Phys 570

Lecture #11

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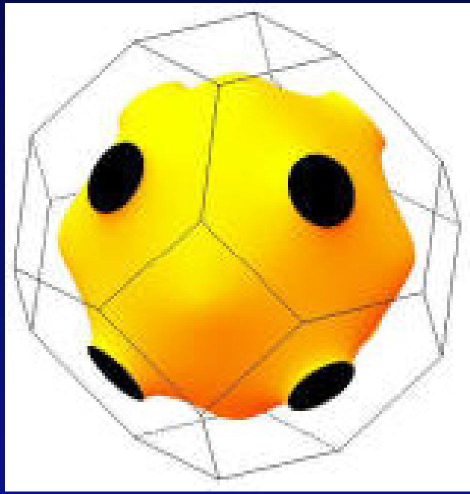
Chapter 9: Fermi Surfaces and Metals

Introduction

- The Fermi surface is the surface of constant energy ε_F in k space.
- The Fermi surface separates the unfilled orbitals from the filled orbitals, at 0 K.
- The electrical properties of the metal are determined by the volume and shape of the Fermi surface.



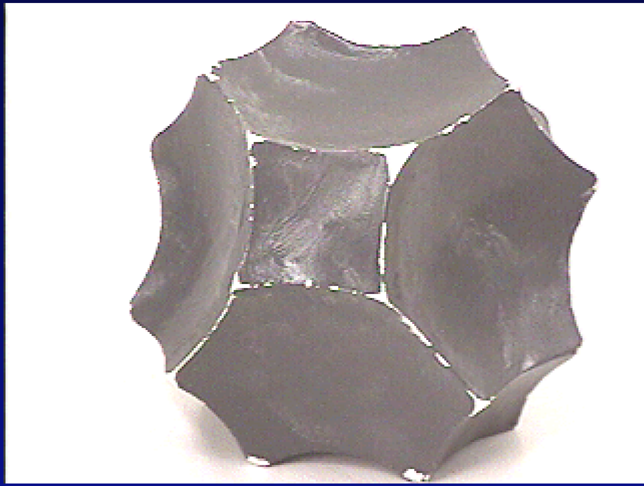
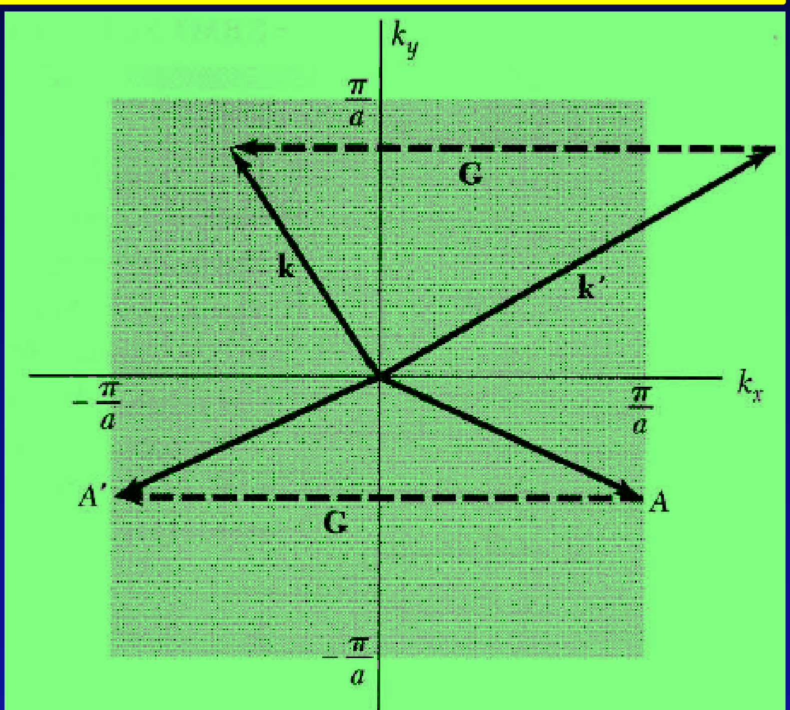


Figure 1 Free electron Fermi surfaces for fcc metals with one (Cu) left and three (Al) right, valence electrons per primitive cell.

Reduced Zone Scheme

- We construct Fermi surfaces from a sphere using the reduced zone schemes. *All vectors are plotted inside the FBZ*.
- It is always possible to select the wavevector k of any Bloch function to lie within the first Brillouin zone. The procedure is known as mapping the band in the reduced zone scheme.

