**Band structure**

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We consider the band structure of the sc, fcc, and bcc lattices.

## 1. sc lattice

$$2\frac{V}{(2\pi)^3}\frac{4\pi}{3}k_F{}^3 = p\frac{V}{a^3}$$

or

$$k_F = \frac{2\pi}{a}\left(\frac{3p}{8\pi}\right)^{1/3}, \qquad \varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left(\frac{3p}{8\pi}\right)^{2/3}$$

where $k_F$ is the Fermi wavenumber, $\varepsilon_F$ is the Fermi energy, $V$ is the volume, and $p$ is the number of electrons per atom.

## 2. fcc lattice

$$2\frac{V}{(2\pi)^3}\frac{4\pi}{3}k_F{}^3 = 4p\frac{V}{a^3}$$

or

$$k_F = \frac{2\pi}{a}\left(\frac{3p}{2\pi}\right)^{1/3}, \qquad \varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left(\frac{3p}{2\pi}\right)^{2/3} = E_0\left(\frac{3p}{2\pi}\right)^{2/3}$$

where $p$ is the number of electrons per atom and $E_0$ is defined by

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

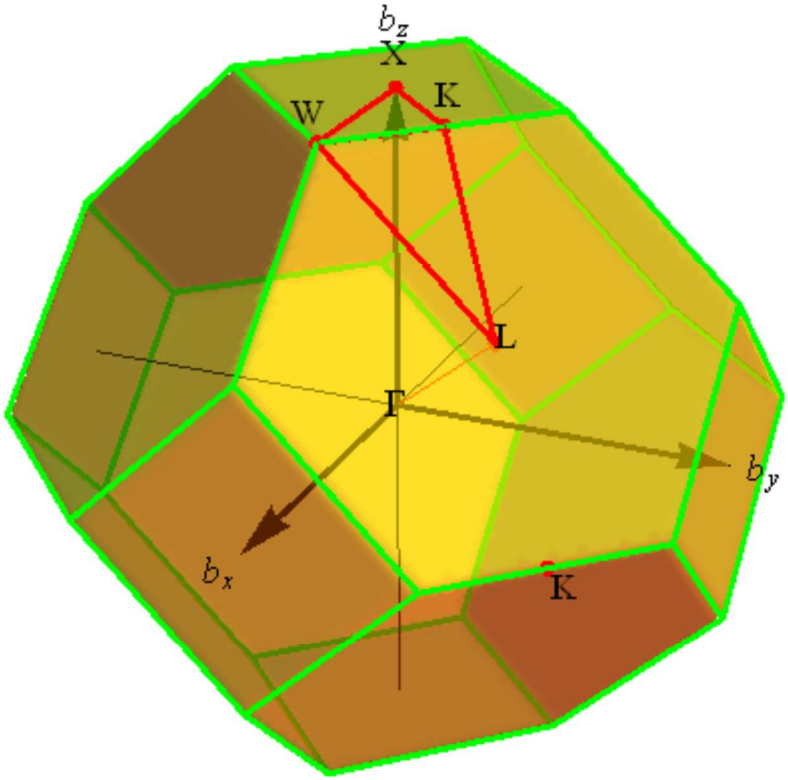
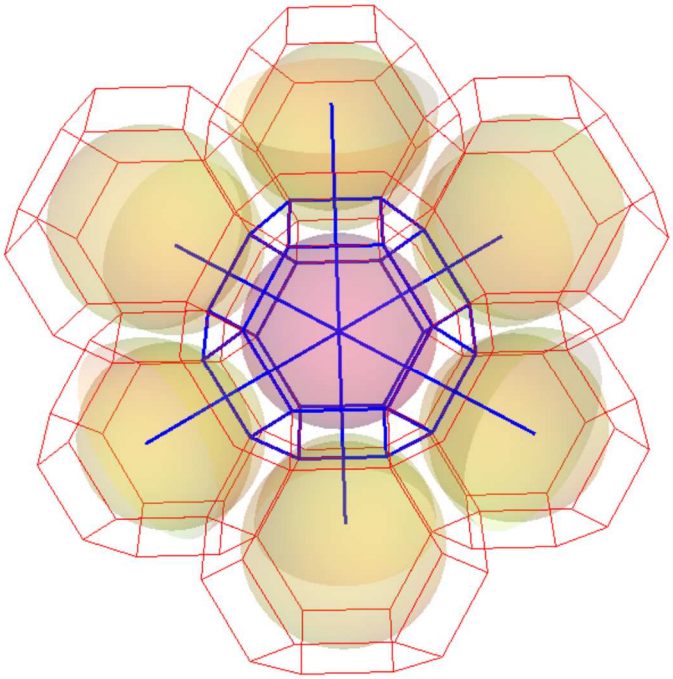



