Condensed Matter Physics

Assignment III

Due: February 5, 2021

1. **Tight-Binding Orbitals**

In the tight binding model we assume that there is a single orbital on atom n which we call $|n\rangle$. Consider these orbitals to be the (1d analogues) of the ground state wavefunction of the hydrogen atom given by

$$|n\rangle = \frac{1}{\sqrt{a_0}} e^{-|x-x_n|/a_0}, \tag{1}$$

where x_n represents the mean position of the n^{th} orbital.

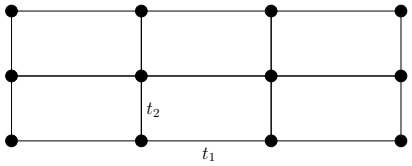
(a) Compute the overlap integral s for electrons on adjacent sites. For what lattice spacing a is the assumption of orthogonality of adjacent orbitals valid? (Use $a_0 = 5.292 \times 10^{-11}$ m).

(b) Plot the effect of systematically increasing the lattice spacing on the dispersion relations.

(25 Marks)

2. **Tight Binding Model in 2d**

Consider an $L \times L$ rectangular lattice in two dimensions as shown in the figure.



Now imagine a tight binding model where there is one orbital at each lattice site, and where the hopping matrix element is $\langle n|H|m\rangle = t_1$ if sites n and m are neighbors in the horizontal direction and is $= t_2$ if n and m are neighbors in the vertical direction. Consider periodic boundary conditions in both directions.

(a) Calculate the dispersion relation for this tight binding model.

(b) What does the dispersion relation look like near the bottom of the band?

(25 Marks)

3. **Cohesive Energy for a Square Well Potential**

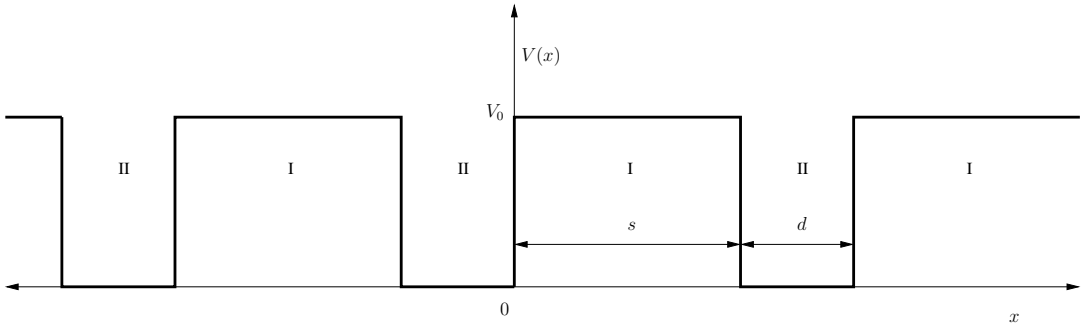
(a) Find an expression for the binding energy of an electron in one dimension in a single square well of depth U_0 and width a. (This is the standard first problem in elementary quantum mechanics.) Assume that the solution is symmetric about the midpoint of the well.

(b) Find a numerical result for the binding energy in terms of U_0 for the special case $|U_0| = 2\hbar^2/ma^2$.

(25 Marks)

4. **Kronig-Penney Model**

Consider a one-dimensional periodic potential $V(x)$ as shown in the figure below. An electron moves in this one-dimensional crystal of length L. The regions denoted II correspond to the positively charged ions of the crystal lattice. The regions denoted I represent the empty spaces between the ions. The lattice parameter is $a = d + s$.



(a) Set up the single-electron Schrödinger equation for this system (in the two regions).

(b) What are the eigenfunctions of this Hamiltonian. Determine the relevant constants using the boundary conditions and the normalization.

(c) What are the conditions for a solution to exist? Plot the energy levels for this system.

(25 Marks)