Empty lattice approximation

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: March 21, 2018)

1. Empty lattice approximation

Actual band structures are usually exhibits as a plot of energy vs wavevector in the first Brillouin zone.

When band energies are approximated fairly well by electron energies

$$\varepsilon_k = \frac{\hbar^2}{2m}\boldsymbol{k}^2$$

It is advsable to start a calculation by carrying the free electron energies back into the first zone. We look for a reciprocal lattice vector $\boldsymbol{G}$ such that

$$\boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{G}$$

where $\boldsymbol{k}'$ is unrestricted and is the true wavevector in the empty lattice,

$$\begin{aligned}\varepsilon_G(\boldsymbol{k}) &= \frac{\hbar^2}{2m}\boldsymbol{k}'^2 \\ &= \frac{\hbar^2}{2m}(\boldsymbol{k} \pm \boldsymbol{G})^2 \\ &= \frac{\hbar^2}{2m}[(k_x \pm G_x)^2 + (k_y \pm G_y)^2 + (k_z \pm G_z)^2]\end{aligned} \quad .$$

with $\boldsymbol{k}$ in the first Brillouin zone and G allowed to run over the appropriate reciprocal lattice points.

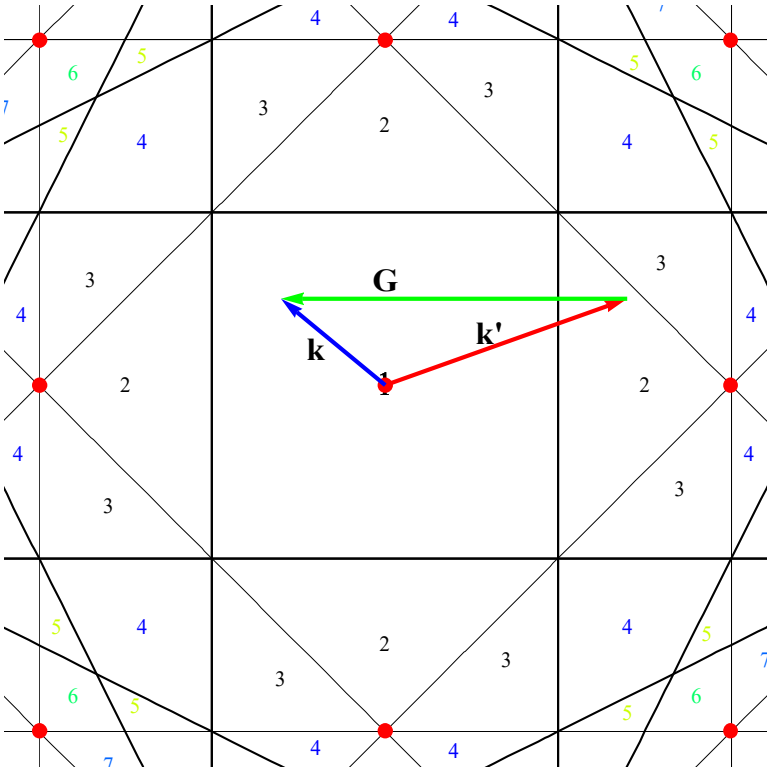


Fig. The Brillouin zone for the 2D square lattice. $\boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{G}$.

2. SC (simple cubic)

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta), \qquad \text{(Cartesian coordinate)}$$

with ξ, η, and, ζ are between -1/2 and 1/2, and

$$\boldsymbol{G} = \frac{2\pi}{a}(h, k, l) = \frac{2\pi}{a}(n_1, n_2, n_3) \qquad \text{(Cartesian coordinate)}$$

with $h = n_1$, $k = n_2$, and, $l = n_3$ are integers.

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2$$
$$= \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 [(\xi - n_1)^2 + (\eta - n_2)^2 + (\varsigma - n_3)^2]$$

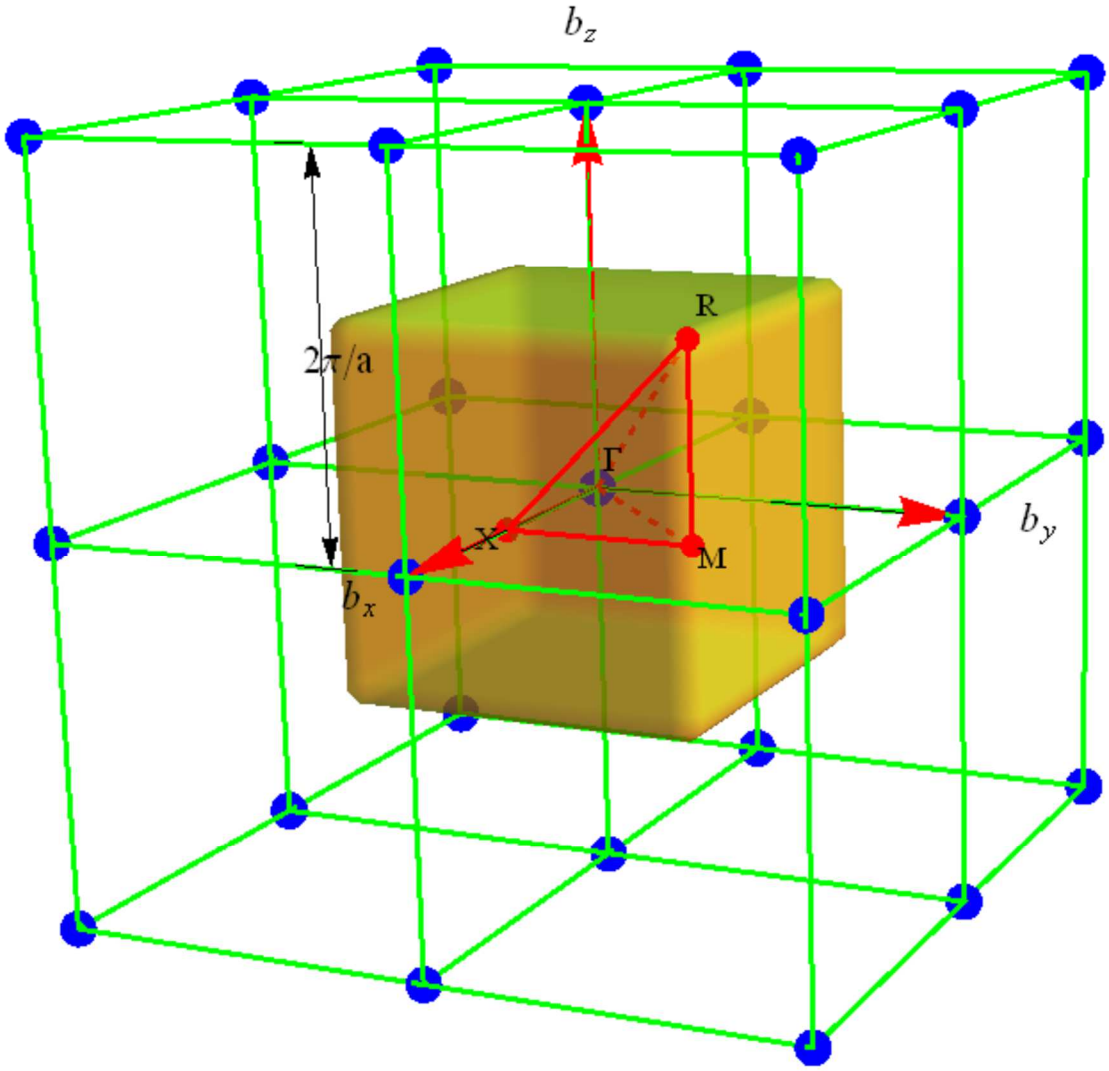


Fig. First Brillouin zone for the simple cubic lattice.

(a) ΓM

$\xi = \eta$, and $\zeta = 0$. $\quad 0 \le \xi \le \frac{1}{2}$.

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{G})^2$$
$$= \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 [(\xi - n_1)^2 + (\xi - n_2)^2 + n_3{}^2]$$

with

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 .$$

(b) MX

$\xi = 1/2$, $\zeta = 0$, and η changes from 1/2 to 0.

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{G})^2$$
$$= \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 [(\frac{1}{2}-n_1)^2 + (\eta - n_2)^2 + {n_3}^2]$$

(c) XΓ

$\eta = \zeta = 0$, and ξ changes from 1/2 to 0.

