Roma la Sapienza
Solid State Physics

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Esercitazione °1

Exercise I : Graphene π-electron band structure and ARPES

Let's consider a simple TB model for the π bands of graphene.

1. Draw the two-dimensional honeycomb lattice of graphene. The C-C bond length is equal to $a = 1.42$ Å. Place one C atom in the origin (atom A) and a nearest neighbor atom (atom B) on the x axis. Draw the unit cell. How many are the atoms contained in the unit cell? Draw the two basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ for the direct lattice (notice that to follow the standard convention for hexagonal lattices, the angle between the two vectors should be 120°, and not 60°). How long are these vectors? Compute and draw the two basis vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ for the reciprocal and the first Brillouin zone. What is the length in Å^{-1} of $\mathbf{b}_1$? The K point and K' point are the two distinct points at the vertex of the Brillouin zone. Compute the distance between Γ and K. Write the coordinates of K and K' in Cartesian coordinates and in terms of $\mathbf{b}_1$ and $\mathbf{b}_2$. The M point is at the mid-distance between two adjacent K and K'. How many distinct M point are there?

2. For the π bands we consider a TB model with one π_z orbital per C site $|\mathbf{R}+\boldsymbol{\tau}_\alpha\rangle$, where $\mathbf{R}$ is a direct lattice vector and $\boldsymbol{\tau}_\alpha$ is the internal coordinate of the atom in the α site. We neglect the overlap between different sites, namely: $\langle \mathbf{R}+\boldsymbol{\tau}_\alpha|\mathbf{R}'+\boldsymbol{\tau}_{\alpha'}\rangle = \delta_{\mathbf{R},\mathbf{R}'}\delta_{\alpha,\alpha'}$. We consider the onsite energy equal to zero, and a hopping integral equal to $-t$ only for the nearest-neighbor atoms. Write the Hamiltonian in the Bloch basis:

$$|\mathbf{k}\alpha\rangle = \sum_{\mathbf{R}} \frac{1}{\sqrt{N}} e^{+i\mathbf{k}\cdot(\mathbf{R}+\boldsymbol{\tau}_\alpha)} |\mathbf{R}+\boldsymbol{\tau}_\alpha\rangle.$$

   Obtain a $\mathbf{k}$ dependent Hamiltonian for the periodic part of the Bloch state $H_{\mathbf{k}}$. Diagonalize the Hamiltonian. Draw the Band structure along the $\Gamma - K - M$ line.

3. Show that the $H_{\mathbf{K}} = H_{\mathbf{K}'} = 0$. Expand the Hamiltonian around K (or around K') keeping the term linear in $\mathbf{q} = (\mathbf{k} - K)$ (or $\mathbf{q} = (\mathbf{k} - K')$). Show that for one of the two points (K or K') the resulting Hamiltonian $\bar{H}_{\mathbf{q}}$ (in the basis $\{|\mathbf{q}+\mathbf{K}\alpha\rangle\}_{\alpha=1,2}$) is given by

$$\bar{H}_{\mathbf{q}} = \hbar v_F \boldsymbol{\sigma}\cdot\mathbf{q}$$

   where $\hbar v_F$ is the Fermi velocity and $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ are the Pauli matrices (notice that, since the σ_y is not symmetric, to obtain this result you have to chose appropriately the order of the two atomic sites $\alpha = 1, 2$). Show that for the other point $\bar{H}_{\mathbf{q}} = -\hbar v_F \boldsymbol{\sigma}^*\cdot\mathbf{q}$.

4. Compare the $\bar{H}_{\mathbf{q}}$ Hamiltonian with that obtained from a Dirac equation setting the mass $m = 0$.

5. Diagonalize $\bar{H}_{\mathbf{q}}$. Compute the eigenenergies and eigenstates. Compare the resulting linearized band structure with that of the original Hamiltonian.

6. Experimentally for graphene $v_F \simeq 10^6 m/s$. Compute the value of t in eV units that gives such a velocity.

7. In the neutral case each carbon atom provides one electron to the crystal. Determine (with justification) the position of the Fermi energy in the neutral case.

8. Consider the case where the Fermi energy is shifted up by $0.3eV$ (as in one of the ARPES experiments). Using the approximated $\bar{H}_{\mathbf{q}}$ Hamiltonians compute the number of extra electrons in graphene per unit surface, where the area is expressed in cm^2.

9. Consider a graphene decorated by Li atoms with stoichiometry LiC_{12}. Using the approximated $\bar{H}_{\mathbf{q}}$ Hamiltonians and supposing that each Li atom donate one electron to graphene, compute the shift of the Fermi energy with respect to the neutral case. Compare the results with the ARPES spectra measured in the bilayer graphene experiment intercalated with Li.

10. For the neutral case and for the two doped case above, (using the approximated Hamiltonian), consider a hole created by a photoemission experiment. Compute and plot the broadening of a hole due to the decay of the hole produced by the emission of a phonon with energy of $0.18eV$. Plot the broadening as a function of the energy distance of the hole from the Fermi energy. Compare the 3 different cases. In which case the decay is more visible? For the Li doped case consider the possibility to decay (with an equal matrix element) into two distinct optical phonons with energy $0.18eV$ and $0.07eV$. Plot the broadening as a function of the energy distance of the hole from the Fermi energy

11. Repeat the above calculations for the case of an inverse photoemission experiment, in which one extra electron is injected above the Fermi energy. Plot the broadening as a function of the energy distance of the electron from the Fermi energy.