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Free Electron Bands In Cubic Crystals

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Introduction

The empty lattice approximation describes a number of properties of energy dispersion relations of non-interacting free electrons in a crystal lattice. The energy of the electrons in the "empty lattice" is the same as the energy of free electrons.

$$E_{\mathbf{q}} = \frac{\hbar^2 q^2}{2m} \tag{1}$$

The structure of the bands are illustrated by plotting energy versus wavevector which are usually shown in reduced zone scheme. When wavevectors happen to be given outside the first zone, they are carried back into the first zone by subtracting a suitable reciprocal lattice vector. So all information is contained in the first Brillouin Zone.

$$\mathbf{q} = \mathbf{k} + \mathbf{K} \tag{2}$$

Calculation

The free electron energy can always be written as

$$\epsilon(k_x, k_y, k_z) = (\hbar^2/2m)(\mathbf{k} + \mathbf{K}) \tag{3}$$

$$\epsilon(k_x, k_y, k_z) = (\hbar^2/2m)[(k_x + K_x)^2 + (k_y + K_y)^2 + (k_z + K_z)^2] \tag{4}$$

where K_x, K_y and K_z for simple cubic, based center cubic and face center cubic can be written using Chapter 5 of Ashcroft.

$$\mathbf{K}_{sc} = (\frac{2\pi}{a})(\hat{x} + \hat{y} + \hat{z}) \tag{5}$$

$$\mathbf{K}_{bcc} = (\frac{2\pi}{a})((k + l)\hat{x} + (h + l)\hat{y} + (h + k)\hat{z}) \tag{6}$$

$$\mathbf{K}_{fcc} = (\frac{2\pi}{a})[(-h + k + l)\hat{x} + (h - k + l)\hat{y} + (h + k - l)\hat{z}] \tag{7}$$

So by using the appropriate $\mathbf{K}$ for the lattice and putting different values for miller indices Eq.4 simplifies to a set of parabolas of $\mathbf{k}$. The bands can be calculated for different direction of $\mathbf{k}$ using Symmetry points in the Brillouin zone.

In the following calculation we set $2\pi/a$ and $\hbar^2/2m$ to one. The simulation was done in Python 3.8.5 using libraries such as mathplotlib, numpy, pandas and itertools.

For putting different miller indices in Eq.4 we must first calculate different family of directions using permutations from itertools library. For the following plots, miller indices in the families of <000>, <100>, <110>, <111>, <200> and <220> was used. A table containing band energy and its corresponding indices is given. The color in each row of the table connects the line in the plot with its corresponding indices.

Link of reprository in Githbu:
https://github.com/hastihojabr/Free-electron-energy-bands---Reduced-zone-scheme.git

