilon_p - 4t_p$, $\varepsilon_{2,3} = \frac{\varepsilon_p + 4t_p + \varepsilon_d}{2} \pm \sqrt{\left(\frac{\varepsilon_p + 4t_p - \varepsilon_d}{2}\right)^2 + 8t_d^2}$

(d) Eigenvalues at Γ are $-3.5eV$, $-2eV$, $\varepsilon_p < \varepsilon_d \Rightarrow$

$$\boxed{\varepsilon_p = -3.5eV,\ \varepsilon_d = -2eV}$$

Lowest and highest eigenvalues at X: assume they are $\varepsilon_{2,3} \Rightarrow$

$\varepsilon_2 + \varepsilon_3 = \varepsilon_p + 4t_p + \varepsilon_d$; $\varepsilon_2 = -6.6eV$, $\varepsilon_3 = +3.6eV$

$\Rightarrow 4t_p = \varepsilon_2 + \varepsilon_3 - \varepsilon_p - \varepsilon_d = 2.5\,eV \Rightarrow \boxed{t_p = 0.625eV}$

$\varepsilon_2 - \varepsilon_3 = 2\sqrt{\left(\frac{\varepsilon_p + 4t_p - \varepsilon_d}{2}\right)^2 + 8t_d^2} \Rightarrow$

$8t_d^2 = \left(\frac{\varepsilon_2 - \varepsilon_3}{2}\right)^2 - \left(\frac{\varepsilon_p + 4t_p - \varepsilon_d}{2}\right)^2 = 26.01eV - 0.25eV$

$\Rightarrow \boxed{t_d = 1.79eV}$

(e) Energies at points Γ, D and X are then:

Γ: $-3.5eV$, $-2eV$

X: $-6.6eV$, $-6eV$, $+3.6eV$

D: $-6.43eV$, $-3.5eV$, $+0.93eV$

(e) Plot of band structure :

Along Γ - X direction, eigenvalues are:

$$\epsilon_1 = \epsilon_p + a$$

$$\epsilon_{2,3} = \frac{\epsilon_p - a + \epsilon_d}{2} \pm \sqrt{\left(\frac{\epsilon_p - a - \epsilon_d}{2}\right)^2 + 2|b_x|^2}$$

