11.1. Folding of the Brillouin zone

11.1.1. 1D

Fig. 1. Dispersion relation \( \epsilon_n(k) \) shown in extended zone, reduced zone and periodic zone.

11.1.2. 2D

Let’s start by considering a very weak square lattice.
Fig. 2. The Fermi sea in extended zone (a square lattice). The solid lines show the zone boundaries. Here we assume that the lattice potential is very weak, so that the Fermi sea is pretty much a sphere.

Fig. 3. The Fermi sea shown in the reduced zone. The first zone is fully filled, while the 2nd and 3rd zones are partially filled. The second zone has a hole pocket and the 3rd zone has an electron pocket.

Fig. 4. Third zone (Fig 3.c) shown in the periodic zone. As we can see here, in the reduced zone, naively speaking, it seems that we have 4 disconnected dark regions (states...
filled by electrons). However, we need to keep in mind that the zone has a periodic structure. If we take into account the periodic structure, we find that in the 3rd zone here, the four seemingly disconnected regions are actually connected. They form one electron pockets.

Fig. 5. If we turn on a weak lattice potential, the sharp corners of the Fermi surfaces will be rounded up and one can prove that when the Fermi surface crosses with a zone boundary, the Fermi surface must be perpendicular to the boundary.

For Fig. 6(b), we have a Fermi sea, which are formed by filling the states inside the Fermi surface using electrons. This filled region is known as an electron pocket and the Fermi surface here is known as an electron orbit.

For the case shown in Fig. 6(a), we have a almost fully-filled band. In some sense, it is exactly opposite to the case 6(b). Here, the Fermi surface enclose a region which is empty. For such a band, we can think the empty states as filled by “holes”. A hole is a missing electron. Since an electron has charge -e, a hole shall have charge +e (missing a charge -e means charge +e). A hole is also a Fermi with spin-1/2. The white region in Fig. 6(a), i.e. the empty states, can be considered as a Fermi sea filled by holes. This Fermi surface is known as a hole orbit. And the (white) region enclosed by the Fermi surface is known as a hole pocket. For this band, the conductivity are contributed by “holes”. Remember that in previous chapters, we discussed the Hall effect. The Hall coefficient is determined by the charge density. For electron pockets, the value is negative because electrons are negatively charged. For hole pockets, they give us a positive Hall coefficient, because the charge are carried by holes with positive charge.

Fig. 6(c) shows another possible case, where the Fermi surface doesn’t form a closed loop inside one zone. This Fermi surface is known as an open orbit.

It is possible to have multiple orbits in one zone and it could even be a combination of different types of orbits.

11.1.3. 3D
We can cut a plane in the 3D reduced zone. Depending on which plane we cut, we may find an electron orbital, a hole orbital or an open orbital in the figure above.

### 11.2. How to see the Fermi surface part I: ARPES: Angle-Resolved Photoemission Spectroscopy

- **Setup**: shoot light (photons) onto the material. When a photon hit a electron (collision) inside the sample, the electron may fly out of the sample (which is known as photoemission) and this electron will be picked up by an detector. The detector can distinguish electrons with different energy and momentum (including both the amplitude and the direction of the momentum, which is a vector). The detector counts the number of electrons which have the energy \( \epsilon \) and the momentum \( \vec{p} \).

- **Basics idea**: we know the energy and momentum of the photon and we can measure the energy and momentum of the out-coming electron. Using energy and momentum conservation, we can get the energy and momentum of the electron before it was hit by the photon. This tells us the relation between \( \epsilon \) and \( \vec{p} \) for an electron inside the material and thus we can get the dispersion relation and to construct the Fermi surfaces.

  The energy conservation tells us that

  \[
  E_p + \epsilon = E_{\text{final}}
  \]  

  (11.1)

  where \( E_p \) is the energy of the photon (light), \( \epsilon \) is the energy of an electron inside the material, and \( E_{\text{final}} \) is the energy of the electron coming out of the sample. \( E_p \) and \( E_{\text{final}} \) can be measures, so that we can determine \( \epsilon \).

  Similarly, we have momentum conservation for the x and y direction. When the electron flies out of the sample, it crosses the surface. When electron crosses the surface, it will lose some momentum along the z-direction. So the z momentum is NOT conserved, but the x and y directions are.

  \[
  \vec{p}_{/p} + \vec{p}_{/\text{final}} = \vec{p}_{/\text{final}}
  \]  

  (11.2)

  Here, \( \vec{p}_{/p} \) is the in plane components of the momentum of the photon, \( \vec{p}_{/\text{in-plane}} \) is the in-plane momentum of the electron (inside the material), and \( \vec{p}_{/\text{final}} \) is the momentum of the final electron flying away from the sample.

  Combining the information obtained above, we get the energy and momentum (in plane) of an electron. There are more complicated techniques that can provide us the z component of the electron. At the end of the day, we can get both \( \epsilon \) and \( \vec{p} \), so we get the dispersion relation \( \epsilon(\vec{p}) \). And