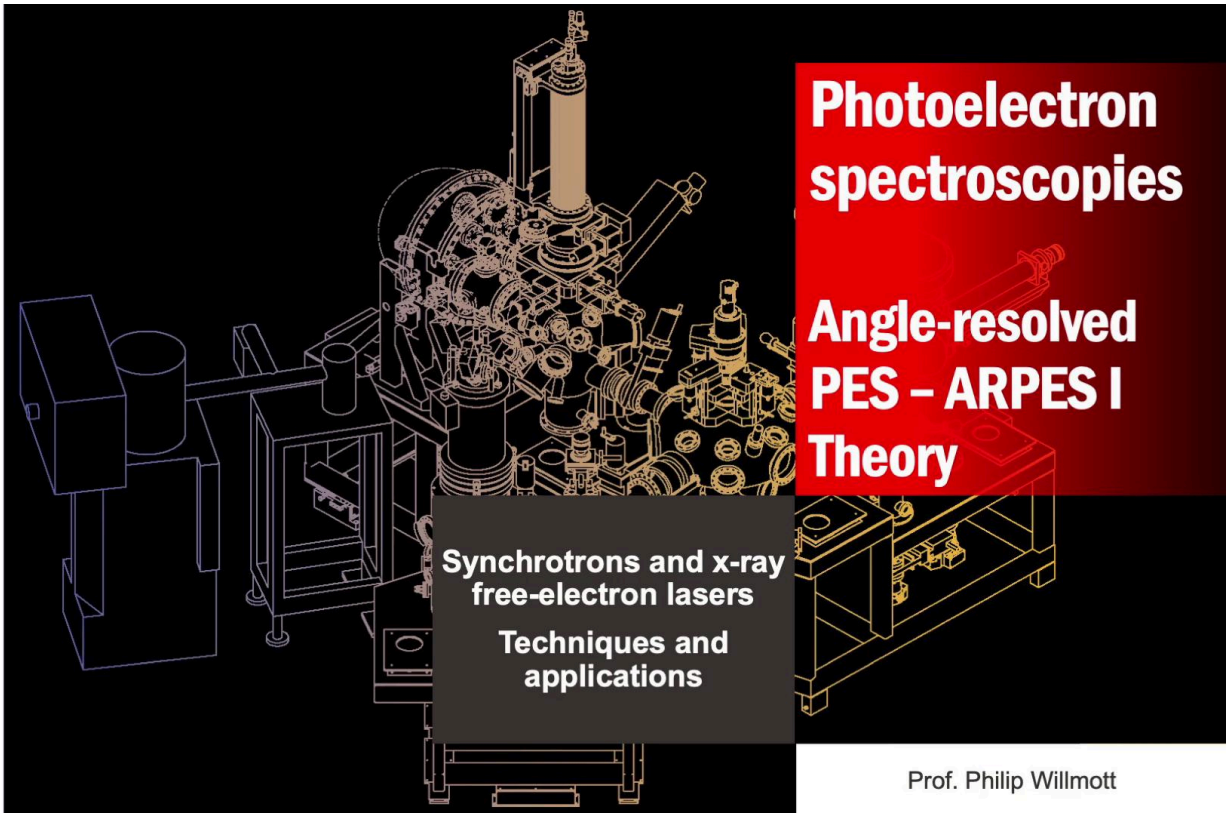

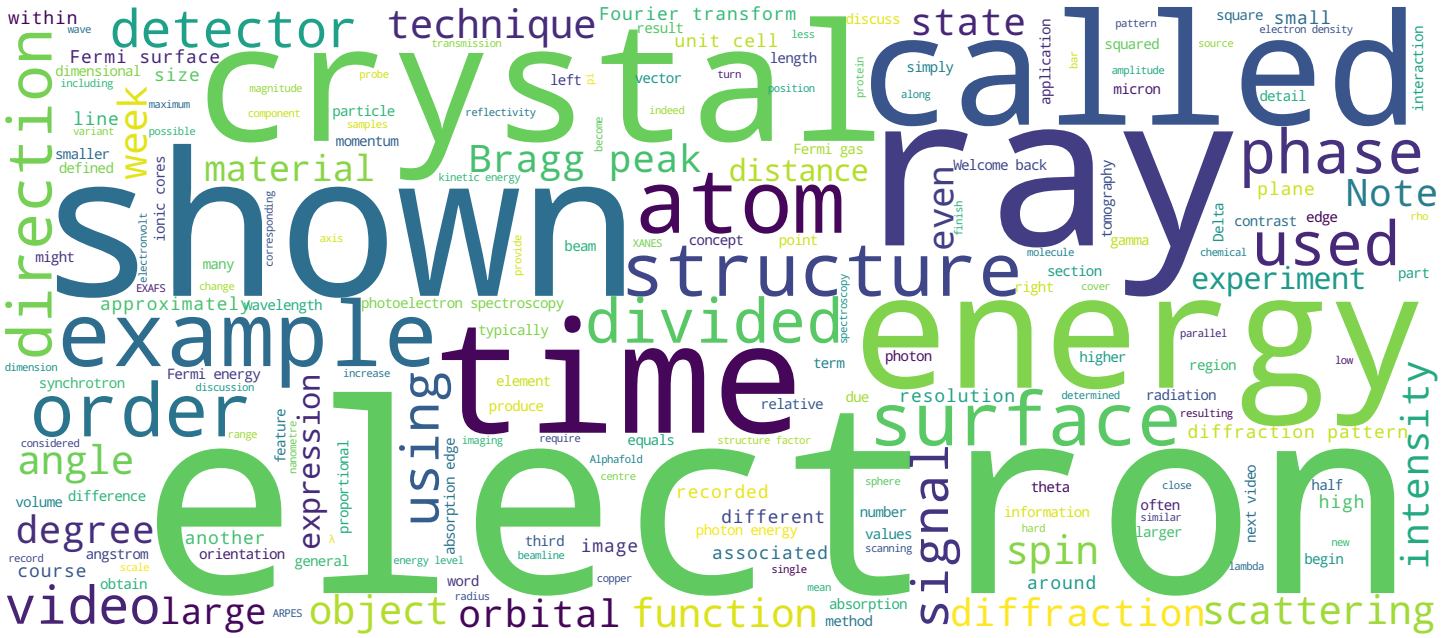

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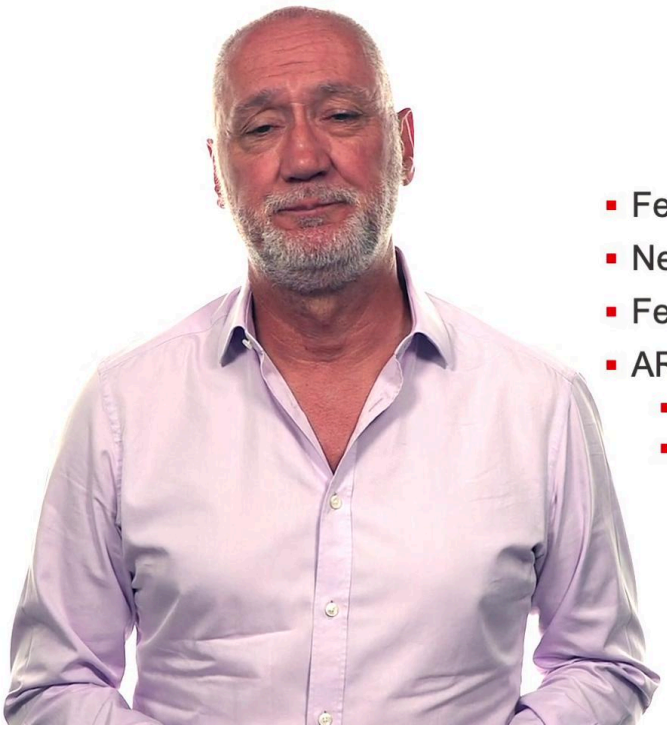
Video

Contents and objectives of this video



- Fermi gas
- Nearly-free electron model
- Fermi surface
- ARPES
  - Experimental aspects
  - Example

Welcome back to Week 4 of this course on synchrotron, XFEL radiation techniques and applications. In this first of two videos on angle-resolved photoelectron spectroscopy, or ARPES, we will consider some theoretical aspects necessary to understand ARPES data. We begin with a description of a gas of free-electrons called a Fermi gas, and then we'll extend this to the case of a nearly-free electron gas that, however, does feel the influence of the regular array of positive charges induced by the ionic cores in a crystal.

