Departments of ECE and MSE, Cornell University

ECE 4070/MSE 5470: Physics of Semiconductor and Nanostructures

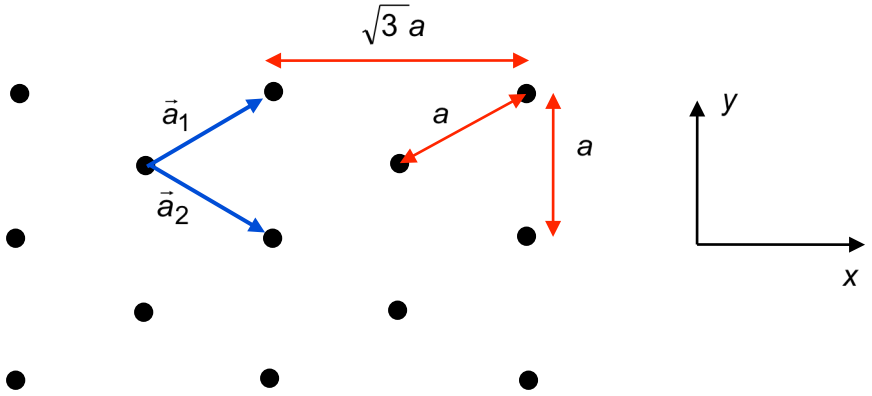
Spring 2015

Homework 4 **Due on March 9, 2015 at 5:00 PM**

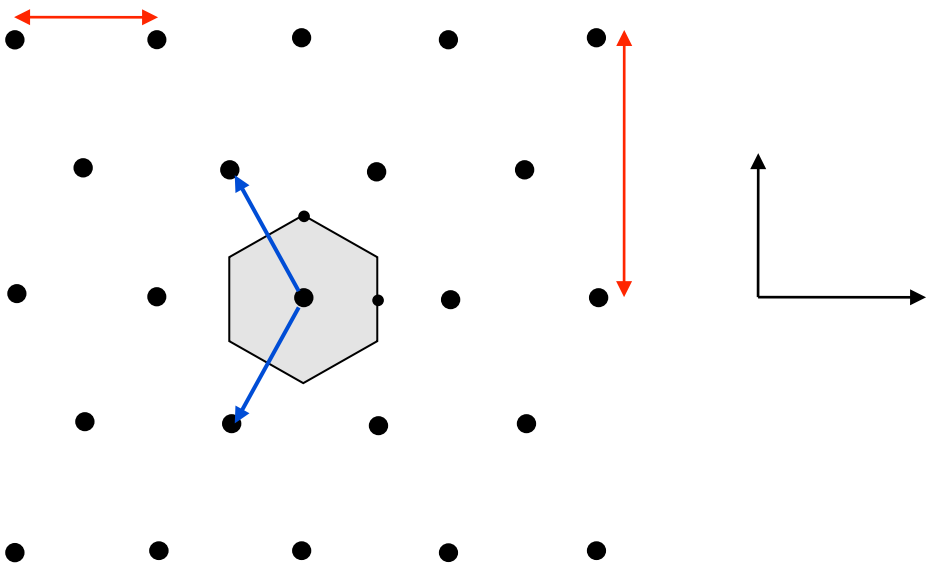
Suggested Readings:
a) Lecture notes
b) Chapter 2 in Kittel (Introduction to Solid State Physics)
c) **Start early** – the last problem involves MATLAB computations

Problem 4.1 (Brillouin zones and energy bands for a hexagonal lattice in 2D)

Consider the following 2D hexagonal lattice from the previous problem along with the primitive lattice vectors:



The corresponding reciprocal lattice with the first BZ is shown below (from Homework 3):