$$a = -4t_p \sin^2 \frac{k_x a}{2}$$

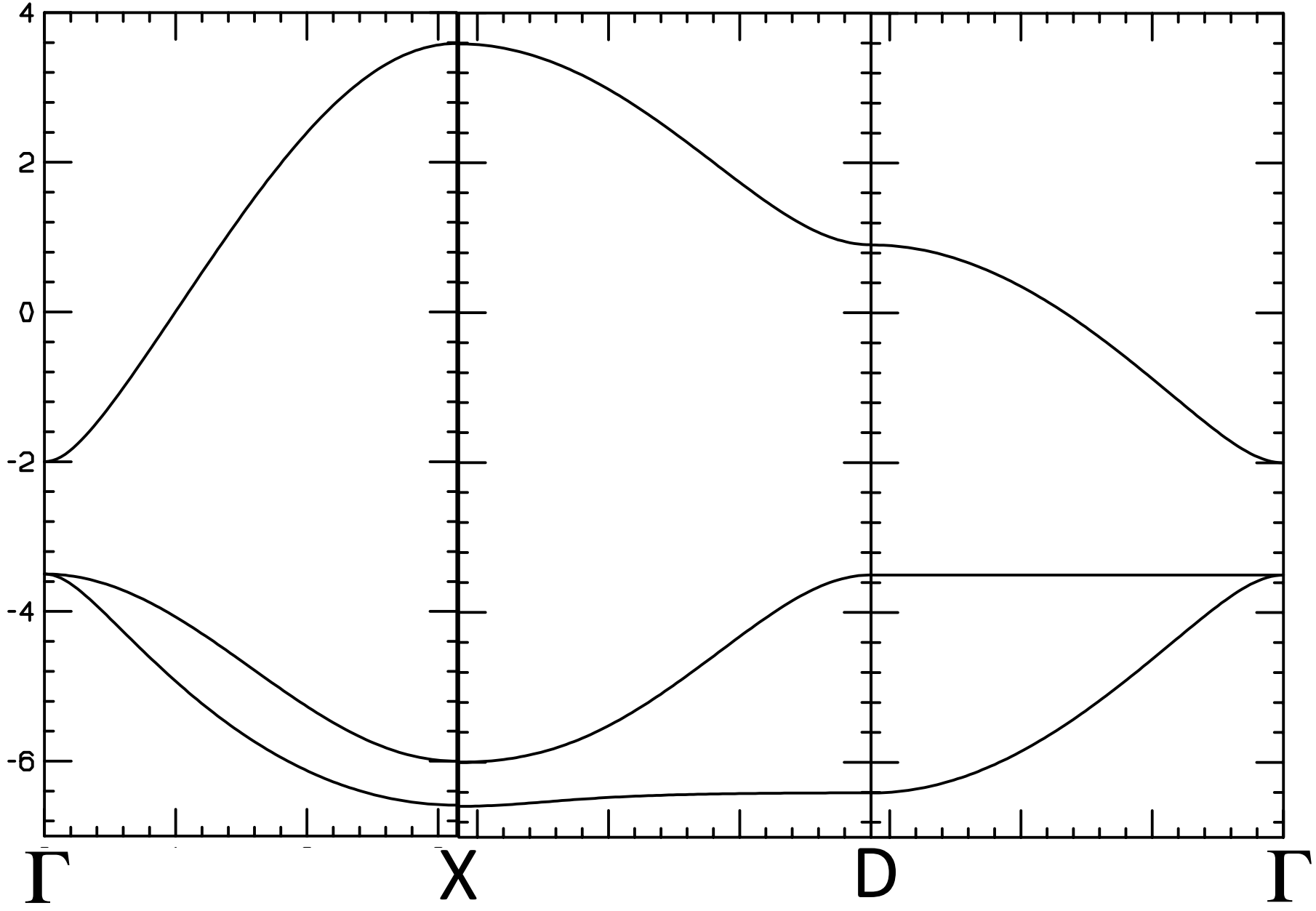
$$b_x = 2it_d \sin \frac{k_x a}{2}$$

Along Γ - D direction, eigenvalues are: since $k_y = 0$, $a = 0$, $b_y = 0$

$$\epsilon_2 = \epsilon_p, \quad \epsilon_{1,3} = \frac{\epsilon_p + \epsilon_d}{2} \pm \sqrt{\left(\frac{\epsilon_p - \epsilon_d}{2}\right)^2 + |b_x|^2}$$

$$b_x = 2it_d \sin \frac{k_x a}{2}$$

Along X - D direction, need to diagonalize 3 x 3 matrix on p. (1) to find eigenvalues numerically.