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{G})^2$$
$$= \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 [(\xi - n_1)^2 + {n_2}^2 + {n_3}^2]$$

4. Numerical calculation (sc)

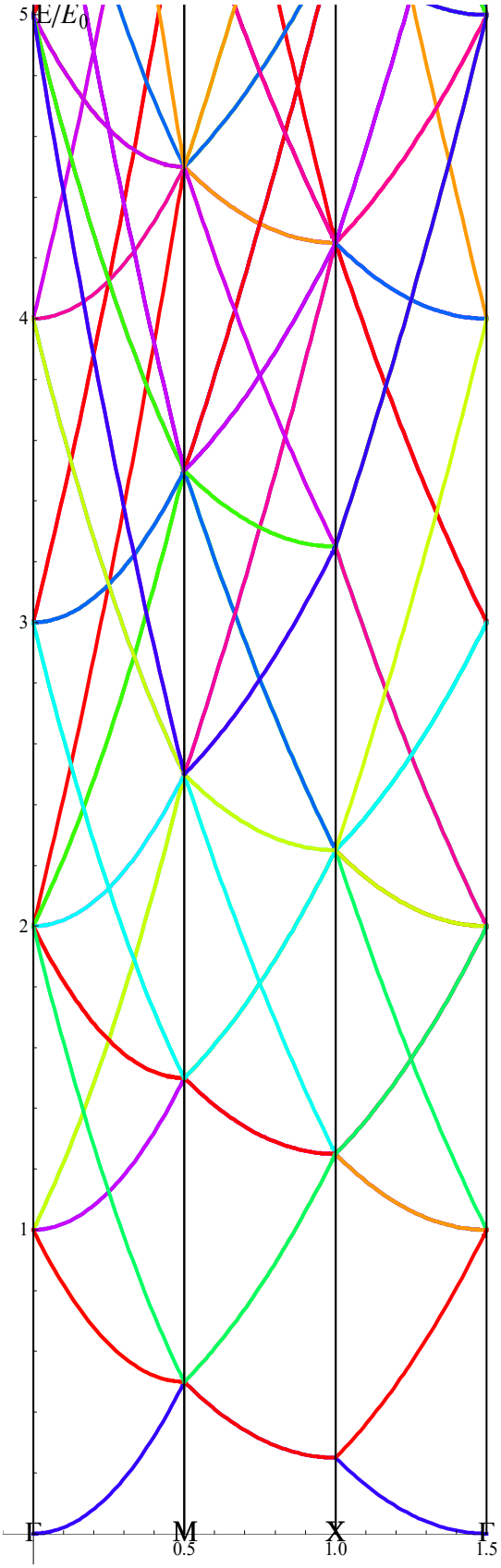

E/E0
5
4
3
2
1
Γ
M
X
Γ
0.5
1.0
1.5

Fig. Energy band of the empty sc lattice along the ΓM, MX, and XΓ line of the first Brillouin zone .

5. fcc (face-centered cubic) lattice

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta), \qquad \text{(Cartesian coordinate)}$$

with ξ, η, and, ζ are between -1/2 and 1/2, and

$$\begin{aligned} \boldsymbol{G} &= \frac{2\pi}{a}(-h+k+l, h-k+l, h+k-l) \\ &= \frac{2\pi}{a}(n_1, n_2, n_3) \end{aligned} \qquad \text{(Cartesian coordinate)}$$

with h, k, and, l are integers.

$$\begin{aligned} \varepsilon_G(\boldsymbol{k}) &= \frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{G})^2 \\ &= \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 [(\xi - n_1)^2 + (\eta - n_2)^2 + (\varsigma - n_3)^2] \end{aligned}$$

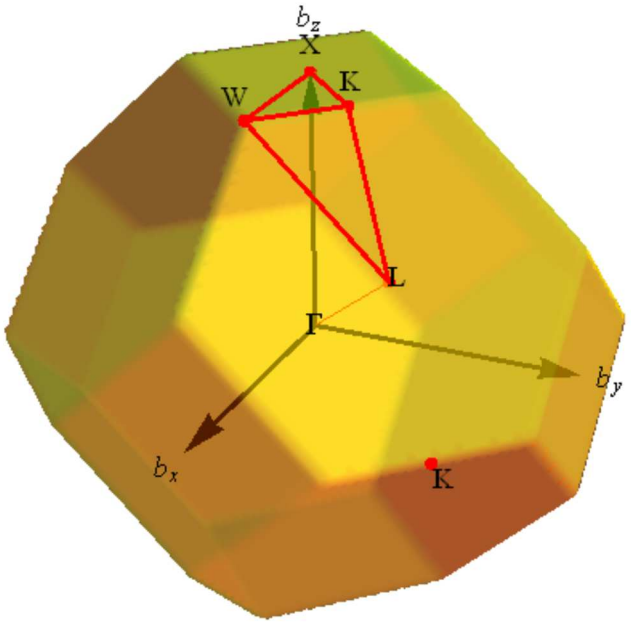


Fig. First Brillouin zone for the fcc lattice. $X = (0,0,1)$, $W=(1/2, 0, 1)$, $L = (1/2, 1/2, 1/2)$, $K = (1/4, 1/4, 1)$ or K = (3/4, 3/4, 0) in the units of $2\pi/a$. $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, $\boldsymbol{b}_z$ are the reciprocal lattice vectors of the conventional unit cell. . $\boldsymbol{b}_x = (2\pi/a)\ (1, 0, 0)$. $\boldsymbol{b}_y = (2\pi/a)\ (0, 1, 0)$. $\boldsymbol{b}_z = (2\pi/a)\ (0, 0, 1)$.

(a) $\Gamma(0,0,0) \rightarrow X(0,0,1)$

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

where

$\xi = 0$ and $\eta = 0$. $0 \le \zeta \le 1$.

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{G})^2$$
$$= E_0[(\xi - n_1)^2 + n_2{}^2 + n_3{}^2]$$

with

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 .$$

(b) X(0,0,1)→W(1/2,0,1)

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

where

$\eta = 0$ and $\zeta = 1$. $0 \le \xi \le 1/2$.

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{G})^2$$
$$= E_0[(\xi - n_1)^2 + n_2{}^2 + (1-n_3)^2]$$

(c) W(1/2,0,1)→L(1/2,1/2,1/2)

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

where

$\zeta = 1 - \eta$ and $\xi = 1/2$. $0 \le \eta \le 1/2$.

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{G})^2$$
$$= E_0[(1/2 - n_1)^2 + (\eta - n_2)^2 + (1-\eta-n_3)^2]$$

(d) Γ(0,0,0)→L(1/2,1/2,1/2)

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

where

$$\xi = \eta = \zeta. \qquad 0 \le \xi \le 1/2 .$$

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2$$
$$= E_0[(1/2 - n_1)^2 + (\eta - n_2)^2 + (1 - \eta - n_3)^2]$$

(e) Γ(0,0,0)→K(3/4,3/4,0)

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

where

$$\xi = \eta,\ \zeta = 0.\ 0 \le \xi \le 3/4 .$$

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2$$
$$= E_0[(\xi - n_1)^2 + (\xi - n_2)^2 + (n_3)^2]$$

(f) K(1/4,1/4,1)→X(0,0,1)

