The free electron energy bands

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Abstract

The purpose of these notes is to explain how to plot the free-electron energy bands for simple cubic, body-centered cubic (bcc), and face-centered cubic (fcc) lattices. After a concise review of the required theory, we outline the necessary routines and examine the technical choices involved in their implementation.

I. INTRODUCTION

In these notes, we address the implementation and plotting of free-electron energy bands for a solid. Our goal is to reproduce a plot akin to Figure 9.5 in Ashcroft and Mermin by building a lightweight Fortran program from scratch to generate the required data. While Fortran is the language used in the companion package containing the complete routines discussed here, the underlying theoretical principles can be implemented in any programming language.

These notes are intended for students who have already covered the fundamentals of the theory presented in Ashcroft and Mermin and need to focus specifically on the practical aspects of generating the plot. This exercise is well-suited for an introductory computational physics course to help students gain familiarity with language compilers, plotting tools, and basic code development.

Finally, these routines mirror those found in more advanced electronic structure codes like Quantum ESPRESSO, serving as a valuable stepping stone for exploring such software.

II. THE BRAVAIS LATTICE

A Bravais lattice is an infinite array of points that appear exactly the same when viewed from any point in the array. It can be generated by three primitive vectors, $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$, by taking all points obtained through integer linear combinations of these three vectors:

$$\mathbf{R}_{n_1,n_2,n_3} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3. \tag{1}$$

To simplify the notation, we denote the triplet of integer indices $\{n_1, n_2, n_3\}$ collectively by the index μ. It is also convenient to impose Born-von Kármán periodic boundary conditions, restricting n_1, n_2, n_3 to a finite region of dimensions $N = N_1 \times N_2 \times N_3$.

Finally, the equilibrium positions of the atoms are given by $\mathbf{R}_I = \mathbf{R}_\mu + \mathbf{d}_s$, where $s = 1, \ldots, N_{at}$ and $\mathbf{d}_s$ is the position of the atoms within one unit cell.

In this exercise, we focus on three specific lattices: The simple cubic lattice is obtained by placing the Bravais lattice points at the corners of a cube. The lattice depends on a parameter a representing the side length of the cube, and its three primitive vectors are:

$$\begin{aligned} \mathbf{a}_1 &= a(1,0,0), \\ \mathbf{a}_2 &= a(0,1,0), \\ \mathbf{a}_3 &= a(0,0,0). \end{aligned} \tag{2}$$

The face-centered cubic (fcc) lattice has lattice points not only at the corners of the cube but also at the centers of its faces. Its primitive vectors can be written, for instance, as:

$$\begin{aligned} \mathbf{a}_1 &= a(0,1/2,1/2), \\ \mathbf{a}_2 &= a(1/2,0,1/2), \\ \mathbf{a}_3 &= a(1/2,1/2,0). \end{aligned} \tag{3}$$

The body-centered cubic (bcc) lattice has lattice points not only at the corners of the cube but also at its center. Its primitive vectors can be chosen as:

$$\begin{aligned} \mathbf{a}_1 &= a(-1/2,1/2,1/2), \\ \mathbf{a}_2 &= a(1/2,-1/2,1/2), \\ \mathbf{a}_3 &= a(1/2,1/2,-1/2). \end{aligned} \tag{4}$$

A volume that fills all space when translated by all vectors of a Bravais lattice is called a unit cell. The volume of the unit cell is given by $\Omega = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$, which evaluates to $\Omega = a^3$ for the simple cubic lattice, $\Omega = a^3/4$ for the fcc lattice, and $\Omega = a^3/2$ for the bcc lattice.

III. THE RECIPROCAL LATTICE

Given a plane wave $f_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}}$, this function is not in general periodic with the periodicity of the Bravais lattice meaning that in general $f_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_\mu) \neq f_{\mathbf{k}}(\mathbf{r})$. However for particular values of $\mathbf{k}$ that we will call $\mathbf{G}$ we have that the $f_{\mathbf{G}}(\mathbf{r}+\mathbf{R}_\mu) = f_{\mathbf{G}}(\mathbf{r})$. This means that $e^{i\mathbf{GR}_\mu} = 1$ for all Bravais lattice points. It turns out that also the $\mathbf{G}$ vectors form a lattice which is called reciprocal lattice. Actually if we define three primitive vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ such that:

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}, \tag{5}$$

the lattice

$$\mathbf{G}_{m_1,m_2,m_3} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3, \tag{6}$$

where $\{m_1, m_2, m_3\}$ are integers, has the property that

$$\mathbf{G}_{m_1,m_2,m_3} \cdot \mathbf{R}_{n_1,n_2,n_3} = 2\pi(m_1n_1 + m_2n_2 + m_3n_3) \tag{7}$$

and $e^{i2\pi(m_1n_1+m_2n_2+m_3n_3)} = 1$.