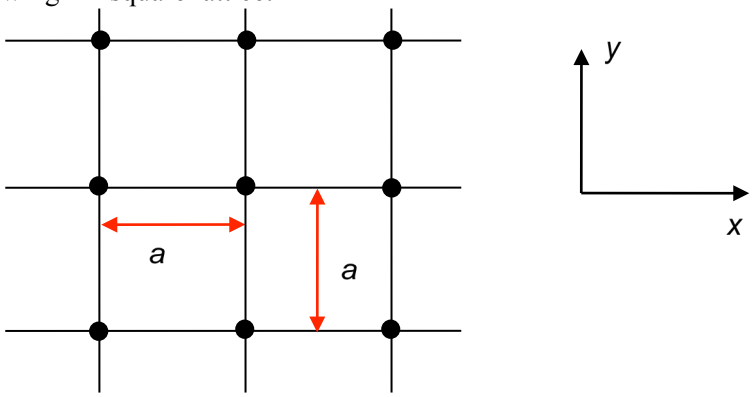


a) Draw the first 3 free-electron energy bands in the first BZ from the Γ-point (0,0) to the M-point ($2\pi/\sqrt{3}a$,0) in k-space, indicate the degeneracy of each band, and indicate on your diagram where bandgaps could open up. In drawing your bands you should use a scientific plotting program like matlab or mathematica (no hand drawings acceptable) and choose energy units such that $\hbar^2/2ma^2 = 1$ for simplicity.

b) Draw the first 3 free-electron energy bands in the first BZ from the Γ-point (0,0) to the K-point (0, $4\pi/3\,a$) in k-space, indicate the degeneracy of each band, and indicate on your diagram where bandgaps could open up. In drawing your bands you should use a scientific plotting program like matlab or mathematica (no hand drawings acceptable) and choose energy units such that $\hbar^2/2ma^2 = 1$ for simplicity.

Problem 4.2 (2D square lattice energy bands and wavefunctions)

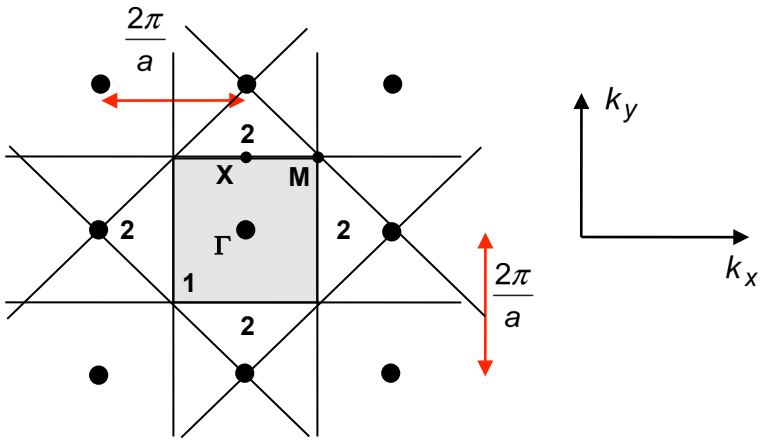
Consider the following 2D square lattice:



Suppose the periodic atomic potential that the electron feels can be written as:

$$V(\vec{r}) = V_o + V_1\cos\left(\frac{2\pi}{a}x\right) + V_2\cos\left(\frac{2\pi}{a}y\right) + V_3\cos\left(\frac{2\pi}{a}x + \frac{2\pi}{a}y\right) + V_3\cos\left(\frac{2\pi}{a}x - \frac{2\pi}{a}y\right)$$
$$+ V_5\cos\left(\frac{4\pi}{a}x\right) + V_6\cos\left(\frac{4\pi}{a}y\right) + V_7\cos\left(\frac{4\pi}{a}x + \frac{4\pi}{a}y\right) + V_8\cos\left(\frac{4\pi}{a}x - \frac{4\pi}{a}y\right)$$

The first and second BZ in the reciprocal lattice, along with a few Bragg lines, are shown below:



There is one Γ-point, four equivalent X-points, and four equivalent M-points in the first BZ, as shown above. In this problem you are to treat the weak periodic potential as a perturbation on the free electron states.

a) In the lecture notes, the first 5 free electron bands from the Γ-point (0,0) to the X-point $(0, \pi/a)$ are drawn and two are degenerate. Draw the first 4 free electron bands from the Γ-point (0,0) to the M-point ($\pi/a, \pi/a$) in the first BZ and indicate the degeneracy of each band. Hint: two bands should be degenerate. In drawing your bands you should use a scientific plotting program like matlab or mathematica (no hand drawings acceptable) and choose energy units such that $\hbar^2/2m\,a^2 = 1$ for simplicity.

b) As a result of the periodic potential, the free electron state with k-vector equal to (π/a,0), which is one of the X-points in the first BZ, is coupled very strongly to one other free electron state. What is the k-vector of this other free electron state?

c) As a result of the periodic potential, the free electron state with k-vector equal to $(0, \pi/a)$, which is also one of the X-points, is coupled very strongly to one other free electron state. What is the k-vector of this other free electron state?