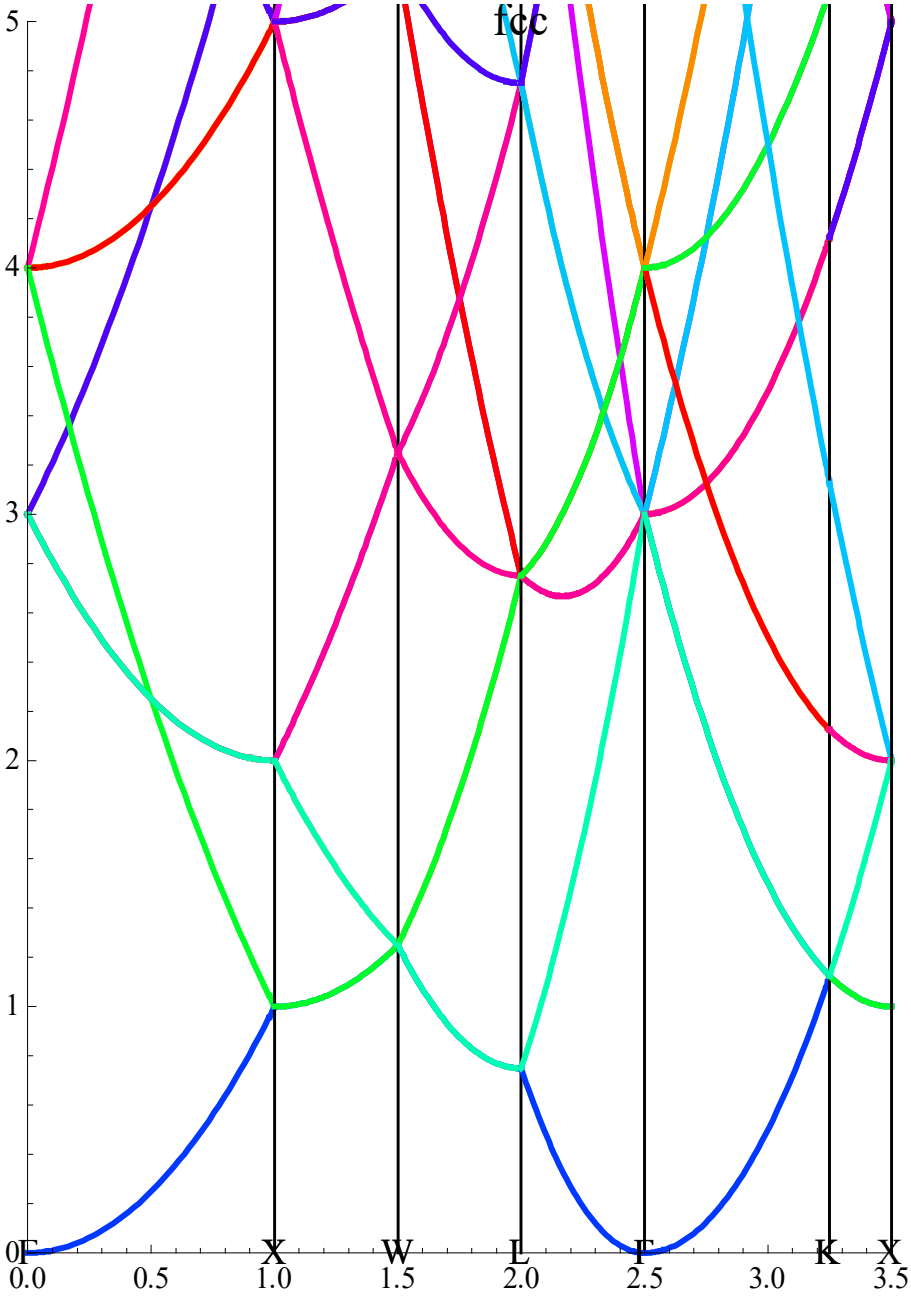
$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

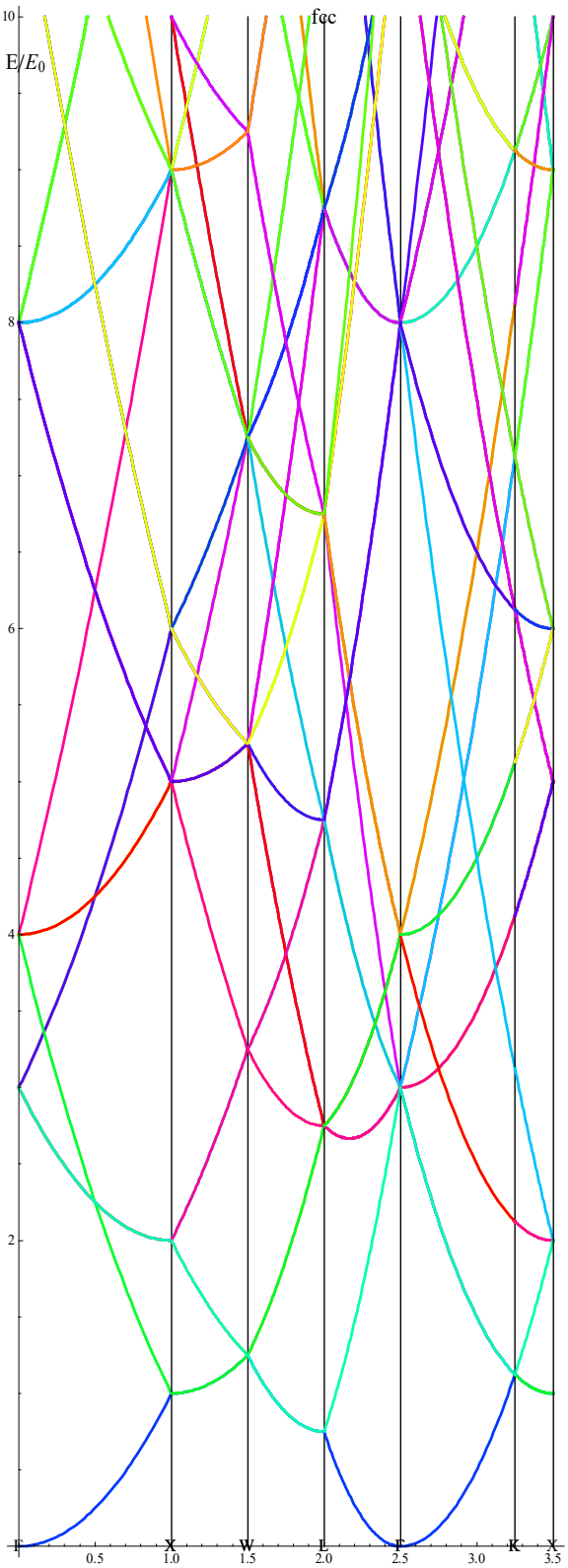
where

$$\xi = \eta,\ \zeta = 1,\ \xi = 1/4 \text{ to } 0.$$

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2$$
$$= E_0[(\xi - n_1)^2 + (\xi - n_2)^2 + (1 - n_3)^2]$$

6. Numerical calculation (fcc)


fcc
5
4
3
2
1
0
Γ
X
W
L
Γ
K
X
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5



7. bcc (body-centered cubic) lattice

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta), \qquad \text{(Cartesian coordinate)}$$

with ξ, η, and, ζ are between -1/2 and 1/2, and

$$\begin{aligned} \boldsymbol{G} &= \frac{2\pi}{a}(k+l, l+h, h+k) \\ &= \frac{2\pi}{a}(n_1, n_2, n_3) \end{aligned} \qquad \text{(Cartesian coordinate)}$$

with h, k, and, l are integers.

$$\begin{aligned} \varepsilon_G(\boldsymbol{k}) &= \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2 \\ &= \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 [(\xi - n_1)^2 + (\eta - n_2)^2 + (\varsigma - n_3)^2] \end{aligned}$$

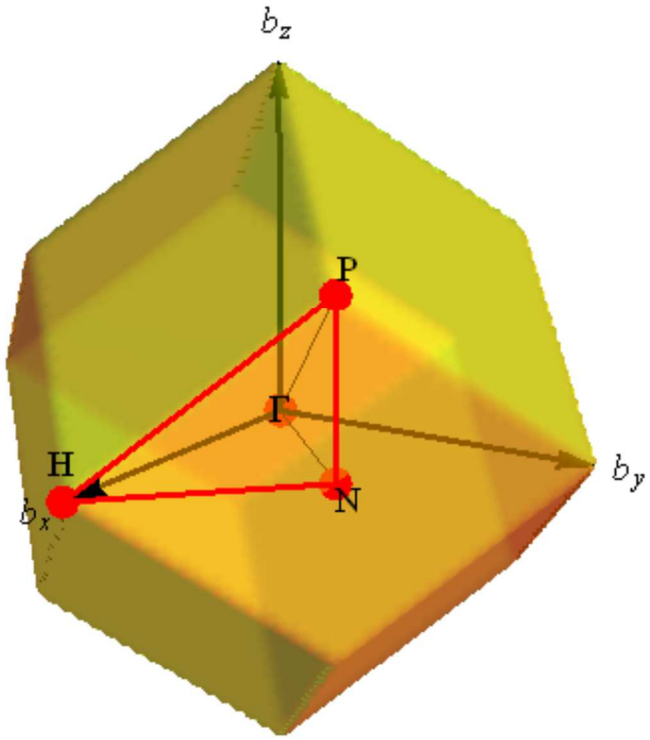


Fig. First Brillouin zone for the bcc lattice. $\Gamma = (0,0,0)$, $H = (1,0,0)$, $N = (1/2, 1/2, 0)$, $P = (1/2, 1/2, 1/2)$, in the units of $2\pi/a$. $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, $\boldsymbol{b}_z$ are the reciprocal lattice vectors of the conventional cubic unit cell. $\boldsymbol{b}_x = (2\pi/a)\ (1, 0, 0)$. $\boldsymbol{b}_y = (2\pi/a)\ (0, 1, 0)$. $\boldsymbol{b}_z = (2\pi/a)\ (0, 0, 1)$.

