

Brillouin Zones and the Fermi Surface

(160)

using theory of electrons in a weak periodic potential
to determine band structure of 3-D crystal

⇒ geometrical constructions of great complexity!

A+M
p. 162

Often, it is most important to look at
the Fermi surface and behavior of $\epsilon_n(\vec{k})$ in its
immediate vicinity

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Fermi surface occurs when the highest occupied
energy level lies within 1 or more bands.

The surface in k -space separating the filled
from the unfilled ~~levels~~ levels.

⇒ Fermi surface

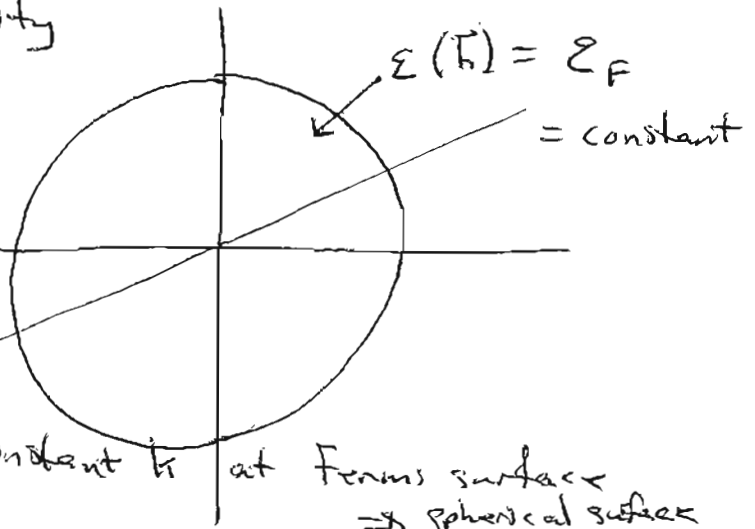
Recall for free electrons, ⇒ Fermi surface
was a sphere

since there is no periodicity

$$\Rightarrow \epsilon_n(\vec{k}) = \frac{\hbar^2 k^2}{2m} = \epsilon_F$$

$$k = |\vec{k}|$$

$$\Rightarrow k = \frac{\sqrt{2m\epsilon_F}}{\hbar} = \text{constant } k \text{ at Fermi surface} \Rightarrow \text{spherical surface}$$



Adding a weak periodic potential results in Bloch wave functions with ϵ_n periodic in \vec{k}

$$\Rightarrow \epsilon_n(\vec{k}) = \epsilon_n(\vec{k} + \vec{K})$$

But by analogy to the free electron case, the Fermi surface still separates the filled from the unfilled states

Let the energy at which that occurs be ϵ_F

$$\Rightarrow \epsilon_n(\vec{k}) = \epsilon_n(\vec{k} + \vec{K}) = \epsilon_F$$

\Rightarrow Fermi surface has periodicity of the reciprocal lattice

can display Fermi surface in either

- a) repeated zone scheme
- or b) reduced zone ~~scheme~~ scheme

Note in passing : Fermi energy is not uniquely determined for a solid with a band gap (unless we talk about chemical potential)

\Rightarrow We do not talk about "Fermi surface" for semiconductors or insulators \rightarrow not defined this way

It is convenient to see the k -dependence or "shape" of the Fermi surface, in case of a weak potential, by defining "Brillouin zones"

1st Brillouin zone we defined already



1st B.Z. consists of all k -space points which lie inside the polyhedron defined by the closest Bragg planes (1st set)

2nd Brillouin zone contains all points which lies outside the first set of Bragg planes but inside the second set of Bragg planes.

3rd B.Z.



n th B.Z. = set of k -points which lie between the $(n-1)$ th set of Bragg planes and the n th set of Bragg planes

Important: to note that all B.Z.'s have the volume of a single primitive cell of reciprocal lattice

and

some B.Z.'s contain points which are discontinuous

Why are B.Z.'s useful (or necessary) to talk about the Fermi surface?

