Introduction to graphene and 2D materials

Homework problem set 1

29.04.2024

1 Carrier density and density of states of graphene

Graphene is a two-dimensional material characterized by a linear dispersion relation: $E = \hbar v_F k$.

(a) The charge carrier density of a material n, also known as carrier concentration, denotes the number of charge carriers per volume (per area in two-dimensional materials). Calculate the charge carrier density of graphene. (Hint: When calculating the charge carrier density remember to include the spin and valley degeneracy).

(b) From the carrier density calculated above and remembering that $n = \int_0^{E_F} g(E)dE$, calculate the density of states of graphene, $g(E)$. Discucss the result.

(c) Calculate numerically the charge carrier density of graphene, for $E_F = 100$ meV. Discucss the result.

2 Dirac Fermions in 1D

Lets imagine that there is a 1D chain of atoms with two atoms per unit-cell and lattice constant $2a$.

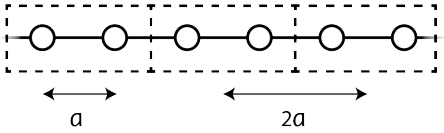

Figure 1: Structure of the imaginary 1D chain of atoms with inter-atomic distance of a and a lattice constant of $2a$. Dashed box outlines the unit cell containing 2 atoms.

(a) Derive the tight binding Hamiltonian assuming that the atoms are identical with only half filled orbitals contributing to the band structure.

(b) Plot the band structure. Comment on the shape of the band structure [* how does it compare to that of graphene?].

(c) Represent the Hamiltonian in terms of Pauli matrices. Comment on the difference between this and graphene.

(d) What is the Fermi velocity in this system?

3 Tight binding calculation of 2D Kagome lattice

Kagome lattices have an interesting crystal structure with a three-point basis that repeat to fill the crystal lattice. In Figure 2 the three atoms that make up the unit-cell are labelled in red (R), green (G) and blue (B), and the vectors connecting the nearest neighbours as $\vec{\delta}_1$, $\vec{\delta}_2$ and $\vec{\delta}_3$. We will calculate the electronic band structure of this Kagome lattice. For simplicity, let's assume that atoms R,G and B are of the same type of an element, and that electrons hop between p_z orbitals of nearest neighbors.

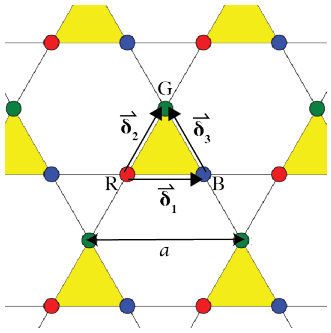

Figure 2: Structure of a Kagome lattice. The unit-cell is highlighted in yellow. Atoms are labeled in red (R), green (G) and blue (B). a is the lattice constant and $\vec{\delta}_{1,2,3}$ the hopping vectors.

(a) Write the hopping vectors $\vec{\delta}_{1,2,3}$ in terms of the lattice constant a.

[* Use $\vec{\delta}_2 = \begin{pmatrix} \cos 60^\circ & -\sin 60^\circ \\ \sin 60^\circ & \cos 60^\circ \end{pmatrix} \vec{\delta}_1$ and $\vec{\delta}_3 = \vec{\delta}_2 - \vec{\delta}_1$]

(b) Solve for the tight binding Hamiltonian.

(c) Solve for the band structure (energy eigenvalues as a function of $k_x,\ k_y,\ k_z$). How many solutions are there?

(d) Plot the band structure of the Kagome lattice. Note the Brillouin Zone boundary. Discuss its band structure in the context of graphene. Where are the Dirac points?

(e) Calculate the Fermi velocities in each of the bands, and comment on your findings.