

EECE 480

Assignment 1

Due date: September 27; hand-in at the beginning of the class.

Objective: To gain familiarity with the concepts of primitive unit cells, energy bands, energy bandgaps, and holes.

1. Consider Fig. 2.2. Remove the middle row of atoms so that the resulting structure is no longer face-centred rectangular, but is simply rectangular. Construct the primitive unit cell for the new lattice. What is the basis?
2. Search beyond the text book for a drawing of the primitive unit cell for a real-space, 3-D, face-centred, cubic lattice. State your source of reference.
Sketch how these primitive unit cells nest together to fill up all of real space (the Bravais Lattice).
3. A new 1-D material, A , has N primitive cells/unit length, 1 atom/primitive cell, and 1 valence electron/atom.
Another new 1-D material, B , has $N/2$ primitive cells/unit length, 2 atoms/primitive cell, and 1 valence electron/atom.
Which of these two materials is a semiconductor?
4. Write a short program (a $.m$ MATLAB file, for example) to plot your own version of Figure 2.4 from Eqn. (2.17), *i.e.*, the equation bounded by a thick red box on slide 6 of Lecture 2. For your numerical answer use $[m_0\beta a/\hbar^2] = 6$, rather than the value of 10 used in the text.
Plot the figure.
5. Imagine that your plot from the previous question applies to a material with a lattice constant of 0.75 nm, and a primitive unit cell that has a basis of 4 atoms, each of which has 2 valence electrons.
Estimate the bandgap of this material.
6. My MATLAB file for generating the data points in Fig. 2.11 is given below.
Run the file and plot the results, with the axes properly labeled.
Imagine, that this plot applies to the material of Question 5.
Show a parabolic fit to near the top of the valence band, and give your estimate (in units of m_0) of the parabolic-band effective mass for holes.
7. The hole-energy E - k relationships for the valence bands of two semiconductor materials, A and B , each with spherical constant-energy surfaces, can be expressed as
$$E_A - 0.7 = \alpha k^2 \quad \text{and} \quad E_B - 1.4 = 2\alpha k^2,$$
respectively, where α is a constant and the energies are in units of eV.
For both materials, the electron-energy E - k relationship for the conduction band is given by
$$E - 0.7 = 2\alpha(k - k')^2,$$
where $k' > 0$, α is a constant, as before, and the energies are in units of eV.
Which material has the higher bandgap?
Which material has the higher hole effective mass?
8. Fig. 2.10b shows the valence band of a semiconductor with one unoccupied state below the top of the band.
If a positive electric field \mathcal{E}_x is now applied, will the empty state move first to a position of higher hole energy or lower hole energy?

Advice:

Make sure that all numerical answers are accompanied by their units.

Matlab code for Fig. 2.11:

```
% bandplot for delta-function results
%uses fbands to get ga for a particular ka
%24APR06
%ka=ka/pi and ga=ga/pi
ka=[0 0.2 0.4 0.6 0.8 1.0];
ga1=[0.8364 0.8500 0.8871 0.9367 0.9814 1.0000];
ga2=[2.0000 1.9637 1.8804 1.7887 1.7171 1.6984];
ga3=[2.5678 2.6099 2.7112 2.8343 2.9475 3.0000];
ga4=[4.0000 3.9331 3.7981 3.6533 3.5285 3.4723];
ga5=[4.3988 4.4681 4.6105 4.7701 4.9205 5.0000];
plot(ka,ga1.^2,'o',-ka,ga1.^2,'o', ka,ga2.^2,'o',-ka,ga2.^2,'o', ...
     ka,ga3.^2,'o',-ka,ga3.^2,'o', ka,ga4.^2,'o',-ka,ga4.^2,'o', ...
     ka,ga5.^2,'o',-ka,ga5.^2,'o')

hold on;
%fitting parabola to valence band

Evb= ..... (fill in your expression);
plot(ka,Evb, -ka,Evb)
```

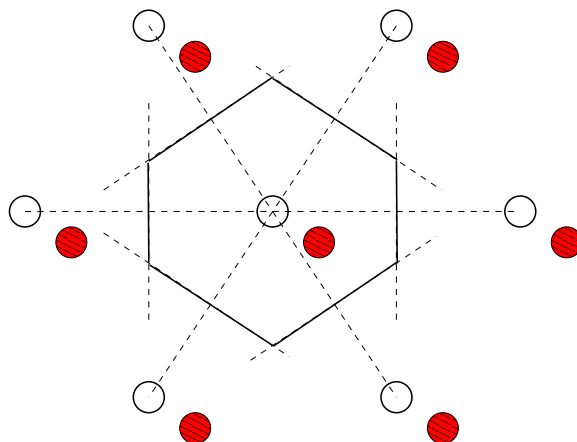


Figure 1: (Fig. 2.2 of text book) Example of a 2-D crystal comprising simple face-centred rectangular arrays of unshaded and shaded atoms. The Wigner-Seitz primitive unit cell is shown by the solid lines. These lines connect the perpendicular bisectors of the lines joining one unshaded atom to each neighbouring unshaded atom. One atom from the shaded array falls within the primitive unit cell; thus, this crystal structure has a basis of two atoms.