The three primitive vectors of the reciprocal lattice can be written as:

$$\begin{aligned}
\mathbf{b}_1 &= 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{\Omega}, \\
\mathbf{b}_2 &= 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{\Omega}, \\
\mathbf{b}_3 &= 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{\Omega}.
\end{aligned} \tag{8}$$

Carrying out this calculation for the simple cubic lattice, we obtain:

$$\begin{aligned}
\mathbf{b}_1 &= \frac{2\pi}{a}(1,0,0), \\
\mathbf{b}_2 &= \frac{2\pi}{a}(0,1,0), \\
\mathbf{b}_3 &= \frac{2\pi}{a}(0,0,1).
\end{aligned} \tag{9}$$

Thus, the reciprocal lattice of the simple cubic lattice is also cubic, with a lattice parameter of $2\pi/a$.

For the fcc lattice, the reciprocal lattice is given by:

$$\begin{aligned}
\mathbf{b}_1 &= \frac{2\pi}{a}(-1,1,1), \\
\mathbf{b}_2 &= \frac{2\pi}{a}(1,-1,1), \\
\mathbf{b}_3 &= \frac{2\pi}{a}(1,1,-1).
\end{aligned} \tag{10}$$

Thus, the reciprocal lattice of an fcc Bravais lattice is a bcc lattice with a cell size of $4\pi/a$.

Similarly, for the bcc lattice, the reciprocal lattice is:

$$\begin{aligned} \mathbf{b}_1 &= \frac{2\pi}{a}(0,1,1), \\ \mathbf{b}_2 &= \frac{2\pi}{a}(1,0,1), \\ \mathbf{b}_3 &= \frac{2\pi}{a}(1,1,0). \end{aligned} \tag{11}$$

Thus, the reciprocal lattice of a bcc Bravais lattice is an fcc lattice with a cell size of $\frac{4\pi}{a}$.

The unit cell of the reciprocal lattice is called the Brillouin zone, and in all cases, its volume is given by $\Omega_{BZ} = \frac{(2\pi)^3}{\Omega}$.

IV. LATTICE PLANES

For the subsequent discussion, we require a result from Ashcroft and Mermin (see page 89) concerning the relation between lattice planes and reciprocal lattice vectors. Rather than presenting the full proof, we simply state the required result. A lattice plane is any plane containing Bravais lattice vectors. A set of parallel lattice planes that contains all points of a Bravais lattice is referred to as a family of lattice planes. This theorem states that for each reciprocal lattice vector $\mathbf{G}$, there is a corresponding family of lattice planes perpendicular to $\mathbf{G}$. The distance between adjacent planes is given by $d = \frac{2\pi}{|\mathbf{G}_1|}$, where $\mathbf{G}_1$ is the shortest reciprocal lattice vector parallel to $\mathbf{G}$. Conversely, for every family of lattice planes separated by a distance d, there is an infinite number of reciprocal lattice vectors $\mathbf{G}$ perpendicular to the planes, the shortest of which has a magnitude of $\frac{2\pi}{d}$.

V. THE BLOCH THEOREM

Bloch's theorem concerns the form of the wavefunction solutions to the one-electron Schrödinger equation when the potential is periodic with the periodicity of the Bravais lattice. One solves the problem:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r}), \tag{12}$$

where $\hbar$ is the Planck constant, m the electron mass and $V(\mathbf{r}+\mathbf{R}_\mu) = V(\mathbf{r})$, yielding solutions that can be classified by a wave vector $\mathbf{k}$ and a band index v. We can write $\psi_i(\mathbf{r}) = \psi_{\mathbf{k}v}(\mathbf{r})$. The wavefunctions themselves are not periodic, but satisfy the

$$\psi_{\mathbf{k}v}(\mathbf{r}+\mathbf{R}_\mu) = e^{i\mathbf{k}\mathbf{R}_\mu}\psi_{\mathbf{k}v}(\mathbf{r}). \tag{13}$$

Equivalently, wavefunctions can be expressed as a phase factor multiplied by a lattice-periodic function:

$$\psi_{\mathbf{k}v}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}}u_{\mathbf{k}v}(\mathbf{r}), \tag{14}$$

where $u_{\mathbf{k}v}(\mathbf{r}+\mathbf{R}_\mu) = u_{\mathbf{k}v}(\mathbf{r})$.

It is clear that $\psi_{\mathbf{k}+\mathbf{G}v}(\mathbf{r})$ shares the same translational property as $\psi_{\mathbf{k}v}(\mathbf{r})$ since

$$\psi_{\mathbf{k}+\mathbf{G}v}(\mathbf{r}+\mathbf{R}_\mu) = e^{i\mathbf{k}\mathbf{R}_\mu}e^{i\mathbf{G}\mathbf{R}_\mu}\psi_{\mathbf{k}+\mathbf{G}v}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{R}_\mu}\psi_{\mathbf{k}+\mathbf{G}v}(\mathbf{r}), \tag{15}$$

and therefore must correspond to one of the wavefunctions at $\mathbf{k}$ for some band index v. We can therefore choose $\mathbf{k}$ in the first Brillouin zone.

