PROBLEM SET #5
"Electronic band structure"
due on 5/19/2021

Physics–172 / Applied Physics–272
Introduction to Solid State Physics
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Comment. In addition, some material in the notes may be more advanced, or will not directly be related to discussions in class. Please view these parts as stimulating extensions, where you are welcome to contact us about questions and relevant references.

Problem 5.1 (δ–Kronig–Penney model— **12 points**)**.** Consider a one dimensional crystal for which the potential is a periodic array of delta-functions,

$$V(x) = \frac{\hbar^2 q}{m} \sum_{n=-\infty}^{\infty} \delta(x - na).$$

where a is the lattice constant.

1. (Exact solution — **7 points**) Compute the energies for this model. Draw a picture of the band structure for positive and negative values of q.

2. (Tight–binding limit — **5 points**) If qa is large and negative, there is a tightly bound Wannier state $w_n(x)$ associated with each delta function. Find zero–order Wannier functions and calculate the width of the energy band within tight–binding approximation. Also, deduce the band width from exact solution you found before and compare the two.

   Hint. Read Chapter 10 in [1] to learn how to derive tight–binding approximation in 1D.

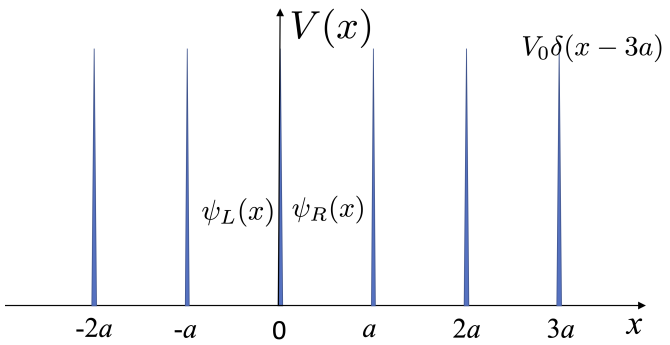


Figure 1: The δ-function Kronig-Penney Model.

Problem 5.2 (Tight–binding chain— **8 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. (**6 points**) Compute the spectrum.
2. (**2 point**) Imagine that you have one electron per node. Is it a metal or an insulator?

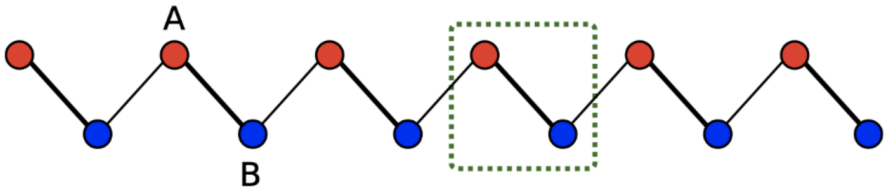


Figure 2: SSH chain with different bonding strength between sublattices.

Problem 5.3 (Graphene spectrum — **9 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 3b). Conductance of such electrons is well-described by tight–binding model.

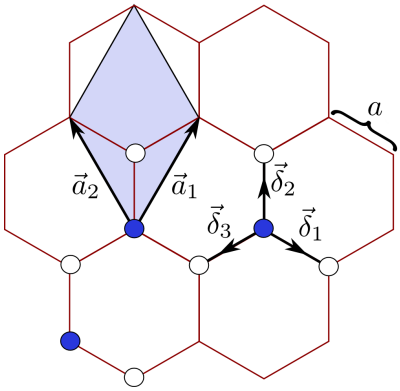
$$\hat{H} = -t \sum_{\langle i,j \rangle} \hat{c}^{+}(\mathbf{r}_i)\hat{c}(\mathbf{r}_j) = -t \sum_{\mathbf{r}}^{\text{SL}} \sum_{j=1}^{3} \hat{c}_A^{+}(\mathbf{r})\hat{c}_B(\mathbf{r} + \boldsymbol{\delta}_j) + \text{h.c.}, \tag{5.3.1}$$

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 3a).

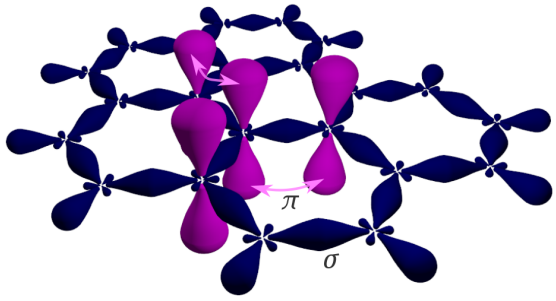
1. (**6 points**) Find the spectrum of Hamiltonian (5.3.1).
2. (**2 points**) Show that there are two points in Brillouin zone $\mathbf{K}$, $\mathbf{K}'$ where energy bands touch each other. In the vicinity of these points (called *valleys*) effective Hamiltonian has the form of 2D Dirac Hamiltonian.

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

   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?



(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 3: Graphene lattice and electron orbitals.

Problem 5.4 (Emery model — **10 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 4. 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 4 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.

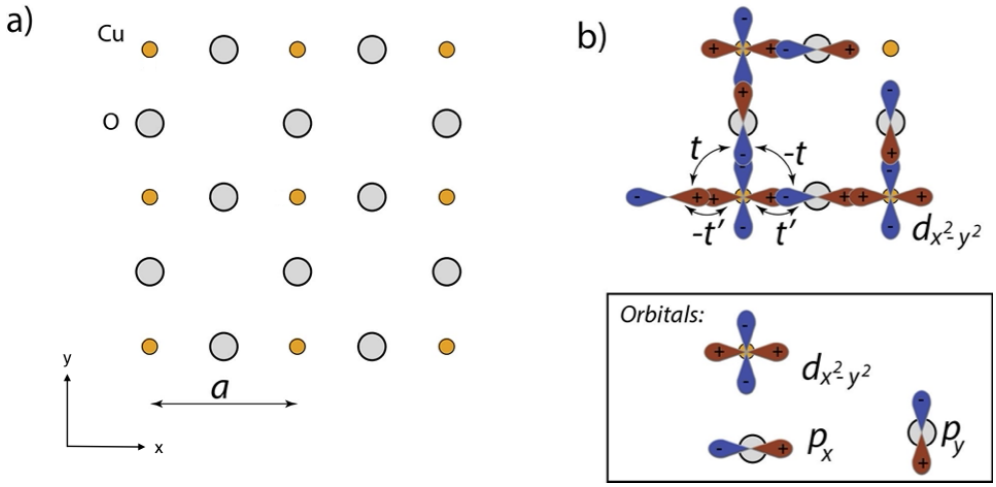


Figure 4: CuO plane and relevant electron orbitals.

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

3. (**4 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. (**3 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?

References

[1] Neil Ashcroft and David Mermin. *Solid state physics*. Harcourt College Publishers, 1976.