Homework 2 Answer

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1 Problem 1

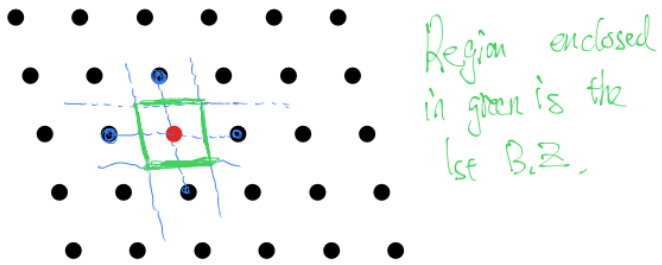

Figure 1: Area enclosed in green is the first BZ

2 Problem 2

From $S_{\mathbf{G}} \equiv \sum_{\text{atoms in unit cell}} f_j(\mathbf{G})\mathbf{e^{iG\cdot x_j}}$, and the question states that: $\mathbf{G} = \mathbf{0}\cdot\mathbf{b_1} + \mathbf{0}\cdot\mathbf{b_2} + \mathbf{l}\cdot\mathbf{b_3}$. Using $\mathbf{b_i}\cdot\mathbf{a_j} = \mathbf{2}\pi\delta_{\mathbf{ij}}$ We get

$$S_{00l} = f_{Ba}e^{i*0} + f_{Ti}e^{i*1/2*l*\mathbf{b_3}\cdot\mathbf{a_3}} + f_O(e^{i*0} + e^{i*1/2*0*\mathbf{b_1}\cdot\mathbf{a_1}+\mathbf{i}*\mathbf{1/2}*\mathbf{l}*\mathbf{b_3}\cdot\mathbf{a_3}} \tag{1}$$

$$+ e^{i*1/2*0*\mathbf{b_2}\cdot\mathbf{a_2}+\mathbf{i}*\mathbf{1/2}*\mathbf{l}*\mathbf{b_3}\cdot\mathbf{a_3}}) \tag{2}$$

$$= f_{Ba} + (e^{i\pi})^l f_{Ti} + [1 + 2(e^{i\pi})^l]f_O \tag{3}$$

$$= f_{Ba} + (-1)^l f_{Ti} + [1 + 2(-1)^l]f_O \quad \square \tag{4}$$