1 Mathematical warming-up

a) Consider the following matrices (with $E, \Delta \in \mathbf{R}$):

$$A_1 = \begin{pmatrix} E & \Delta \\ \Delta & E \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad A_3 = \begin{pmatrix} 0 & 2 & 1 & 0 & 0 & 1 & 2 \\ 2 & 0 & 2 & 1 & 0 & 0 & 1 \\ 1 & 2 & 0 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 0 & 2 & 1 & 0 \\ 0 & 0 & 1 & 2 & 0 & 2 & 1 \\ 1 & 0 & 0 & 1 & 2 & 0 & 2 \\ 2 & 1 & 0 & 0 & 1 & 2 & 0 \end{pmatrix}.$$

Do you notice any particular properties of these matrices?

b) Find the eigenvalues and eigenvectors of A_1, A_2, A_3, using your favorite mathematical software if necessary.

c) Sketch how the two eigenvalues of A_1 evolve as a function of Δ.

d) For all three matrices, verify $\mathrm{Tr}\, A = \sum_i \lambda_i$, with λ_i the eigenvalues of A.

e) Consider the following matrices:

$$T_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad T_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad T_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Verify that the T_j are unitary. The T stands for *translation*, can you explain why?

f) Show $[A_j, T_j] = 0$ for $j = 1, 2, 3$.

The following exercises apply to any dimension N, with the above examples corresponding to $N = 2, 6, 7$. It can be helpful to do the exercises for specific examples before giving proofs for general N.

g) An N-dimensional vector space has the standard basis e_a with $a \in [0, 1, \ldots N-1]$. We now wish to define a new basis v^k, with $k \in [0, 1, \ldots N-1]$, namely as $v^k_a = \frac{1}{\sqrt{N}} \exp(\frac{2\pi i a k}{N})$. In this definition, v^k_a stands for the a-th component of the vector v^k, i.e., $v^k = \sum_a v^k_a e_a$. Show that the vectors v^k are orthonormal (and as a result, they indeed form a basis).

j) We define the translation matrix T as $T_{mn} = 1$ if $n - m = 1$ modulo N and $T_{mn} = 0$ otherwise (verify that this is consistent with **e)**). What is Te_a?

i) Show that the v^k are eigenvectors of T and draw the eigenvalues in the complex plane.

j) Show that T is unitary, $T^{-1} = T^\dagger$.

k) How would this help with **a)**?

Interpretation: v^k are plane waves (here: in a discrete, periodic system), they are eigenvectors of the translation operator, with complex eigenvalues of magnitude 1. In other words, they are functions that do not change in magnitude (only in phase) if you translate them.

If a Hamiltonian H is translationally invariant, i.e., commutes with a translation operator T, then H and T have a basis of common eigenvectors. Since the eigenvectors of T are known, this greatly simplifies the eigenanalysis of H.

(In these examples, the matrices A_j have an additional symmetry: spatial inversion.)

2 Hamilton operator in Bloch representation

Consider the Hamilton operator from the lecture,

$$H_{\mathbf{GG}'}(\mathbf{k}) = \delta_{\mathbf{GG}'} \frac{\hbar^2(\mathbf{k}+\mathbf{G})^2}{2m} + V(\mathbf{G}-\mathbf{G}') \equiv (\mathbf{H}(\mathbf{k}))_{\mathbf{GG}'}$$

Show that $\mathbf{H}(\mathbf{k})$ and $\mathbf{H}(\mathbf{k}+\mathbf{G})$ have the same eigenvalues for every $\mathbf{G}$ from the reciprocal lattice.

3 Cosine potential

Consider the one-dimensional potential

$$V(x) = v_0 \cos(2\pi \frac{x}{a}).$$

a) Calculate the corresponding Fourier transformed potential V_G.

b) Write down the corresponding Hamilton operator in the Bloch representation.

c) Sketch the band structure for sufficiently small v_0. What is the magnitude of the band gap at the Brillouin Zone boundary?

d) For which v_0 does this approximation break down?

4 Artificial graphene

Consider the honey comb lattice. The reciprocal lattice is a hexognal lattice with $\mathbf{G}_1 = (1,0)$, $\mathbf{G}_2 = (\cos(\pi/3), \sin(\pi/3))$. In terms of the previous exercise, the lowest-order non-zero Fourier components are

$$V_{\pm\mathbf{G}_1} = V_{\pm\mathbf{G}_2} = V_{\pm\mathbf{G}_1\mp\mathbf{G}_2} = V$$

a) Sketch the reciprocal lattice in the first Brillouin Zone.

b) Consider the corner $\mathbf{K}_0 = 1/3\mathbf{G}_1 + 1/3\mathbf{G}_2$ of the Brillouin Zone. Show that there are two reciprocial lattice vectors $\mathbf{G}_a \neq \mathbf{G}_b$ with

$$\mathbf{K}_0^2 = (\mathbf{K}_0 - \mathbf{G}_a)^2 = (\mathbf{K}_0 - \mathbf{G}_b)^2 .$$

What does this degeneracy say about the band structure at this point for free electrons ($V = 0$)?

c) Write the explicit Fourier transformed Schrödinger equation for $\mathbf{k}$ close to $\mathbf{K}_0$ for the lowest energy subspace (The Hamilton operator should be a 3×3 matrix.

d) Consider $\mathbf{k} = \mathbf{K}_0$. Diagonalize the Hamiltonian. What is the degeneracy?

e) Calculate the band structure for $\mathbf{k} = \mathbf{K}_0 + \delta\mathbf{k}$ for small $\delta\mathbf{k}$. Do this by diagonalizing the 3×3 Hamilton operator numerically and calculate the dispersion graphically for $\delta\mathbf{k} = d \cdot (1,1)$ with $d \in [-1,1]$.