8.231 Physics of Solids I — Fall 2017
Problem Set 4

Posted: Tuesday, Sep 26, 2017
***Due:* Tuesday, Oct 3, 2017**

Readings (Optional)

- Simon, Steven H. *The Oxford Solid State Basics*, Chapter 15-16.

Note: Bonus problems are more challenging. It is fine you do not solve them. By solving them you can earn extra credits.

Problem 1

Tight-binding Chain Done Right

In solving the one-dimensional tight-binding chain, we made several approximations:

- This atomic orbitals at different sites are orthogonal $\langle m|n\rangle = \delta_{mn}$.
- The overlapping integral only non-vanishes when $|m-n| \leq 1$:

$$\langle m|H|n\rangle = \begin{cases} \mathcal{E}, & n = m, \\ -t, & |n-m| = 1, \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

In this problem, we explore the effect when these restrictions are relaxed.

(a) Relax the nearest-neighbour hopping restriction. Suppose now the next-nearest-neighbour hopping is allowed, i.e.,

$$\langle m|H|n\rangle = \begin{cases} \mathcal{E}, & n = m, \\ -t_1, & |n-m| = 1, \\ -t_2, & |n-m| = 2, \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

Solve the band structrue. Sketch the band dispersion when $t_1 = t_2$. What happens if d-th-nearest-neighbour hopping is allowed?

(b) (Bonus) Relax the orthogonality relation. Suppose

$$\langle n|m\rangle = \begin{cases} A, & n = m, \\ B, & |n-m| = 1, \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

Suppose the Hamiltonian matrix element is still given by Eq. (1). Solve the band structure.

Problem 2

Tight-binding Model for Polyacetylene

Hideki Shirakawa, Alan Heeger, and Alan MacDiarmid are awarded Nobel Prize in Chemistry in 2000 "for their discovery and development of conductive polymers". One of the most important (and simplest) conductive polymers is polyacetylene. The structural diagram of trans-polyacetylene, which is thermodynamically more stable than cis-polyacetylene, is as follows:

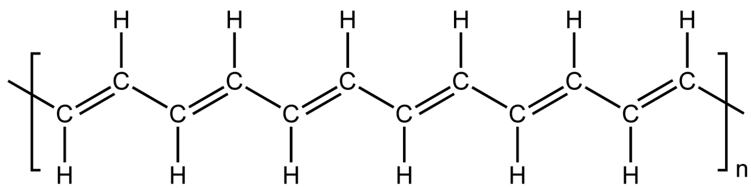

Figure 1: The structural diagram of trans-polyacetylene.

The σ bonding (sp^2 hybrids) connects carbon and hydrogen atoms. What is responsible for the electric conduction is the π bonding (p_z orbital) of carbon atoms, which can be modeled by a tight-binding chain as follows:

Suppose the spacing between the carbon atoms is a. The on-site energy for carbon atom (i.e., the diagonal term in the Hamiltonian matrix) is $\mathcal{E}$. The nearest-neighbour electron hopping strengths (i.e., the off-diagonal term in the Hamiltonian matrix) are t and t' for "single" and "double" bonds in Figure 1.

(a) Without doing any calculation, what are the band structures in the limit (i)$t = t'$ and (ii)$t \neq 0, t' = 0$. Sketch $E(k)$ in the Brillouin zone $k \in [-\frac{\pi}{2a}, \frac{\pi}{2a}]$.

(b) Solve the band structure for the general case. Sketch the band structure.

(c) Subtracting the three electrons for sp^2 hybridization, there is only one electron left per carbon atom for the p_z orbital. How are the bands filled? Is it an insulator or a metal? In order for the polyacetylene to be conductive, it is necessary to dope polyacetylene with I, Br or Cl. In this way, the conductivity can increase by seven orders of magnitude. Why?

Problem 3

Phonons in the Diatomic Chain

Consider a diatomic chain consists of two kinds of atoms, with masses m_A and m_B respectively:

$$-A - B - A - B - A - B-$$

They are connected by a spring whose equilibrium length is a. The spring constant is κ.

(a) Solve and sketch the phonon bands.

(b) At $k = 0$, sketch the atom motion of the two bands by examining the eigenvectors you obtained in (a).

(c) Phonons in the lower branch are called the "acoustic phonons". As suggested by its name, they are responsible for the sound propagating. What is the sound velocity in the long wavelength limit $k \to 0$?

(d) Phonons in the upper band are called the "optical phonons". If the material is ionic, they are responsible for optical properties of the lattice. To see this, suppose atom A and B take charges $+q$ and $-q$ respectively. An alternating electric field $E = E_0 e^{-i\omega t}$ is applied to the lattice. In the $k \to 0$ limit, solve the equations of motion. What is the electric susceptibility χ_e? With this, we can derive optical properties as you have already done in Problem 2 of Pset 2.