Figure 2 FBZ of a square lattice of side *a*. *k'* can be carried into the first zone by forming k'+G. The wavevector at a point *A on* the zone boundary is carried by G to the point *A'* on the opposite boundary. A and A' are connected by a reciprocal lattice vector, we count them as *one identical point in the zone*.



Chapter 9: Fermi Surfaces and Metals

Periodic Zone Scheme

- We can repeat a given Brillouin zone periodically through all of wavevector space. To repeat a zone, we translate the zone by a reciprocal lattice vector.
- If we can translate a band from other zones into the first zone, we can translate a band in the first zone into every other zone. In this scheme the energy $\boldsymbol{\varepsilon_k}$ of a band is a periodic function in the reciprocal lattice:

$$\varepsilon_k = \varepsilon_{k+G} \qquad (2)$$

- Here ε_{k+G} is understood to refer to the same energy band ε_k. The result of this construction is known as the periodic zone scheme. Three different zone schemes are useful (see next slide for the figure): *Extended, Reduced and Periodic Zone Schemes*

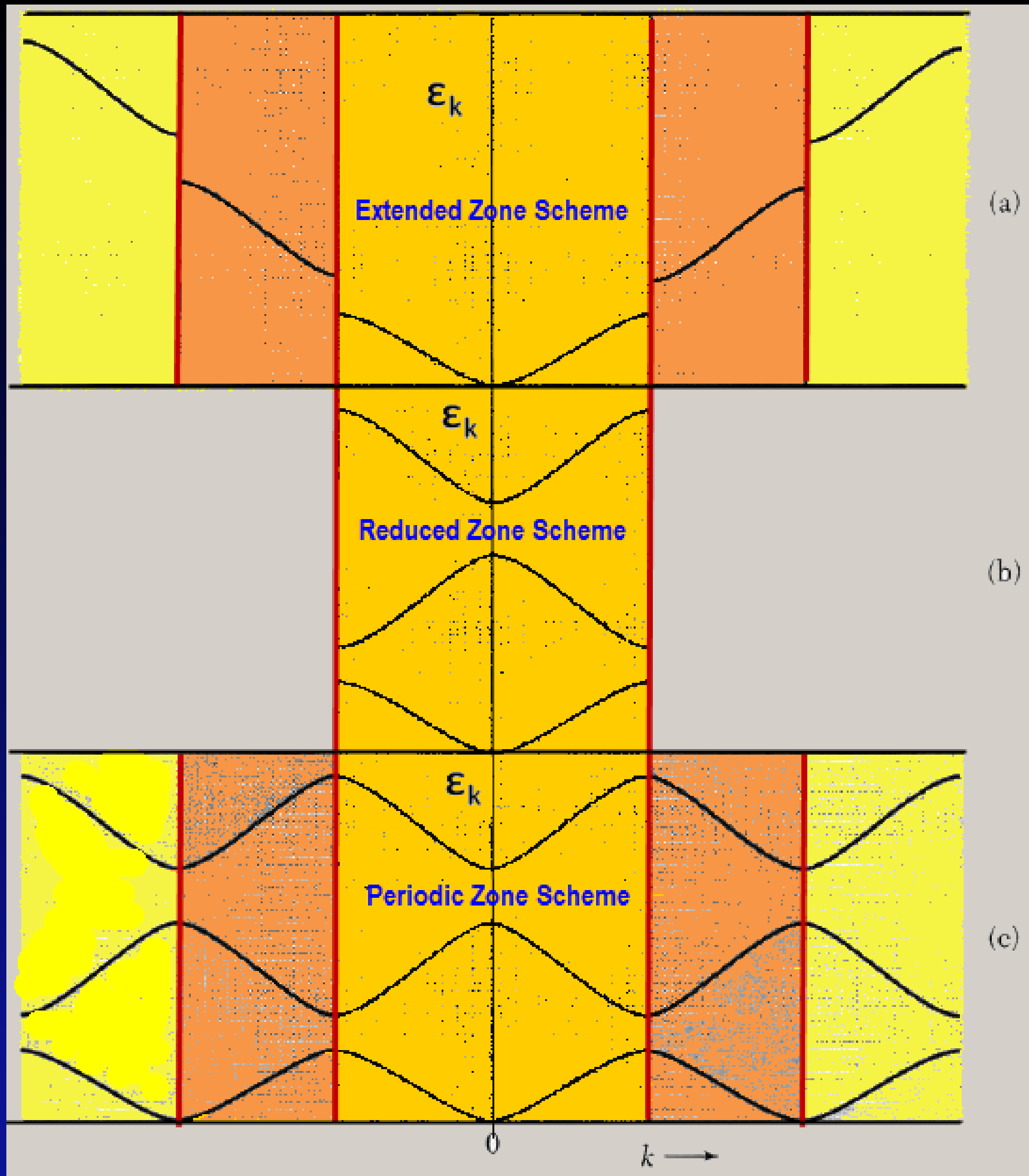
Figure 4:

Three energy bands of a linear lattice plotted in:

(a) The extended Brillouin Zone Scheme

(b) Reduced Brillouin Zone Scheme.