d) As a result of the periodic potential, the free electron state with k-vector equal to ($\pi/a, \pi/a$), which is one of the M-points in the first BZ, is coupled very strongly to three other degenerate free electron states. What are the k-vectors of these other free electron states? Note that the M-point is located at the intersection of 3 different Bragg planes and therefore the free electron state here becomes strongly coupled to 3 other free electron states.

e) Write the variational solution for the actual electron wavefunction at the X-point (π/a,0) as a superposition of two degenerate free electron states, obtain a 2x2 matrix energy eigenvalue equation, and then solve it to obtain:

i) the energies of the 2 energy bands at the X-point (π/a,0) and,
ii) the actual wavefunctions of the electron at the X-point (π/a,0) corresponding to the 2 energy bands

f) Write the solution for the actual electron wavefunction at the X-point $(0, \pi/a)$ as a superposition of two degenerate free electron states, obtain a 2x2 matrix energy eigenvalue equation, and then solve it to obtain:

i) the energies of 2 energy bands at the X-point $(0, \pi/a)$ and,

ii) the actual wavefunctions of the electron at the X-point $(0, \pi/a)$ corresponding to the 2 energy bands

g) Write the solution for the actual electron wavefunction at the M-point $(\pi/a, \pi/a)$ as a superposition of four degenerate free electron states, obtain a 4x4 matrix energy eigenvalue equation, and then solve it to obtain:

i) the energies of 4 energy bands at the M-point $(\pi/a, \pi/a)$ and,

ii) the actual wavefunctions of the electron at the M-point $(\pi/a, \pi/a)$ corresponding to the 4 energy bands

A software program, such as matlab or mathematica, will be useful here. However, the 4 energy values can even be obtained analytically.

h) If you did parts (a) and (g) correctly, you should see that the four bands that were all degenerate in part (a) at the M-point are no longer degenerate. Has the degeneracy been completely or partially lifted?

Problem 4.3 (Exact numerical solution for a 1D lattice)

Consider a 1D lattice of lattice constant a equal to 5 Angstroms. In this problem you will find an almost exact numerical solution to the problem of an electron in a periodic 1D lattice and compare this solution with approximate analytical methods discussed in the lecture. Matlab or Mathematica will be needed.

Suppose the lattice potential can be written as:

$$V(x) = 2\,V_1 \cos\left(\frac{2\pi}{a}x\right)$$

where V_1 equals 0.2 eV.

The exact solution for any wavevector k in the FBZ can be written as a superposition of plane waves in the form:

$$|\psi_k\rangle = \sum_{m=-\infty}^{\infty} c_k(G_m)\,|\phi_{k+G_m}\rangle = \sum_{m=-\infty}^{\infty} c_k(G_m)\sqrt{\frac{1}{L}}\,e^{i(k+G_m)x}$$

Where:

$$G_m = m\frac{2\pi}{a}$$

A good approximation to the exact can be obtained by terminating the series above at both ends, as follows:

$$|\psi_k\rangle = \sum_{m=-N}^{N} c_k(G_m)\,|\phi_{k+G_m}\rangle$$

Where N is some large number, say 10. Now the solution looks more like a variational solution.

a) Plug the assumed form of the solution in the Schrodinger equation and show that the resulting matrix equation looks like as shown below.

$$\begin{bmatrix} \ddots & & & & & & & \\ & e(k+G_{-2}) & V_1 & & & & & \\ & V_1 & e(k+G_{-1}) & V_1 & & & & \\ & & V_1 & e(k) & V_1 & & & \\ & & & V_1 & e(k+G_1) & V_1 & & \\ & & & & V_1 & e(k+G_2) & & \\ & & & & & & \ddots & \end{bmatrix} \begin{bmatrix} \vdots \\ c(G_{-2}) \\ c(G_{-1}) \\ c(0) \\ c(G_{-1}) \\ c(G_{-2}) \\ \vdots \end{bmatrix}$$

$$= E(k) \begin{bmatrix} \vdots \\ c(G_{-2}) \\ c(G_{-1}) \\ c(0) \\ c(G_{-1}) \\ c(G_{-2}) \\ \vdots \end{bmatrix}$$

The advantage of this approach is that now one can solve the matrix eigenvectors and eigenvalues numerically, and in the limit N becomes large the solution obtained is pretty much the exact solution. For numerical solution, you will need to use software like Matlab or Mathematica.

b) Assume N=10. For each value of k in the FBZ from $-\pi/a$ to π/a, numerically solve for the smallest three eigenvalues of the matrix above. This will give you the energies, $E_1(k)$, $E_2(k)$, and $E_3(k)$ of the lowest three bands. Plot these energies vs the k-vector from $-\pi/a$ to π/a.

