University of Anbar
College of Science
Department of Physics

فيزياء الحالة الصلبة

Solid state Physics

المرحلة الرابعة

الكورس الثاني

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Brillouin zones. مناطق برليون

If we draw the normal planes which bisect the reciprocal lattice vectors, the regions enclosed between these planes form the various Brillouin zones.

اذا رسمنا المستويات الاعتيادية التي تقسم متجهات الشبيكة التبادلية فان المناطق المغلقة بين هذه المستويات تشكل مناطق برليون المختلفة.

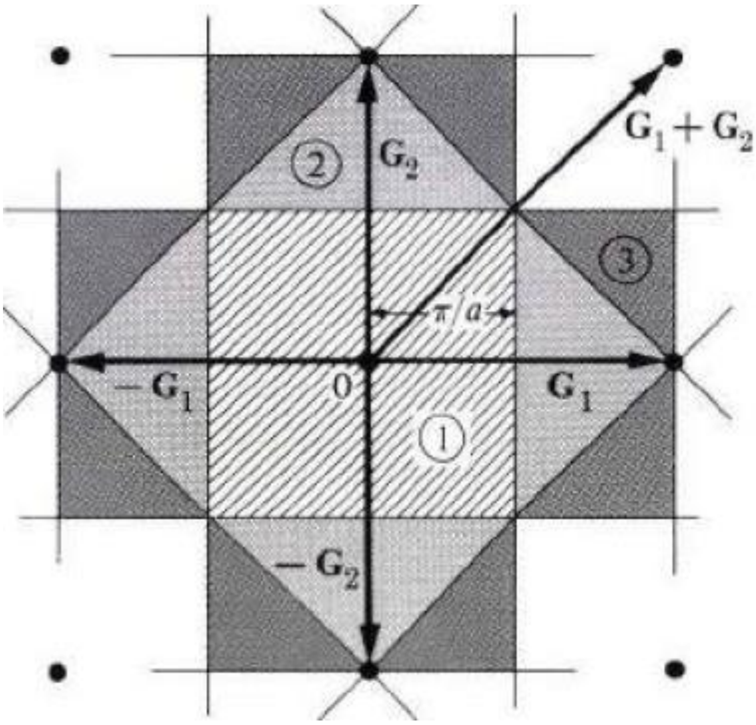

Figure 1

Figure 1 shows that the first three Brillouin zones of the square lattice: First zone (cross-hatched), second zone (shaded) and third zone (screened). Numbers indicate indices of zones.

ان الشكل واحد يوضح اول ثلاث مناطق برليون للشبيكة المربعة. المنطقة الاولى(cross-hatched) والمنطقة الثانية(shaded) والمنطقة الثالثة(screened)

Consider the square lattice whose reciprocal-also a square lattice of edge equal to $2\pi/a$ is shown, in Figure 1, which also shows the reciprocal vectors G_1, $-G_1$, G_2, and $-G_2$, etc., as well as the corresponding normal bisectors.

The smallest enclosed region centred around the origin (the crosshatched area) is the first zone.

The shaded area (composed of four separate half diamond-shaped pieces enclosed between the normal bisectors to G1, G2, and G1 + G2, etc.) forms the second zone. Similarly, the screened area (eight parts) forms the third zone.

➢ <u>The zone scheme types</u>

- Extended zone scheme
  The extended zone scheme in which different bands are drawn in different zones in wavevector space
- Reduced Zone Scheme
  The reduced zone scheme in which all bands are drawn in the first Brillouin zone.
- Periodic Zone Scheme
  The periodic zone scheme in which every hand is drawn in every zone.