(a) $\Gamma(0,0,0) \rightarrow H(1,0,0)$

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

where

$\eta = 0$ and $\zeta = 0$. $0 \le \xi \le 1$.

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2$$
$$= E_0[(\xi - n_1)^2 + n_2{}^2 + n_3{}^2]$$

with

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2.$$

(b) $H(1,0,0) \rightarrow P(1/2,1/2,1/2)$

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

where

$$\boldsymbol{\xi} = 1 - \eta,\ \eta = \zeta.\ 0 \le \eta \le 1/2.$$

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2$$
$$= E_0[(1 - \eta - n_1)^2 + (\eta - n_2)^2 + (\eta - n_3)^2]$$

(c) $P(1/2,1/2,1/2) \rightarrow \Gamma(0,0,0)$

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

where

$\xi = \eta = \zeta$, where ξ changes from 1/2 to 0

$$\varepsilon_G(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2$$
$$= E_0[(\xi - n_1)^2 + (\xi - n_2)^2 + (\xi - n_3)^2]$$

(d) $\Gamma(0,0,0) \rightarrow N(1/2,1/2,0)$

$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

where

$$\xi = \eta,\ \zeta = 0 \le \xi \le 1/2 .$$

$$\begin{aligned} \varepsilon_G(\boldsymbol{k}) &= \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2 \\ &= E_0[(\xi - n_1)^2 + (\xi - n_2)^2 + (n_3)^2] \end{aligned}$$

(e) $N(1/2,1/2,0) \rightarrow H(1,0,0)$

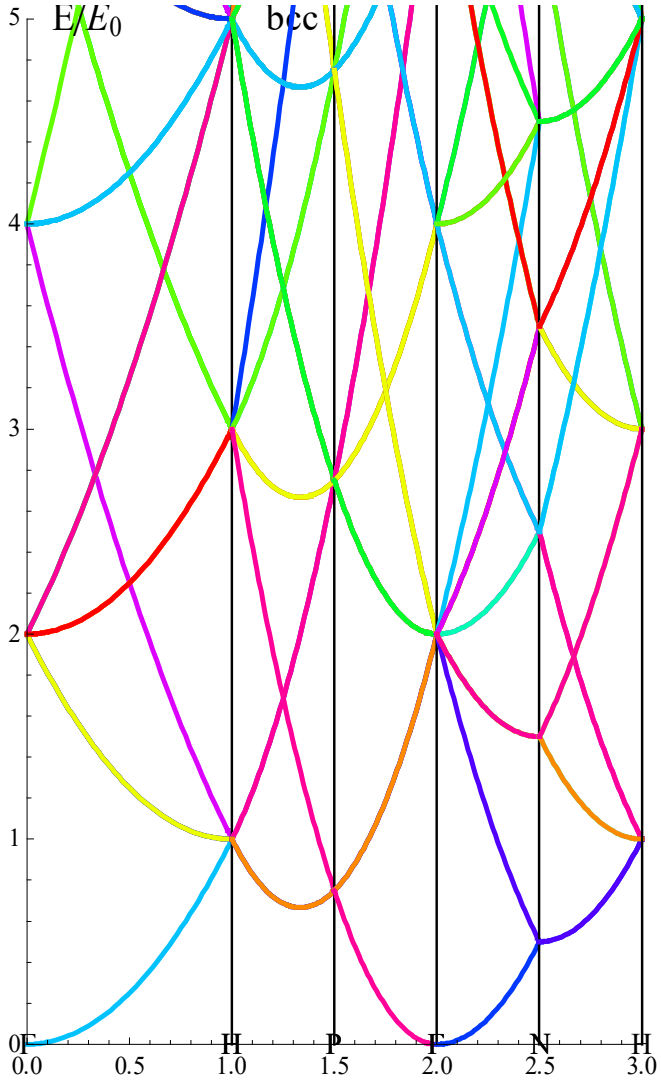
$$\boldsymbol{k} = \frac{2\pi}{a}(\xi, \eta, \zeta),$$

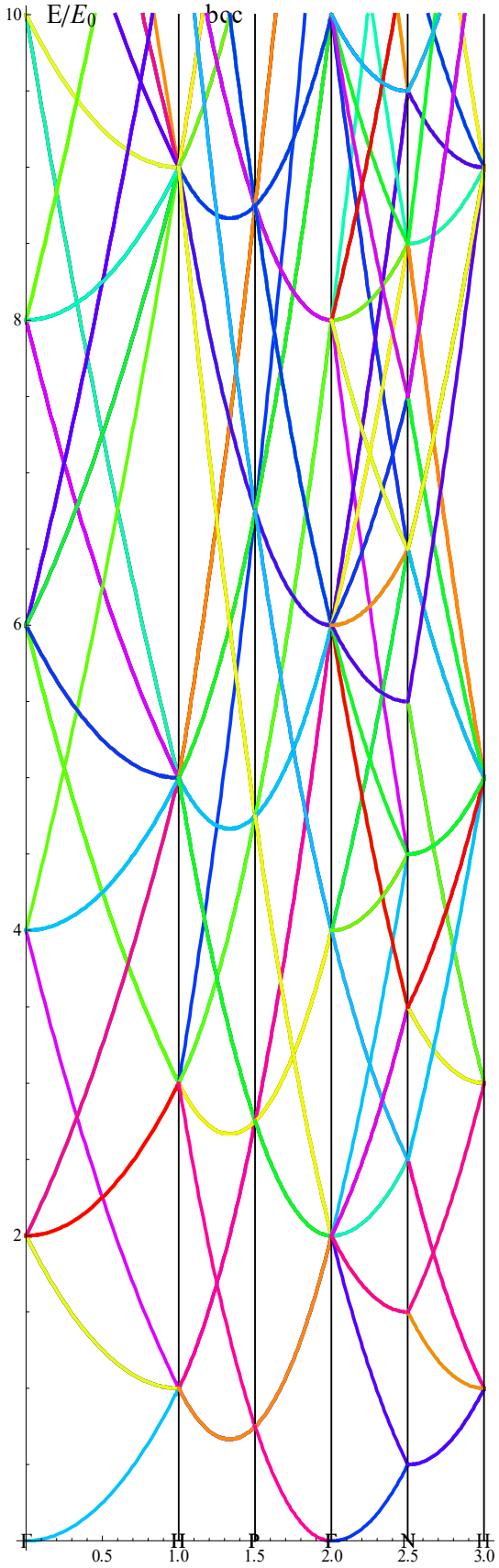
where

$$\xi + \eta = 1,\ \zeta = 0.\ 1/2 \le \xi \le 1.$$

$$\begin{aligned} \varepsilon_G(\boldsymbol{k}) &= \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{G})^2 \\ &= E_0[(\xi - n_1)^2 + (1 - \xi - n_2)^2 + (n_3)^2] \end{aligned}$$

