PHYS*4150: Problem Set 4

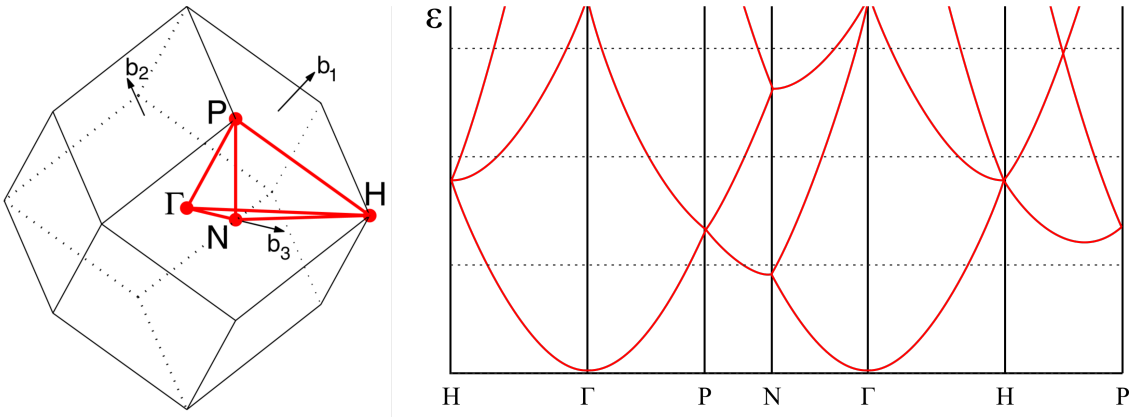
Distributed: Monday March 4, 2019
Due: Friday March 15, 2019 at 10:30am

Problem 1 (10 pts): Density of States

Ashcroft & Mermin question 8.2 parts a) and b). You can do c) for practice, but no need to hand it in.

Problem 2 (10 pts): Nearly free electron

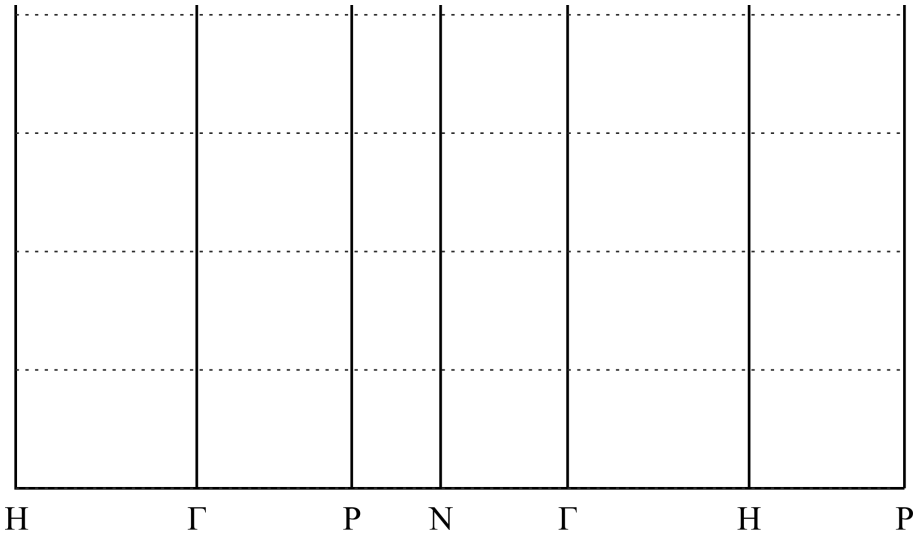
The 1st Brillouin Zone of a BCC lattice is shown below (Note: the *direct* lattice is BCC). To the right, the band structure is plotted between high symmetry points under the empty lattice approximation.



The introduction of a periodic potential causes a modification to the band structure of the solid. If the potential is weak, the modification is small, but qualitatively significant. This is called the *nearly free electron* model.

In the context of the nearly free electron model, explain the nature of the changes to the band structure of the BCC lattice above. Discuss the regions both near and far from degenerate bands and/or the Brillouin Zone boundary. This discussion should be qualitative for the most part.

On the empty plot below, sketch your estimate of the BCC band structure in the nearly free electron model. This should be qualitative only - don't be concerned with specific values of band-gap energies. Note: you will not be judged on the absolute accuracy of your diagram. Rather, do your best to apply the qualitative principles of the nearly free electron model to the BCC band structure.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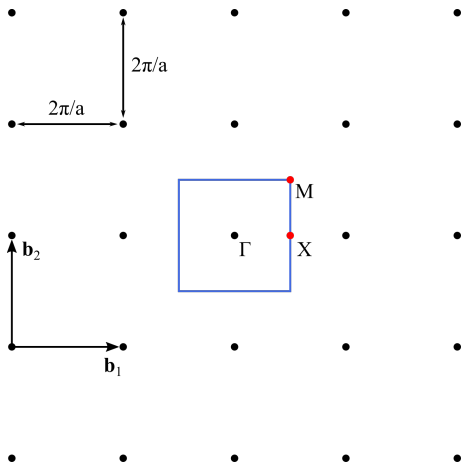
Problem 3 (30 pts): 2D Empty Lattice Approximation

Consider the simple square reciprocal lattice shown below (Note: the corresponding *direct* lattice is a simple square with side length a).