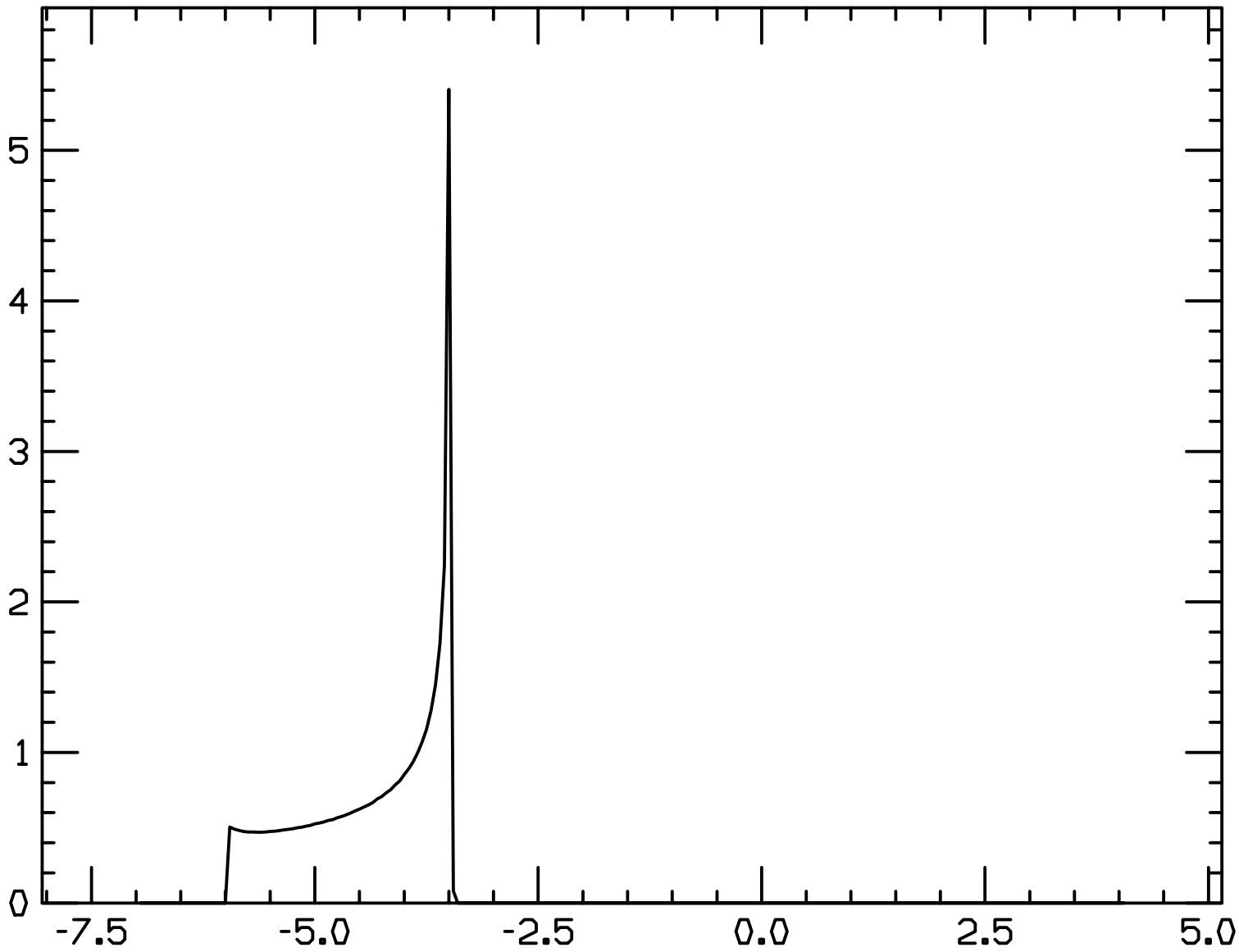

4
2
0
-2
-4
-6
Γ
X
D
Γ

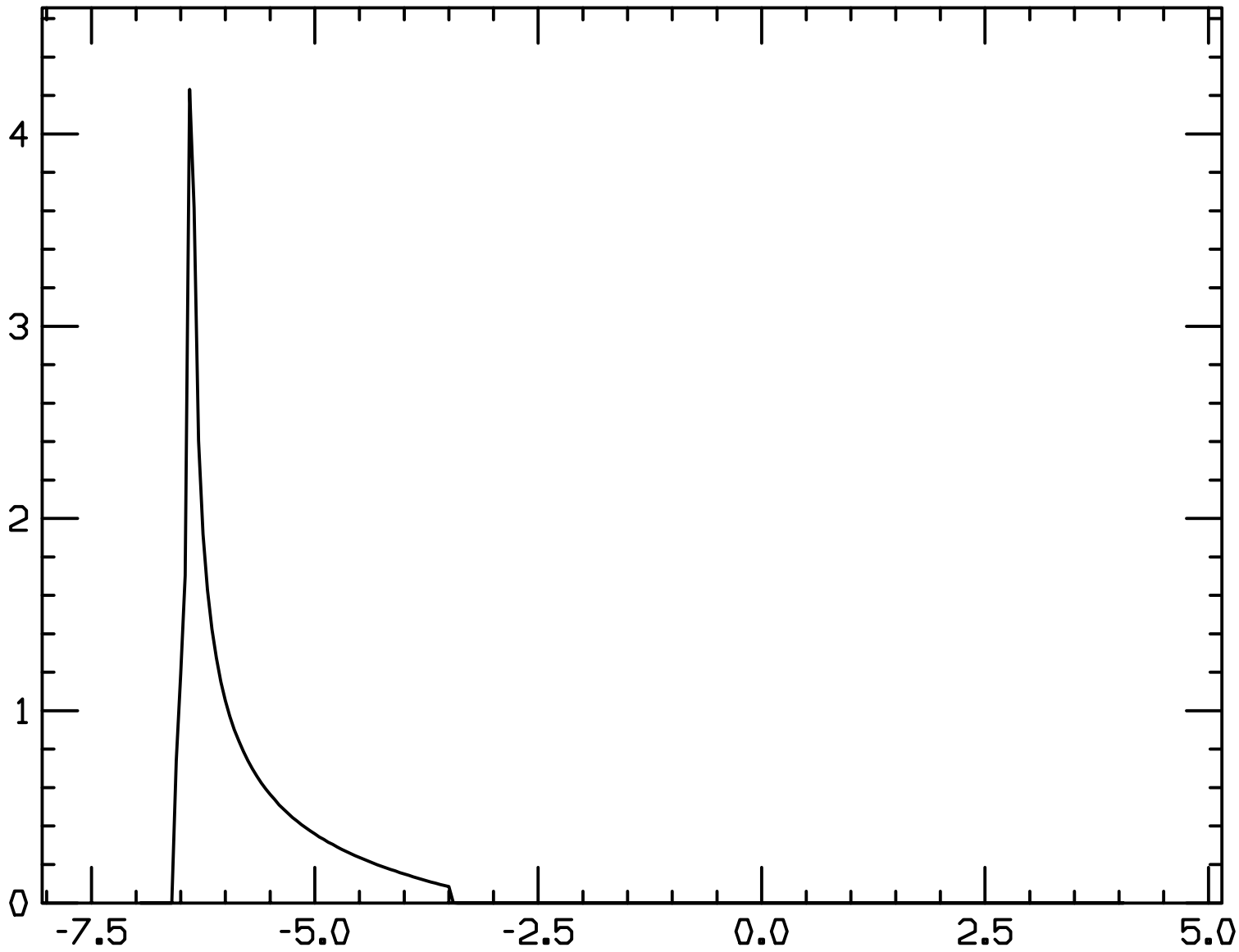
(g) electron density:
sum over k-states in the Brillouin zone that have energy < \epsilon_F. Each state is occupied by 2 electrons. Divide by # of k-states in BZ, to get electrons per unit cell