(c) Periodic Brillouin Zone Scheme.



CONSTRUCTION OF FERMI SURFACES

- We will use square lattice and use diffraction condition:

$$2k.G+G^2=0$$

- ***k*** satisfied if terminates on the plane normal to ***G*** at the midpoint of ***G***. From this equation we can construct the Fermi Surface.
- The first Brillouin zone of the square lattice is the area enclosed by the perpendicular bisectors of $\boldsymbol{G_1}$ and of the three reciprocal lattice vectors equivalent by symmetry to $\boldsymbol{G_1}$ in Fig. 5a. These four reciprocal lattice vectors are $\pm(2\pi/a)\boldsymbol{k}_x$ *and* $\pm(2\pi/a)\boldsymbol{k}_y$.
- The second zone is constructed from $\boldsymbol{G_2}$ and the three vectors equivalent to it by symmetry, and similarly for the third zone. The pieces of the second and third zones are drawn in Fig. 5b.

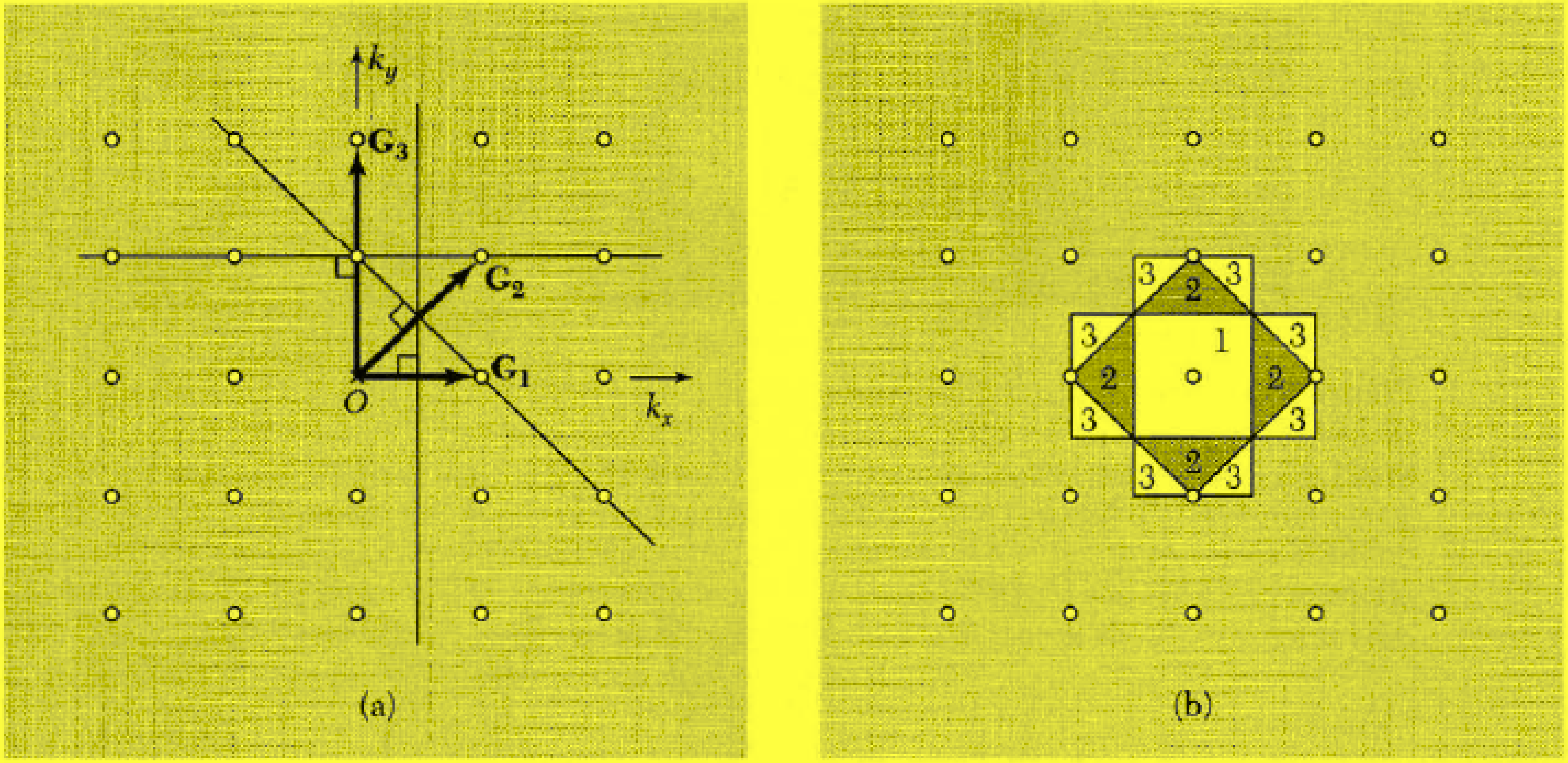


Figure 5 (a) Construction in **k** space of the first three Brillouin zones of a square lattice. The three shortest forms of the reciprocal lattice vectors are indicated as $\mathbf{G}_1$, $\mathbf{G}_2$, and $\mathbf{G}_3$. The lines drawn are the perpendicular bisectors of these **G**'s. (b) On constructing all lines equivalent by symmetry to the three lines in (a) we obtain the regions in **k** space which form the first three Brillouin zones. The numbers denote the zone to which the regions belong; the numbers here are ordered according to the length of the vector **G** involved in the construction of the outer boundary of the region.

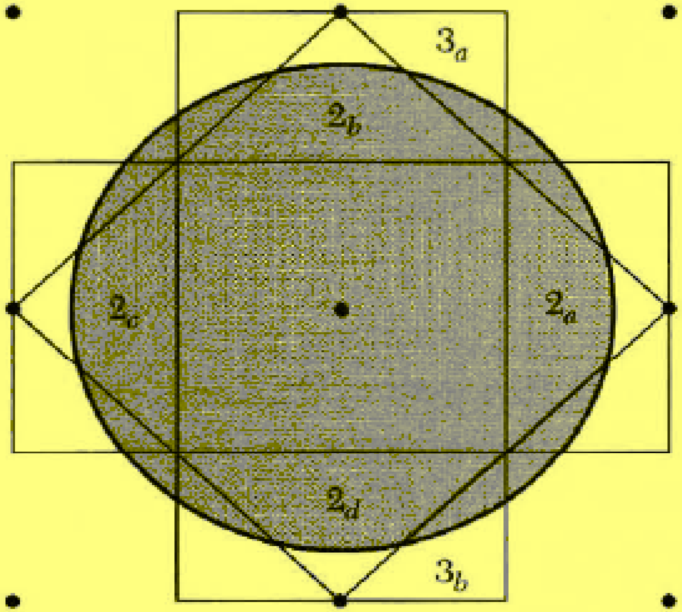


Figure 6 Brillouin zones of a square lattice in two dimensions. The circle shown is a surface of constant energy for free electrons; it will be the Fermi surface for some particular value of the electron concentration. The total area of the filled region in **k** space depends only on the electron concentration and is independent of the interaction of the electrons with the lattice. The shape of the Fermi surface depends on the lattice interaction, and the shape will not be an exact circle in an actual lattice. The labels within the sections of the second and third zones refer to Fig. 7.