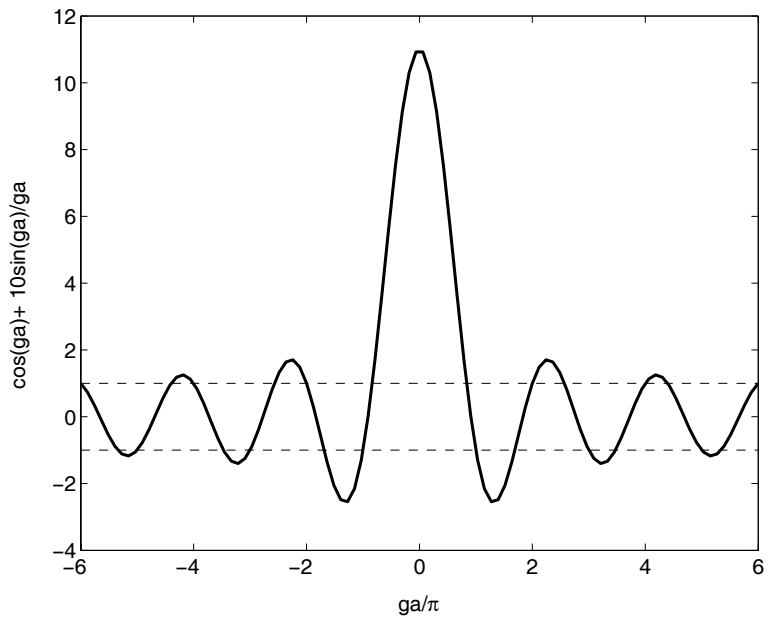


Figure 2: (Fig. 2.4 of text book) Plot of Eqn. 2.17 for $\left[\frac{m_0\beta a}{\hbar^2}\right] = 10$, showing the allowed values of ga , *i.e.*, those within the dashed lines. The forbidden values of ga lie in the areas outside the dashed lines.

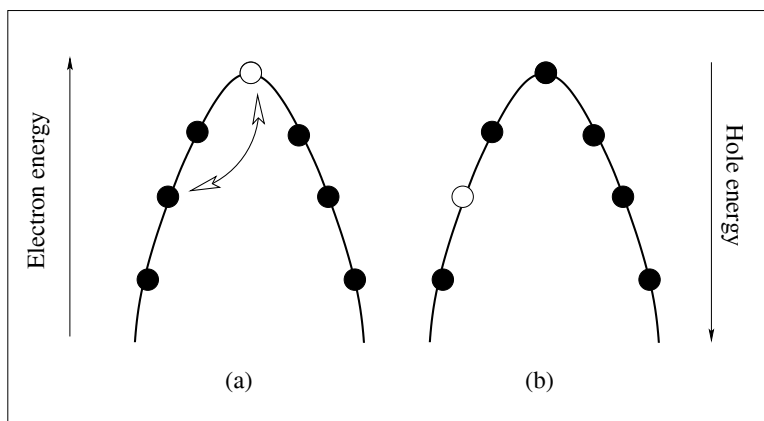


Figure 3: (Fig. 2.10 of text book) Hole energy. (a) Excitation of an electron to a higher energy state in the valence band. (b) After the excitation, the hole can be viewed as having gained energy, *i.e.*, the hole energy increases downwards.

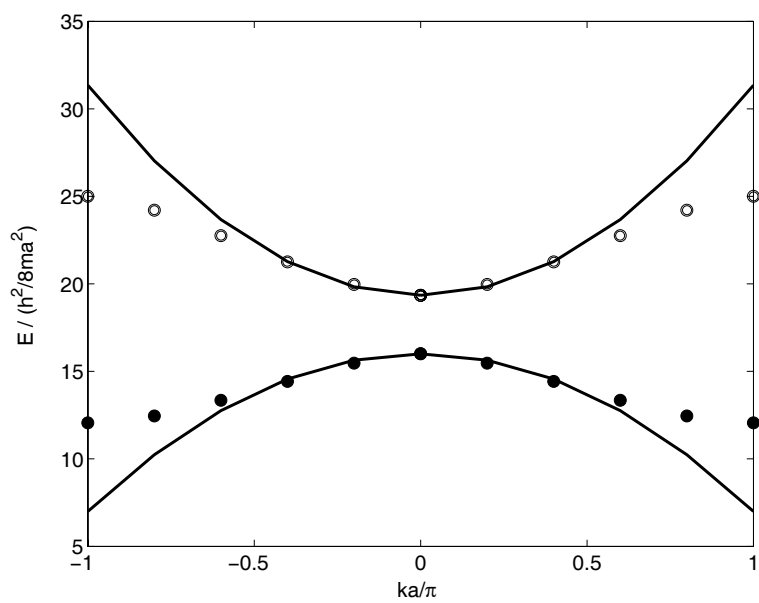


Figure 4: (Fig. 2.11 of text book) Fitting of parabolae to the 4th and 5th bands of Fig. 2.6.