Considering a model of a solid with a finite volume $N\Omega$ and Born-von Kármán periodic boundary conditions, we must have

$$\begin{aligned}
\psi_{\mathbf{k}v}(\mathbf{r}+N_1\mathbf{a}_1) &= \psi_{\mathbf{k}v}(\mathbf{r}),\\
\psi_{\mathbf{k}v}(\mathbf{r}+N_2\mathbf{a}_2) &= \psi_{\mathbf{k}v}(\mathbf{r}),\\
\psi_{\mathbf{k}v}(\mathbf{r}+N_3\mathbf{a}_3) &= \psi_{\mathbf{k}v}(\mathbf{r})
\end{aligned} \tag{16}$$

Combined with Bloch's theorem, this yields $e^{i\mathbf{k}N_i\mathbf{a}_i} = 1$. We can write $\mathbf{k} = \frac{l_1}{N_1}\mathbf{b}_1 + \frac{l_2}{N_2}\mathbf{b}_2 + \frac{l_3}{N_3}\mathbf{b}_3$, where $\{l_1, l_2, l_3\}$ are integers that take N distinct values. We can conclude that there are N allowed $\mathbf{k}$ points in the Brillouin zone, each occupying a volume equal to $\frac{(2\pi)^3}{N\Omega}$. As N approaches infinity, in the thermodynamic limit, $\mathbf{k}$ becomes continuous.

VI. FREE ELECTRONS IN 1D

We start by considering the problem of solving the Bloch equation in one dimension for free electrons. Free electrons imply that $V(\mathbf{r}) = 0$. This represents a special case of a periodic potential, where we can view free electrons as an unperturbed system that is subsequently subjected to a periodic potential. We therefore consider the equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_i(x) = \epsilon_i\psi_i(x) \tag{17}$$

For free electrons, solutions can be found for any value of x. However, analogously to our discussion of Bloch's theorem, it is convenient to choose a large length L for the interval $0 < x < L$ and apply Born-von Kármán periodic boundary conditions for the other x. Letting $K^2 = \frac{\epsilon_K 2m}{\hbar^2}$, we solve the equation:

$$\frac{d^2}{dx^2}\psi_K(x) = -K^2\psi_K(x), \tag{18}$$

which has the solutions

$$\psi_K(x) = \frac{1}{\sqrt{L}}e^{iKx}, \tag{19}$$

with eigenvalue

$$\epsilon_K = \frac{\hbar^2 K^2}{2m}. \tag{20}$$

Born von Kármán periodic boundary conditions imply that $\psi_K(x + L) = \psi_K(x)$, therefore

$$e^{iKL} = 1, \tag{21}$$

or $K = 2\pi l/L$, where l is an integer.

Bloch's theorem also introduces a Bravais lattice. In one dimension, we have a lattice parameter a and impose the condition $L = Na$, where a is determined by the perturbing potential we intend to introduce. The reciprocal lattice vectors are given by $G_m = \frac{2\pi}{a}m$, where m is an integer. Let us consider three specific reciprocal lattice vectors: G_0, $G_1 = \frac{2\pi}{a}$, and $G_{-1} = -\frac{2\pi}{a}$. The first Brillouin zone is defined as the set of points closer to G_0 than to any other reciprocal lattice vector. Identifying the points at $G_1/2 = \pi/a$ and $G_{-1}/2 = -\pi/a$, the Brillouin zone spans the interval $-\pi/a < K \leq \pi/a$.

Over this interval, the energy forms a parabola from 0 to:

$$\epsilon_{\frac{\pi}{a}} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2. \tag{22}$$

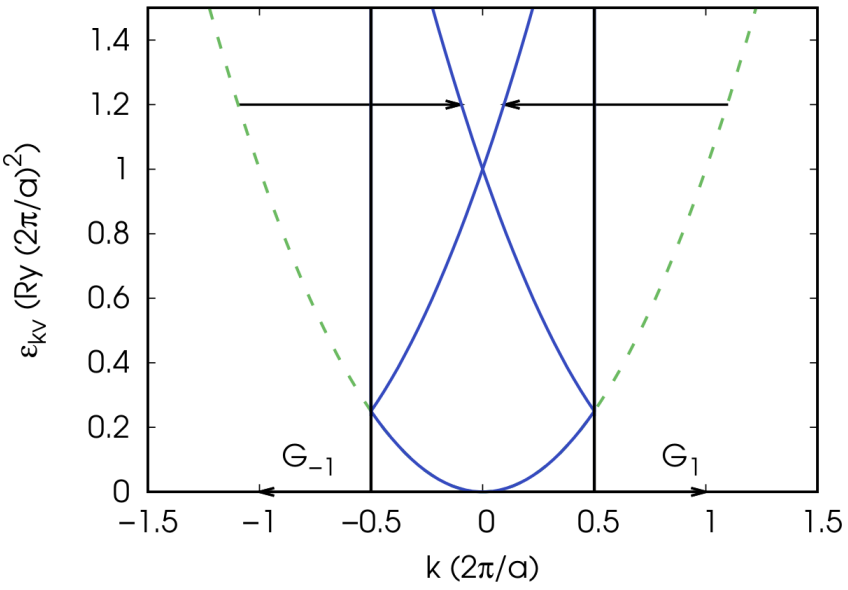


FIG. 1. Free electron bands in one dimension.

