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# Allowed wavevectors under the application of incommensurate periodic boundary conditions

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## Abstract

While the energy bands of solids are often thought of as continuous functions of the wavevector,  $\mathbf{k}$ , they are in fact discrete functions, due to the periodic boundary conditions applied over a finite number of primitive cells. The traditional approach enforces periodicity over a volume containing  $N_i$  primitive unit cells along the direction of the primitive lattice vector  $\mathbf{a}_i$ . While this method yields a simple formula for the allowed  $\mathbf{k}$ , it can be problematic computer programs for lattices such as face-centred cubic (FCC) where the boundary faces of the primitive cell are not orthogonal. The fact that  $\mathbf{k}$  is discrete is of critical importance for supercell calculations since they include only a finite number of unit cells, which determines the number of wavevectors, and have a given geometry, which determines their spacing. Rectangular supercells, with the faces orthogonal to the Cartesian axes, are computationally simplest but are not commensurate with the FCC unit cell, so that the traditional approach for determining the allowed  $\mathbf{k}$ -values is no longer useful. Here, we present a simple method for finding the allowed  $\mathbf{k}$ -values when periodic boundary conditions are applied over a rectangular supercell, answering the question in both its practical and pedagogical aspects.

## 1. Introduction

The problem of finding the allowed wavevectors in the first Brillouin zone is a seemingly simple one, treated in solid state physics texts [1–4]. The traditional presentation quite correctly asserts that bulk properties such as the energy bands cannot be sensitive to the exact boundaries over which periodic conditions are enforced so long as the volume of the repeated cell (i.e., supercell) can completely fill all space when replicated. The supercell in real space

is taken to consist of  $N_i$  primitive unit cells along the direction of the primitive lattice vector  $\mathbf{a}_i$ . For this supercell, the allowed wavevectors are shown to be of the form [1–4]

$$\mathbf{k} = \frac{n_1}{N_1}\mathbf{b}_1 + \frac{n_2}{N_2}\mathbf{b}_2 + \frac{n_3}{N_3}\mathbf{b}_3, \quad n_i \text{ integers} \quad (1)$$

where  $\mathbf{b}_i$  are primitive reciprocal lattice vectors such that  $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{i,j}$ . In addition, using this definition it is a straightforward exercise to show that there is one  $\mathbf{k}$  in the first zone for each primitive cell in the supercell, for a total of  $N_c = N_1N_2N_3$  wavevectors, where  $N_c$  is the number of primitive cells in the supercell.

This presentation is often sufficient and satisfactory for most students and professors, so that other shapes for supercells are hardly ever considered; for the simple cubic lattice no other supercell would be realistically contemplated. The face-centred cubic (FCC) lattice is another matter entirely. This technologically important lattice (it is the Bravais lattice for both the diamond and zinc blende crystals) has non-orthogonal primitive direct lattice translation vectors. Curious students might wonder about the allowed wavevectors when the supercell is rectangular (i.e., a rectangular parallelepiped), so this issue clearly has pedagogical relevance.

Finding the allowed wavevectors for a rectangular supercell is especially important since this shape supercell is the easiest to implement in a computer program. The details of the supercell determine both number of allowed  $\mathbf{k}$  (equal to  $N_c$ ) and the spacing between the  $\mathbf{k}$ , which equation (1) shows is determined by the supercell geometry. Hence, bulk solids simulated with supercell programs produce energies only at certain  $\mathbf{k}$ , and it is essential to know exactly which  $\mathbf{k}$  should be found on projecting bulk states out of the supercell states [5]. This step is also important in verifying supercell programs. The issue of allowed  $\mathbf{k}$ -values is thus of significant practical interest as well.