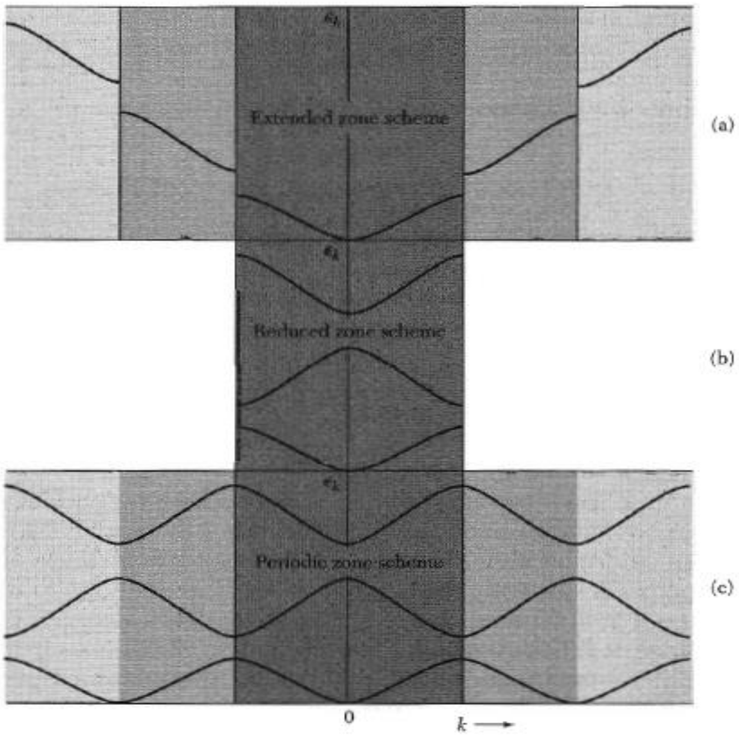

Figure 2

Figure 2 shows that the three energy bands of a linear lattice plotted in (a) the extended (Brillouin), (b) reduced, and (c) periodic zone schemes.

Fermi surfaces.

The Fermi surface is the surface of constant energy E_f in k space. The Fermi surface separates the unfilled orbitals from the filled orbitals, at absolute zero (0k). The electrical properties of the metal are determined by the volume and shape of the Fermi surface, because the current is due to changes in the occupancy of states near the Fermi surface. For free electron model Fermi surface is a perfect sphere.

Construction of Fermi surfaces:

- **For free electron:**

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.

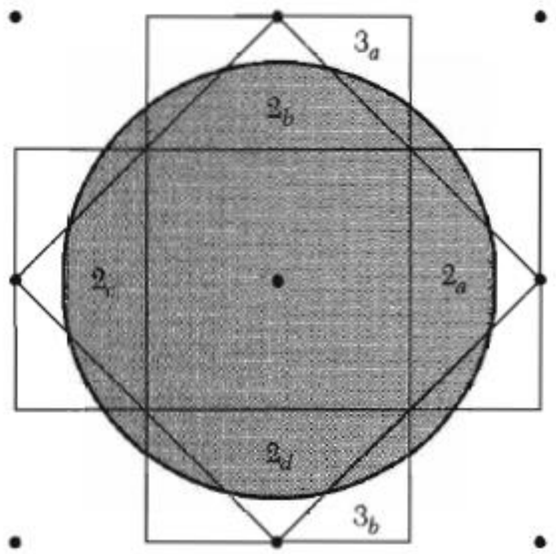

Figure 3

Mapping of the first, second, and third Brillouin zones in the reduced zone scheme are shown in figure 4. The sections of the second zone, in Fig. 4 , 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.

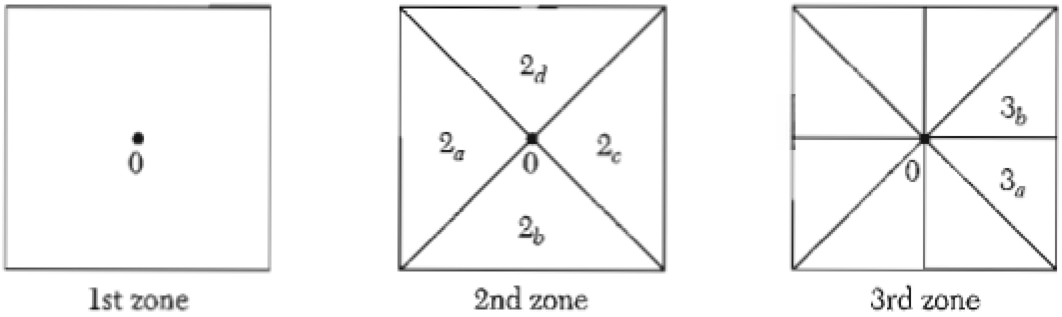

Figure 4

In figure 5, the free electron Fermi surface of 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.

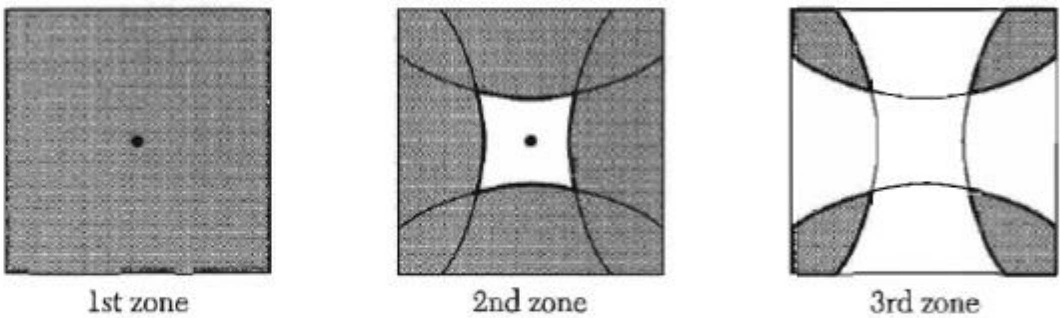

Figure 5

- **For nearly free electrons:**

How do we go from Fermi surfaces for **free electrons** to Fermi surfaces for **nearly free electrons**? We can make approximate constructions freehand by the use of four facts:

- The interaction of the electron with the periodic potential of the crystal creates energy gaps at the zone boundaries.
- The Fermi surface will intersect zone boundaries perpendicularly.
- The crystal potential will round out sharp comers in the Fermi surfaces.
- The total volume enclosed by the Fermi surface depends only on the electron concentration and is independent of the details of the lattice interaction.