Answer

Added together, the Brillouin zones fill all of k-space reciprocal lattice

$$\sum_n (B.Z.)_n = N \times V_k$$

N = number of primitive cells
 V_k = ^{k-}volume of 1 reciprocal primitive cell

Therefore,

the Fermi surface will cut through potentially many different B.Z.'s

The pieces of k-space surfaces which are the intersection of the "spherical-like" Fermi sphere with the n^{th} B.Z.,

when translated back into the 1^{st} B.Z. through 1 or more reciprocal lattice vectors \vec{K} ,

result in what can be referred to as the n^{th} zone Fermi surface

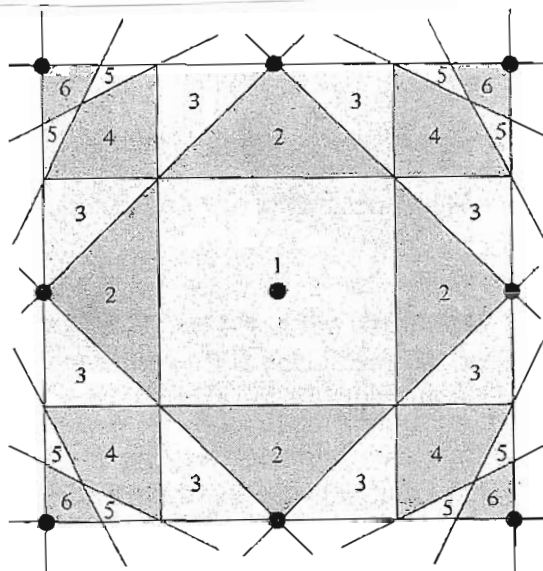
in the reduced zone scheme,

Take an example in 2-D

2-D square Bravais lattice

Figure 9.7

Illustration of the definition of the Brillouin zones for a two-dimensional square Bravais lattice. The reciprocal lattice is also a square lattice of side b . The figure shows all Bragg planes (lines, in two dimensions) that lie within the square of side $2b$ centered on the origin. These Bragg planes divide that square into regions belonging to zones 1 to 6. (Only zones 1, 2, and 3 are entirely contained within the square, however.)

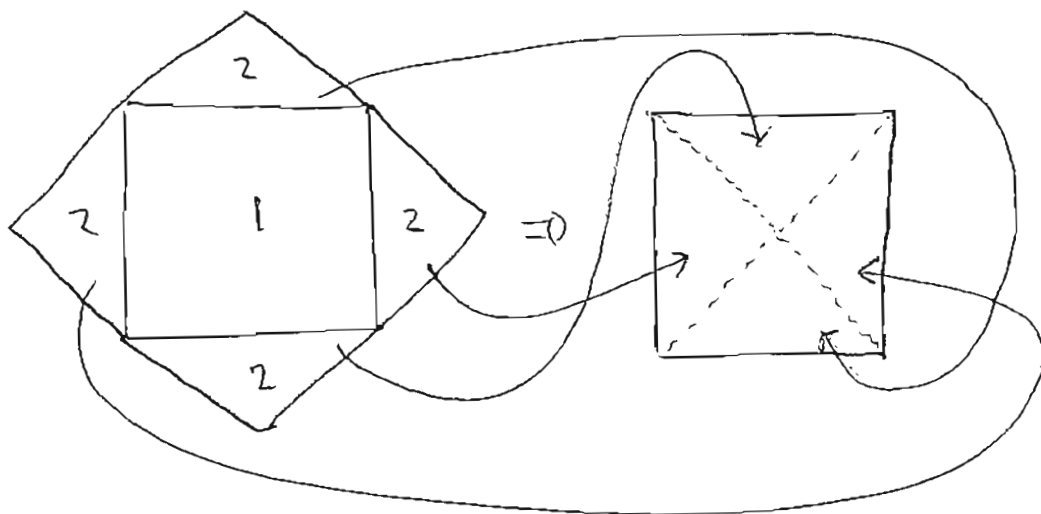


Ashcroft & Mermin,
p. 163
"Solid State Physics"