8. Numerical calculation for bcc


E/E0
bcc
5
4
3
2
1
0
Γ
H
P
Γ
N
H
0.0
0.5
1.0
1.5
2.0
2.5
3.0


E/E_0
bcc
10
8
6
4
2
Γ
H
P
Γ
N
H
0.5
1.0
1.5
2.0
2.5
3.0

9. Radius of Fermi sphere for the fcc lattice

Fermi wavenumber k_F:

$$2\frac{V}{(2\pi)^3}\frac{4\pi}{3}{k_F}^3 = \frac{V}{V_c}n\,,$$

where

n: electrons per primitive cell (fcc), or number of electrons per atom.
V_c: volume of primitive cell (fcc)

$$V_c = \frac{1}{4}a^3\,.$$

Then we get

$$2\frac{1}{(2\pi)^3}\frac{4\pi}{3}{k_F}^3 = \frac{4}{a^3}n$$

or

$${k_F}^3 = \frac{12\pi^2}{a^3}n$$

or

$$k_F = \frac{2\pi}{a}\left(\frac{3n}{2\pi}\right)^{1/3}$$

The Fermi energy is

$$\varepsilon_F = \frac{\hbar^2}{2m}{k_F}^2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left(\frac{3n}{2\pi}\right)^{2/3} = E_0\left(\frac{3n}{2\pi}\right)^{2/3}$$

with

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 .$$

In summary,

$$\frac{\varepsilon_F}{E_0} = \left(\frac{3n}{2\pi}\right)^{2/3}$$

Table

n	$(\frac{3n}{2\pi})^{2/3}$
1	0.610887
2	0.969723
3	1.2707
4	1.53934
5	1.78624
6	2.0171
7	2.23542
8	2.44355
9	2.64315
10	2.83549
11	3.0215
12	3.20195
13	3.37746
14	3.54851
15	3.71554

10. Radius of Fermi sphere for the bcc lattice

Fermi wavenumber k_F:

$$2\frac{V}{(2\pi)^3}\frac{4\pi}{3}k_F{}^3 = \frac{V}{V_c}n ,$$

where

n: electrons per primitive cell (bcc), or number of electrons per atom.
V_c: volume of primitive cell (fcc)

$$V_c = \frac{1}{2}a^3 .$$

Then we get

$$2\frac{1}{(2\pi)^3}\frac{4\pi}{3}k_F{}^3 = \frac{2}{a^3}n$$

or

$$k_F{}^3 = \frac{6\pi^2}{a^3}n$$

or

$$k_F = \frac{2\pi}{a}\left(\frac{3n}{4\pi}\right)^{1/3}$$

The Fermi energy is

$$\varepsilon_F = \frac{\hbar^2}{2m}k_F{}^2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left(\frac{3n}{4\pi}\right)^{2/3} = E_0\left(\frac{3n}{4\pi}\right)^{2/3}$$

with

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2.$$

In summary,

$$\frac{\varepsilon_F}{E_0} = \left(\frac{3n}{4\pi}\right)^{2/3}$$

Table

n	$\left(\frac{3n}{4\pi}\right)^{2/3}$
1	0.384835
2	0.610887
3	0.800488
4	0.969723
5	1.12526
6	1.2707
7	1.40823
8	1.53934
9	1.66508
10	1.78624
11	1.90343
12	2.0171
13	2.12766
14	2.23542
15	2.34064

11. Energy band of real systems: comparison with the empty lattice approximation

(i) Na (bcc)

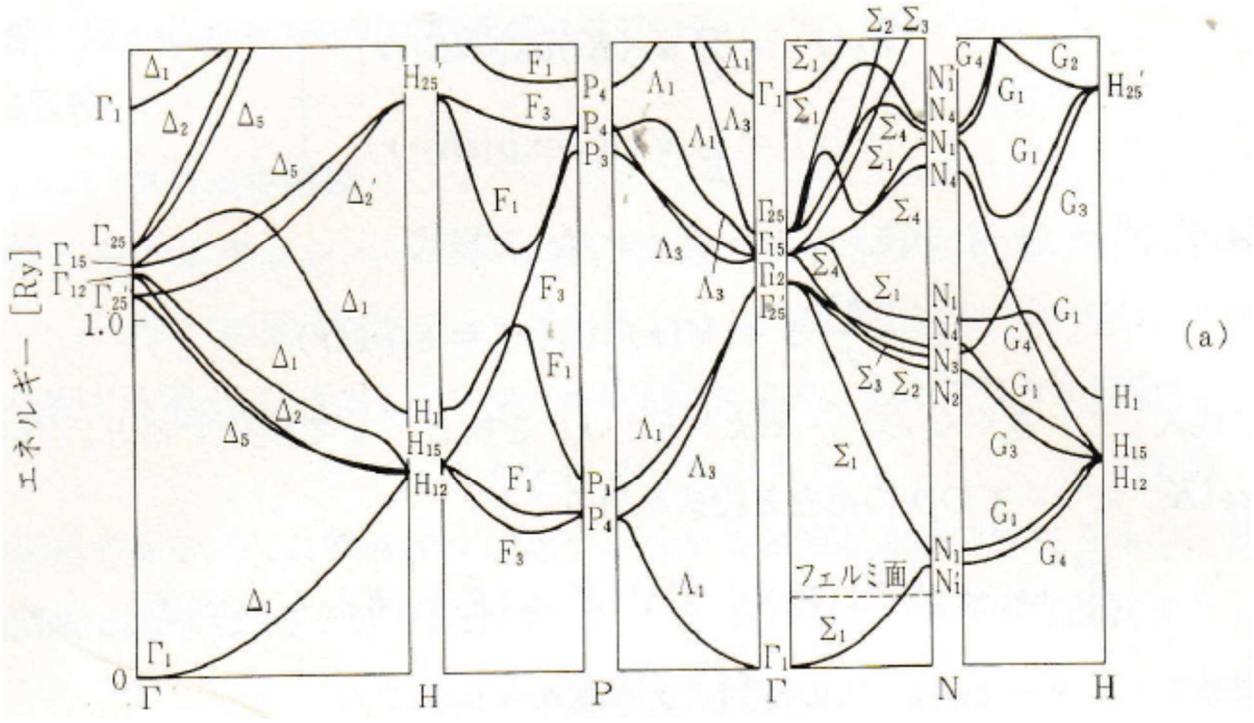


Fig. Energy dispersion of Na (bcc). J. Yamashita, The theory of Electrons in Metals (Asakura, 1973, in Japanese)

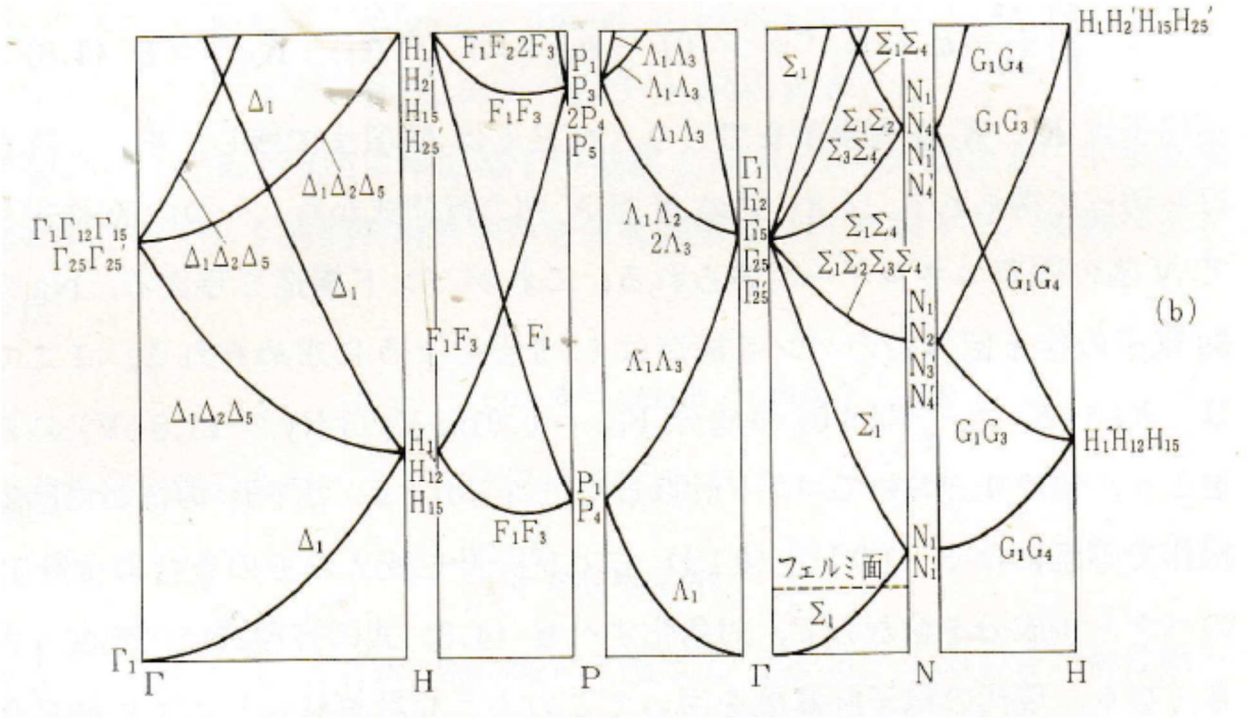


Fig. Energy dispersion (the empty lattice approximation) for thr bcc metal. J. Yamashita, The Theory of Electrons in Metals (Asakura, 1973, in Japanese)