Notes

Summary

0m 05s

Pro memoria – The Fermi gas

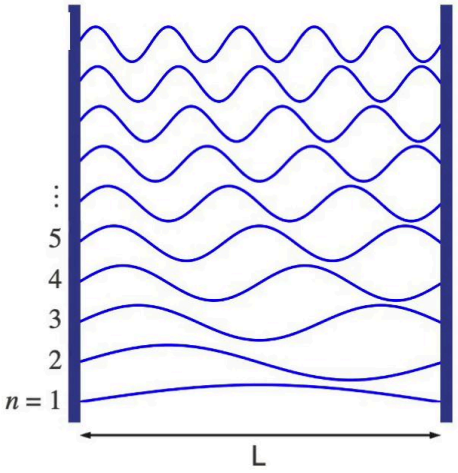
- Describes free electrons in a metal
- 1D box, electrons trapped inside
  - EM-theory demands zero E-field at boundary ⇒ $\lambda = 2L/n$
  - Energy level given by λ (or k)

$$E = \frac{p^2}{2m_e} = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2 n^2 \pi^2}{2m_e L^2}$$

  - Pauli exclusion principle allows maximum 2 electrons per level (spin up and spin down)
  - N electrons. Highest energy = E_F @ 0K

$$E_F^{(1D)} = \frac{\hbar^2 \pi^2}{2m_e L^2}\left(\frac{N}{2}\right)^2$$

$\lambda = 2L/n;\ n = 1, 2, 3, \cdots$



Now, last week we were introduced to the concept of the Fermi gas. The Fermi gas model starts off by assuming that the conduction electrons are completely free to move as they please without any influence from the ionic cores of the atoms, or indeed without any interaction with one another. We considered a one-dimensional case corresponding to a single line of regularly separated metal atoms of length L. Electromagnetic theory demands that the electric field at the boundaries to the one-dimensional box be zero, resulting in standing waves emerging from electrons with periodicity 2L divided by n. But the momentum of the electron is P equals h divided by λ, which in turn is equal to $\hbar$ times k, where k is the wave vector equal to 2π divided by λ. The electron kinetic energy is P^2 divided by $2m_e$, which is therefore equal to $\hbar^2$ k^2 divided by $2m_e$. Using our expression for λ, we then obtained an expression for the energy of the n^{th} electron in a metal to be E is equal to $\hbar^2$ n^2 π^2 divided by $2m_e$ L^2. Now, the Pauli Exclusion Principle allows a maximum of only two electrons per energy level, one with spin up, the other with spin down.

Notes

Summary

0m 45s

Pro memoria – The Fermi gas

- Describes free electrons in a metal
- 1D box, electrons trapped inside
  - EM-theory demands zero E-field at boundary ⇒ $\lambda = 2L/n$
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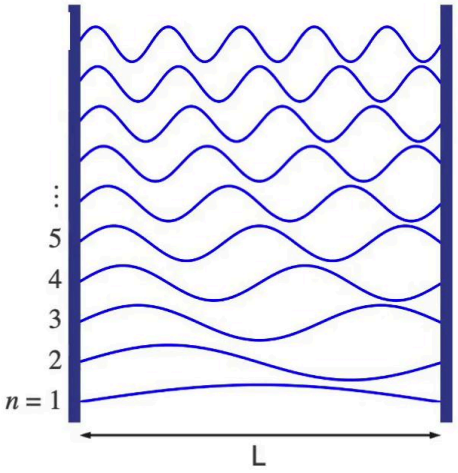
  - Pauli exclusion principle allows maximum 2 electrons per level (spin up and spin down)
  - N electrons. Highest energy = E_F @ 0K

$$E_F^{(1D)} = \frac{\hbar^2 \pi^2}{2m_e L^2}\left(\frac{N}{2}\right)^2$$

$\lambda = 2L/n;\ n = 1, 2, 3, \cdots$



If we say there are N electrons in total, there will be N divided by two energy levels, each level occupied by these two electrons spin up and spin down. The highest energy, which is called the Fermi energy, is therefore equal to $\hbar^2$, π^2 divided by $m_e L^2$, multiplied by n^2, upon 2, squared.

Notes

Summary

2m 37s

Pro memoria – The Fermi gas in 3D

- In 3D

$$E^{(3D)} = \frac{\hbar^2\pi^2}{2m_eL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