It is convenient here to introduce the Bohr radius $a_B = \frac{\hbar^2 4\pi\epsilon_0}{me^2}$, which corresponds to the radius of the ground state of the hydrogen atom in Bohr's theory. Here ϵ_0 is the vacuum electric permittivity. Expressing the unit cell size in Bohr units as $a = \bar{a}a_B$, we can write:

$$\epsilon_{\frac{\pi}{a}} = \frac{\hbar^2}{2ma_B^2}\left(\frac{\pi}{\bar{a}}\right)^2 = \frac{E_H}{2}\left(\frac{2\pi}{\bar{a}}\right)^2\frac{1}{4}, \tag{23}$$

where we have introduced the Hartree energy $E_H = \frac{\hbar^2}{ma_B^2}$, an energy unit frequently used in electronic structure calculations. This energy is twice the ground-state energy of the hydrogen atom. Often, the Rydberg energy-equal to $E_H/2$, which corresponds exactly to the ground-state energy of the hydrogen atom-is used instead. Thus, if we adopt as our energy unit the Rydberg energy multiplied by $(2\pi/\bar{a})^2$, the energy is obtained simply as k^2, with k expressed in units of $2\pi/\bar{a}$.

Outside the first Brillouin zone, we can write $K = k + G_m$. To plot the energy $\epsilon_{k+G_m} = \frac{\hbar^2(k+G_m)^2}{2m}$ as a function of k, we introduce a band index to distinguish the different G_m values at the same k (see Fig. 1).

VII. FREE ELECTRONS IN 3D

Now we can solve the case $V(\mathbf{r}) = 0$ in three dimensions. The Schrodinger equation become

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\psi_{\mathbf{K}}(x,y,z) = \epsilon_{\mathbf{K}}\psi_{\mathbf{K}}(x,y,z) \tag{24}$$

The problem is separable. We can search the solution as:

$$\psi_{\mathbf{K}}(x,y,z) = \psi_{K_1}(x)\psi_{K_2}(y)\psi_{K_3}(z), \tag{25}$$

and we obtain three separate equations identical to the one dimensional problem:

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{K_1}(x) &= \epsilon_{K_1}\psi_{K_1}(x), \\ -\frac{\hbar^2}{2m}\frac{d^2}{dy^2}\psi_{K_2}(y) &= \epsilon_{K_2}\psi_{K_1}(y), \\ -\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\psi_{K_3}(z) &= \epsilon_{K_3}\psi_{K_3}(z). \end{aligned} \tag{26}$$

where $K_1^2 = \frac{2m\epsilon_{K_1}}{\hbar^2}$, $K_2^2 = \frac{2m\epsilon_{K_2}}{\hbar^2}$, and $K_3^2 = \frac{2m\epsilon_{K_3}}{\hbar^2}$. We obtain

$$\psi_{\mathbf{K}}(x) = Ae^{i(K_1x+K_2y+K_3z)} = Ae^{i\mathbf{K}\mathbf{r}}, \tag{27}$$

and eigenvalues

$$\epsilon_{\mathbf{K}} = \epsilon_{K_1}+\epsilon_{K_2}+\epsilon_{K_3} = \frac{\hbar^2}{2m}\mathbf{K}^2. \tag{28}$$

To determine the normalization constant A we can consider the volume $V = N\Omega$ with Born von Kármán boundary conditions and request that the integral of the square modulus of the wavefunction integrated in this volume is normalized to 1. We obtain $A = \frac{1}{\sqrt{V}}$.

For the energy units we can do as in the one dimensional case and give the energy in units of Ry $(\frac{2\pi}{\bar{a}})^2$. The energy will be equal to $\mathbf{K}^2$ if the three components of $\mathbf{K}$ are given in units of $\frac{2\pi}{\bar{a}}$.

We can now choose a path inside the first Brillouin zone and along this path the energy will be $\mathbf{k}^2$ for $\mathbf{K}$ inside the first Brillouin zone. For $\mathbf{K}$ outside the first Brillouin zone we should write $\mathbf{K} = \mathbf{k}+\mathbf{G}_m$ and plot in each $\mathbf{k}$, $|\mathbf{k}+\mathbf{G}_m|^2$ where the different $\mathbf{G}_m$ will give the different bands.

