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Exercise 1: Electronic density of states (Written)

Consider the following tight binding dispersion

$$E(\boldsymbol{k}) = -2t \sum_{i=1}^{d} \cos(k_i a) \tag{1}$$

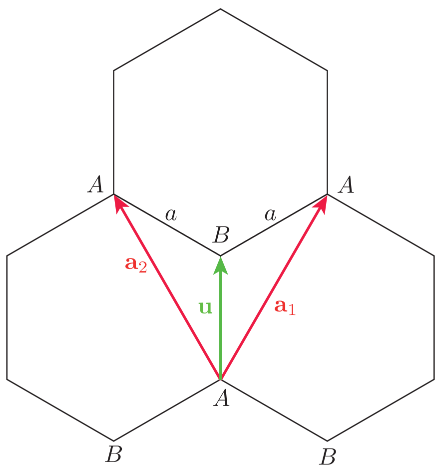
where t is the hopping integral and a is the lattice spacing.

Calculate the density of states (DOS) for $d = 1$ and discuss the algebraic form of the van Hove singularities at $E = \pm 2t$.

Exercise 2: Dispersion of graphene (Oral)

Consider a honeycomb lattice with a distance a between any neighboring sites. Such a lattice consists of two interpenetrating triangular sublattices A and B and hence has 2 different sites per unit cell. The lattice is invariant under translations of the form $\boldsymbol{R}_j = j_1\boldsymbol{a}_1 + j_1\boldsymbol{a}_2$ with j_1,j_2 integers and

$$\begin{aligned} \boldsymbol{a}_1 &= a \begin{pmatrix} \sqrt{3}/2 \\ 3/2 \end{pmatrix}, \\ \boldsymbol{a}_2 &= a \begin{pmatrix} -\sqrt{3}/2 \\ 3/2 \end{pmatrix}. \end{aligned} \tag{2}$$



In the following, we consider a tight-binding model with localized states $|\boldsymbol{R}_j, n\rangle$, where j denotes the unit cell at position $\boldsymbol{R}_j$, $\boldsymbol{R}_j$ a lattice vector, and $n = 0, 1$ corresponds to the site in the unit cell with $n = 0 \Leftrightarrow A$ and $n = 1 \Leftrightarrow B$. The states $|\boldsymbol{R}_j, n\rangle$ are orthogonal and normalized according to

$$\langle \boldsymbol{R}_j, n | \boldsymbol{R}_i, m\rangle = \delta_{i,j}\delta_{n,m} \,. \tag{3}$$

The matrix elements with the Hamiltonian are given by

$$\begin{aligned}
\langle \boldsymbol{R}_i, 0|H|\boldsymbol{R}_j, 0\rangle &= \langle \boldsymbol{R}_i, 1|H|\boldsymbol{R}_j, 1\rangle = 0, \quad \forall\, i, j \\
\langle \boldsymbol{R}_j, 0|H|\boldsymbol{R}_j, 1\rangle &= -t\,, \\
\langle \boldsymbol{R}_j, 1|H|\boldsymbol{R}_j + \boldsymbol{a}_1, 0\rangle &= \langle \boldsymbol{R}_j, 1|H|\boldsymbol{R}_j + \boldsymbol{a}_2, 0\rangle = -t\,, \\
\langle \boldsymbol{R}_j, 0|H|\boldsymbol{R}_j - \boldsymbol{a}_1, 1\rangle &= \langle \boldsymbol{R}_j, 0|H|\boldsymbol{R}_j - \boldsymbol{a}_2, 1\rangle = -t\,,
\end{aligned} \tag{4}$$

i.e. there is particle hopping from A sites to B sites and vice versa.

We further introduce the Bloch states

$$|\boldsymbol{k}, n\rangle = \frac{1}{\sqrt{V}} \sum_j e^{i\boldsymbol{k}(\boldsymbol{R}_j + n\boldsymbol{u})} |\boldsymbol{R}_j, n\rangle\,, \tag{5}$$

which are orthonormal, $\langle \boldsymbol{k}, n|\boldsymbol{q}, m\rangle = \delta_{\boldsymbol{k},\boldsymbol{q}}\delta_{n,m}$ and provide a basis.

a) Calculate the dispersion relation for the tight-binding model (4).
Hint: Consider the general eigenvalue equation $H|\psi\rangle = E|\psi\rangle$ and decompose $|\psi\rangle$ into the Bloch states (5). Project the resulting Schrödinger equation onto the localized states $|i, n\rangle$. The corresponding matrix is block diagonal in $\boldsymbol{k}$ and the dispersion relation can be calculated by diagonalizing the remaining 2×2 block matrices.

b) Show that there are two points $\boldsymbol{K}$ and $\boldsymbol{K'}$ (which are symmetry points of the lattice) where the dispersion is degenerate and vanishes. These points are called *Dirac points*.

c) Plot the dispersion over the first Brillouin zone and along the path $\Gamma - M - K - \Gamma$. (You may use the computer for this task.) Show that around the Dirac points, the dispersion is linear.

d) Discuss whether this system is an insulator or a conductor.