## 2. Method for the FCC lattice

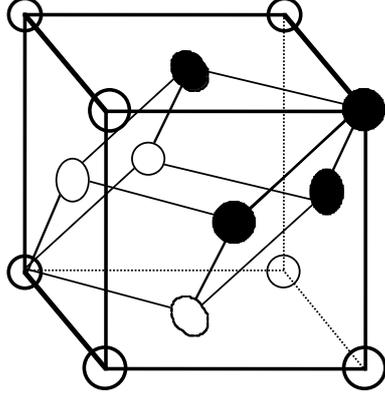
### 2.1. Determination of the wavevectors

Basic geometry shows that the rectangular supercell, which has a fixed number of cubes  $N_\alpha$ ,  $\alpha \in \{x, y, z\}$ , along each of the Cartesian axes, is not commensurate with a fixed number of FCC primitive cells along each of the non-orthogonal primitive cell directions  $\mathbf{a}_i$ . (For example, the number of cells along  $\mathbf{a}_3$  at a boundary is in general a function of the number of cells along the other two directions on the boundary.) Equation (1) thus no longer applies, and another approach is necessary. Observe that if one can determine the allowed wavevectors when periodic boundary conditions are applied over the conventional (non-primitive) cubic unit cell containing four (4) primitive cells, one can find them for any rectangular supercell. This follows from the fact that periodicity over the conventional cube is commensurate with periodicity over an integral number of such cubes along each Cartesian axis.

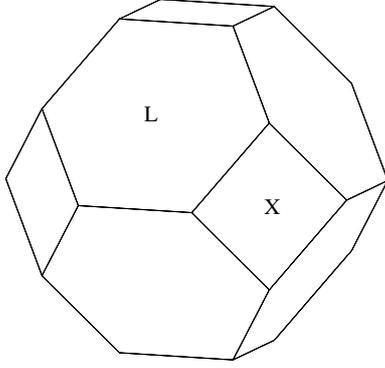
Figure 1 shows the conventional FCC unit cell, a cube of side  $a$ , which contains four (4) lattice points (one set of four points is indicated by solid balls). Enforcing wavefunction periodicity over this cube results in the following relations for the wavevectors,  $\mathbf{q}$ :

$$a\mathbf{e}_\alpha \cdot \mathbf{q} = 2\pi n_\alpha \Rightarrow q^{(\alpha)} = \frac{2\pi n_\alpha}{a}, \quad \alpha \in \{x, y, z\}, n_\alpha \text{ integer.} \quad (2)$$

Obviously the zero vector,  $n_x = n_y = n_z = 0$ , is allowed. Examination of the FCC first Brillouin zone (figure 2) reveals that there are three additional allowed values. These are the triples  $\mathbf{n} = (1, 0, 0)$ ,  $(0, 1, 0)$ ,  $(0, 0, 1)$ , which correspond to three of the X-points,  $\mathbf{k} = 2\pi\mathbf{e}_x/a$ ,  $2\pi\mathbf{e}_y/a$ ,  $2\pi\mathbf{e}_z/a$ . (The remaining three X-points are related to these by FCC



**Figure 1.** Conventional (non-primitive) cubic unit cell (side  $a$ ) for FCC. The cube contains four primitive cells; a set of four lattice points for these cells is indicated by solid balls in the figure. A rhombohedral FCC primitive cell is shown inside the conventional cube. Although it appears larger, its volume is  $a^3/4$ , as one can verify from the formula  $volume = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$ , where the FCC primitive lattice vectors are:  $\mathbf{a}_1 = a(\mathbf{e}_y + \mathbf{e}_z)/2$ ,  $\mathbf{a}_2 = a(\mathbf{e}_x + \mathbf{e}_z)/2$  and  $\mathbf{a}_3 = a(\mathbf{e}_x + \mathbf{e}_y)/2$ .



**Figure 2.** First Brillouin zone for the FCC lattice. The point labelled  $X$  has  $\mathbf{k} = (2\pi/a)\mathbf{e}_y$  while that labelled  $L$  has  $\mathbf{k} = (\pi/a)(\mathbf{e}_x + \mathbf{e}_y + \mathbf{e}_z)$ . Note that the  $X$ -point  $\mathbf{k} = -(2\pi/a)\mathbf{e}_y$  is not in the first zone as it differs from  $(2\pi/a)\mathbf{e}_y$  by the FCC reciprocal lattice vector  $\mathbf{b}_1 + \mathbf{b}_3 = (4\pi/a)\mathbf{e}_y$ . From the values of the  $X$ - and  $L$ -points it is clear that only the triples  $\mathbf{n} = (1, 0, 0)$ ,  $(0, 1, 0)$ ,  $(0, 0, 1)$  in equation (2) yield nonzero wavevectors in the first zone. This figure (without labels) was generated with MAPLE 8 using the *TruncatedOctahedron* and *draw* commands.