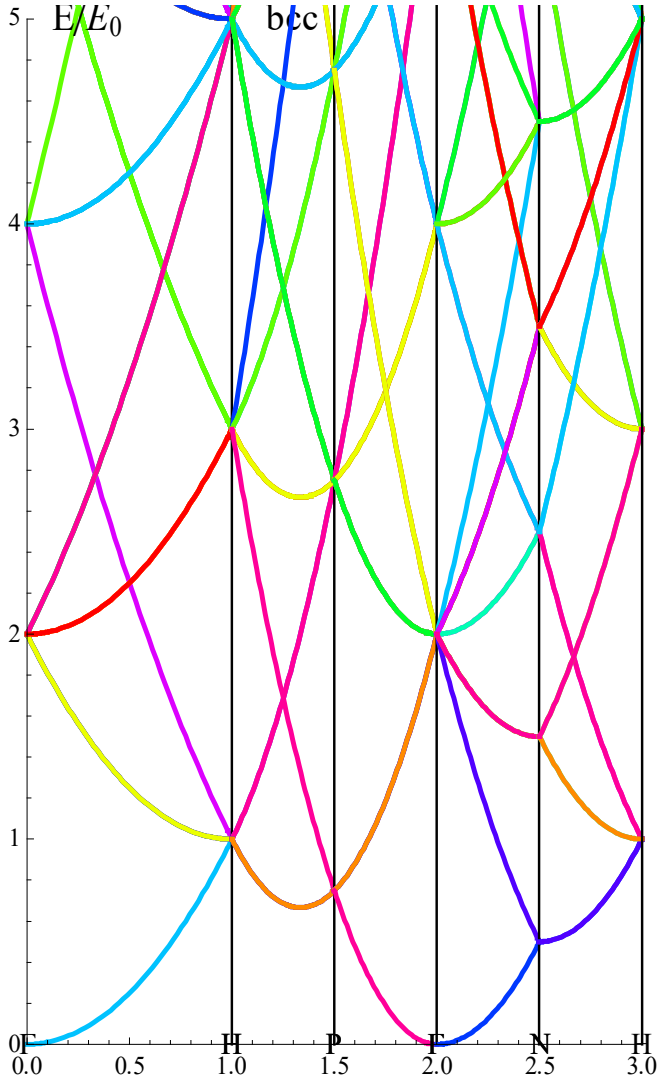


Fig. Energy dispersion of bcc from the empty lattice approximation (the present result).

(ii) Al (fcc)

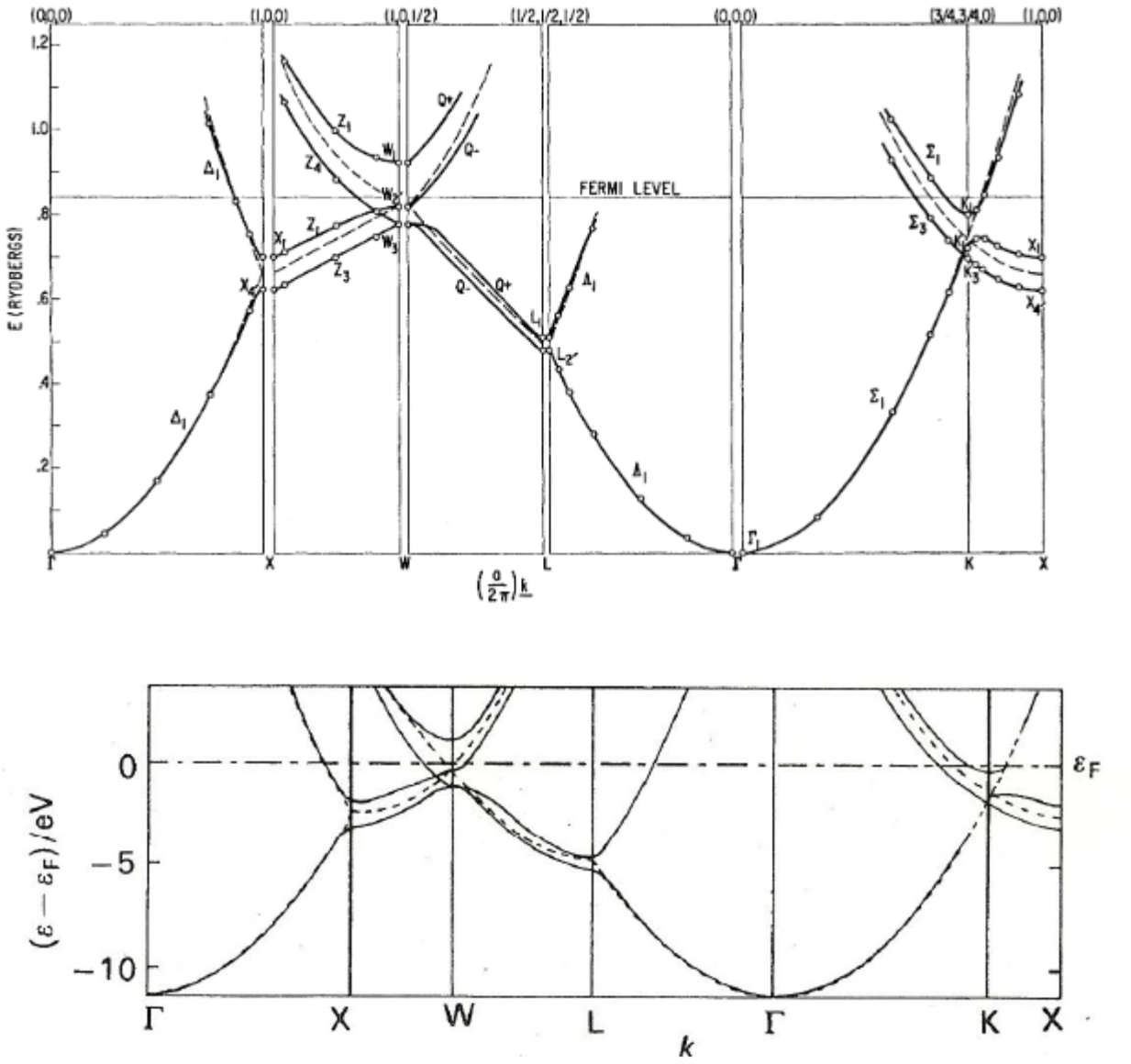


Fig. Energy dispersion of Al (fcc, full lines) compared with the free electron fcc metal (broken lines) [After Segal (1961), Phys. Rev.124, 1797]. R.G. Chambers, Electrons in Metals and Semiconductors (Chapman and Hall, 1990).