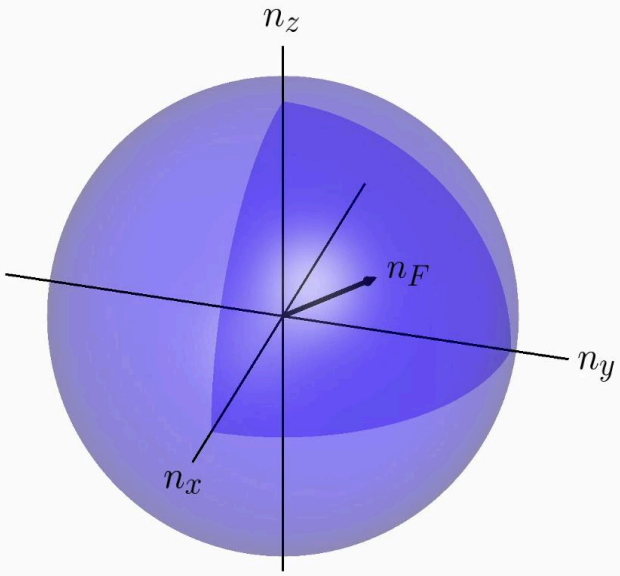
- But

$$N = 2 \times \frac{1}{8} \times \frac{4}{3}\pi n_F^3$$

$$\Rightarrow n_F = \left(\frac{3N}{\pi}\right)^{1/3}$$

$$\Rightarrow E_F = \frac{\hbar^2\pi^2}{2m_eL^2}\left(\frac{3N}{\pi}\right)^{2/3}$$

$$= \frac{\hbar^2}{2m_e}\left(\frac{3\pi^2N}{V}\right)^{2/3} \quad (V = L^3)$$



Now, in three dimensions, the energy depends on n_x, n_y, and n_z independently, corresponding to the three orthogonal axes of the box. We only consider positive N. Therefore, the total number of electrons, N, is equal to 2 times the volume of an octant of a spherical volume of radius nF or 2 times one-eighth times four-thirds π nF^3, which is equal to πnF^3 divided by 3. From this, we can say that nF is equal to 3n divided by π to the third, and therefore, that EF is equal to $\hbar^2\pi^2$ divided by $2m_eL^2$ multiplied by 3N divided by π to the two-thirds, which in turn is equal to $\hbar^2$ divided by $2m_e$, multiplied by $3\pi^2$ N divided by V, all to the two-thirds, whereby V is equal to L^3, the volume of the box. Feel free to rewind a bit to take your time in understanding this relatively straightforward derivation, but perhaps as yet novel argument and difficult to follow.

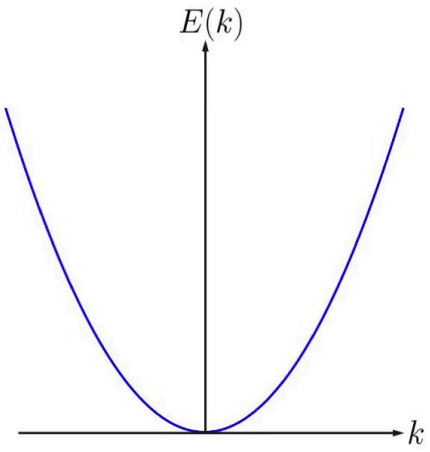
Notes

Summary

3m 04s

Pro memoria – The Fermi gas in 3D

$$E = \frac{p^2}{2m_e} = \frac{\hbar^2 k^2}{2m_e}$$



We therefore, see that the energy of an electron is proportional to the square of its momentum or k vector, if that electron is completely free.

