PROBLEM SET #6
"Electrons in crystal"
due on 5/23/2021

Physics–172 / Applied Physics–272
Introduction to Solid State Physics
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Problem 6.1 (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?

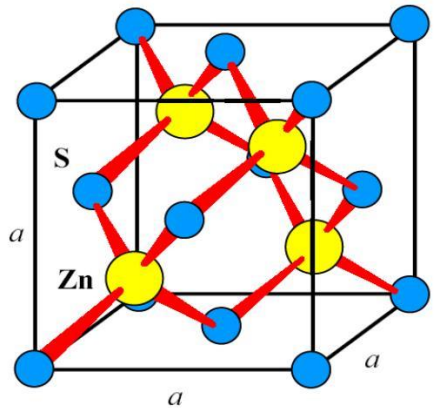
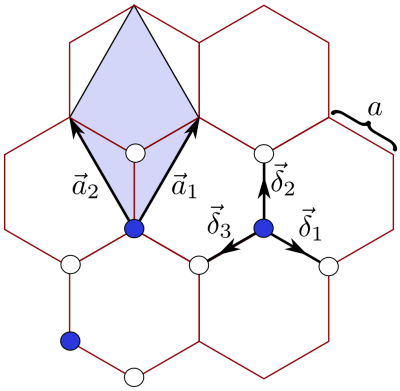


Figure 1: Zinc blende lattice

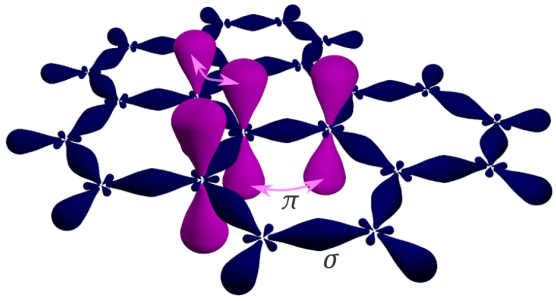
Problem 6.2 (Graphene spectrum — **6 points**)**.** In graphene, three out of four $n = 2$ electrons of Carbon sp^2–hybridize and form strong in–plane valence σ–bond, while forth electron's wave function barely overlaps with other electrons via so–called π–bonding (see Figure 2b). Conductance of such electrons is well-described by tight–binding model.

$$\hat{H} = -t \sum_{\langle i,j \rangle} \hat{c}^{+}(\mathbf{r}_i)\hat{c}(\mathbf{r}_j) = -t \sum_{\mathbf{r}}^{\mathrm{SL}} \sum_{j=1}^{3} \hat{c}_A^{+}(\mathbf{r})\hat{c}_B(\mathbf{r} + \boldsymbol{\delta}_j) + \text{h.c.}, \tag{6.2.1}$$

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. (**3 points**) Find the spectrum of Hamiltonian (6.2.1).

2. (**1 point**) Show that there are two points in Brillouin zone **K**, **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. (**1 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?

Problem 6.3 (Emery model — **6 points**)**.** It turns out that electronic properties of copper–based high-T_c superconductors (a.k.a cuprates) are well described by valence electrons in Cu–O plane.

Consider a two dimensional square lattice illustrated on Figure 3. Imagine that the only relevant electron are those on $d_{x^2-y^2}$ orbitals of copper and p_x and p_y orbitals of oxygen. Hopping amplitudes t_{ij} are either $\pm t$ for jumps between neighboring oxygen atoms or $\pm t'$ for neighboring copper and oxygen atoms. Figure 3 explains what determines the relative sign of these amplitudes.

$$\hat{H} = \sum_i \begin{Bmatrix} \varepsilon_{\mathrm{Cu}} \\ \varepsilon_{\mathrm{O}} \end{Bmatrix} \hat{c}^+(\mathbf{r}_i)\hat{c}(\mathbf{r}_i) + \sum_{\langle i,j \rangle}^{\text{Cu–O}} (\pm t')\hat{c}^+(\mathbf{r}_i)\hat{c}(\mathbf{r}_j) + \sum_{\langle i,j \rangle}^{\text{Oxygen}} (\pm t)\hat{c}^+(\mathbf{r}_i)\hat{c}(\mathbf{r}_j).$$

Here $\varepsilon_{\mathrm{Cu}}$ and ε_{O} are self–energies of electrons on copper and oxygen atoms respectively. Following the steps outlined below, find electronic energy spectrum in cuprates.

