

# Physics 195 / Applied Physics 195 — Assignment #3

Professor: Donhee Ham

Teaching Fellows: Brendan Deveney and Laura Adams

Date: Sep. 29, 2017

Due: 12:45pm + 10 min grace period, October 6, 2017 at the dropbox outside Maxwell-Dworkin Room 131.

## Problem 1 (100 pt): 1D metal with tight binding

Consider the 1D crystal of Lecture Note #5, with a crystal length  $L$ , a unit cell length  $a$ , one atom per unit cell, and a total number of unit cells  $N$  (which, in this case with one atom per unit cell, is the same as the total number of atoms).  $L = Na$ . As we studied, if we consider only the nearest-neighbor hopping in the tight-binding approximation, the matrix element of the Hamiltonian  $H$  for an electron in the periodic potential due to the 1D crystal lattice can be written as

$$\langle n|H|m\rangle = \epsilon_0\delta_{nm} - t[\delta_{n-1,m} + \delta_{n+1,m}] \quad (m = 1, 2, 3, \dots, N; n = 1, 2, 3, \dots, N) \quad (1)$$

in the basis of atomic ground states  $\{|n\rangle\}$  ( $n = 1, 2, 3, \dots, N$ ).  $\epsilon_0$  and  $t$  ( $> 0$ ) are as we defined in class/note. Assume that there is one valence electron per atom.

(a) Following the recipe of Lecture #5, show that the single-electron energy eigenstates and their corresponding energy eigenvalues are given by

$$|\psi_k\rangle = N^{-1/2} \sum_{n=1}^N e^{ikna} |n\rangle \quad (2)$$

$$\epsilon(k) = \epsilon_0 - 2t \cos(ka) \quad (3)$$

where you should also show that  $k$ , the state index, is discretized as  $k = (2\pi/L) \times$  integers.  $\epsilon(k)$  represents a band. Identify the 1st Brillouin zone. Find the total number of  $k$ -states (*i.e.*, states labeled by  $k$ ) and the total number of quantum states available in this band. Show the orthogonality of the energy eigenstates, *i.e.*,  $\langle \psi_k | \psi_{k'} \rangle = 0$  for  $k \neq k'$ . Calculate the effective electron mass  $m^*$  near  $ka \ll 1$ .

(b) Show that, in contrast to the free electron Fermi gas, the energy eigenstate  $|\psi_k\rangle$  here is not in general a momentum eigenstate<sup>1</sup>. Is this consistent with the commutation relation between Hamiltonian  $H$  and momentum operator  $p$ ?

(c) Calculate the density of states  $D(\epsilon)$ .

(d) Argue that this crystal is a metal. How much total electronic energy lowering is achieved by bringing together the  $N$  atoms into the 1D crystal? That is, what is the cohesive energy contributed by the valence electrons? For this calculation, assume  $T = 0$ .

(e) Calculate the chemical potential  $\mu(T)$  and the total electronic energy  $U(T)$  both to the second order of  $T$ , assuming  $k_B T \ll t$ . Calculate the specific heat  $C(T)$ .

(f) Now consider the electron hopping (strength  $\delta > 0$ ) between the 2nd nearest-neighbor atoms as well, *i.e.*:

$$\langle n|H|m\rangle = \epsilon_0\delta_{nm} - t[\delta_{n-1,m} + \delta_{n+1,m}] - \delta[\delta_{n-2,m} + \delta_{n+2,m}]. \quad (4)$$

Calculate the new band dispersion  $\epsilon(k)$ . Within the 1st Brillouin zone, plot this new  $\epsilon(k)$  in juxtaposition with  $\epsilon(k)$  of Eq. (3) (assume  $\delta \sim 0.1t$ ). Do you see that the additional hopping increases the bandwidth? Do you understand why?

---

<sup>1</sup>So  $\hbar k$  is not momentum any more (in contrast to the free electron Fermi gas); it is called crystal momentum.