The qualitative impression of the effect of a weak periodic crystal potential on the Fermi surface of figure 5 is shown in figure 6.

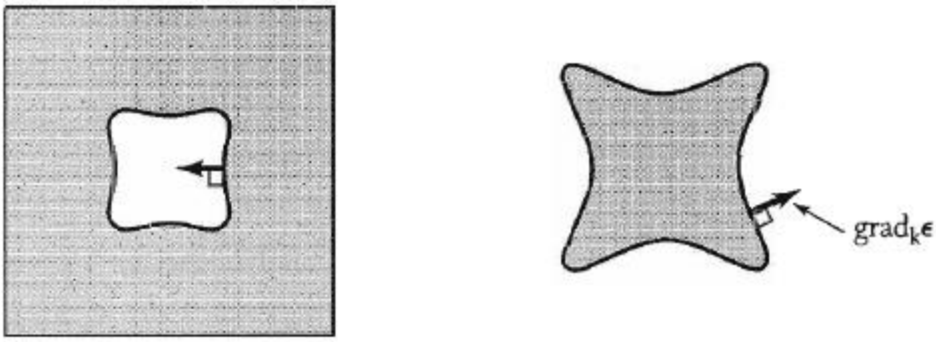

Figure 6

At one point on each Fermi surface we have shown the vector grad$_k$€. In the second zone the energy increases toward the interior of the figure, and in the third zone the energy increases toward the external. The shaded regions are filled with electrons and are lower in energy than the unshaded regions.

Effective mass.

Consider an electron in a periodic solid which is subject to an external electric field E.

Acceleration $a = \frac{dV}{dt} = \frac{dV}{dk} \cdot \frac{dk}{dt} \ldots\ldots\ldots \quad (1)$

$$V = \frac{d\omega}{dk}$$

$$\because E = \hbar\omega, \qquad \omega = \frac{E}{\hbar} \qquad\qquad V = \frac{1}{\hbar} \cdot \frac{dE}{dk} \ldots\ldots\ldots(2)$$

$$\therefore \frac{dV}{dk} = \frac{1}{\hbar} \cdot \frac{d^2E}{dk^2} \ldots\ldots\ldots(3)$$

$$\because E = F \cdot x \qquad\qquad \therefore dE = F \cdot dx$$

$$dE = F \cdot Vdt$$

$$\therefore \frac{dE}{dt} = F \cdot V$$

$$\frac{dE}{dk} \cdot \frac{dk}{dt} = F \cdot V \ldots\ldots\ldots(4)$$

Substitute equation (2) in equation (4)

$$\hbar \frac{dk}{dt} = F \;\ldots\ldots\ldots(5)$$

By substitute equation (3) and (5) in equation (1)

$$a = \frac{dV}{dk} \cdot \frac{dk}{dt} = \frac{1}{\hbar} \cdot \frac{d^2E}{dk^2} \cdot \frac{F}{\hbar}$$

$$\because a = \frac{F}{m} \qquad \therefore a = \frac{F}{m^*}$$

$$\boxed{\therefore m^* = \frac{\hbar^2 dk^2}{d^2E}}$$

The effective mass of an electron near the top of a band is negative. Negative effective mass means that on going from state k to state k+ Δk the momentum transfer from the lattice to electron is opposite to and larger than the momentum transfer from the applied force to the electron.

الكتلة الفعالة للإلكترون بالقرب من أعلى النطاق تكون سالبة.الكتلة السالبة الفعالة تعني أنه عند الانتقال من الحالة k الى الحالة k + Δk فإن انتقال الزخم من الشبكة إلى الإلكترون هو عكس وأكبر من نقل الزخم من القوة المطبقة إلى الإلكترون

Although k is increased by Δk by the applied electric field, the consequent approach to Bragg reflection can result in an overall decrease in the forward momentum of the electron, if this happens the effective mass is described as negative.

على الرغم من ان زيادة k يزداد بمقدار Δk بواسطة المجال الكهربائي المسلط, فان التقريب التالي لانعكاس Bragg يمكن ان يؤدي الى انخفاض عام في الزخم الامامي للالكترون, اذا حدث هذا فان الكتلة الفعالة توصف بانها سالبة.