VIII. CODE LAYOUT

Thus, the overall strategy of the code will be:

1. Choose a path of $\mathbf{k}$ points in the first Brillouin zone.

2. For each $\mathbf{k}$, calculate all vectors $\mathbf{k} + \mathbf{G}_{m_1,m_2,m_3}$ for a set of $\mathbf{G}_{m_1,m_2,m_3}$ vectors chosen to obtain all bands within the desired energy window.

3. For instance, one can set a cut-off energy E_{cut} and include all bands such that

$$|\mathbf{k} + \mathbf{G}_{m_1 m_2 m_3}|^2 < E_{cut} \tag{29}$$

4. Once all bands at a given $\mathbf{k}$ are obtained, order them from lowest to highest energy.

5. Finally, write to the output file the lowest number of bands, N_b, requested by the user.

To carry out these tasks, we need a few auxiliary routines:

1. A routine that generates $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$.

2. A routine that calculates $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$.

3. A routine that generates an appropriate set of $\mathbf{G}$ vectors. In particular, it is convenient to choose a sphere of radius $|\mathbf{G}_{max}|$ that encompasses all spheres defined by $|\mathbf{k}+\mathbf{G}|^2 < E_{cut}$.

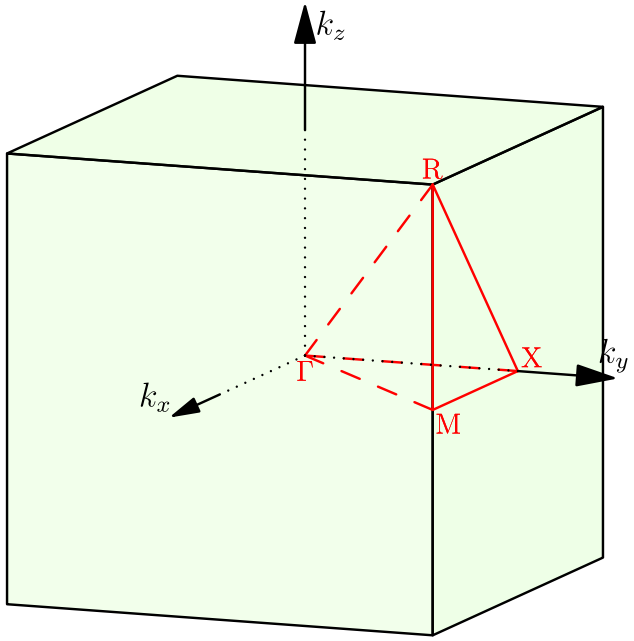


FIG. 2. Brillouin zone of the simple cubic lattice. High symmetry lines and points are also indicated.

IX. THE BRILLOUIN ZONES OF THE SIMPLE CUBIC, FCC AND BCC LATTICES

The Brillouin zones of the three lattices chosen for this exercise are shown in the following Figs. 2, 4, and 6. In the same figures we also indicate a few high symmetry lines and some points of high symmetry.

The path that one can choose in the simple cubic case is Γ – X – M – Γ – R. The coordinates of these points are written in Fig. 3 and can be easily verified for a cubic lattice.

The path needed to reproduce Fig.9.5 of Ascroft and Mermin with the free electron bands of the fcc lattice is Γ – X – W – L – Γ – K – X. The positions of these points are shown in Fig. 4. The coordinates of these points can be easily found noticing that the plane passing through L bisects the vector $\mathbf{G}_{111} = (1, 1, 1)$ and is perpendicular to it. Therefore it has equation:

$$k_x + k_y + k_z = 3/2, \tag{30}$$

and it crosses the plane $k_z = 0$, along the line

$$k_x + k_y = 3/2, \quad k_z = 0. \tag{31}$$

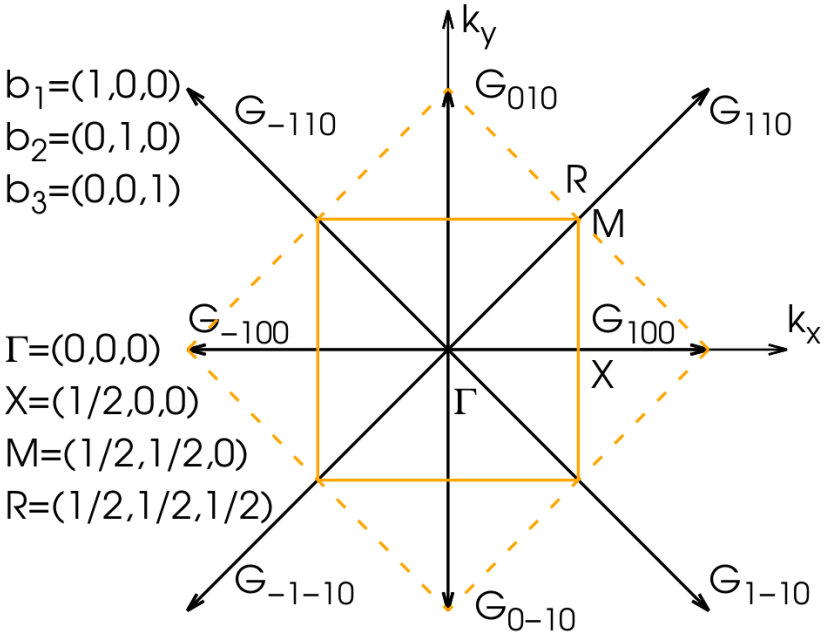


FIG. 3. View of the simple cubic Brillouin zone in the k_x-k_y plane. **k** points coordinates and reciprocal lattices are given in units of $\frac{2\pi}{a}$.