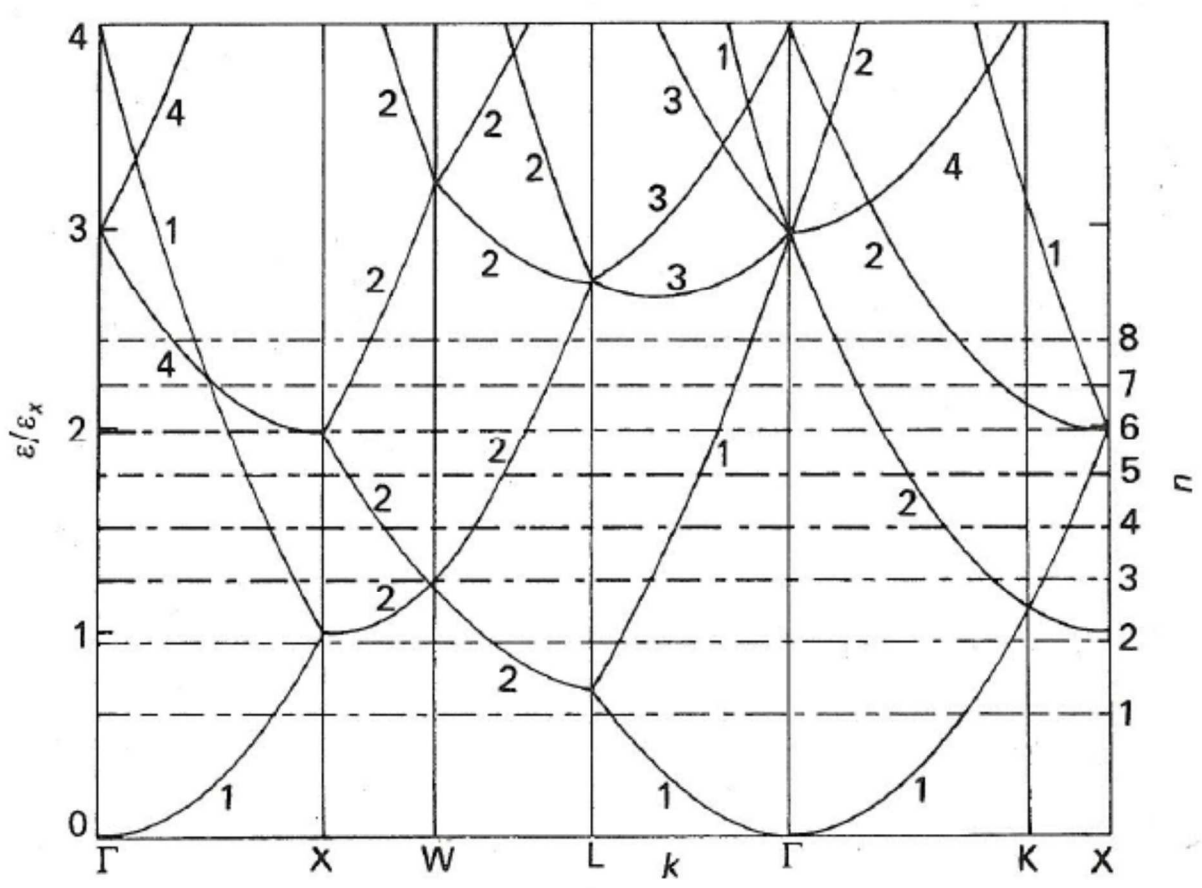


Fig. Energy dispersion of free electron fcc metal (empty lattice approximation) [Herman (1967), in An Atomic Approach to the Nature and Properties of Materials (ed. Pask), Wiley, New York]. R.G. Chambers, Electrons in Metals and Semiconductors, Chapman and Hall, 1990.

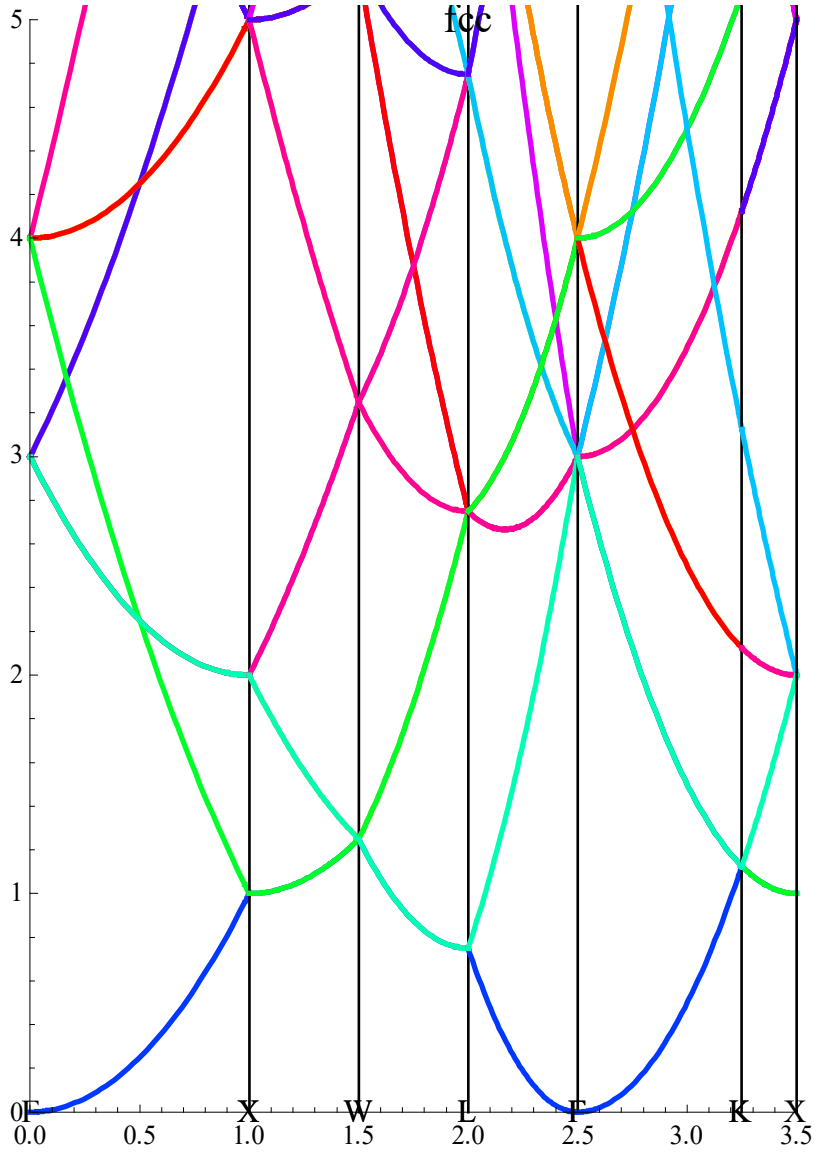


Fig. Energy dispersion of fcc from the empty lattice approximation (the present result).

APPENDIX

2D square lattice

$$\varepsilon = \frac{\hbar^2}{2m}[(k_x - \frac{2\pi}{a}h)^2 + (k_y - \frac{2\pi}{a}k)^2]$$