The B.Z.'s are labeled

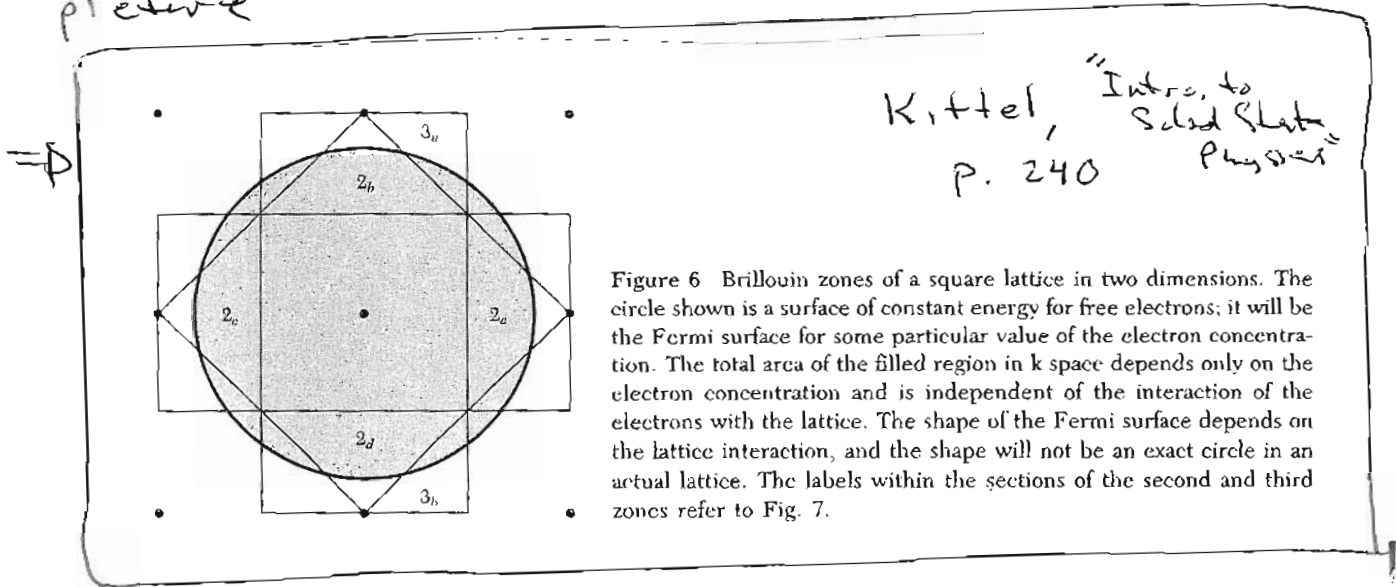
Note that area of 2nd zone = area of 1st zone
etc.

Note that, if translated back into the 1st zone,
any zone will completely fill up the 1st zone



Now, how many valence electrons per primitive unit cell will determine ϵ_F

Add a free-electron Fermi sphere to the picture



Note that this particular Fermi sphere "cuts" through zones 2, 3, and 4.