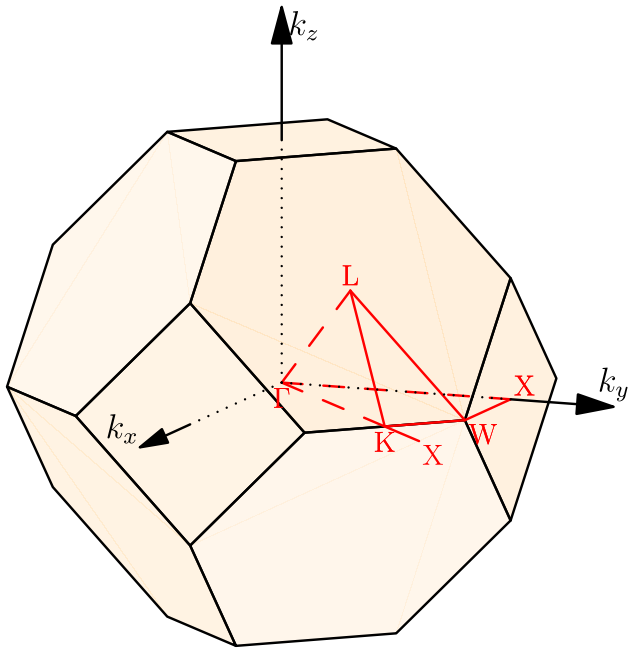


FIG. 4. Brillouin zone of the face-centered cubic lattice. High symmetry lines and points are also indicated.

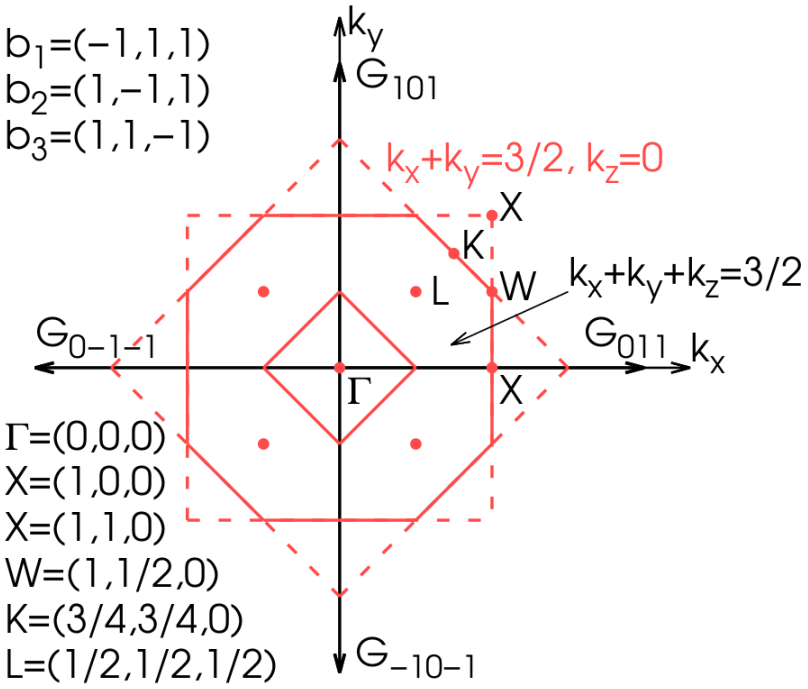


FIG. 5. View of the face-centered cubic Brillouin zone in the k_x-k_y plane. **G** vectors are indicated with the notation $\mathbf{G}_{m_1m_2m_3}$.**k** points Cartesian coordinates and primitive reciprocal lattices are given in units of $\frac{2\pi}{\bar{a}}$.

The plane $k_z = 1$ is instead crossed along the line

$$k_x + k_y = 1/2, \quad k_z = 1. \tag{32}$$

We refer to Fig. 5 for the coordinates of the points.