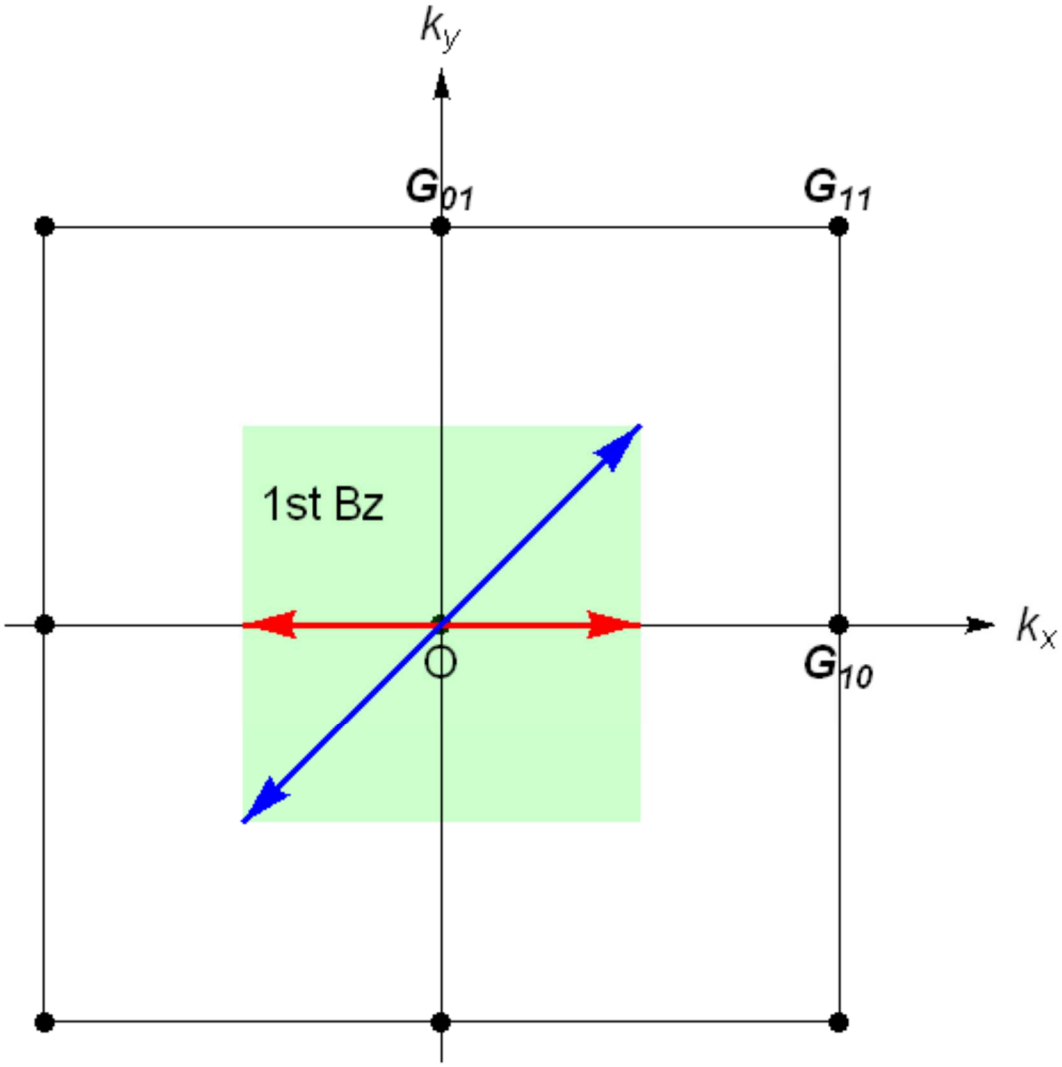
Here we put

$$k_x = \frac{2\pi}{a}\xi, \quad k_y = \frac{2\pi}{a}\eta,$$

Thus we have the resulting energy dispersion as

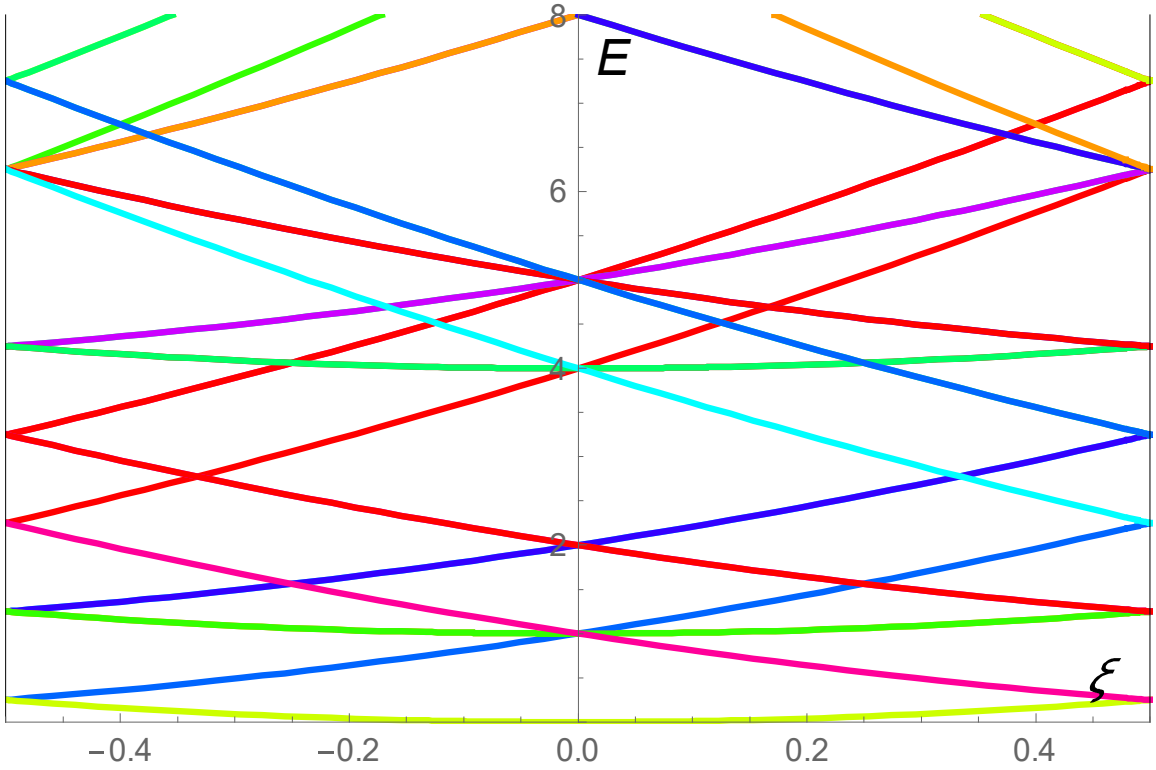
$$E(\xi,\eta)=\frac{1}{\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2}\sum_{h,k}[(\xi-h)^2+(\eta-k)^2]$$

where $h=0,\ \pm1,\ \pm2,....$, and $k=0,\ \pm1,\ \pm2,....$



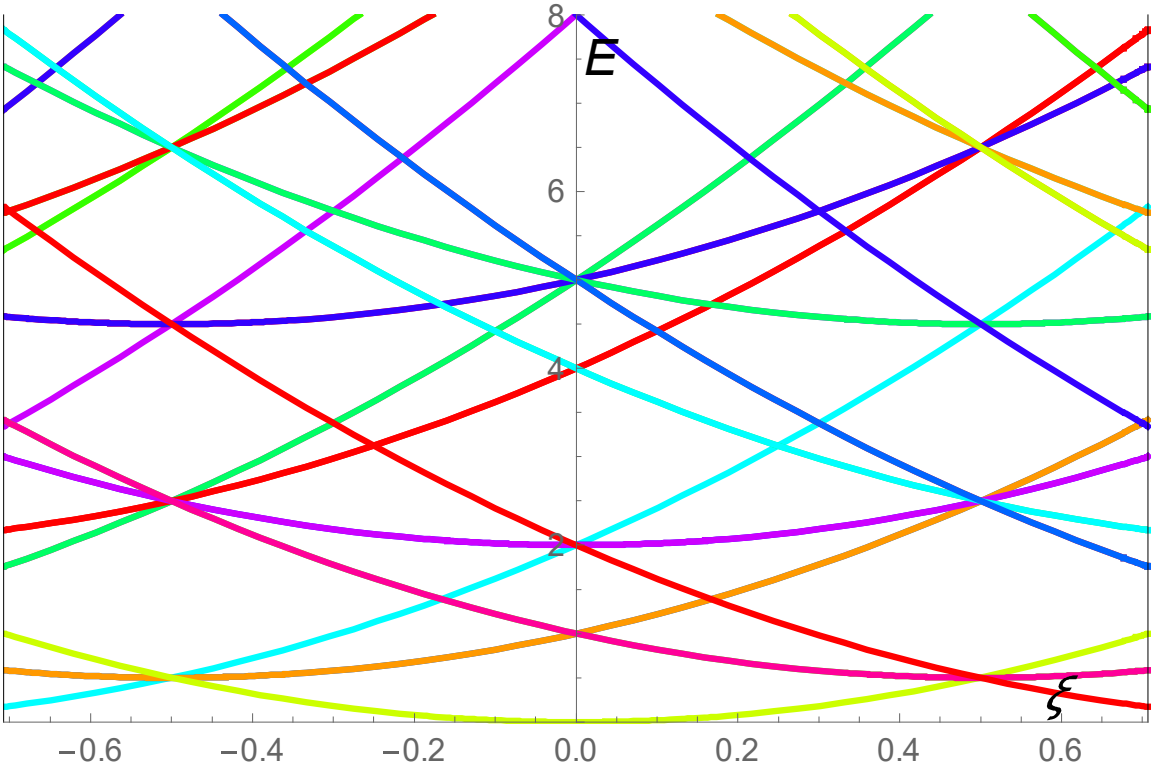
(a) Energy dispersion along the $(k_x,0)$ direction (denoted by red arrow)

We make a plot of $E(\xi,0)$ as s function of ξ for $|\xi|\le\frac{1}{2}$



(b) Energy dispersion along the (k_x, k_x) direction (denoted by blue arrow)

We make a plot of $E(\xi,\xi)$ as s function of ξ for $|\xi| \le \frac{\sqrt{2}}{2}$


E
8
6
4
2
ξ
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6