**Problem 2 (100 pt): 1D crystal tight binding with 2 orbitals per unit cell**

We again consider the 1D crystal of Problem 1 and Lecture #5—a crystal length  $L$ , a unit cell length  $a$ , one atom per unit cell, and a total number of unit cells  $N$ . But we now seek to delocalize not only the atomic ground states but also their first excited states. We denote the ground and first excited states of the  $n$ -th atom as  $|n_L\rangle$  and  $|n_H\rangle$ , and their energies as  $\epsilon_L$  and  $\epsilon_H$  ( $\epsilon_H > \epsilon_L$ ). Using the tight-binding approximation, and considering only the nearest neighbor hopping, the matrix elements of the single-electron Hamiltonian  $H$  in the 1D crystal in the basis of the ground and first excited atomic states may be expressed as:

$$\langle n_L|H|m_L\rangle = \epsilon_L\delta_{nm} - t_{LL}[\delta_{n-1,m} + \delta_{n+1,m}]; \quad (5)$$

$$\langle n_H|H|m_H\rangle = \epsilon_H\delta_{nm} + t_{HH}[\delta_{n-1,m} + \delta_{n+1,m}]; \quad (6)$$

$$\langle n_H|H|m_L\rangle = t_{LH}[\delta_{n-1,m} + \delta_{n+1,m}]; \quad (7)$$

$$\langle n_L|H|m_H\rangle = t_{HL}[\delta_{n-1,m} + \delta_{n+1,m}], \quad (8)$$

where  $n, m = 1, 2, 3, \dots, N$ . Here:  $t_{LL} > 0$  is the hopping strength between the ground states of two neighboring atoms (this is  $t$  of Problem 1 and Lecture #5);  $t_{HH} > 0$  is the hopping strength between the first excited states of two neighboring atoms; and  $|t_{LH}| = |t_{HL}|$  is the hopping strength between the ground state of one atom and the first excited state of a neighboring atom. For simplicity, assume that:  $t_{LL} = t_{HH} \equiv t > 0$  (although the equality is unrealistic);  $t_{LH}$  and  $t_{HL}$  are real and  $t_{LH} = t_{HL} \equiv s$  (although we can treat more generally with complex numbers); and  $\epsilon_H = -\epsilon_L \equiv \epsilon_0 > 0$  (this is achieved by shifting the energy reference).

(a) Solve the Schrödinger equation  $H|\psi_k\rangle = \epsilon(k)|\psi_k\rangle$  by using the following  $k$ -labeled ket

$$|\psi_k\rangle = \sum_{n=1}^N e^{ikna} [c_L(k)|n_L\rangle + c_H(k)|n_H\rangle] \quad (9)$$

as an eigenstate ansatz. Demonstrate the formation of 2 bands. For each band, find  $\epsilon(k)$  and corresponding  $|\psi_k\rangle$  (*i.e.*, find  $c_L(k)$  and  $c_H(k)$ ). Show that  $k$  is again discretized as  $k = (2\pi/L)\times$  integers. Identify the 1st Brillouin zone, and count the total number of quantum states available in each band.

(b) Show that for  $s = 0$  (no mixing between different types of atomic orbitals), one band originates from the delocalization of the atomic ground states only, and the other band arises from the delocalization of the first excited atomic states only (this corresponds to the situation described on Page 6, Lecture #5). What is the condition (in terms of  $\epsilon_0$  and  $t$ ) for no energy overlap between the two bands? Under this condition, sketch  $\epsilon(k)$  for both bands.

(c) Show that for  $s \neq 0$ , each band originates from the delocalization of mixture of the atomic ground states and first excited states.

**Problem 3 (100 pt): Stabilization by distortion**

In Problems 1 and 2 above and in Lecture #5, we have studied the single-electron eigen energy problem in the 1D crystal lattice of Fig. 1(A), with a crystal length  $L$ , a unit cell length  $a$ , one atom per unit cell, a total number of unit cells  $N$ , and thus a total number of atoms  $N$  ( $L = Na$ ). If the atomic ground states (energy  $\epsilon_0$ ) are delocalized with the hopping strength  $t > 0$  between two neighboring atoms in tight-binding approximation, a single band of energy is formed with the dispersion relation given by

$$\epsilon(k) = \epsilon_0 - 2t \cos(ka). \quad (10)$$

In the present problem we distort the 1D crystal of Fig. 1(A) into that of Fig. 1(B). The total number of atoms and the crystal length remain the same at  $N$  and  $L$ , respectively. But atoms are paired up and brought closer, while every other atom is repeated with distance  $2a \equiv d$ . In this distorted crystal of Fig. 1(B), a unit cell contains 2 atoms, the total number of unit cells is  $N/2$ , and the unit cell length is  $d$ . We denote the ground states of the 1st and 2nd atom of the  $n$ -th unit cell as  $|n, 1\rangle$  and  $|n, 2\rangle$ , where each of