reciprocal lattice vectors and hence are not in the first zone.) There are thus four (4) allowed wavevectors, one per primitive cell in the conventional cube, and we may take them to be

$$\mathbf{q}_0 = \mathbf{0}, \quad \mathbf{q}_1 = \frac{2\pi}{a}\mathbf{e}_x, \quad \mathbf{q}_2 = \frac{2\pi}{a}\mathbf{e}_y, \quad \mathbf{q}_3 = \frac{2\pi}{a}\mathbf{e}_z. \quad (3)$$

We remark that for body-centred cubic (BCC), the conventional cube has only two primitive cells, and only two allowed wavevectors ( $\mathbf{q}_0$  and, say,  $\mathbf{q}_1$ ) since  $\mathbf{q}_2$  and  $\mathbf{q}_3$  differ from  $\mathbf{q}_1$  by BCC reciprocal lattice vectors.

Having found the allowed wavevectors for a single conventional cube, we need only enforce wavefunction periodicity over the rectangular supercell of  $N_\alpha$ ,  $\alpha \in \{x, y, z\}$  cubes

along each of the Cartesian axes. The customary calculation leads to allowed supercell wavevectors,

$$\mathbf{K}_{\mathbf{n}} = \frac{2\pi}{a} \left[ \frac{n_x}{N_x} \mathbf{e}_x + \frac{n_y}{N_y} \mathbf{e}_y + \frac{n_z}{N_z} \mathbf{e}_z \right] \quad (4)$$

where the integers  $n_\alpha$ ,  $\alpha \in \{x, y, z\}$ , satisfy

$$n_\alpha = \begin{cases} -\frac{(N_\alpha - 1)}{2}, \dots, \frac{(N_\alpha - 1)}{2}; & N_\alpha \text{ odd} \\ -\frac{(N_\alpha - 2)}{2}, \dots, \frac{N_\alpha}{2}; & N_\alpha \text{ even.} \end{cases} \quad (5)$$

As noted above, the wavevectors  $\mathbf{q}_j$  are automatically compatible with periodicity enforced over an integral number of cubes along each Cartesian axis. It therefore follows that any wavevector  $\mathbf{K}_{\mathbf{n}} + \mathbf{q}_j$  is also compatible with these boundary conditions. Thus, for each of the  $N_x N_y N_z$  wavevectors  $\mathbf{K}_{\mathbf{n}}$  there are four independent wavevectors

$$\mathbf{k}_{\mathbf{n},j} = \mathbf{K}_{\mathbf{n}} + \mathbf{q}_j, \quad j = 0, 1, 2, 3 \quad (6)$$

so that the total number of allowed wavevectors in the first Brillouin zone equals the number of FCC primitive cells in the supercell,  $N_c = 4N_x N_y N_z$ .

It is useful to rewrite the wavevectors, equation (6), in terms of the FCC primitive reciprocal lattice vectors [4],

$$\mathbf{b}_1 = \frac{2\pi}{a} (-\mathbf{e}_x + \mathbf{e}_y + \mathbf{e}_z), \quad \mathbf{b}_2 = \frac{2\pi}{a} (\mathbf{e}_x - \mathbf{e}_y + \mathbf{e}_z), \quad \mathbf{b}_3 = \frac{2\pi}{a} (\mathbf{e}_x + \mathbf{e}_y - \mathbf{e}_z). \quad (7)$$