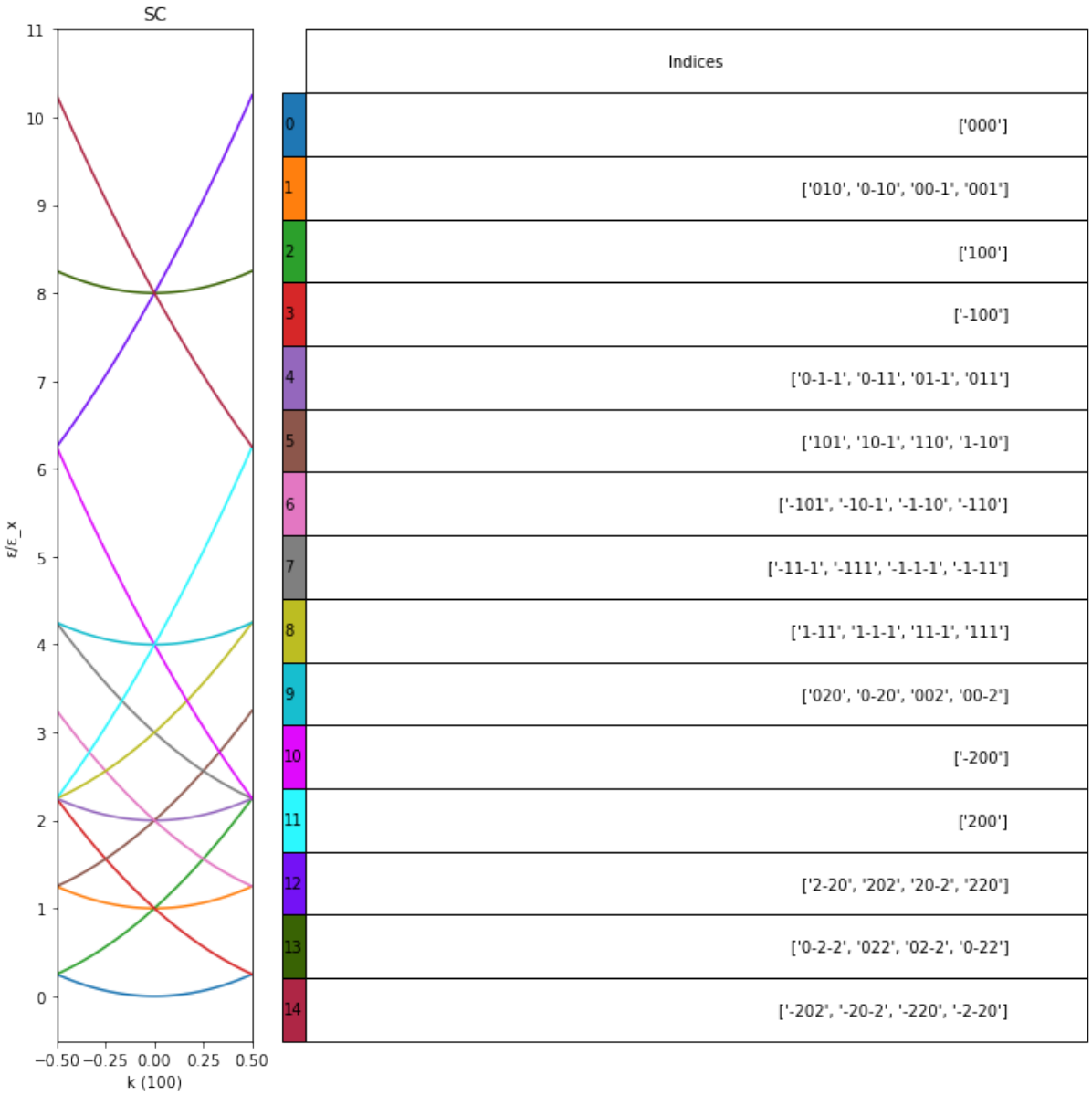

Figure 1: Free electron energy bands for SC lattice in 100 direction

Results and Analysis

Face Centered Cubic

Considering the symmetry points given in table 1, we can find band structures for different directions.

Symmetry points	[kx,ky,kz]
Γ	$[0, 0, 0]$
X	$[0, 2\pi/a, 0]$
L	$[\pi/a, \pi/a, \pi/a]$
W	$[\pi/a, 2\pi/a, 0]$
U	$[\pi/2a, 2\pi/a, \pi/2a]$
K	$[3\pi/2a, 3\pi/2a, 0]$

Table 1: Directions

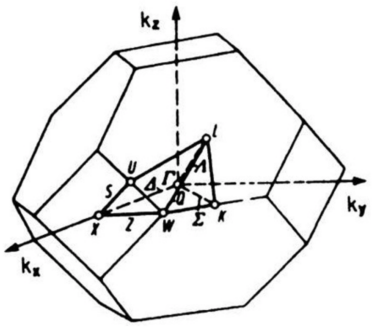

Figure 2: First Brillouin zone of the fcc structure

For example for **ΓX**, k can be written as

$$\mathbf{k} = (2\pi/a)(\mu, 0, 0)\,; \quad 0 \leq \mu \leq 1 \tag{8}$$

On the other hand for directions that do not start from the center such as **XW**, the direction of vector k change between **ΓX** and **ΓW**. So **k** is linear combination of theses two vectors such as the coefficient of **ΓX** is 1 when **k** is in the same direction of **ΓX** and as the vector goes towards direction of **ΓW** it decreases to zero.

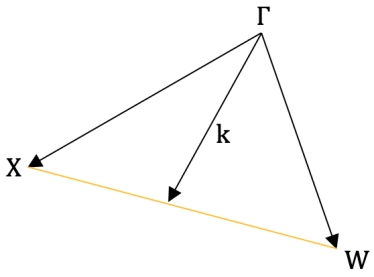

Figure 3: **XW**

So we can write **k** as

$$\mathbf{k}_{XW} = (1-\mu)\,\mathbf{\Gamma X} + \mu\,\mathbf{\Gamma W}\,; \quad 0 \leq \mu \leq 1 \tag{9}$$

$$\mathbf{k}_{XW} = (1, \mu/2, 0)\,\mathbf{\Gamma W}\,; \quad 0 \leq \mu \leq 1 \tag{10}$$

Free electron band structure for the path $\mathbf{\Gamma - X - W - L - \Gamma - K - X}$ is shown in Fig.4.