The first Brillouin Zone is drawn in blue and the high symmetry points Γ, X, and M are labelled. These points can be written as the vectors:

$$\Gamma = (0, 0) \tag{1a}$$
$$\mathrm{X} = (1/2, 0) \tag{1b}$$
$$\mathrm{M} = (1/2, 1/2) \tag{1c}$$

Note: in this notation, the reciprocal lattice vectors are expressed as $\mathbf{b_1} = (1, 0)$ and $\mathbf{b_2} = (0, 1)$. In this problem you will draw the band structure for this 2D lattice along the path $\Gamma \to \mathrm{X} \to \mathrm{M} \to \Gamma$ under the Empty Lattice Approximation.

The energy of a free electron in a crystal lattice is given by

$$\varepsilon_n(\mathbf{k}) = \frac{\hbar^2}{2m}(\mathbf{k} - \mathbf{G}_n)^2 \tag{2}$$

where $\mathbf{G}_n$ is a reciprocal lattice vector and characterizes a specific *band*. Equation 2 is referred to as a *dispersion relation* and it relates the energy of a band to the wave vector $\mathbf{k}$. Notationally, the band index n represents a set of integers, h and k, defining the reciprocal lattice vector $\mathbf{G}_{hk}$:

$$\mathbf{G}_n = \mathbf{G}_{hk} = h\mathbf{b_1} + k\mathbf{b_2} = (h, k). \tag{3}$$

For every $\mathbf{G}_{hk}$ in the reciprocal lattice there is a corresponding dispersion relation (Eq. 2).

Plot the band structure (i.e. dispersion relations) of this lattice on the diagram below along the direction $\Gamma \to \mathrm{X} \to \mathrm{M} \to \Gamma$. Label each band as (hk). Explicitly show the dispersion relation for each band along each Brillouin Zone direction. To get you started, the lowest band along each direction has been plotted and labelled. It is useful to parameterize $\mathbf{k}$ along the specific direction you are considering:

$$\Gamma \to \mathrm{X}: \quad \mathbf{k} = (u, 0) \tag{4a}$$
$$\mathrm{X} \to \mathrm{M}: \quad \mathbf{k} = (1/2, u) \qquad 0 < u < \frac{1}{2} \tag{4b}$$
$$\Gamma \to \mathrm{M}: \quad \mathbf{k} = (u, u) \tag{4c}$$

You can confirm this by check that the correct vector $\mathbf{k}$ is reproduced at the points Γ, X, and M. Follow the example below to familiarize yourself with the procedure of calculating the band structure. Repeat this procedure for each of the Brillouin Zone directions Γ → X, X → M, and M → Γ. Plot enough bands to fill the diagram, i.e. up to band energies around $4 - 5\epsilon_0$. Note that some bands may be degenerate along certain paths (see bands (00) and (01) along path X→M on the diagram) - label them appropriately.

Example: Γ → X, $\mathbf{G}_{00}$ band. Along the path Γ → X, $\mathbf{k}$ takes the form $\mathbf{k} = u(1, 0)$ where $0 < u < 1/2$. This can be confirmed by noting that $\mathbf{k}(\Gamma) = (0, 0)$ and $\mathbf{k}(\mathrm{X}) = (1/2, 0)$. The general dispersion relation along this direction is then:

$$\varepsilon_{hk}(\mathbf{k}) = \frac{\hbar^2}{2m}|(u - h, -k)|^2 \tag{5}$$

Now, let us examine the $\mathbf{G}_{00} = (0, 0)$ band. It follows that:

$$\varepsilon_{00} = \frac{\hbar^2}{2m}|(u, 0)|^2 \tag{6}$$

For the square lattice $|\mathbf{b_1}|^2 = |\mathbf{b_2}|^2 = (2\pi/a)^2$, and $\mathbf{b_i} \cdot \mathbf{b_j} = \delta_{ij}$, therefore the dispersion relation can be written as:

$$\varepsilon_{00} = \epsilon_0 u^2 \tag{7}$$

where the constants have been grouped together as follows:

$$\epsilon_0 \equiv \frac{2\pi^2\hbar^2}{ma^2}. \tag{8}$$

The dispersion relation ε_{00} is plotted in blue on the diagram below and is labelled as (00). Note that at point Γ (where $u = 0$), $\varepsilon_{00} = 0$; at point X (where $u = 1/2$), $\varepsilon_{00} = \frac{1}{4}\epsilon_0$.