For the bcc lattice we can choose the path Γ – H – N – Γ – P – H. The position of these points is illustrated in Fig. 6. To find the coordinates of these points we refer to Fig. 7. The plane perpendicular to $\mathbf{G}_{001} = (1, 1, 0)$ is vertical, bisect $\mathbf{G}_{001}$ and has equation:

$$k_x + k_y = 1. \tag{33}$$

Therefore $N = \mathbf{G}_{001}/2 = (1/2, 1/2, 0)$. The plane perpendicular to $\mathbf{G}_{010} = (1, 0, 1)$ that bisect it has equation

$$k_x + k_z = 1. \tag{34}$$

The intersection of the two planes is the set of point that satisfy both equations. P is above N and has $k_x = 1/2$, $k_y = 1/2$ and since it is on the intersection line it must have $k_z = 1/2$. Finally H is the point that bisects the vector $\mathbf{G}_{-111} = (2, 0, 0)$ so $H = \mathbf{G}_{-111}/2 = (1, 0, 0)$.

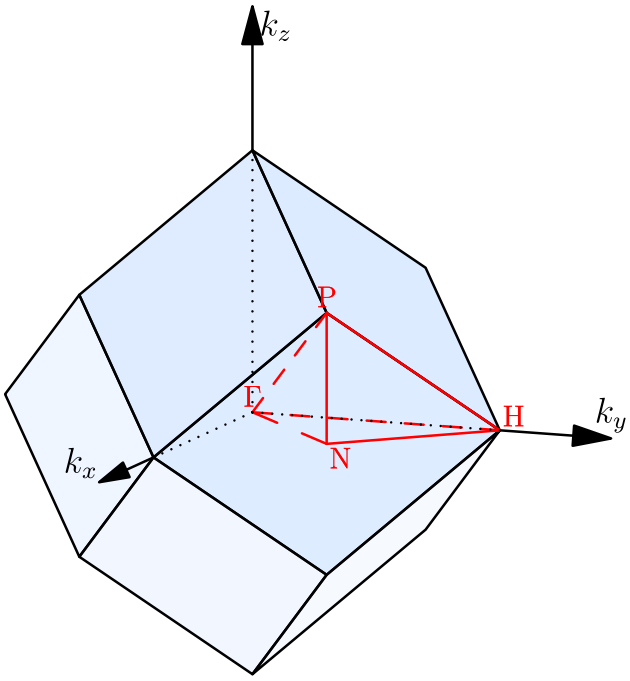


FIG. 6. Brillouin zone of the body centered cubic lattice. High symmetry lines and points are also indicated.

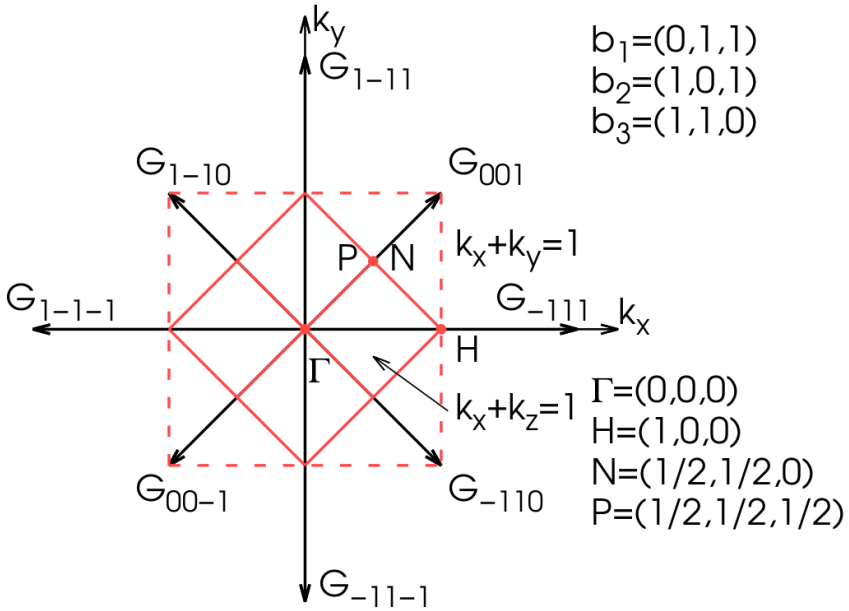


FIG. 7. View of the body-centered cubic Brillouin zone in the k_x-k_y plane. **G** vectors are indicated with the notation $\mathbf{G}_{m_1 m_2 m_3}$. **k** points Cartesian coordinates and primitive reciprocal lattices are given in units of $\frac{2\pi}{a}$.

X. THE G VECTORS GENERATION

To limit the number of $\mathbf{G}$ vectors used in the calculation, one considers a sphere centered at the origin with a given radius $|\mathbf{G}_{max}|$. This sphere must encompass all spheres of radius $\sqrt{E_{cut}}$ centered at the various $\mathbf{k}$ points. Given the maximum value of the modulus of $\mathbf{k}$, $|\mathbf{k}_{max}|$, it is easy to see that we should take $|\mathbf{G}_{max}| \geq |\mathbf{k}_{max}| + \sqrt{E_{cut}}$.