Doing so, we find

$$\mathbf{k}_{\mathbf{n},0} = \frac{1}{2} \left( \frac{n_y}{N_y} + \frac{n_z}{N_z} \right) \mathbf{b}_1 + \frac{1}{2} \left( \frac{n_x}{N_x} + \frac{n_z}{N_z} \right) \mathbf{b}_2 + \frac{1}{2} \left( \frac{n_x}{N_x} + \frac{n_y}{N_y} \right) \mathbf{b}_3 \quad (8)$$

$$\mathbf{k}_{\mathbf{n},1} = \frac{1}{2} \left( \frac{n_y}{N_y} + \frac{n_z}{N_z} \right) \mathbf{b}_1 + \frac{1}{2} \left( \frac{n_x}{N_x} + \frac{n_z}{N_z} + 1 \right) \mathbf{b}_2 + \frac{1}{2} \left( \frac{n_x}{N_x} + \frac{n_y}{N_y} + 1 \right) \mathbf{b}_3 \quad (9)$$

$$\mathbf{k}_{\mathbf{n},2} = \frac{1}{2} \left( \frac{n_y}{N_y} + \frac{n_z}{N_z} + 1 \right) \mathbf{b}_1 + \frac{1}{2} \left( \frac{n_x}{N_x} + \frac{n_z}{N_z} \right) \mathbf{b}_2 + \frac{1}{2} \left( \frac{n_x}{N_x} + \frac{n_y}{N_y} + 1 \right) \mathbf{b}_3 \quad (10)$$

$$\mathbf{k}_{\mathbf{n},3} = \frac{1}{2} \left( \frac{n_y}{N_y} + \frac{n_z}{N_z} + 1 \right) \mathbf{b}_1 + \frac{1}{2} \left( \frac{n_x}{N_x} + \frac{n_z}{N_z} + 1 \right) \mathbf{b}_2 + \frac{1}{2} \left( \frac{n_x}{N_x} + \frac{n_y}{N_y} \right) \mathbf{b}_3. \quad (11)$$

Note the contrast between equations (8)–(11) and equation (1), especially the fact that the spacing between allowed wavevectors differs considerably from the commensurate supercell case.

## 2.2. Independence of the wavevectors

Using equations (8)–(11), it is straightforward to establish that none of the  $\mathbf{k}_{\mathbf{n},j}$  differ by a FCC reciprocal lattice vector. For fixed  $\mathbf{n}$  any two  $\mathbf{k}_{\mathbf{n},j}$  differ by  $(1/2)(\mathbf{b}_j \pm \mathbf{b}_{j'})$ ,  $j \neq j'$ , which is clearly not a reciprocal lattice vector. Establishing that the difference  $\mathbf{k}_{\mathbf{n},j} - \mathbf{k}_{\mathbf{n}',j'}$  is not a reciprocal lattice vector involves treating only two cases, say  $\mathbf{k}_{\mathbf{n},1} - \mathbf{k}_{\mathbf{n}',0}$  and  $\mathbf{k}_{\mathbf{n},3} - \mathbf{k}_{\mathbf{n}',2}$ , as the others follow using the cyclic permutations  $x \rightarrow y \rightarrow z \rightarrow x$ ,  $\mathbf{b}_1 \rightarrow \mathbf{b}_2 \rightarrow \mathbf{b}_3 \rightarrow \mathbf{b}_1$ , etc. In either case, the coefficient of each reciprocal lattice vector  $\mathbf{b}_j$  must be an integer if the

difference is to be a reciprocal lattice vector. Consider first the difference  $\mathbf{k}_{\mathbf{n},1} - \mathbf{k}_{\mathbf{n},0}$ : if this is to be a reciprocal lattice vector, then

$$\begin{aligned}\frac{n_y - n'_y}{N_y} + \frac{n_z - n'_z}{N_z} &= 2m_1, \\ \frac{n_x - n'_x}{N_x} + \frac{n_z - n'_z}{N_z} + 1 &= 2m_2, \\ \frac{n_x - n'_x}{N_x} + \frac{n_y - n'_y}{N_y} + 1 &= 2m_3\end{aligned}\quad (12)$$

where  $m_j$  are integers. Adding the first two of equations (12), subtracting the third and dividing by 2 yields

$$\frac{n_z - n'_z}{N_z} = m_1 + m_2 - m_3. \quad (13)$$

From the limits in equation (5) it is clear that the only possible solution of this equation is  $n'_z = n_z$ . In this case, however, the first of equations (12) likewise implies  $n'_y = n_y$  for the same reason. The last two of equations (12) now imply  $(n_x - n'_x)/N_x = 2m_2 - 1 = 2m_3 - 1$  which is impossible since  $m_j$  are integers and  $(n_x - n'_x)/N_x$  cannot be a nonzero integer.