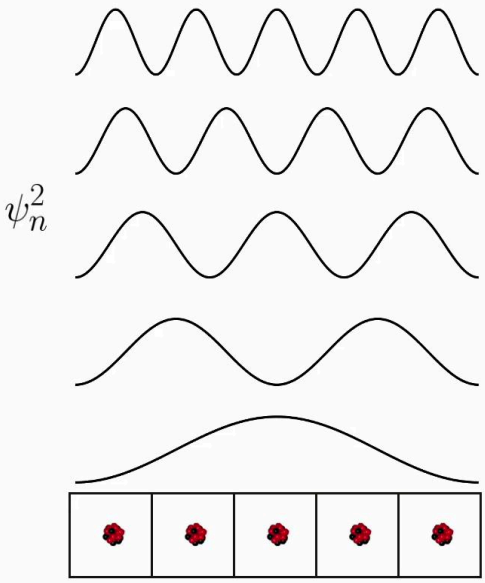
Notes

Summary

4m 34s

Adding an interaction with the core

- 1D case



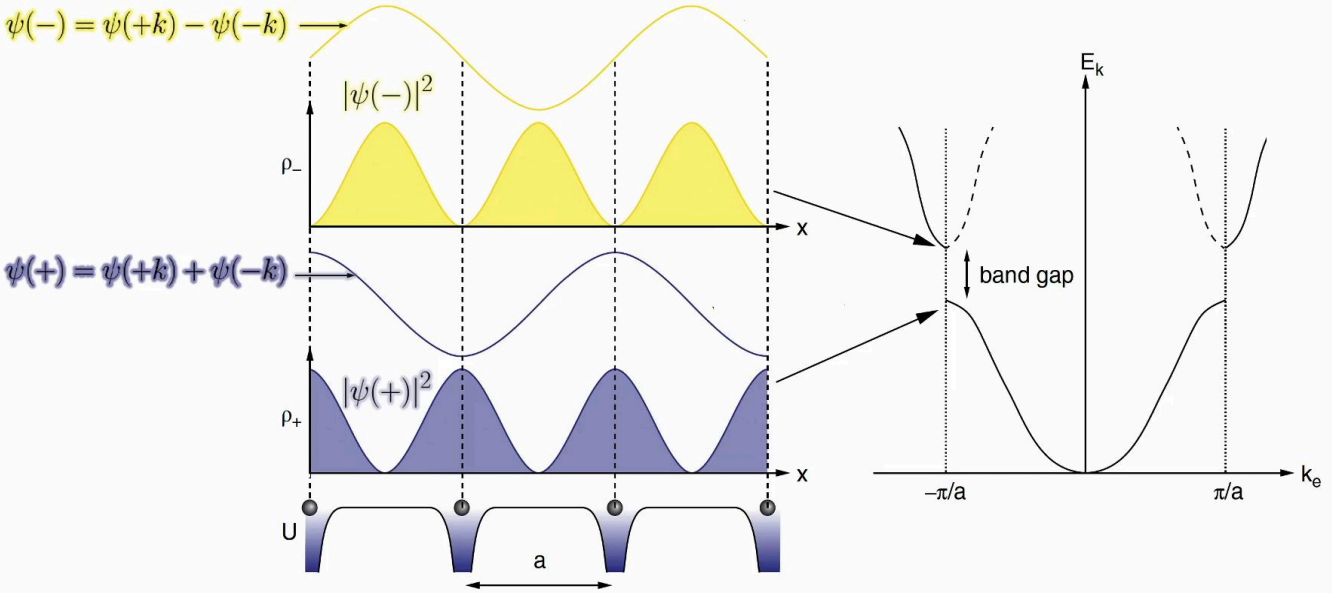
We now add an interaction with the ionic cores. Let's consider the first allowed five wave functions of the electrons in a 1D row of five-unit cells. The probability distribution is simply the squares of these shown here. Note that the fifth probability distribution, $\Psi 5^2$, has a periodicity which is equal to that of the 1D crystal, while the wave function, $\Psi 5$, has a periodicity λ equal to twice the crystal periodicity.

Notes

Summary

4m 44s

Nearly-free electron model



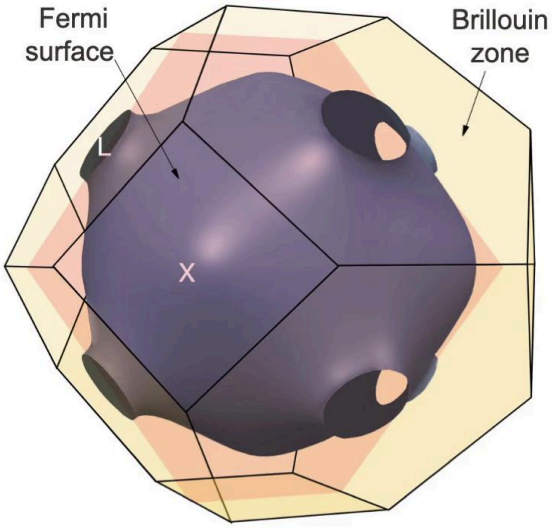
But there are two allowed solutions to this, one in which the electrons tend to pile up on top of the ionic cores, and one in which they line up between the cores. The former we designate with a plus sign and the latter with a minus sign. Now, when we consider these two functions on the energy versus wavevector graph, instead of having the same energy, the interaction with the cores means that the Ψ plus function is more energetically stable, as the electrons have a larger probability of being located at, and coulombically attracted to, the positively-charged ions, while the Ψ minus function is correspondingly higher in energy due to its unfavourable distribution. As a consequence, there arises a band gap at the Fermi energy at k values of plus or minus π divided by a.