**Fig.** Brillouin zone of the fcc lattice. ***X*** = (0,0,1), ***W*** = (1/2, 0, 1), ***L*** = (1/2, 1/2, 1/2), ***K*** = (1/4, 1/4, 1) or ***K*** = (3/4, 3/4, 0). $\Gamma L = \sqrt{3}/2 = 0.866$, in the units of $2\pi/a$.

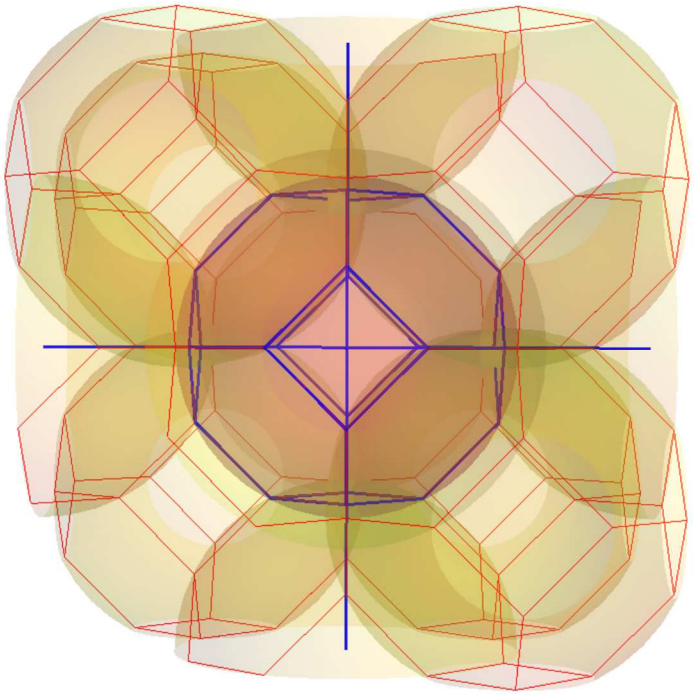
**Table** $k_F/(2\pi/a)$ and $\varepsilon_F / E_0$ for the fcc lattice

| p | $k_F/(2\pi/a)$ | $\epsilon/E_0$ |
|---|---|---|
| 1. | 0.781593 | 0.610887 |
| 2. | 0.984745 | 0.969723 |
| 3. | 1.12725 | 1.2707 |
| 4. | 1.2407 | 1.53934 |
| 5. | 1.3365 | 1.78624 |
| 6. | 1.42025 | 2.0171 |
| 7. | 1.49513 | 2.23542 |
| 8. | 1.56319 | 2.44355 |
| 9. | 1.62578 | 2.64315 |
| 10. | 1.68389 | 2.83549 |

(1) $p = 1$



(2) $p = 3$



W.A. Harrison Phys. Rev. **118**, 1190 (1960).

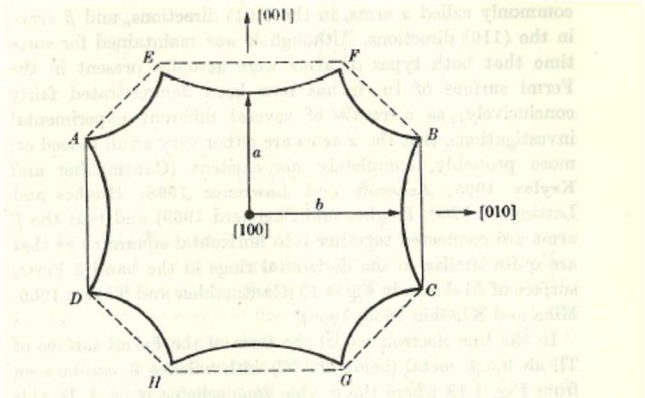



FIG. 4.17. Cross section of the free-electron Fermi surface of In in band 2 (Rayne 1963).