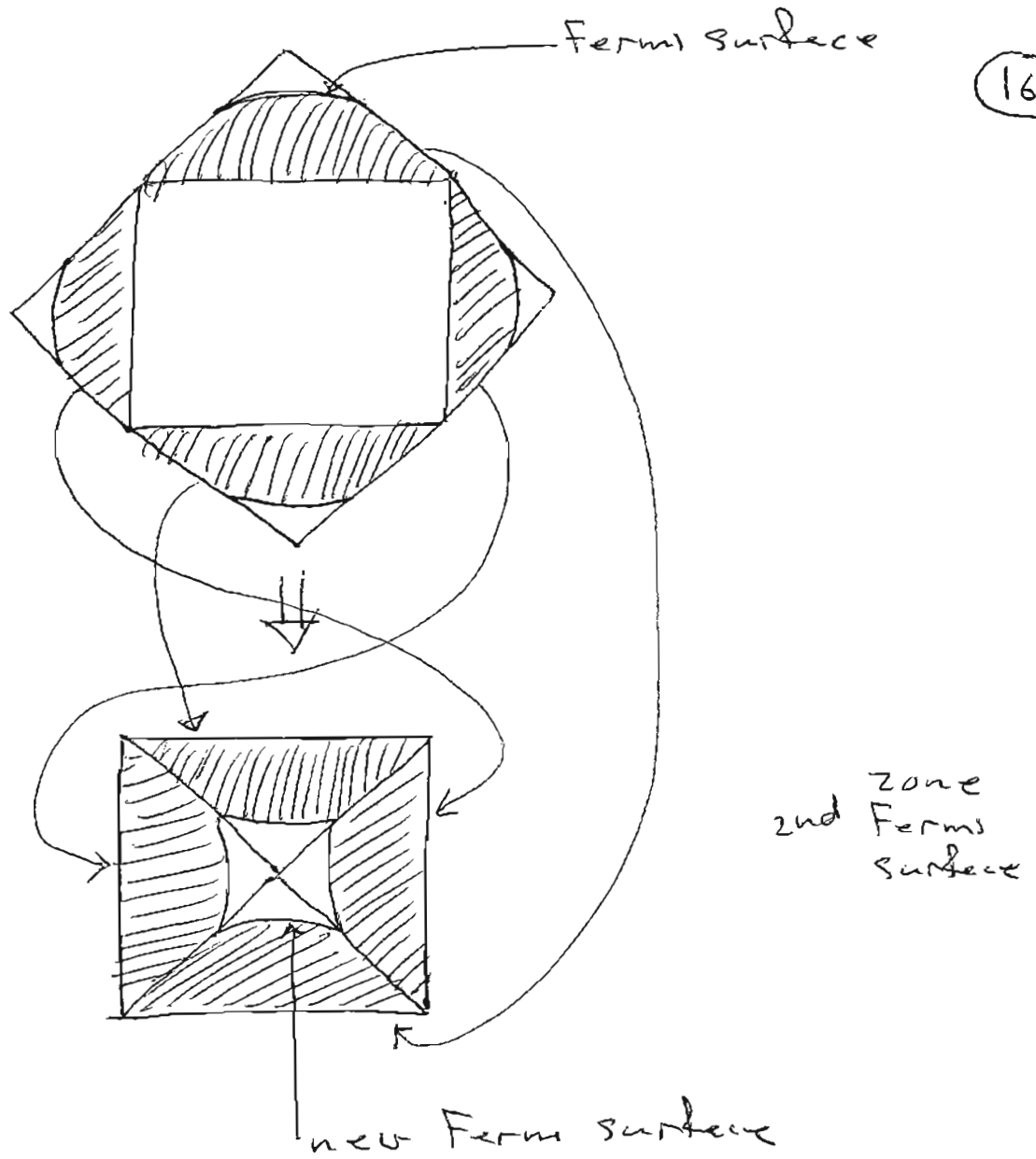
Zone 1 is completely occupied

But zones 2, 3, and 4 are not completely occupied

To see the different parts of the Fermi surface,

\Rightarrow translate the pieces of the Fermi sphere surface defined by the zones back into the first zone

(reduced zone scheme)



