PROBLEM SET #7
"Electrons in crystal"
due on 5/24/2021

Physics–172 / Applied Physics–272
Introduction to Solid State Physics
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Problem 7.1 (Zinc blende — **2 points**)**.** Crystalline structure of ZnS is drawn on Figure 1.

1. (**1 point**) Identify Bravias lattice, primitive unit cell and primitive translation vectors $\mathbf{a}_i$. Calculate the volume of the primitive unit cell. Lattice constant a is defined on Figure 1.

2. (**1 point**) Compute primitive translation vectors $\mathbf{b}_i$ of reciprocal lattice $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$. What Bravias type does reciprocal lattice belong to?

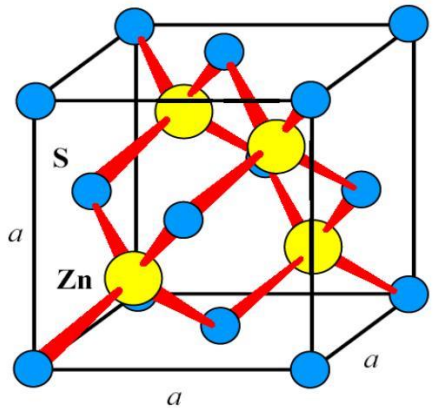


Figure 1: Zinc blende lattice

Problem 7.2 (Tight–binding chain— **4 points**)**.** Consider one–dimensional chain of nodes with alternating hopping amplitudes between nearest neighbors t_1, $t_2 \in \mathbb{R}$. Such system is known in the literature as Su-Schrieffer-Heeger model.

$$\mathcal{H} = \sum_{i=-\infty}^{\infty} t_1 c^+_{2i+1} c_{2i} + t_2 c^+_{2i+1} c_{2i+2} + \text{h.c.}$$

Here h.c. stands for hermitian conjugate and c_i are fermionic annihilation operators on site i.

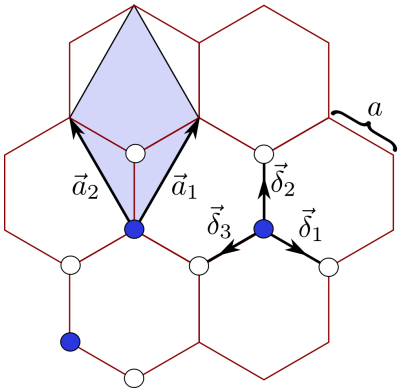
1. (**3 points**) Compute the spectrum.

2. (**1 point**) Imagine that you have one electron per node. Is it a metal or an insulator?

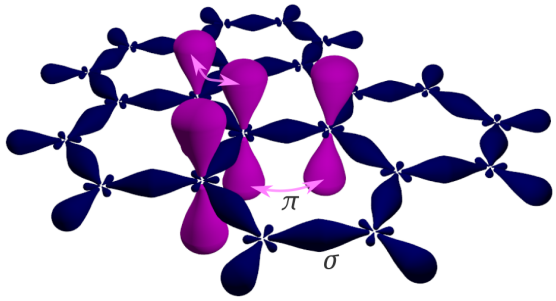
Problem 7.3 (Graphene spectrum — **8 points**)**.** In graphene, three out of four $n = 2$ electrons of Carbon sp^2–hybridize and form strong in–plane valence σ–bond, while forth electron's wave function barely overlaps with other electrons via so–called π–bonding (see Figure 2b). Conductance of such electrons is well-described by tight–binding model.

$$\hat{H} = -t \sum_{\langle i,j \rangle} \hat{c}^+(\mathbf{r}_i)\hat{c}(\mathbf{r}_j) = -t \sum_{\mathbf{r}}^{\text{SL}} \sum_{j=1}^{3} \hat{c}_A^+(\mathbf{r})\hat{c}_B(\mathbf{r} + \boldsymbol{\delta}_j) + \text{h.c.}, \tag{7.3.1}$$

Here $t = 3$ eV is the nearest–neighbor hopping amplitude. Hexagonal (or honeycomb) lattice could be described as two triangular sublattices symmetrically displaced with respect to each other (see Figure 2a).



(a) Primitive unit cell (blue) and translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$ of the hexagonal lattice.



(b) Illustration of in–plane σ–bonds and out–of–plane π–bonds that are formed by valence electrons.

Figure 2: Graphene lattice and electron orbitals.

1. (**4 points**) Find the spectrum of Hamiltonian (7.3.1).

2. (**1 point**) Show that there are two points in Brillouin zone $\mathbf{K}$, $\mathbf{K}'$ where energy bands touch each other. In the vicinity of these points (called *valleys*) effective Hamiltonian has the form of 2D Dirac Hamiltonian.

   $$\mathcal{H}_{\mathbf{K}+\mathbf{k}} \approx \hbar v_F(\sigma_x k_x + \sigma_y k_y).$$

   Calculate numerical value of Fermi velocity v_F if hopping amplitude $t = 3$ eV and carbon–carbon distance $a = 1.42$ Å.

3. (**1 point**) Where is the Fermi level in graphene? Is it a metal or an insulator?

4. (**2 points**) Introduce next nearest–neighbor hopping (with amplitude $t' = 0.3$ eV). Describe how it modifies electronic spectrum. Does it change the position of Fermi energy with respect to the conical points? Does it change Fermi velocity?