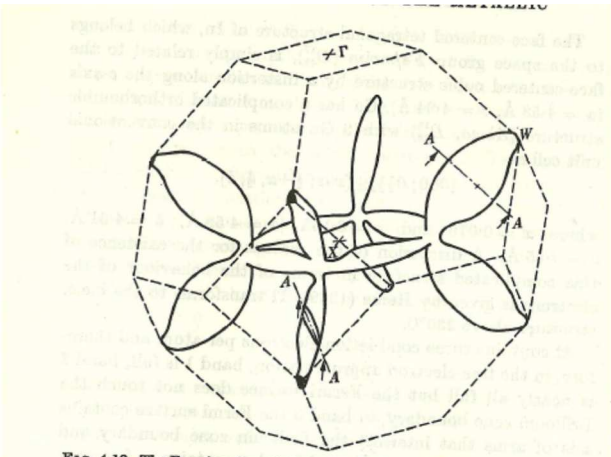



FIG. 4.12. The Fermi surface of electrons of Al in band 3 proposed by Harrison (1959); note that $X$ and not $\Gamma$ is at the centre of the zone.

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## 3. bcc lattice

$$2\frac{V}{(2\pi)^3}\frac{4\pi}{3}k_F{}^3 = 2p\frac{V}{a^3}$$

or

$$k_F = \frac{2\pi}{a}\left(\frac{3p}{4\pi}\right)^{1/3}, \qquad \varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left(\frac{3p}{4\pi}\right)^{2/3} = E_0\left(\frac{3p}{4\pi}\right)^{2/3}$$

where $p$ is the number of electrons per atom

**Table** $k_F/(2\pi/a)$ and $\varepsilon_F / E_0$ for the bcc lattice

| p | $k_F/(2\pi/a)$ | $\epsilon/E_0$ |
|---|---|---|
| 1. | 0.62035 | 0.384835 |
| 2. | 0.781593 | 0.610887 |
| 3. | 0.8947 | 0.800488 |
| 4. | 0.984745 | 0.969723 |
| 5. | 1.06078 | 1.12526 |
| 6. | 1.12725 | 1.2707 |
| 7. | 1.18669 | 1.40823 |
| 8. | 1.2407 | 1.53934 |
| 9. | 1.29038 | 1.66508 |
| 10. | 1.3365 | 1.78624 |

