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.

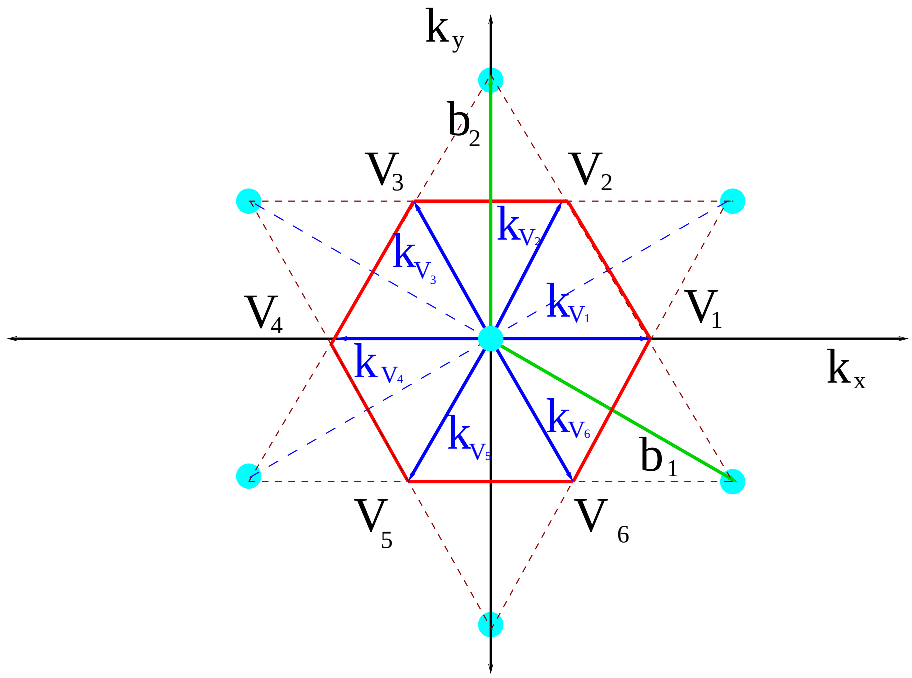


FIG. 1: The primitive vectors are indicated in green and the FBZ is indicated in red.

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)

See Fig. 1.

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)

We see that

$$p \cos 30^o = p\frac{\sqrt{3}}{2} = \frac{b_1}{2} = \frac{b_2}{2} = \frac{4\pi}{3a}\frac{\sqrt{3}}{2}, \tag{1}$$

then,

$$p = \frac{4\pi}{3a}. \tag{2}$$

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

We know that the energy of a free electron with momentum $\mathbf{k}$ is given by $\epsilon^0_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$, then a free electron with momentum $\mathbf{k}_{V_1} = (\frac{4\pi}{3a}, 0)$ has energy

$$\epsilon^0_{\mathbf{k}_{V_i}} = \frac{\hbar^2 k^2_{V_i}}{2m} = \frac{8\pi^2\hbar^2}{9ma^2}. \tag{3}$$

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)

We see that all 6 vertices of the FBZ are equidistant from the origin because the FBZ is an equilateral hexagon. This means that these 6 points have crystal momenta with the same magnitude as $V_1$, i.e. $k_{V_i} = \frac{4\pi}{3a}$ for $i = 1, 2, 3, 4, 5, 6$. The crystal momentum for each point is given by:

$$\mathbf{k}_{V_1} = \frac{4\pi}{3a}(1, 0), \tag{4}$$

$$\mathbf{k}_{V_2} = \frac{4\pi}{3a}(\frac{1}{2}, \frac{\sqrt{3}}{2}), \tag{5}$$

$$\mathbf{k}_{V_3} = \frac{4\pi}{3a}(-\frac{1}{2}, \frac{\sqrt{3}}{2}), \tag{6}$$

$$\mathbf{k}_{V_4} = \frac{4\pi}{3a}(-1, 0), \tag{7}$$

$$\mathbf{k}_{V_5} = \frac{4\pi}{3a}(-\frac{1}{2}, -\frac{\sqrt{3}}{2}), \tag{8}$$

$$\mathbf{k}_{V_6} = \frac{4\pi}{3a}(\frac{1}{2}, -\frac{\sqrt{3}}{2}). \tag{9}$$

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)

We need to evaluate $\mathbf{k}_j - \mathbf{k}_{V_1}$ for $j = V_2, V_3, V_4, V_5$ and $V_6$:

$$\mathbf{k}_{V_2} - \mathbf{k}_{V_1} = \frac{4\pi}{3a}(\frac{1}{2}, -\frac{\sqrt{3}}{2}) = \frac{1}{3}\mathbf{b}_1. \tag{10}$$

We see that the above is not a vector of the reciprocal lattice because it cannot be expressed in terms of the primitive vectors with integer coefficients. We also see that the magnitude of $\mathbf{k}_{V_2} - \mathbf{k}_{V_1}$ is smaller than the magnitude of the primitive vectors.

$$\mathbf{k}_{V_3} - \mathbf{k}_{V_1} = \frac{4\pi}{3a}(-\frac{3}{2}, \frac{\sqrt{3}}{2}) = -\mathbf{b}_1 = \mathbf{K}_3. \tag{11}$$

We see that $\mathbf{K}_3$ is a vector of the reciprocal lattice.