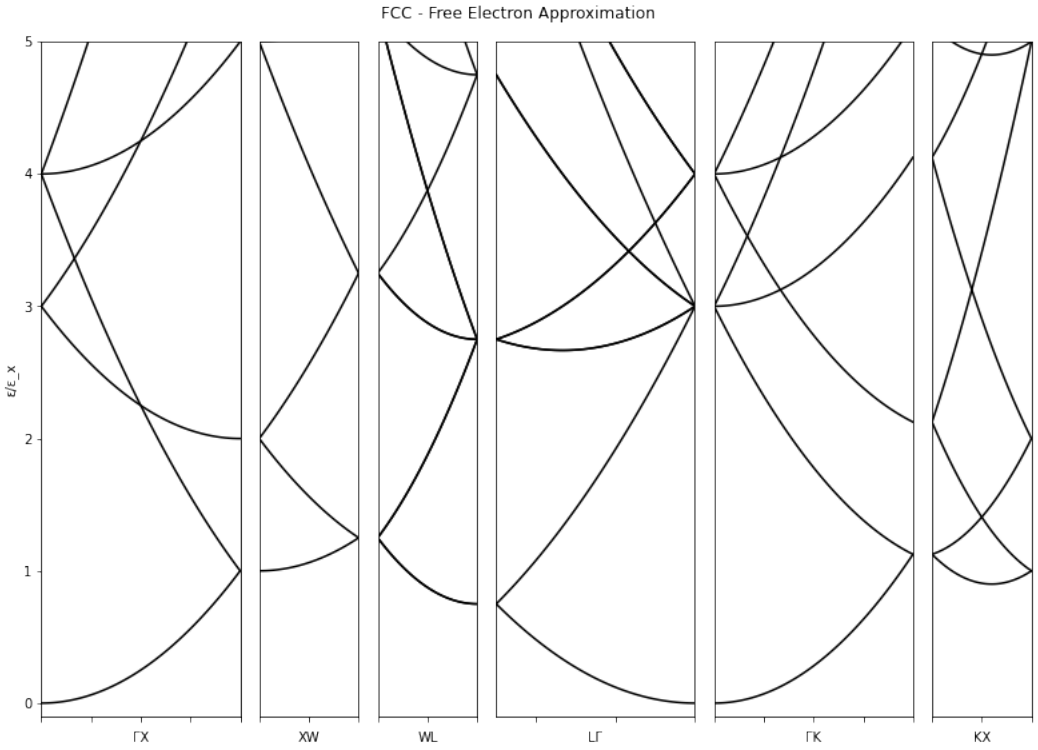

Figure 4: Free electron bands of the fcc structure. The letters on the bottom of the graphs correspond to letters in Fig.2 and indicate specific symmetry points in k-space.

Base Centered Cubic

Considering the symmetry points given in table 2, we can find band structures for different directions.

Symmetry points	[kx,ky,kz]
Γ	$[0, 0, 0]$
H	$[0, 0, 2\pi/a]$
P	$[\pi/a, \pi/a, \pi/a]$
N	$[0, 0, \pi/a]$

Table 2: Directions

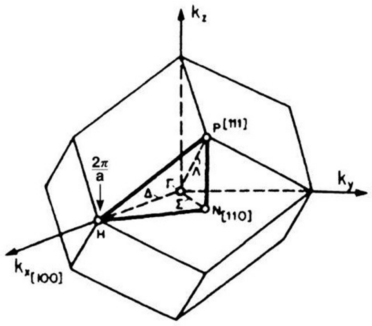

Figure 5: First Brillouin zone of the bcc structure

The same method was used for finding different directions. Free electron band structure for the path $\mathbf{H} - \mathbf{\Gamma} - \mathbf{P} - \mathbf{N} - \mathbf{\Gamma} - \mathbf{H} - \mathbf{P}$ is shown in Fig.4.

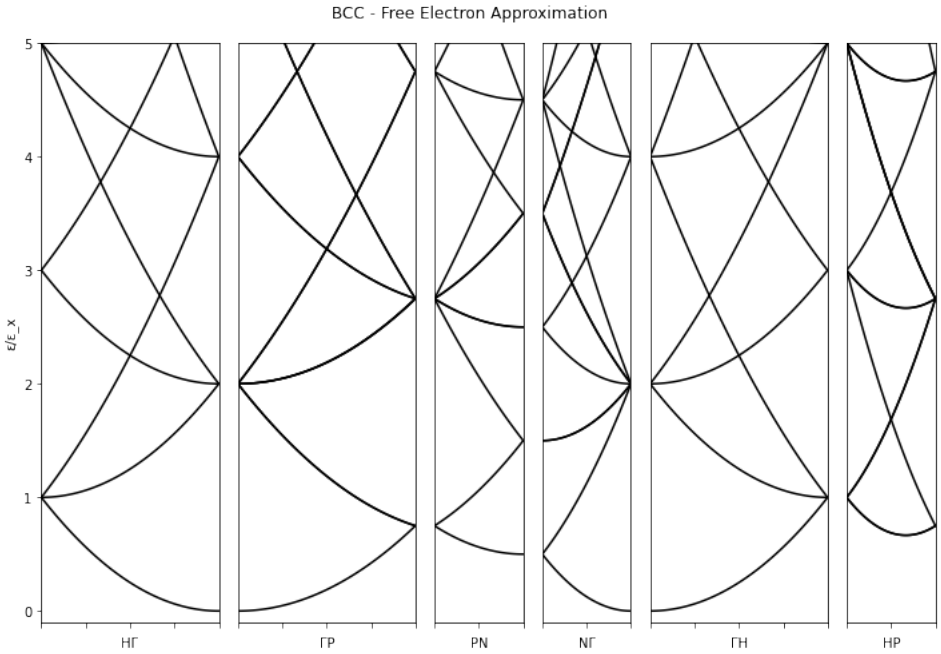

Figure 6: Free electron bands of the bcc structure. The letters on the bottom of the graphs correspond to letters in Fig.5 and indicate specific symmetry points in k-space.