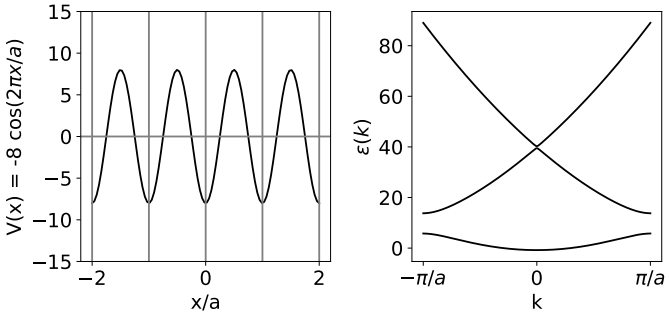
Exercise for Computational Materials Sciences

Exercise 3, November 19th, 2024. Discussion on Decmeber 3rd, 2024

1) Wannier functions for the 1D cosine potential

Recall question 4 from problem set 1. You used Bloch's theorem to numerically calculate the band structure of electrons in a 1D cosine potential. The lowest band is separated from the rest by a gap of width v_0. In this exercise, you will find the Wannier function corresponding to the lowest band. Choose $v_0 < 0$.



1. The Bloch Hamiltonian takes the form of a 3×3 matrix $\hat{H}(k)$ in the basis of plane waves $\varphi_{k,G}(x)$ around $G = 0, \pm G_0$, where $G_0 = 2\pi/a$:

$$\varphi_{k,G}(x) = e^{i(k+G)x} \equiv \{e^{i(k-G_0)x}, e^{ikx}, e^{ik+G_0x}\} \tag{1}$$

   Plot the three-component eigenvector $C^n_{k,G}$ corresponding to the lowest energy band as a function of k in the first Brillouin zone. Do all three components vary smoothly? If not, perform a gauge transformation to make the wavefunction of the lowest band *smooth* in k.

   Hint: Look at both the real and imaginary parts of the coefficients.

2. The three-component eigenvector $C^n_{k,G}$ of the matrix $\hat{H}(k)$ corresponding to the nth eigenvalue is related to the real-space wave function $\psi^n_k(x)$ through:

$$\psi^n_k(x) = \sum_G c^n_{k,G}\, \varphi_{k,G} \tag{2}$$

   Plot the lowest energy eigenvalue for a few different values of k in the first Brillouin zone.

3. Compute the Wannier function $w(x)$ centered at $x = 0$ of the lowest band by integrating the wavefunction $\psi^0_k(x)$ over the first Brillouin zone. Is the Wannier function exponentially localized?

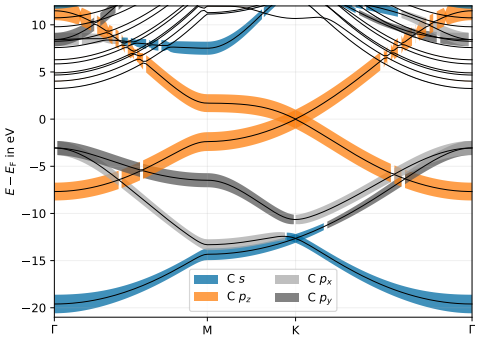
4. Shift the Wannier function by one lattice constant by correctly applying the phase factor e^{-ika} in the Brillouin zone integration. Do you reproduce $w(x - a)$?

5. When $v_0 < 0$, there is a potential minimum at the lattice sites. What happens if you run your Wannierization routine for $v_0 > 0$?

In real materials, it is much more complicated to find the optimal smooth gauge to get well-localized Wannier functions. Practicaly, we choose the gauge implicitly using a so-called *projection method*. In the next exercise, you will get acquainted with the software `Wannier90` that implemements this method.

2) Graphene — Wannier functions

Coming back to graphene, you can find a so-called *projected bands* plot on the right (often referred to as fat bands). It is a crucial step in understanding the electronic structure of materials and how the projectors in a Wannier construction can possibly be chosen.
The width of the colored bands shows the spectral weight of the dominant orbital for the given band. Other contributions are not shown and there is no distinction between the two carbon atoms in the basis.



a) Discuss from the fat-bands plot, which subsets of bands might be possible choices for a Wannier construction. Give reasoning how you reach your conclusions.

b) Start by extracting a five-band model from the *ab initio* band structure, using projectors to p_z and sp^2 orbitals. Compare the Wannier bands with the DFT bands obtained before.

In order to do this, a SCF and nSCF run has to be completed first. From there, the necessary inputs for the Wannier90 code are calculated, i.e. the overlaps and initial projections

$$M_{mn}^{\vec{k},\vec{b}} = \left\langle u_{m\vec{k}} \middle| u_{n\vec{k}+\vec{b}} \right\rangle , \qquad A_{mn}^{\vec{k}} = \langle \psi_{m\vec{k}} | g_n \rangle \ ;$$

where u denotes the cell periodic part of Bloch states, ψ are the full Bloch states and g are trial states. As a final step, the Wannier construction can be done. Here only a disentanglement by minimisation of the gauge invariant spread of the Wannier states is performed.

c) Next up, you will try to reduce the effective subspace. Drop the sp^2 orbitals in order to obtain a description of the two bands crossing the Fermi energy from an initial guess of p_z orbitals. Compare to the *ab initio* band structure and the five-band Wannierisation.

To do so, copy the Wannier input file ending in `win` and adapt the number of Wannier states as well as the initial projections as stated. Change the values set for the frozen window, too. Specifically, the input parameters for `dis_win_min/max` should be chosen such that within this window only energy states of the targeted sub-manifold are present.

d) From both Wannier constructions extract information on the initial and final spreads. What differences do you observe? Can you explain your observation?