$$\mathbf{k}_{V_4} - \mathbf{k}_{V_1} = \frac{4\pi}{3a}(-2, 0) = -\frac{4}{3}\mathbf{b}_1 - \frac{2}{3}\mathbf{b}_2. \tag{12}$$

We see that the above is not a vector of the reciprocal lattice because it cannot be expressed in terms of the primitive vectors with integer coefficients.

$$\mathbf{k}_{V_5} - \mathbf{k}_{V_1} = \frac{4\pi}{3a}(-\frac{3}{2}, -\frac{\sqrt{3}}{2}) = -\mathbf{b}_1 - \mathbf{b}_2 = \mathbf{K}_5. \tag{13}$$

We see that $\mathbf{K}_5$ is a vector of the reciprocal lattice.

$$\mathbf{k}_{V_6} - \mathbf{k}_{V_1} = \frac{4\pi}{3a}(-\frac{1}{2}, -\frac{\sqrt{3}}{2}) = -\frac{1}{3}\mathbf{b}_1 - \frac{2}{3}\mathbf{b}_2. \tag{14}$$

We see that the above is not a vector of the reciprocal lattice because it cannot be expressed in terms of the primitive vectors with integer coefficients.

Thus, only $V_3$ and $V_5$ are connected to $V_1$ by a vector of the reciprocal lattice.

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)

From the results of part (e) we see that the components of the wave function with momentum $\mathbf{k}_{V_1}$ will be strongly connected with the components with momentum $\mathbf{k}_{V_3}$ and $\mathbf{k}_{V_5}$.

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

We have a system of three equations:

$$\frac{\hbar^2 k_{V_1}^2}{2m}\Psi(\mathbf{k}_{V_1}) + U_{\mathbf{k}_{V_1}-\mathbf{k}_{V_3}}\Psi(\mathbf{k}_{V_3}) + U_{\mathbf{k}_{V_1}-\mathbf{k}_{V_5}}\Psi(\mathbf{k}_{V_5}) = \epsilon\Psi(\mathbf{k}_{V_1}), \tag{15}$$

$$\frac{\hbar^2 k_{V_3}^2}{2m}\Psi(\mathbf{k}_{V_3}) + U_{\mathbf{k}_{V_3}-\mathbf{k}_{V_1}}\Psi(\mathbf{k}_{V_1}) + U_{\mathbf{k}_{V_3}-\mathbf{k}_{V_5}}\Psi(\mathbf{k}_{V_5}) = \epsilon\Psi(\mathbf{k}_{V_3}), \tag{16}$$

$$\frac{\hbar^2 k_{V_5}^2}{2m}\Psi(\mathbf{k}_{V_5}) + U_{\mathbf{k}_{V_5}-\mathbf{k}_{V_3}}\Psi(\mathbf{k}_{V_3}) + U_{\mathbf{k}_{V_5}-\mathbf{k}_{V_1}}\Psi(\mathbf{k}_{V_1}) = \epsilon\Psi(\mathbf{k}_{V_5}). \tag{17}$$

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)

$$\begin{vmatrix} \epsilon^0_{\mathbf{k}_{V_1}} - \epsilon & U_{-\mathbf{K}_3} & U_{-\mathbf{K}_5} \\ U_{\mathbf{K}_3} & \epsilon^0_{\mathbf{k}_{V_3}} - \epsilon & U_{-\mathbf{K}_{53}} \\ U_{\mathbf{K}_{53}} & U_{\mathbf{K}_5} & \epsilon^0_{\mathbf{k}_{V_5}} - \epsilon \end{vmatrix} = 0, \tag{18}$$

where

$$\mathbf{K}_{53} = \mathbf{k}_{V_5} - \mathbf{k}_{V_3} = \frac{4\pi}{3a}(0, -\sqrt{3}) = -\mathbf{b}_2. \tag{19}$$

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)

Let's rewrite the determinant using the hint, i.e., that all the values of $U_{\mathbf{K}} = U$ and the fact that $\epsilon^0_{\mathbf{k}_{V_1}} = \epsilon^0_{\mathbf{k}_{V_3}} = \epsilon^0_{\mathbf{k}_{V_5}} = \epsilon_0$. Then the matrix now becomes

$$\begin{vmatrix} \epsilon_0 - \epsilon & U & U \\ U & \epsilon_0 - \epsilon & U \\ U & U & \epsilon_0 - \epsilon \end{vmatrix} = 0. \tag{20}$$

The determinant in Eq. 20 leads to the cubic equation:

$$(\epsilon_0 - \epsilon)^3 + 2U^3 - 3(\epsilon_0 - \epsilon)U^2 = 0. \tag{21}$$

We see that $\epsilon_1 = \epsilon_0 + U$ is a root of the equation. Dividing the cubic polynomial by $\epsilon - \epsilon_1$ we obtain the quadratic equation

$$-\epsilon^2 + (2\epsilon_0 - U)\epsilon + (2U^2 - \epsilon_0^2 + \epsilon_0 U) = 0, \tag{22}$$

which has solutions $\epsilon_2 = \epsilon_0 + 2U$ and $\epsilon_3 = \epsilon_0 - U$. Thus, $\epsilon_1$, $\epsilon_2$, and $\epsilon_3$ are the possible values that an electron with momentum $\mathbf{k}_{V_1}$ in the periodic potential may have. The triple degeneracy is lifted and 3 separate energy bands develop.