Similarly,

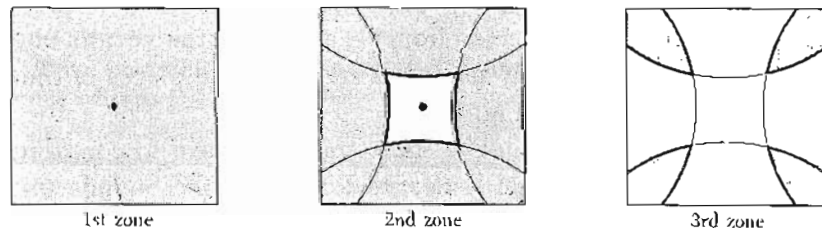
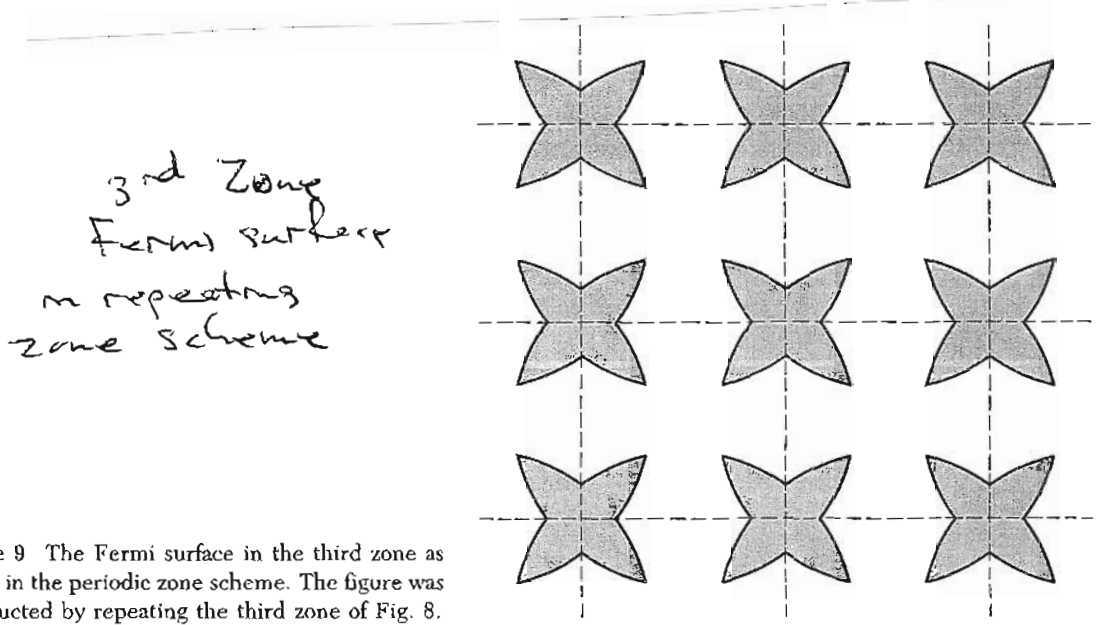


Figure 8 The free electron Fermi surface of Fig. 6, as viewed in the reduced zone scheme. The shaded areas represent occupied electron states. Parts of the Fermi surface fall in the second, third, and fourth zones. The fourth zone is not shown. The first zone is entirely occupied.

Kittel,
p. 240
"Intro to
Solid State
Physics"

By repeating those 1st zone pictures into all other zones
 ⇒ repeating zone picture for the nth Fermi surface

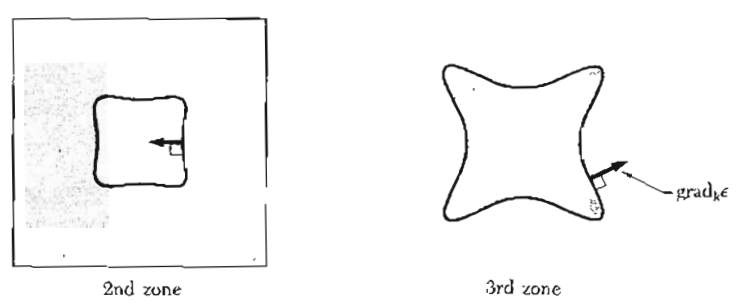


3rd Zone Fermi surface
 in repeating zone scheme

Figure 9 The Fermi surface in the third zone as drawn in the periodic zone scheme. The figure was constructed by repeating the third zone of Fig. 8.

Kittel, Intro to Sol. State Physics, p. 241

Another important aspect is the effect of the weak periodic potential on the shape of the nth zone Fermi surfaces



Kittel, Intro to Solid State Physics, p. 241

Figure 10 Qualitative impression of the effect of a weak periodic crystal potential on the Fermi surface of Fig. 8. At one point on each Fermi surface we have shown the vector $\text{grad}_k \epsilon$. In the second zone the energy increases toward the interior of the figure, and in the third zone the energy increases toward the exterior. The shaded regions are filled with electrons and are lower in energy than the unshaded regions. We shall see that a Fermi surface like that of the third zone is electronlike, whereas one like that of the second zone is holelike. It is said that electrons sink and holes float.

