Sheet 5

a) The equations $\langle \phi_1 | \Delta u_1 | \psi \rangle = E(\vec{k}) \langle \phi_1 | \psi \rangle$ and for ϕ_2 respectively can be rewritten using the expressions for $\langle \phi_1 | \Delta u_1 | \psi \rangle, \langle \phi_1 | \psi \rangle$ given on the sheet.

$$\hookrightarrow \langle \phi_1 | \Delta u_1 | \psi \rangle = E(\vec{k}) \langle \phi_1 | \psi \rangle$$

$$b_2 \gamma_1 \alpha(\vec{k}) = E(\vec{k}) \left(b_1 + b_2 \gamma_0 \alpha(\vec{k}) \right)$$

and $\langle \phi_2 | \Delta u_2 | \psi \rangle = E(\vec{k}) \langle \phi_2 | \psi \rangle$

$$\Leftrightarrow b_1 \gamma_1 \alpha^*(\vec{k}) = \left(b_2 + b_1 \gamma_0 \alpha^*(\vec{k}) \right) E(\vec{k})$$

b) This condition for E can be written into a matrix equation:

$$\begin{pmatrix} E(\vec{k}) & (\gamma_1 + \gamma_0 E(\vec{k})) \alpha(\vec{k}) \\ (\gamma_1 + \gamma_0 E(\vec{k})) \alpha^*(\vec{k}) & E(\vec{k}) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

c) These equation yields a non-trivial solution if the determinant of the matrix vanishes

$$\hookrightarrow E^2(\vec{k}) = (\gamma_1 + \gamma_0 E(\vec{k}))^2 |\alpha(\vec{k})|^2$$

Using the approximation $\gamma_0 \approx 0$, we receive the dispersion relation

$$E(\vec{k}) = \pm \gamma_1 |\alpha(\vec{k})|$$

Thus the dispersion relation depends also partly by the sign of γ_1. It is apparent that E behaves the same for negative and positive energies despite that it is mirrored at the perpendicular plane dividing $E>0$ and $E<0$.

d)

$$|\alpha(\vec{k})|^2 = 1 + e^{i\vec{k}\vec{a}_1} + e^{i\vec{k}\vec{a}_2} + e^{-i\vec{k}\vec{a}_1} + e^{-i\vec{k}\vec{a}_2}$$

$$+ 2 + e^{i\vec{k}(\vec{a}_1 - \vec{a}_2)} + e^{-i\vec{k}(\vec{a}_1 - \vec{a}_2)}$$

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

$$+ 2\cos(k_x a)$$

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

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

$$\Rightarrow E(\vec{k}) = \pm\gamma_1\sqrt{1 + 4\cos^2\left(\frac{a}{2}k_x\right) + 4\cos\left(\frac{a}{2}k_x\right)\cos\left(\frac{a}{2}\sqrt{3}k_y\right)}$$

with $\cos\left(\frac{2}{3}\pi\right) = -0{,}5$ we get for $\vec{k} = (1, 0) \cdot \frac{4\pi}{3a}$

$E_1(\vec{k}) = \pm\gamma_1\sqrt{1 + 1 - 2} = 0$. Thus we find there a zero band gab between E_1 and E_2.

for $\vec{k} = 0$ we find $E(0) = \gamma_1$