1. (**1 point**) Determine primitive cell and translation vectors. How many atoms are in the primitive cell? Find dual vectors and determine the form of Brillouin zone.

2. (**1 point**) Produce Fourier transform and obtain 3×3 Bloch Hamiltonian $\mathcal{H}$.

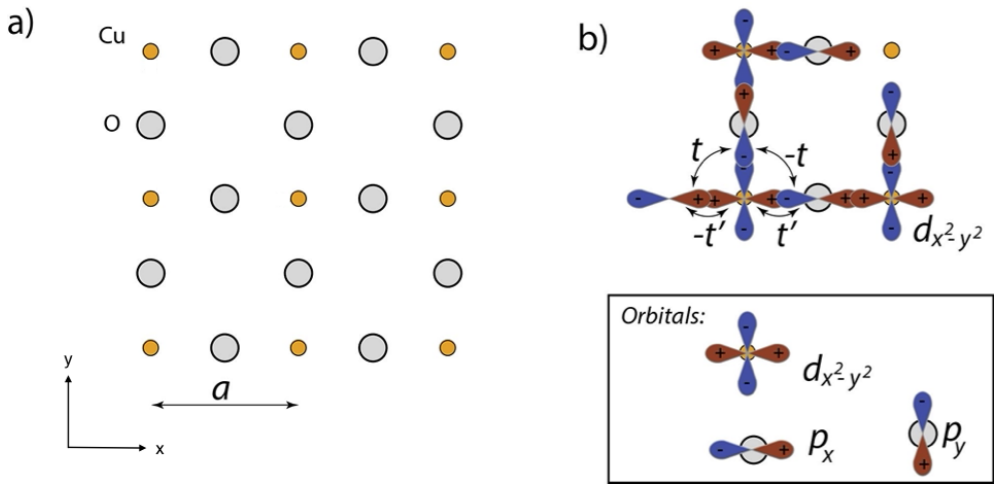


Figure 3: CuO plane and relevant electron orbitals.

3. (**2 points**) Let $\varepsilon_{\mathrm{Cu}} = \varepsilon_{\mathrm{O}} = 0$ and $t' = t$. Find energy bands. Instead of writing cumbersome analytical expression, you're encouraged to provide a plot of $\varepsilon(\mathbf{k})$ for an answer. Since 3D plots are hard to read, we recommend using contour plots, color maps or plot of energy slices between the high–symmetry points (Γ, X, M).

4. (**2 points**) Still assume $\varepsilon_{\mathrm{Cu}} = \varepsilon_{\mathrm{O}} = 0$ and $t' = t$. Imagine that there are 8/3 electrons per unit cell. At what energy is Fermi level located?

Problem 6.4 (Landau levels in graphene — **4 points**)**.** Solve stationary Schrödinger problem[1] for electrons in graphene in the presence of the magnetic field $\mathbf{B} = B\hat{z}$, $B > 0$.

$$\hat{\mathcal{H}} = v\left(\hat{\boldsymbol{\sigma}}, \hat{\mathbf{p}} + \frac{|e|}{c}\mathbf{A}\right), \qquad \mathbf{A} = (-By, 0, 0).$$

1. (**3 points**) Find energies ε_n and eigenvectors $\psi_{n,k}$. You can use harmonic oscillator functions (a.k.a normalized Hermite functions) $\psi_n^{\mathrm{osc}}(x)$ in your answer.

$$\psi_n^{\mathrm{osc}}(x) = \frac{e^{-x^2/2}H_n(x)}{\sqrt{2^n n!\sqrt{\pi}}}.$$

   Pay attention to zeroth Landau level. Which eigenvector does it correspond to?

2. (**1 points**) Compute energy difference between zeroth and first Landau level at $B = 1$ T. Express your answer in Kelvins.

[1] In case you are interested how to justify the Hamiltonian above, read on the Peierls substitution.