The difference  $\mathbf{k}_{\mathbf{n},3} - \mathbf{k}_{\mathbf{n},2}$  is treated in a like manner. If this difference is to be a reciprocal lattice vector, then

$$\begin{aligned}\frac{n_y - n'_y}{N_y} + \frac{n_z - n'_z}{N_z} &= 2m_1, \\ \frac{n_x - n'_x}{N_x} + \frac{n_z - n'_z}{N_z} + 1 &= 2m_2, \\ \frac{n_x - n'_x}{N_x} + \frac{n_y - n'_y}{N_y} - 1 &= 2m_3\end{aligned}\quad (14)$$

where again  $m_j$  are integers. Adding the last two of equations (14), subtracting the first and dividing by 2 yields

$$\frac{n_x - n'_x}{N_x} = m_2 + m_3 - m_1. \quad (15)$$

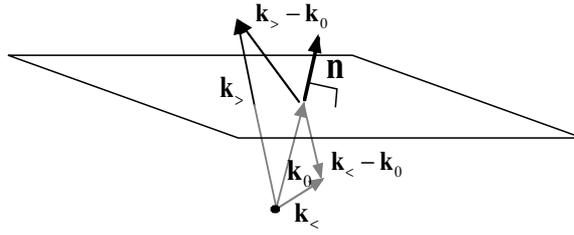
As before the only possible solution is  $n'_x = n_x$ . However, the second of equations (14) now implies  $(n_z - n'_z)/N_z = 2m_2 - 1$  which is impossible for the reasons stated above. Likewise, the third of equations (14) now implies  $(n_y - n'_y)/N_y = 2m_3 + 1$  which is again impossible. Hence, equations (8)–(11) indeed define independent  $\mathbf{k}$ -vectors.

### 2.3. Shifting wavevectors back into the first zone

We briefly mention that some of the  $\mathbf{k}_{\mathbf{n},j}$  as written in equations (8)–(11) might fall outside the FCC first Brillouin zone, but are easily shifted back into the zone by adding the proper FCC reciprocal lattice vector. One method for determining the required reciprocal lattice vector takes advantage of the fact that a wavevector  $\mathbf{k}$  lying on the Brillouin zone face satisfies

$$(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{n} = 0 \quad (16)$$

where  $\mathbf{k}_0$  is a fixed point on the face and  $\mathbf{n}$  is the outward normal to the face. For FCC,  $\mathbf{k}_0$  is one of the six  $X$ -points or eight  $L$ -points (e.g.,  $\mathbf{k}_0 = \pi(\mathbf{e}_x + \mathbf{e}_y + \mathbf{e}_z)/a$ ) and  $\mathbf{n} = \mathbf{k}_0/|\mathbf{k}_0|$ . If  $\mathbf{k}$  is outside the zone then  $(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{n} > 0$ , as shown for the vector  $\mathbf{k}_>$  in figure 3. Likewise,



**Figure 3.** Geometrical construction for determining whether a wavevector lies above or below a plane. The wavevector  $\mathbf{k}_>$  lies above so that  $(\mathbf{k}_> - \mathbf{k}_0) \cdot \mathbf{n} > 0$ , while  $\mathbf{k}_<$  lies below so that  $(\mathbf{k}_< - \mathbf{k}_0) \cdot \mathbf{n} < 0$ .

if  $\mathbf{k}$  is inside the zone then  $(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{n} < 0$ , as shown for the vector  $\mathbf{k}_<$  in figure 3. Thus, a wavevector  $\mathbf{k}_{n,j}$  is tested against each of the Brillouin zone faces as in equation (16) and if it is outside the appropriate reciprocal lattice vector is added to shift it back inside.

### 3. Conclusions

We have therefore shown how to find the allowed wavevectors for a rectangular supercell in the FCC lattice. By decomposing the problem into first a wavevector due to periodicity enforced over the conventional cubic unit cell and second a wavevector due to periodicity enforced over the supercell, we have shown that the number of wavevectors equals the number of primitive cells in the supercell, as required. This procedure also gives explicit formulae for the allowed wavevectors. We have also shown a simple method for shifting any wavevectors falling outside the first Brillouin zone back inside.

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