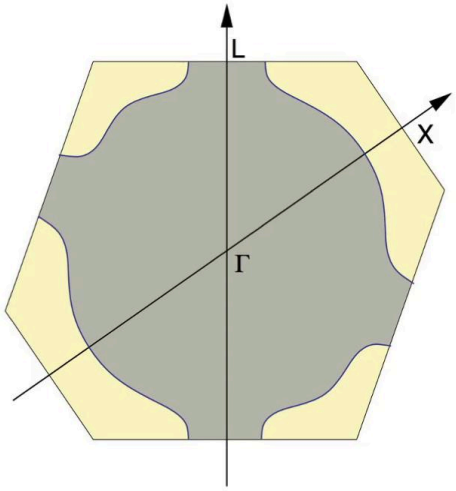
Notes

Summary

5m 22s

Band structure and the Fermi surface





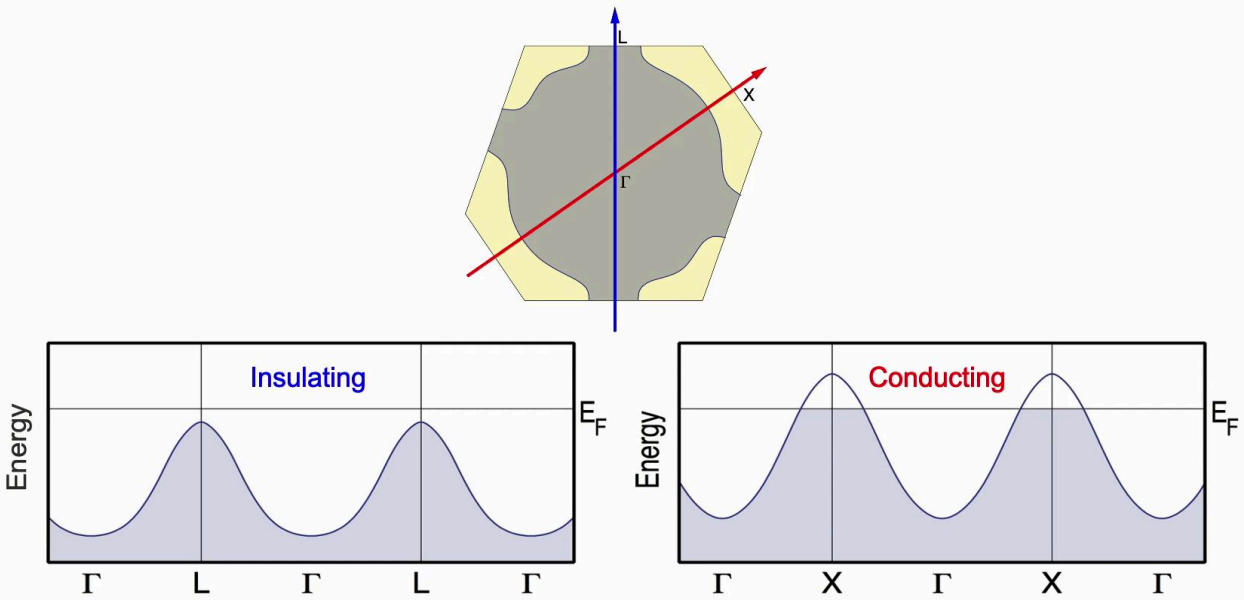
In the case of a completely interaction-free Fermi gas, the Fermi surface, that is, the shape of the 2D surface at the Fermi energy is simply that of a sphere. In reality, however, the Fermi surface changes according to which direction the electron is moving through the crystal, which is determined by kx, ky, and kz, and depends on the interaction between it and the ionic electrostatic potential in that direction. Even for the most simple, elemental, metals such as copper, the Fermi surface can assume complex forms, as shown here. The repeat structure in reciprocal or momentum space is called the Brillouin zone. We see a cut through the Fermi surface on the right-hand side. The centre of this, which has zero momentum, is called the gamma point, while the two crystallographic directions; 1, 1, 1, denoted L, and 1, 0, 0, denoted X, are also shown.

Notes

Summary

6m 22s

Band structure and the Fermi surface



Looking at this in more detail, if we look along the gamma L and gamma X directions, the Fermi surface never crosses the gamma L line, and in this direction, all the states are, therefore, below the Fermi energy, and a gap opens up between the occupied states and unoccupied states in this direction. In contrast, in the gamma X direction, the Fermi surface does cross the Fermi energy, and copper is thus conducting in this direction.

Notes

Summary

7m 26s

In the next video...

In the next video, we will look at ultraviolet photoelectron spectroscopy and specifics of angle-resolved photoelectron spectroscopy, or ARPES, a hugely important technique used to investigate the electronic properties of crystalline materials.

Notes

Summary

7m 59s