ECE 4070/MSE 5470
Physics of Semiconductors and Nanostructures
Exam 2, April 14, 2015

Debdeep Jena (djena@cornell.edu), Depts. of ECE and MSE, Cornell University

Instructions:

- There are **THREE** problems in this exam
- Every problem must be done in the blue booklet
- Only work done on the blue exam booklets will be graded. Do not attach your own sheets to the exam booklets under any circumstances
- To get partial credit you must show all the relevant work
- Correct answers with wrong reasoning will not get points
- All questions do not carry equal points
- All questions do not have the same level of difficulty, use your time judiciously

DO NOT WRITE IN THIS SPACE

1 Bandstructure of a 2D Semiconductor [40 points]

As shown in Figure 1, in the **k**-space of a 2D square lattice (lattice constant: a), denote the points Γ : (k_x, k_y)=(0,0), X : $(\pi/a, 0)$, and W : $(\pi/a, \pi/a)$. The nearly free electron bandstructure assumes no crystal potential, but a lattice.

(a) Draw the nearly free-electron bandstructure from the BZ center in the $\Gamma - W$ direction slightly beyond the BZ edge. Identify the magnitude of k at the BZ edge, and express the energy in terms of $F = \hbar^2\pi^2/ma^2$. Include reciprocal lattice vectors smaller than $2\times 2\pi/a$.

(b) Label each band with the reciprocal lattice vector it is associated with. Clearly point out the *degeneracies* of each band.

Consider now that the basis atoms produce a 2-D potential

$$V(x, y) = -4V_0 \cos(\frac{2\pi x}{a}) \cos(\frac{2\pi y}{a}). \tag{1}$$

(c) Find the bandgap at the W point due to this potential. Be judicious in choosing the basis set.

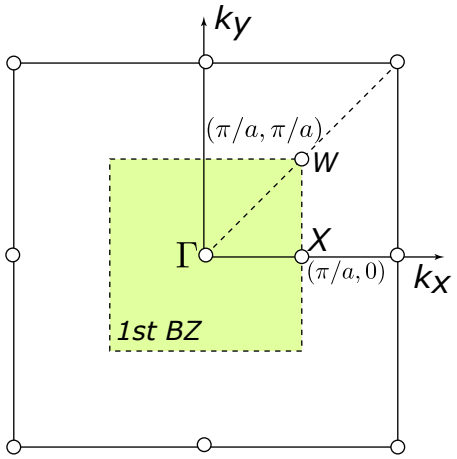

Figure 1: 2D reciprocal lattice.

(d) The lowest energy at the Γ : $(k_x, k_y) = (0, 0)$ point *before* the potential was turned on was $E_\Gamma(0, 0) = 0$ eV. Give an estimate of the change in this energy eigenvalue due to the periodic potential.

2 2-Dimensional Boron Nitride [40 points]

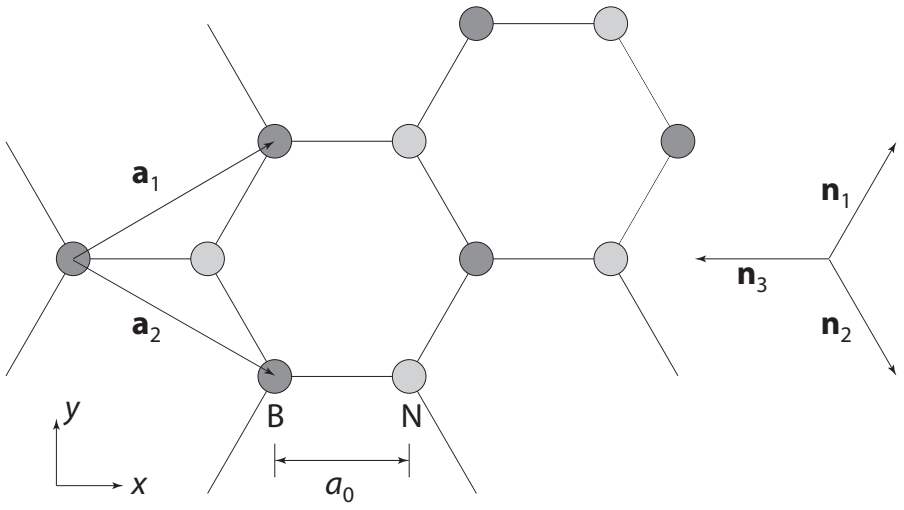

Figure 2: The Boron Nitride 2D crystal.

You have extensively solved the bandstructure details of graphene in class. In this problem, we look at a closely related material, where we replace the two carbon-atom basis of graphene with Boron and Nitrogen - to form a monolayer 2D crystal hexagonal Boron Nitride. Figure 2 shows the crystal, the primitive lattice vectors $\mathbf{a_1}, \mathbf{a_2}$, the distance between the B and N atoms is a_0, and three related vectors $\mathbf{n_1}, \mathbf{n_2}, \mathbf{n_3}$ are shown to assist you in this problem.

(a) Write $\mathbf{a_1}, \mathbf{a_2}$ in terms of a_0, and $\mathbf{n_1}, \mathbf{n_2}, \mathbf{n_3}$ also in terms of a_0. Find the reciprocal lattice vectors, and sketch the 1st Brillouin Zone.

(b) *Qualitatively* outline a process to find the tight-binding bandstructure of BN.

(c) Of most interest for electronic and photonic properties are the bands formed by the *out-of-plane* p_z orbitals attached to each atom in the crystal. Sketch the orbitals and put signs on the lobes.

(d) In graphene, these orbitals had same energies because all atoms were carbon. Let E_B be the energy of the p_z orbitals on the B sites, and E_N the energy of the p_z orbitals on the N sites. Let $V_{pp\pi}$ be the relevant overlap integral. Write down the tight-binding Hamiltonian for the bands formed by these p_z orbitals.

(e) Find the energy bandgaps at the $\Gamma-$ point ($k_x = 0, k_y = 0$), and at the *vertices* of the 1st BZ edge you sketched in part (a) of this problem.

3 Defect States in the Kronig-Penney Model [20 points]

We have discussed about the Kronig-Penney crystal model, and how defect states cause energy eigenvalues to split off from band-edges. For simplicity, we are going to solve this problem for $k = 0$ (the Γ point), and neglect all other $k-$points. Let us say that a perfect Kronig-Penney crystal of lattice constant a has N eigenvalues E_i with $i = 1...N$ in a band at Γ. All other energy bands are very far in energy, and may be neglected. We have shown in class that if at one of the lattice sites, a defect changes the delta function strength by U_0, then the new *exact* eigenvalues are given by solving

$$\frac{a}{U_0} = \text{Trace}[G(E)] = \sum_{i=1}^{N} \frac{1}{E - E_i}, \tag{2}$$

for allowed energies E, where U_0 is in eV-nm units, $G(E)$ is the Green's function, the Trace of which is just the inverse sum on the right.

(a) Argue why the equation above is correct if no defect is present.

(b) Show *graphically* that if the eigenvalues themselves are widely separated, and $U_0 >> 0$, the eigenvalue that splits off the band due to the defect has energy $E_s^+ \approx E_N + \frac{U_0}{a}$.

(c) Using your graph of part (b), show that if $U_0 << 0$, the eigenvalue that splits off the band due to the defect has energy $E_s^- \approx E_1 + \frac{U_0}{a}$.