One gets several effects

1. energy gaps at zone boundaries
2. typical intersection of Fermi surface perpendicular to zone boundaries

⇒ 3. rounding out of sharp corners of Fermi surface

Next, we consider 3-D cases

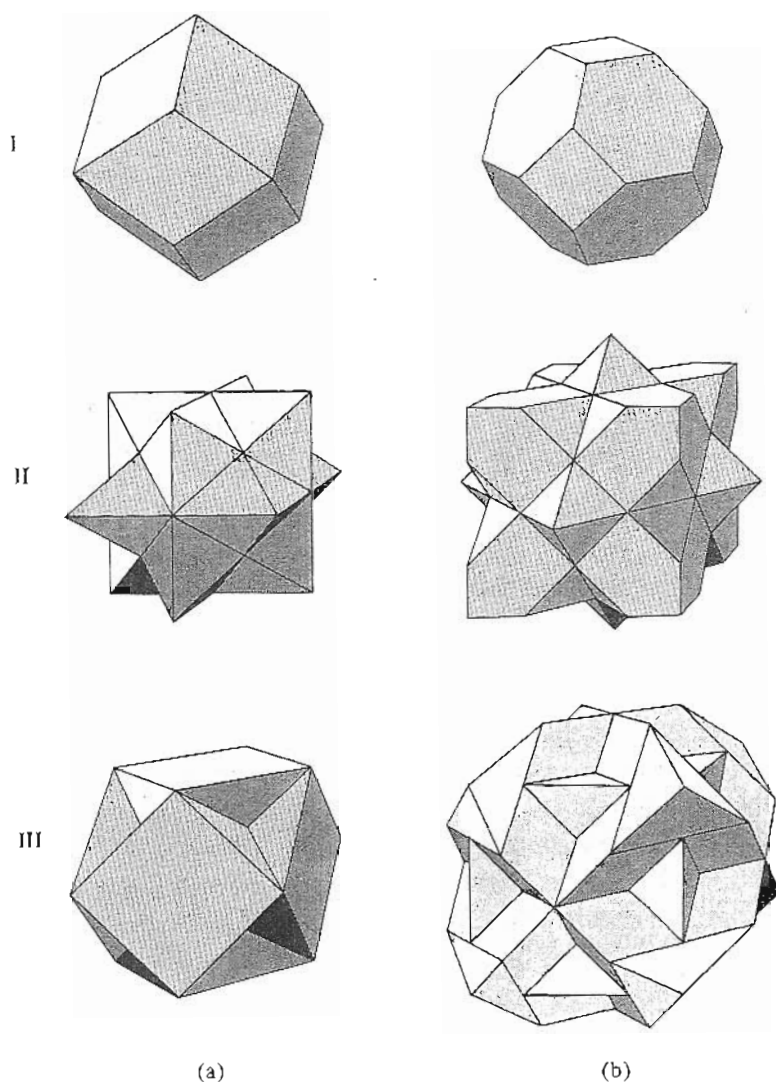


Figure 9.8

Surfaces of the first, second, and third Brillouin zones for (a) body-centered cubic and (b) face-centered cubic crystals. (Only the exterior surfaces are shown. It follows from the definition on page 163 that the interior surface of the n th zone is identical to the exterior surface of the $(n - 1)$ th zone.) Evidently the surfaces bounding the zones become increasingly complex as the zone number increases. In practice it is often simplest to construct free electron Fermi surfaces by procedures (such as those described in Problem 4) that avoid making use of the explicit form of the Brillouin zones. (After R. Lück, doctoral dissertation, Technische Hochschule, Stuttgart, 1965.)

Ascroft & Mearns,
Solid State Physics,
p. 164

Brillouin zones are quite complex!

The procedure for 3-D cases is similar to that for 2-D, just more complicated.