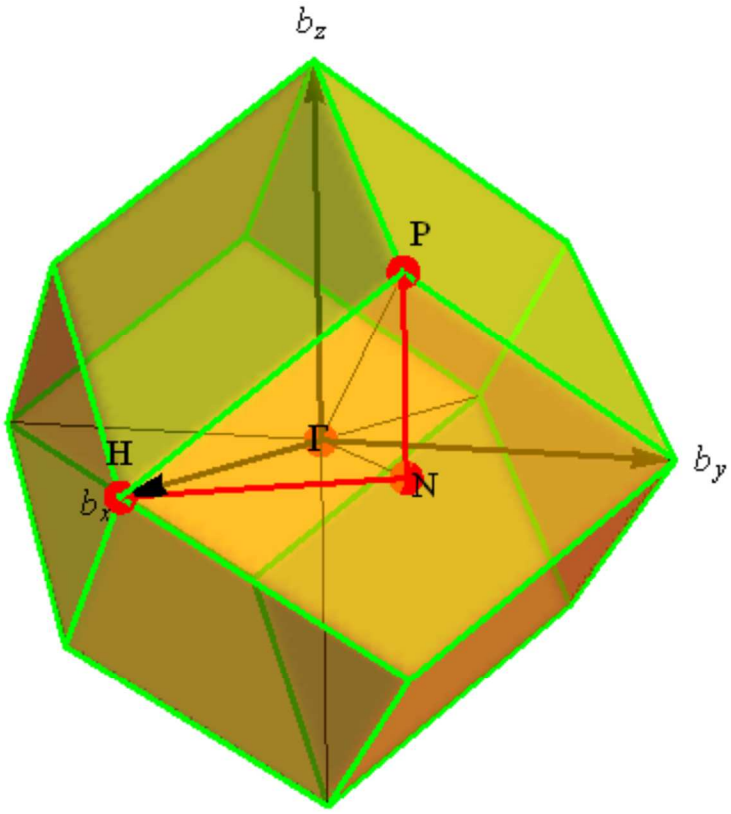


**Fig.** First Brillouin zone of bcc lattice. $\boldsymbol{\Gamma}$= (0,0,0), $\boldsymbol{H}$ = (1,0,0), $\boldsymbol{P}$ = (1/2, 1/2, 1/2), $N$ = (1/2, 1/2, 0), $\Gamma H$ =1, $\Gamma N = \sqrt{2}/2$, and $\Gamma P = \sqrt{3}/2$, $\boldsymbol{b}_x$ = (1, 0, 0). $\boldsymbol{b}_y$ = (0, 1, 0), and $\boldsymbol{b}_z$ = (0, 0, 1), in the units of $2\pi/a$:

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## 4. Alkali metal:

| | |
|---|---|
| Li: | $1s^2 2s^1$ |
| Na: | $[Ne]3s^1$ |
| K: | $[Ar]4s^1$ |
| Rb | $[Xr]5s^1$ |
| Cs: | $[Xe]6s^1$ |

The bcc lattice has one atom per primitive cell. (2) The bcc lattice has two atoms per conventional cell. There is one electron per atom. The Fermi wavenumber is given by

$$k_F = 0.620\left(\frac{2\pi}{a}\right).$$

The first Brillouin zone is illustrated below

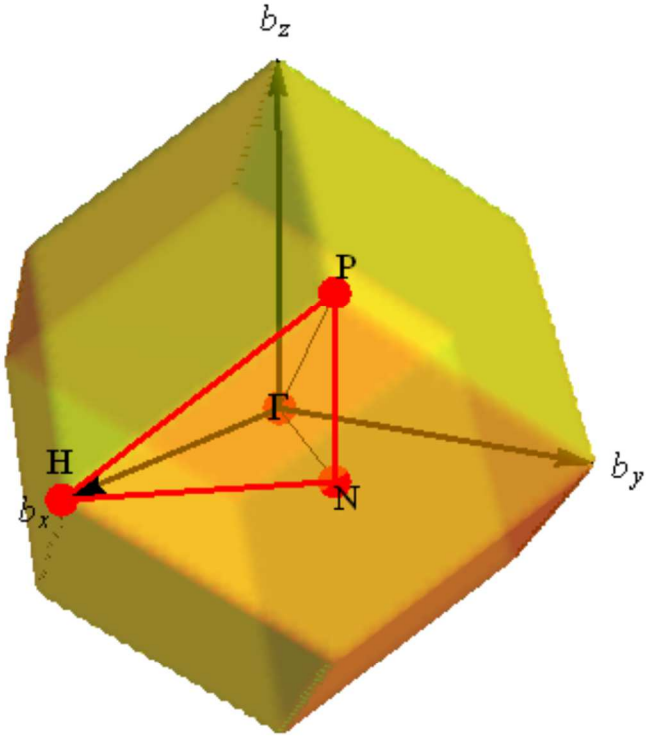



**Fig.** First Brillouin zone of bcc lattice. $\Gamma = (0,0,0)$, $H = (1,0,0)$, $P = (1/2, 1/2, 1/2)$, $N = (1/2, 1/2, 0)$, $\Gamma H = 1$, $\Gamma N = \sqrt{2}/2$, and $\Gamma P = \sqrt{3}/2$, $\boldsymbol{b}_x = (1, 0, 0)$. $\boldsymbol{b}_y = (0, 1, 0)$, and $\boldsymbol{b}_z = (0, 0, 1)$, in the units of $2\pi/a$:

The shortest distance from the center of the zone to a zone face is

$$\Gamma N = \frac{\sqrt{2}}{2}\frac{2\pi}{a} = 0.707\frac{2\pi}{a},$$

Since $k_F < \Gamma N$, the free electron sphere is entirely contained within the first zone, approaching it most closely in the direction $\Gamma N$, where it reaches a fraction

$$k_F/\Gamma N = 0.877,$$

of the way to the zone face. dHvA measurements of Fermi surface confirm this free electron picture to a remarkable degree of precision, especially in Na and K.

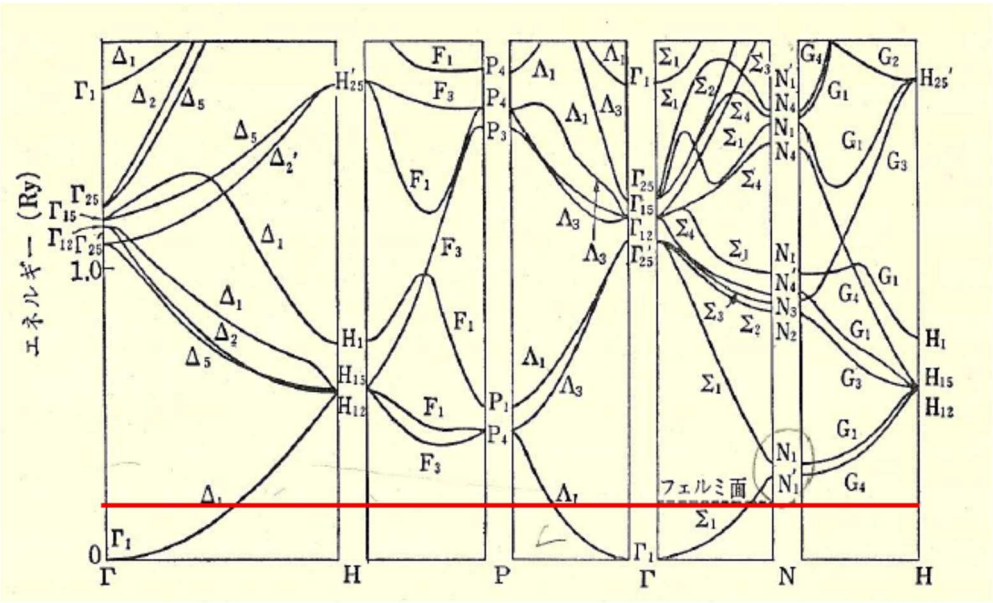



**Fig.** Band structure of Na (bcc)

The band structure of Na illustrates that a fairly substantial energy gap at the Bragg plane (N) is possible, even though the bands are indistinguishable from free electron bands at $k_F = 0.877\ \Gamma N$.