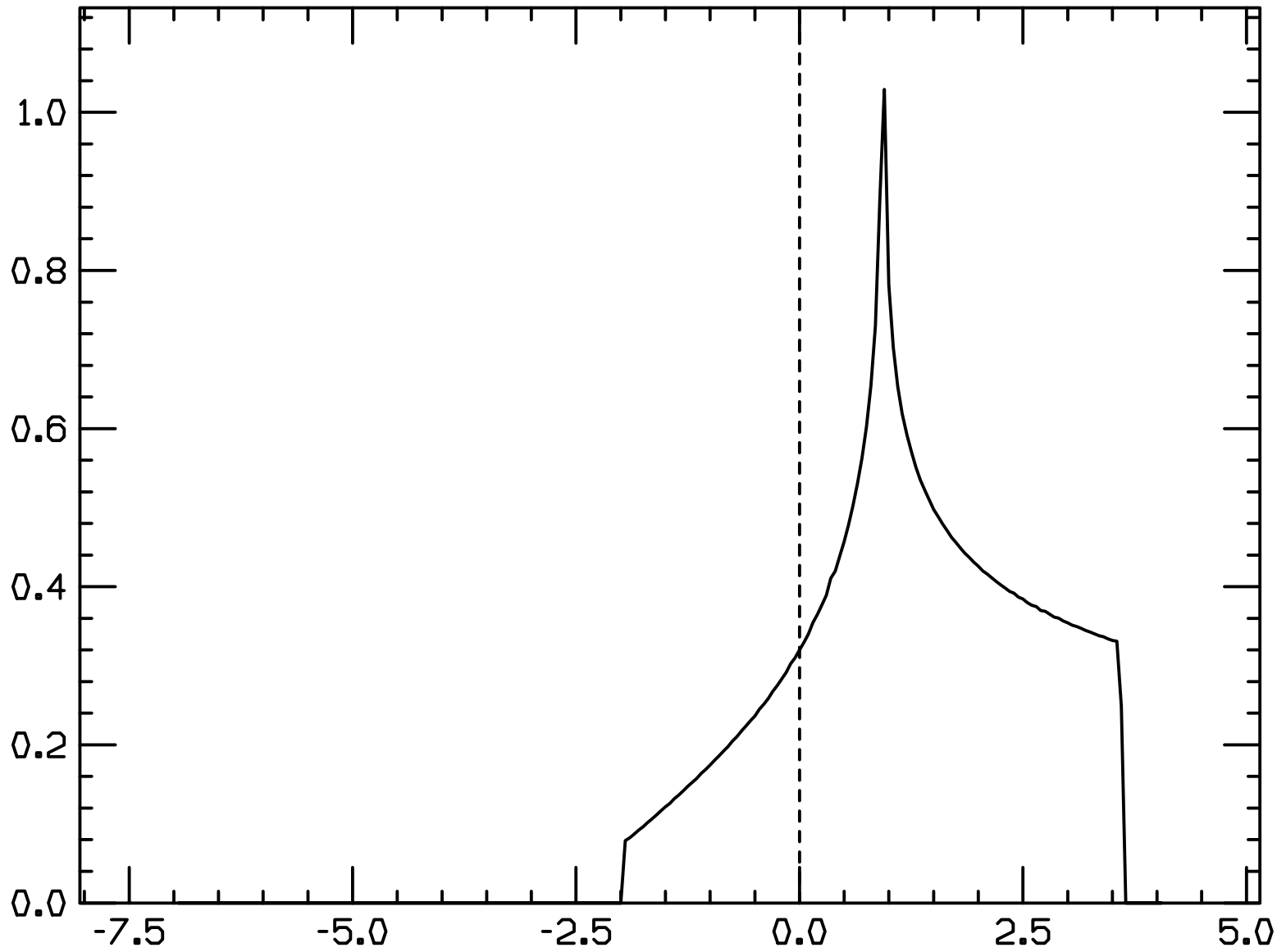
band 1: 2 electrons/unit cell
band 2: 2 electrons/unit cell
band 3: 0.37 electrons/unit cell
total: 4.37 electrons/unit cell