We generate all $\mathbf{G}$ vectors using the expression:

$$\mathbf{G}_{m_1,m_2,m_3} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3 \tag{35}$$

This raises the question: what range of m_1, m_2, and m_3 is necessary to generate all $\mathbf{G}$ vectors contained within a sphere of radius $|\mathbf{G}_{max}|$? Let us first consider the range for m_1. By varying m_2 and m_3, we generate a family of lattice planes perpendicular to the direct lattice vector $\mathbf{a}_1$. The distance between adjacent planes in this family is given by $\frac{2\pi}{|\mathbf{a}_1|}$. Consequently, within the radius $|\mathbf{G}_{max}|$, we have $\frac{|\mathbf{G}_{max}||\mathbf{a}_1|}{2\pi}$ positive values for m_1 and an equal number of negative values must be sampled to contain all the sphere.

Similarly, the possible positive values for m_2 will be $\frac{|\mathbf{G}_{max}||\mathbf{a}_2|}{2\pi}$, and those for m_3 will be $\frac{|\mathbf{G}_{max}||\mathbf{a}_3|}{2\pi}$.

Since within the code $|\mathbf{G}_{max}|$ is expressed in units of $\frac{2\pi}{\bar{a}}$ and $|\mathbf{a}_1|$ in units of $\bar{a}$, the factor of 2π in the denominator is omitted.

TABLE I. Fermi level as a function of the number of electrons in the unit cell.

N_{el}	sc ($\alpha = 1$)	fcc ($\alpha = 4$)	bcc ($\alpha = 2$)
1	0.2424	0.6109	0.3848
2	0.3848	0.9697	0.6109
3	0.5043	1.2707	0.8005
4	0.6109	1.5393	0.9697

XI. COMPUTATION OF THE FERMI LEVEL.

Suppose there are N_{el} electrons in the unit cell. To calculate the radius of the Fermi sphere, denoted by k_F, we note that it encloses a volume $\Omega_F = \frac{4\pi}{3}k_F^3$. Since each $\mathbf{k}$ point occupies a volume of $\frac{(2\pi)^3}{N\Omega}$, the total number of available states (accounting for a factor of two for spin) is:

$$\frac{8\pi k_F^3 N\Omega}{3(2\pi)^3}. \tag{36}$$

Equating this to the total number of electrons NN_{el}, we obtain:

$$k_F = \left(\frac{3\pi^2 N_{el}}{\Omega}\right)^{1/3}. \tag{37}$$

Expressing the unit cell volume as $\Omega = \frac{a^3}{\alpha}$, where $\alpha = 1, 4$, and 2 for the simple cubic, fcc, and bcc cases, respectively, we have:

$$E_F = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left(\frac{3\alpha N_{el}}{8\pi}\right)^{2/3}. \tag{38}$$

Thus, in units of Rydberg times $(\frac{2\pi}{\bar{a}})^2$, the Fermi energy to be plotted in the graph is:

$$E_F = \left(\frac{3\alpha N_{el}}{8\pi}\right)^{2/3}. \tag{39}$$

The values of the Fermi level for the three lattices, corresponding to $N_{el} = 1, 2, 3, 4$ electrons, are summarized in Table I.

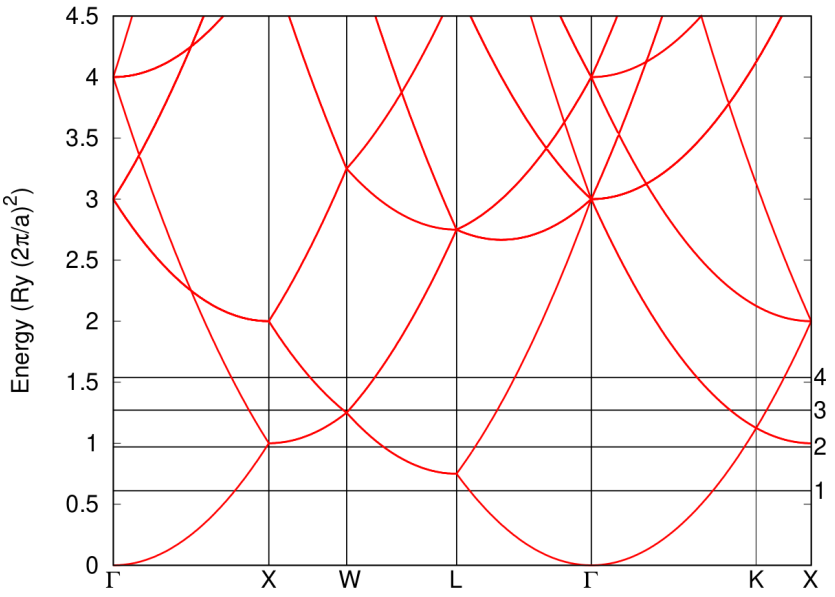


FIG. 8. Free electron bands of the fcc lattice produced by the code.

XII. FREE ELECTRON BANDS OF THE FCC LATTICE

The free electron bands of the fcc lattice are shown in Fig. 8