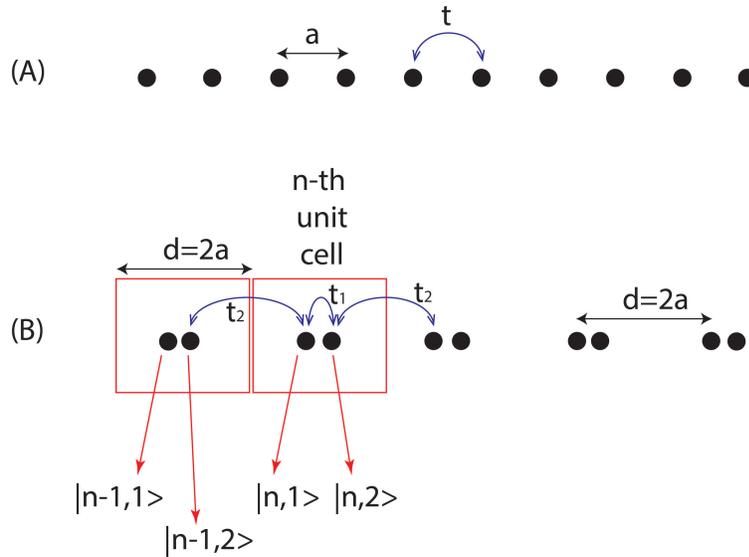


Figure 1: Problem 3

these states has the same energy  $\epsilon_0$ . Ignore higher energy atomic orbitals. The strength of electron hopping between any two closer adjacent atoms is  $t_1 > 0$ , and that between any two farther adjacent atoms is  $t_2 > 0$ . Ignore all other hopping possibilities.

(a) Express the matrix elements for the single-electron Hamiltonian  $H$  in this distorted crystal under tight-binding approximation.

(b) By using the following  $k$ -labeled ket

$$|\psi_k\rangle = \sum_{n=1}^N e^{iknd} [c_1(k)|n, 1\rangle + c_2(k)|n, 2\rangle] \quad (11)$$

as an eigenstate ansatz<sup>2</sup> for the Schrödinger equation  $H|\psi_k\rangle = \epsilon(k)|\psi_k\rangle$ , demonstrate the formation of 2 bands. For each band, calculate  $\epsilon(k)$ . Express the bandgap size. Sketch  $\epsilon(k)$  for both bands, while identifying the 1st Brillouin zone. How does this 1st Brillouin zone differ from the 1st Brillouin zone of the 1D crystal of Fig. 1(A)? More generally, how does the band structure of this distorted crystal differ from the band structure Eq. (10) of the undistorted crystal? How many quantum states are available in each band for this distorted crystal?

(c) Assume one valence electron per atom. Argue that while the crystal of Fig. 1(A) is a metal, that of Fig. 1(B) is an insulator. Argue that the distorted crystal can have a lower total electron energy than the undistorted crystal, and is thus more energetically favorable. Such distortion has been observed.

**Problem 4 (0 pt) — This is an extra challenge, and will not be graded.**

In the crystal lattice of Problem 1, derive  $\epsilon(k)$  of Eq. (3) and  $|\psi_k\rangle$  of Eq. (2) without resorting to the ansatz-based approach of Lecture #5, but by directly solving the energy eigen problem with the  $N \times N$  tight-binding Hamiltonian matrix  $H$  (as we did with the  $3 \times 3$  tight-binding Hamiltonian matrix in Homework #1 and with the  $2 \times 2$  tight-binding Hamiltonian matrix in Lecture #1).

<sup>2</sup>Do you understand why we use  $e^{iknd}$  instead of  $e^{ikna}$ ?