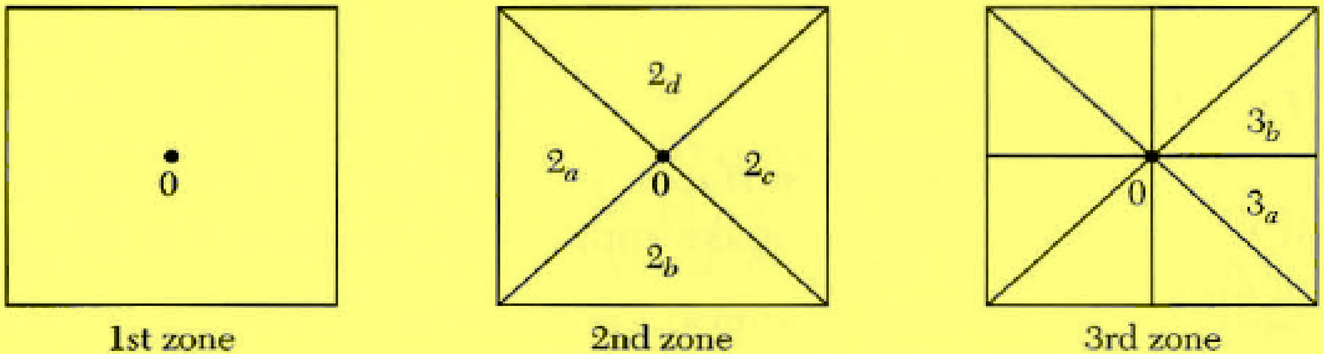


Figure 7 Mapping of the first, second, and third Brillouin zones in the reduced zone scheme. The sections of the second zone in Fig. 6 are put together into a square by translation through an appropriate reciprocal lattice vector. A different **G** is needed for each piece of a zone.

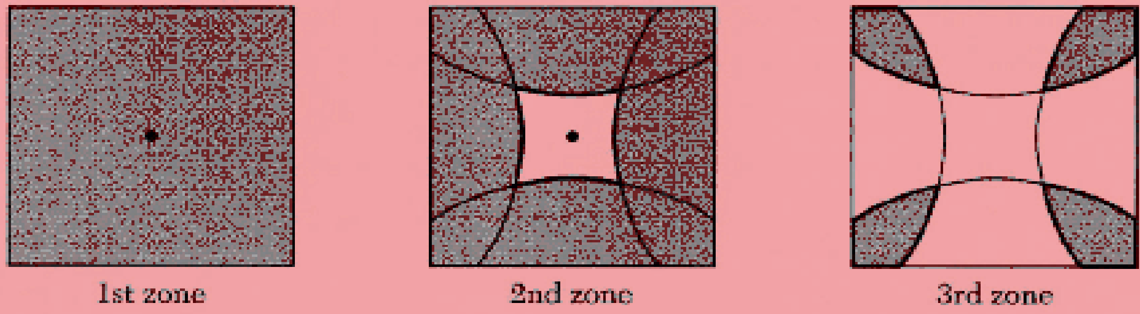


Figure 8 The free electron Fermi surface of Fig. 6, as viewed in the reduced zone scheme. The shaded areas represent occupied electron states. Parts of the Fermi surface fall in the second, third, and fourth zones. The fourth zone is not shown. The first zone is entirely occupied.

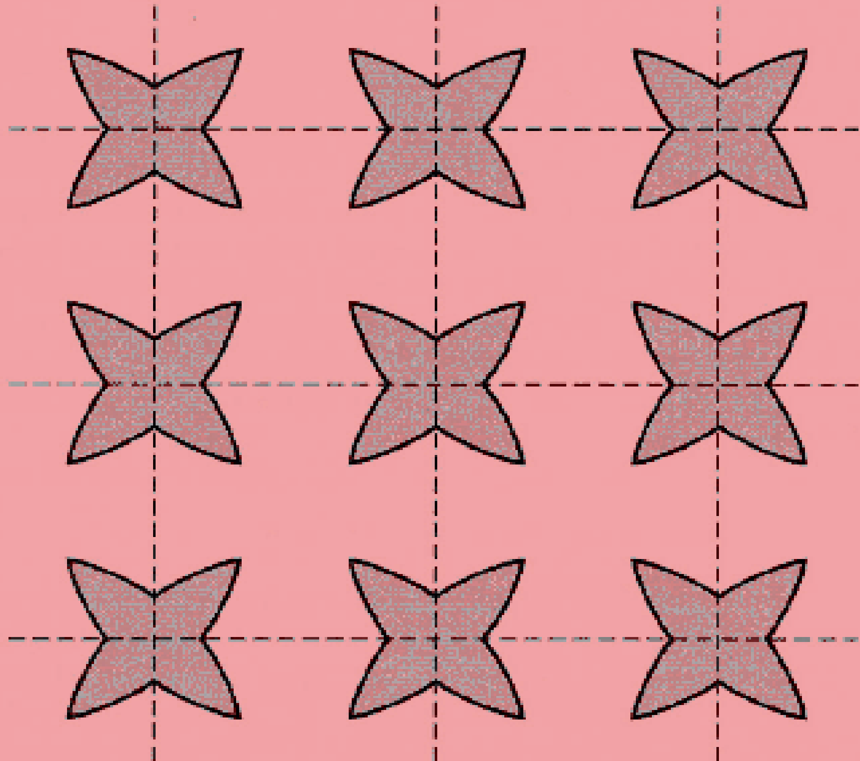


Figure 9 The Fermi surface in the third zone as drawn in the periodic zone scheme. The figure was constructed by repeating the third zone of Fig. 8.