Exercise 5 (online: 22.05.2023. Return by: **Mo 05.06.2023 10:00**) **8P**

1. **Band structure of graphene based on the tight-binding-model** 8P

   To find the dispersion relation in graphene one should generally speaking solve the eigenvalue problem $\hat{H}\psi_{\boldsymbol{k}} = E(\boldsymbol{k})\psi_{\boldsymbol{k}}$, where

   $$\psi_k(\boldsymbol{x}) = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\boldsymbol{R}}\phi(\boldsymbol{x}-\boldsymbol{R}) = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\boldsymbol{R}}\left[b_1\phi_1(\boldsymbol{x}-\boldsymbol{R}) + b_2\phi_2(\boldsymbol{x}-\boldsymbol{R})\right], \tag{1}$$

   with ϕ_1 and ϕ_2 the wavefunctions of atom A and atom B in graphene. Technically, it is easier to project this equation onto ϕ_1 and ϕ_2, *i.e.*,

   $$\langle\phi_1|\Delta U_1|\psi\rangle = E(\boldsymbol{k})\langle\phi_1|\psi\rangle, \text{ and } \langle\phi_2|\Delta U_2|\psi\rangle = E(\boldsymbol{k})\langle\phi_2|\psi\rangle. \tag{2}$$

   If we consider the effect of each atom's potential $V_{\text{at}}(\boldsymbol{x}-\boldsymbol{x}_i-\boldsymbol{R})$ $(i=1,2)$ only on the wave function ϕ_i of the neighboring three nodes (instead of the infinite sum over $\boldsymbol{R}$ in (1)), the above $\langle\ldots\rangle$ can be reduced to the following:

   $$\begin{aligned}
   \langle\phi_1|\psi\rangle &= b_1 + b_2\gamma_0\left[1 + e^{-i\boldsymbol{k}\boldsymbol{a}_1} + e^{-i\boldsymbol{k}\boldsymbol{a}_2}\right] = b_1 + b_2\gamma_0\alpha(\boldsymbol{k}); &\text{(3a)}\\
   \langle\phi_2|\psi\rangle &= b_2 + b_1\gamma_0\left[1 + e^{+i\boldsymbol{k}\boldsymbol{a}_1} + e^{+i\boldsymbol{k}\boldsymbol{a}_2}\right] = b_2 + b_1\gamma_0\alpha^*(\boldsymbol{k}); &\text{(3b)}\\
   \langle\phi_1|\Delta U_1|\psi\rangle &= b_2\gamma_1\left[1 + e^{-i\boldsymbol{k}\boldsymbol{a}_1} + e^{-i\boldsymbol{k}\boldsymbol{a}_2}\right] = b_2\gamma_1\alpha(\boldsymbol{k}); &\text{(3c)}\\
   \langle\phi_2|\Delta U_2|\psi\rangle &= b_1\gamma_1\left[1 + e^{i\boldsymbol{k}\boldsymbol{a}_1} + e^{i\boldsymbol{k}\boldsymbol{a}_2}\right] = b_1\gamma_1\alpha^*(\boldsymbol{k}), &\text{(3d)}
   \end{aligned}$$

   where $\gamma_0 = \langle\phi_1|\phi_2\rangle = \langle\phi_2|\phi_1\rangle$ and $\gamma_1 = \langle\phi_1|\Delta U_1|\phi_2\rangle = \langle\phi_2|\Delta U_2|\phi_1\rangle$ and

   $$\alpha(\boldsymbol{k}) \equiv 1 + e^{-i\boldsymbol{k}\boldsymbol{a}_1} + e^{-i\boldsymbol{k}\boldsymbol{a}_2}, \tag{4}$$

   with the lattice vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$.

   (a) Write out explicitly both of the eqs. (2) by inserting the expressions from (3).(1P)

   (b) Bring the results into the form: (1P)

   $$\begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix} \cdot \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{5}$$

   (c) The nontrivial solution of Eq. (5) exists when the determinant of the matrix vanishes. Derive the corresponding equation and determine $E(\boldsymbol{k})$ by using the approximation $\gamma_0 \simeq 0$. What dependence is found for $E(\alpha(\boldsymbol{k}))$? How do the dispersion relations behave for negative (valence band) compared to positive (conductance band) energies?(3P)

   (d) Express $E(\boldsymbol{k})$ as a function of $\sin(\boldsymbol{k}\boldsymbol{a}_i)$, $\cos(\boldsymbol{k}\boldsymbol{a}_i)$ (calculated from α). Insert the vectors

   $$\boldsymbol{a}_1 = \frac{a}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \quad \boldsymbol{a}_2 = \frac{a}{2}\begin{pmatrix} -1 \\ \sqrt{3} \end{pmatrix} \tag{6}$$

   and write down $E(\boldsymbol{k})$ as a function of k_x, k_y.(2P)

   (e) Determine the value of $E(\boldsymbol{K})$ for the corner of the first Brillouin zone at $\boldsymbol{K} = \frac{4\pi}{3a}(1,0)$. What is the energy $E(\boldsymbol{k})$ for $\boldsymbol{k} = 0$?(1P)