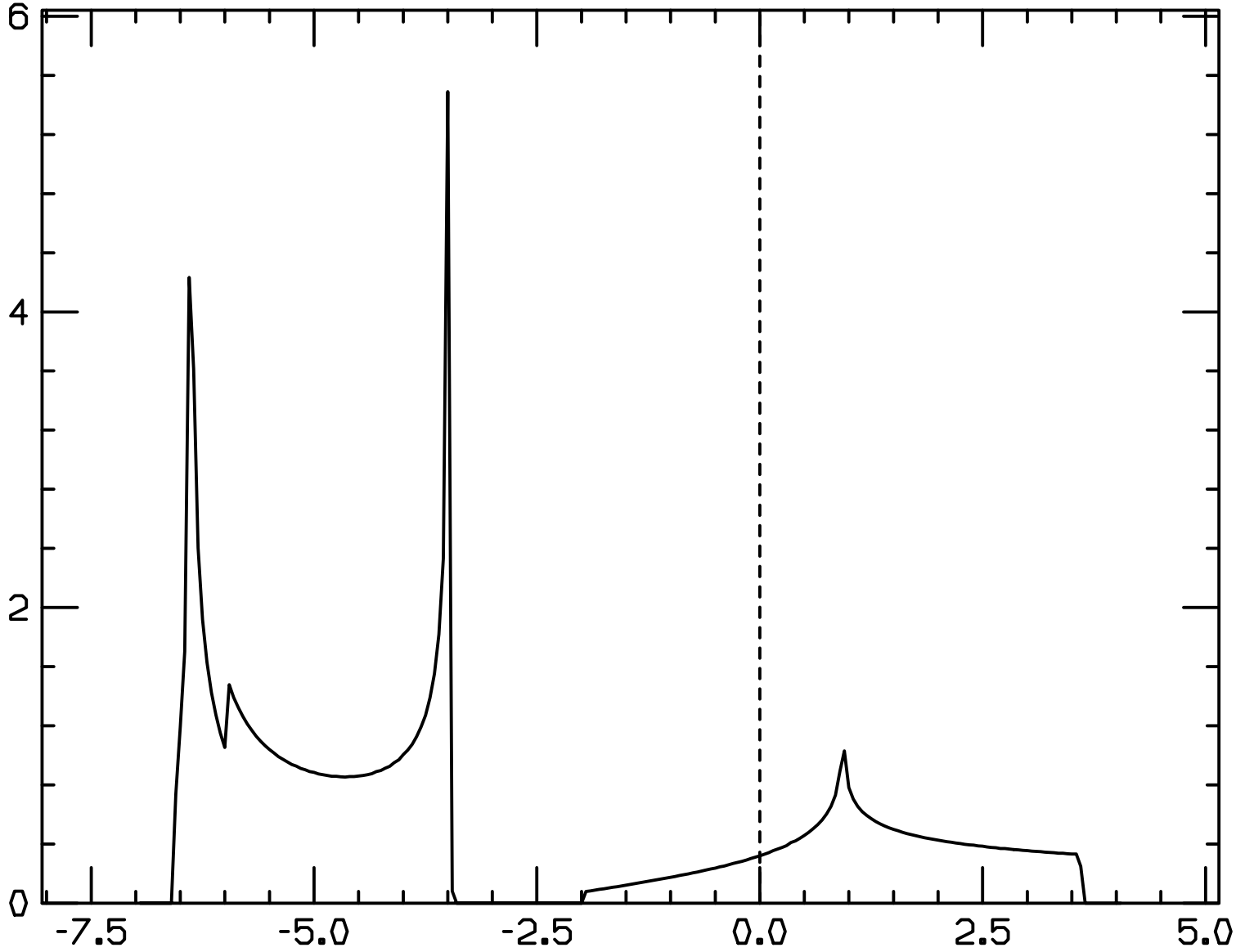
unit cell area = $(2.5A)^2$. n=electrons/unit cell/unit cell area
==> electron density n =0.70 $x10^{16}$ electrons/cm^2

(h) Density of states per eV per unit cell versus energy in eV is given in following graphs for band 1, band 2, band 3, and total.
Fermi energy is dashed line. Integral of density of states over each band gives 2.
For band 3, integral up to Fermi level gives 0.37.


5
4
3
2
1
0
-7.5
-5.0
-2.5
0.0
2.5
5.0


4
3
2
1
0
-7.5
-5.0
-2.5
0.0
2.5
5.0


1.0
0.8
0.6
0.4
0.2
0.0
-7.5
-5.0
-2.5
0.0
2.5
5.0


6
4
2
0
-7.5
-5.0
-2.5
0.0
2.5
5.0