P555

April 1, 2021 SHOW ALL YOUR WORK TO GET FULL CREDIT!

Problem 1: In Fig. 1 you can see the reciprocal lattice for an hexagonal Bravais lattice with primitive vectors $\mathbf{a}_1 = a(1,0)$ and $\mathbf{a}_2 = a(1/2, \sqrt{3}/2)$. The primitive vectors of the reciprocal lattice $\mathbf{b}_1 = 2\pi/a(1, -\sqrt{3}/3)$ and $\mathbf{b}_2 = 4\pi/a(0, \sqrt{3}/3)$ are indicated in the figure.

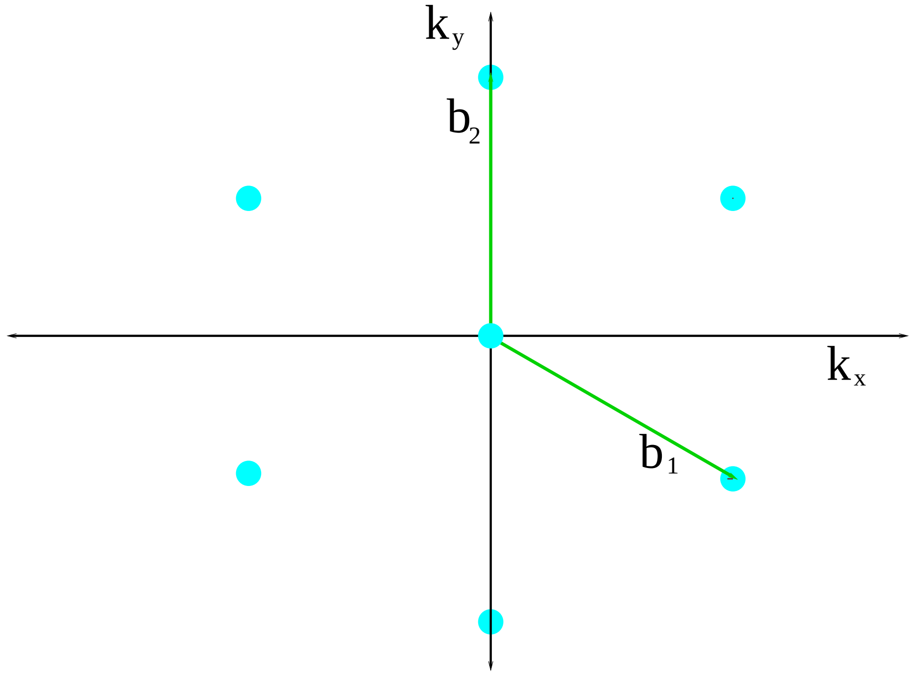

FIG. 1: The primitive vectors are indicated in green.

a) Draw the FBZ in Fig. 1 and label the vertices of the FBZ V_1, V_2,...,V_n with V_1 indicating the vertex along the positive k_x axis, V_2 the next vertex in a counterclockwise direction, etc. n is the number of vertices in the FBZ. (10 points)

b) In your graph V_1 labels a point with momentum $\mathbf{k}_{V_1} = (p, 0)$. Provide the value of p in terms of the lattice constant a.(5 points)

c) What is the energy $\epsilon^0_{V_1}$ of a free electron with momentum $\mathbf{k}_{V_1}$? (5 points)

d) Identify all the points in the FBZ in which a free electron will have the same energy as in point V_1 and provide the crystal momentum $\mathbf{k}$ for each of the points. (10 points)

e) Identify which of the points found in (d) have a momentum $\mathbf{k}_j$ satisfyng $\mathbf{k}_j - \mathbf{k}_{V_1} = \mathbf{K}_j$ where $\mathbf{K}_j$ is a vector of the reciprocal lattice and j is an index that labels the point that satisfy the condition. Provide the points and the vector $\mathbf{K}_j$ for each of the points in terms of the primitive vectors $\{\mathbf{b}_i\}$ given at the beginning of the problem. (10 points)

f) Now a periodic potential $U(\mathbf{r}) = \sum_{\mathbf{K}} U_{\mathbf{K}} e^{i\mathbf{K}.\mathbf{r}}$ is introduced. For $\mathbf{k} = \mathbf{k}_{V_1}$ to which components of the wave function $\Psi(\mathbf{q})$ will $\Psi(\mathbf{k}_{V_1})$ be strongly coupled? (5 points)

g) Write the Schrödinger's equation in the subspace involving only the components of Ψ named in part (f). (10 points)

h) Write the matrix whose determinant needs to be zero in order to find the possible energies that an electron in the periodic potential may have when its crystal momentum is $\mathbf{k}_{V_1}$. (10 points)

Bonus (to do at home): provide the energy values that result from solving the equation in part (h). Hint: assume that $U_{\mathbf{K}} = U$ for all the values of $\mathbf{K}$ that appear in your equation. (10 points)