## 5. Noble metals

fcc lattice

Cu: [Ar]$3d^{10}4s^1$
Ag: [Kr]$4d^{10}5s^1$
Au: [Xe]$4f^{14}5d^{10}6s^1$

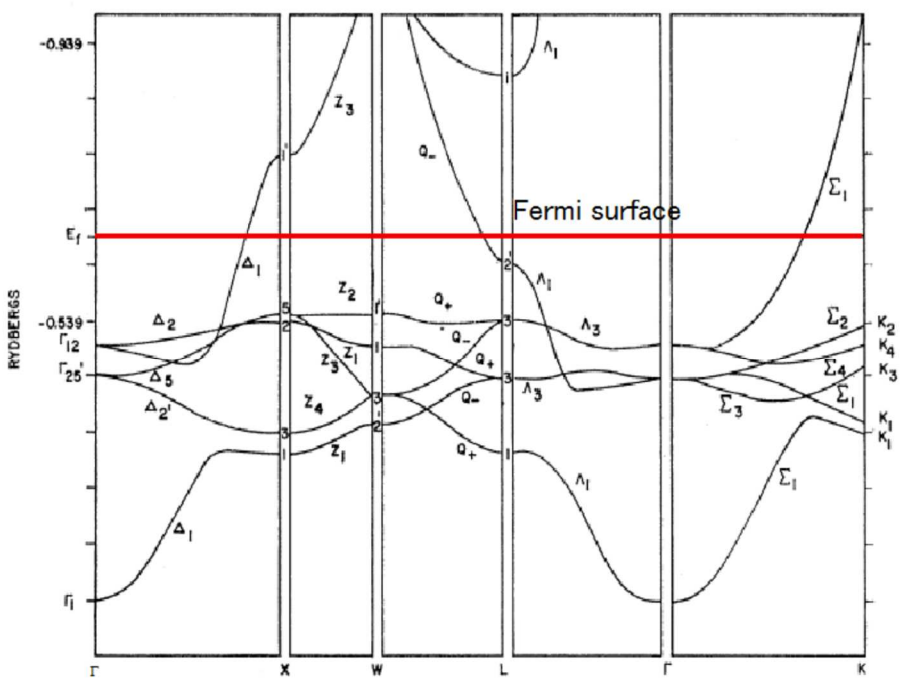
((**Comaparison**))

K: [Ar] $4s^1$
Rb: [Kr] $5s^1$
Cs: [Xe] $6s^1$

[Ar] =[$1s^2 2s^2 2p^6 3s^2 3p^6$] gives rise to very tightly bound bands, lying well below the energies of any of the remaining electroniclevels in the metal. The electrons in these low-lying levels can be considered as part of the inert ion cores.

$Cu^{11+}$ + 11 electrons ($3d^{10}4s^1$) per primitive cell. So there are 11*N* electrons (or simply 11 electrons). Note that there are 2*N* states (or simply 2 electrons) per each band (*N*: number of primitive cells). Then at least six band are required to accomodate the eleven additional electrons. It is convenient to refer to the set of five narrow bands as the *d*-band, and the remaining set of levels as the *s*-band.

Band structure of Cu




G.A. Burdick, Phys. Rev. 129, 138 (1963)

**Fig.** Band structure of Cu (fcc) by G.A. Burdick, Phys. Rev. **129**, 138 (1963).

For almost all $k$, the six bands can be seen to separate into five lying in a relatively narrow range of energies from about 2 - 5 eV below $\varepsilon_F$, and a sixth with an energy anywhere from about 7 eV above to 8 eV. It is convenient to refer to the set of five narrow bands as the d-band, and the remaining set of levels as the s band. The s-band intersects the Fermi level. Note that the $\boldsymbol{k}$-dependence of the s-band levels, except they approach the $d$-band (the hybrization effect occurs between the s-band and d-band), bears a remarkable resemblance to the lowest free electron band for a fcc lattice.

