

Assignment 2.1

1. Show/Proof that $n(x)$ written as a Fourier series (equation 4) has a periodicity of a .
2. Show/Proof that the complex Fourier series given by equation (5) is only real if n_p is the complex conjugated of n_p .
3. Show/Proof that the values of the constants n_p can be calculated from $n(x)$ using equation (10).

Read the reciprocal lattice vector section on page 29 and 32 and then answer the following questions:

4. Explain why Kittel's definition of b_1 , b_2 , and b_3 , is the same as the following definition that is more common in literature:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_2 \cdot \vec{a}_3 \times \vec{a}_1}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_3 \cdot \vec{a}_1 \times \vec{a}_2}$$

5. Why would we call \mathbf{b}_1 , \mathbf{b}_2 , and \mathbf{b}_3 reciprocal lattice vectors? Explain reciprocal!
6. Show/prove that the 3D electron density function $n(\mathbf{r})$ is periodic in \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 or any linear combination of those lattice vectors.
7. Work problem 1 at the end of chapter 2.
8. Work Problem 4 at the end of chapter 2.