NOTE: In Matlab the routine to use is "eigs", and "[V,D]=eigs(A,3,'SM')" will give the smallest three eigenvalues of the matrix A as diagonal components of the matrix D and the corresponding eigenvectors will be the column vectors of the matrix V.

c) See if bandgaps open up anywhere in the plots you generated in part (a). What is the magnitude (in eV) of these bandgaps? How does the values of the bandgaps compare to the approximate theoretical values of the bandgaps?

d) Assume N=10 and assume $k = \pi/2a$ (a specific value in the middle of the FBZ) and numerically solve for the smallest three eigenvalues of the matrix above. The matrix "V" contains the corresponding eigenvectors arranged in each of its columns. Take the first eigenvector and plot the square magnitude of its components. The matlab command "stem" should prove useful here in plotting. Specifically,
"stem([-N:1:N],abs(V(:,1)).^2)"
should do the job. Remember the eigenvector gives the expansion coefficients of the plane waves that make up your solution,

$$|\psi_k\rangle = \sum_{m=-\infty}^{\infty} c_k(G_m) |\phi_{k+G_m}\rangle = \sum_{m=-\infty}^{\infty} c_k(G_m) \sqrt{\frac{1}{L}}\, e^{i(k+G_m)x}$$

You will note that the component with the largest value will be $c_k(G_m = 0)$ which means that the original plane wave of the free-electron is hardly modified by the periodic potential.

e) Assume N=10 and assume $k = \pi/a$ (right at the Bragg point) and numerically solve for the smallest three eigenvalues of the matrix above. Take the first eigenvector and plot the square magnitude of its components. You will note that there will be two components with the largest values which means that your solution is essentially made up of two plane waves. Explain how/why your results agree or do not agree with your expectations.

Now assume that the potential has an extra term:

$$V(x) = 2V_1 \cos\left(\frac{2\pi}{a}x\right) + 2V_2 \cos\left(\frac{4\pi}{a}x\right)$$

Where V_2 equals 0.4 eV.

f) Plug the assumed form of the solution in the Schrodinger equation and show the resulting matrix equation in the form given above for part (a).

g) Assume N=10. For each value of k in the FBZ from $-\pi/a$ to π/a, numerically solve for the smallest three eigenvalues of the matrix above. This will give you the energies, $E_1(k)$, $E_2(k)$, and $E_3(k)$ of the lowest three bands. Plot these energies vs the k-vector from $-\pi/a$ to π/a.

h) See if bandgaps open up anywhere in the plots you generated in part (d). What is the magnitude (in eV) of these bandgaps? How does the values of the bandgaps compare to the approximate theoretical values of the bandgaps?

i) Now for something interesting. We make the periodic potential ten times stronger so that simple first order perturbation theory would not work anymore. Suppose the lattice potential can be written as:

$$V(x) = 2\,V_1 \cos\left(\frac{2\pi}{a}x\right)$$

where V_1 equals 2.0 eV.

Assume N=10. For each value of k in the FBZ from $-\pi/a$ to π/a, numerically solve for the smallest three eigenvalues of the matrix above. This will give you the energies, $E_1(k)$, $E_2(k)$, and $E_3(k)$ of the lowest three bands. Plot these energies vs the k-vector from $-\pi/a$ to π/a.

You will note that bandgaps will open up at the second Bragg point, at $k = 2\pi/a$ in the unfolded zone scheme, or equivalently at $k = 0$ in the folded zone scheme, even though the potential has no Fourier component at $G_{\pm 2}$ (i.e. $V(G_{\pm 2}) = 0$. This happens because now the potential is strong enough so that multiple scattering events can occur in which an electron initially with wavevector $k = 2\pi/a$ gets scattered to $k = -2\pi/a$ via scattering twice in succession from the periodic potential and each scattering adds a reciprocal lattice vector G_{-1} to the electron wavevector. This multiple scattering is captured in second order and higher order perturbation theory which we will not cover in this course. But your almost exact numerical variational solution here does capture it.