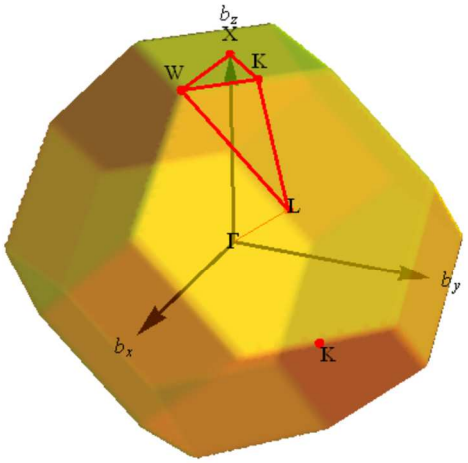


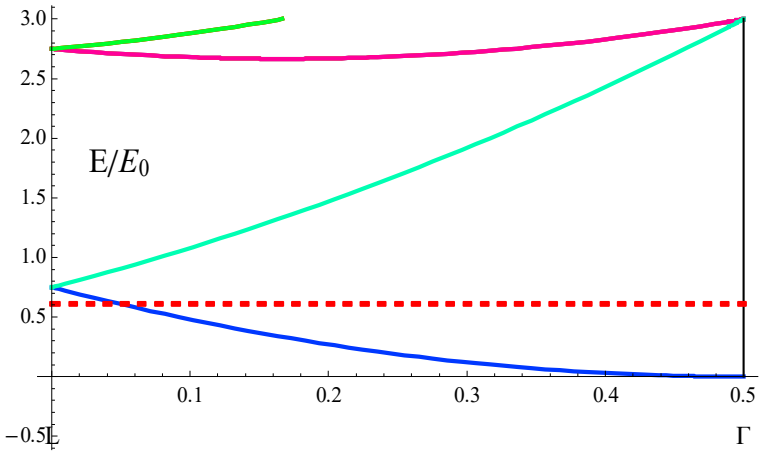

**Fig.** First Brillouin zone for the fcc lattice. $\boldsymbol{X}$ = (0,0,1), $\boldsymbol{W}$=(1/2, 0, 1), $\boldsymbol{L}$ = (1/2, 1/2, 1/2), $\boldsymbol{K}$ = (1/4, 1/4, 1) or $\boldsymbol{K}$ = (3/4, 3/4, 0). $\Gamma L = \sqrt{3}/2$. $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, $\boldsymbol{b}_z$ are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

The Fermi energy of the fcc lattice is evaluated as

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

where $E_0 = \frac{\hbar^2}{2m}(\frac{2\pi}{a})^2$, $p$ is the number of electrons per atom (there is one atom per primitive fcc cell). For $p = 1$, we have

$$\frac{\varepsilon_F}{E_0} = \left(\frac{3p}{2\pi}\right)^{2/3} = 0.610887$$




The Fermi level intersects the $\varepsilon$ vs $k$ at

$$\frac{0.451253}{0.5} = 0.90251 \quad (\Gamma L)$$

in the ***L*** direction.

The Fermi surface for a single half-filled free electron free electron band in a fcc lattice is a sphere entirely contained within the first Brillouin zone, approaching the surface of the zone closely in the <111> direction (*L* point), where it reaches 0.90251 of the distance from the origin to the center of the hexagonal face (L point).

((**Experimental result**))
dHvA effect in the noble metal.

The Fermi surface is closely related to the free electron sphere. In the <111> directions contact is actually made with the zone faces.

((**Fermi surface of Cu**))

(i) A.B. Pippard p.68 Dynamics of conduction electrons

$$\frac{\varepsilon}{\alpha} = [-3 + \sum \cos(\frac{k_x a}{2}) \cos(\frac{k_y a}{2})] + 0.0995[-3 + \sum \cos(k_x a)] = -3.63$$

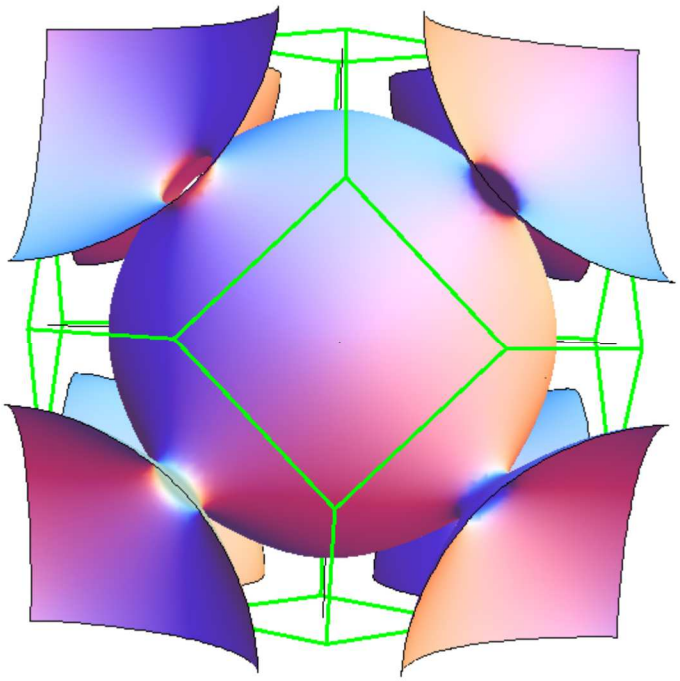


Fig. ContourPlot of the Fermi surface for Cu.