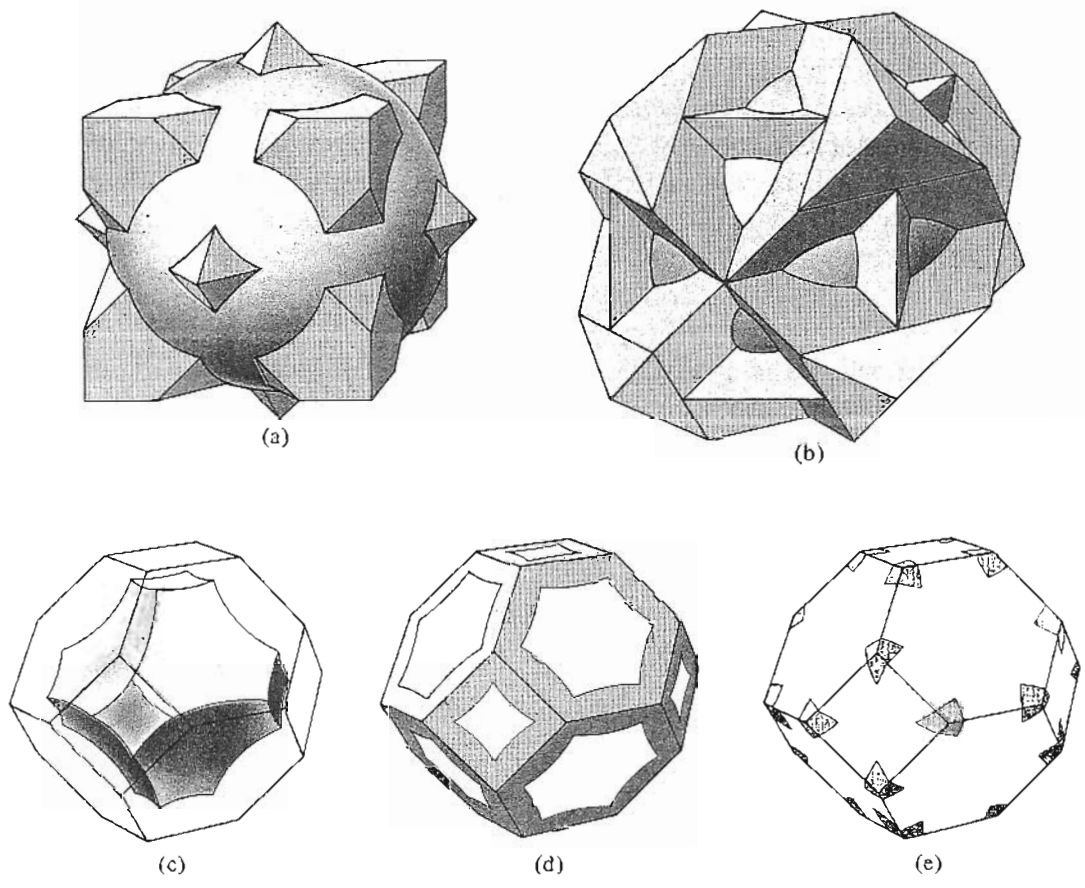


Figure 9.9

The free electron Fermi sphere for a face-centered cubic metal of valence 4. The first zone lies entirely within the interior of the sphere, and the sphere does not extend beyond the fourth zone. Thus the only zone surfaces intersected by the surface of the sphere are the (exterior) surfaces of the second and third zones (cf. Figure 9.8b). The second-zone Fermi surface consists of those parts of the surface of the sphere lying entirely within the polyhedron bounding the second zone (i.e., all of the sphere except the parts extending beyond the polyhedron in (a)). When translated through reciprocal lattice vectors into the first zone, the pieces of the second-zone surface give the simply connected figure shown in (c). (It is known as a "hole surface"; the levels it encloses have higher energies than those outside). The third-zone Fermi surface consists of those parts of the surface of the sphere lying outside of the second zone (i.e., the parts extending beyond the polyhedron in (a)) that do not lie outside the third zone (i.e., that are contained within the polyhedron shown in (b)). When translated through reciprocal lattice vectors into the first zone, these pieces of sphere give the multiply connected structure shown in (d). The fourth-zone Fermi surface consists of the remaining parts of the surface of the sphere that lie outside the third zone (as shown in (b)). When translated through reciprocal lattice vectors into the first zone they form the "pockets of electrons" shown in (e). For clarity (d) and (e) show only the intersection of the third and fourth zone Fermi surfaces with the surface of the first zone. (From R. Lück, *op. cit.*)

Ashcroft & Mermin, Solid State Physics, p. 165