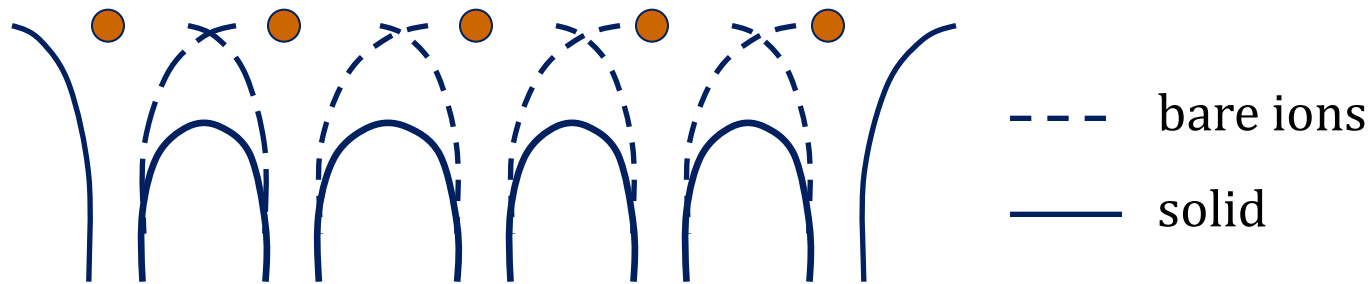


# Dynamics of Bloch Electrons

- A. Energy Bands
- B. Equations of Motion
- C. Effective Mass
- D. De Haas-van Alphen Effect
- E. Angle-Resolved Photoemission Spectroscopy (ARPES)
- F. Bloch Oscillation

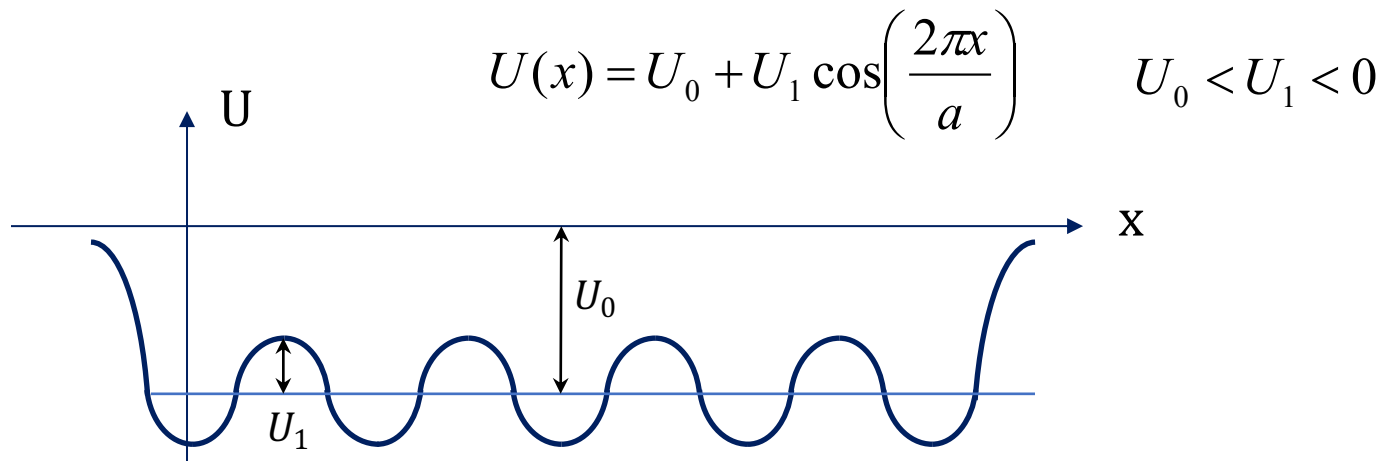
# Energy Band Gap in a Periodic Potential

Recall the electrostatic potential energy in a crystalline solid along a line passing through a line of atoms:



Along a line parallel to this but running between atoms, the divergences of the periodic potential energy are softened.

A simple 1D model that captures the periodicity of such a potential is:



# Electron Wavefunctions in a Periodic Potential

Consider the following cases:

$U_1 = 0$  Wavefunctions are plane waves and energy bands are parabolic:  $\psi = Ae^{i(kx-\omega t)}$   $E = \frac{\hbar^2 k^2}{2m}$

$U_1 \neq 0$  Electrons wavelengths much larger than  $a$ , so wavefunctions and energy bands are nearly the same as above  
 $k \ll \frac{\pi}{a}$

$U_1 \neq 0$  Electrons wavelengths approach  $a$ , so waves begin to be strongly back-scattered :  
 $k \leq \frac{\pi}{a}$   $\psi_{\pm} = Ae^{i(kx-\omega t)} \pm Be^{-i(kx-\omega t)}$   $B < A$

$U_1 \neq 0$  Electrons waves are strongly back-scattered (Bragg scattering) so standing waves are formed:  
 $k = \frac{\pi}{a}$

$$\psi_{\pm} = C \left[ e^{i(kx-\omega t)} \pm e^{-i(kx-\omega t)} \right] = \frac{1}{\sqrt{2}} A \left[ e^{ikx} \pm e^{-ikx} \right] e^{-i\omega t}$$

# Bloch Theorem and Wavefunctions

Bloch theorem is one of the most important formal results in all of solid state physics because it tells us the mathematical form of an electron wavefunction in the presence of a periodic potential energy.

In independent-electron approximation, the time-independent Schrodinger equation (SE) for an electron in a periodic potential is:

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right] \psi = E \psi$$

where the potential energy is invariant under a lattice translation vector  $\mathbf{T}$ :

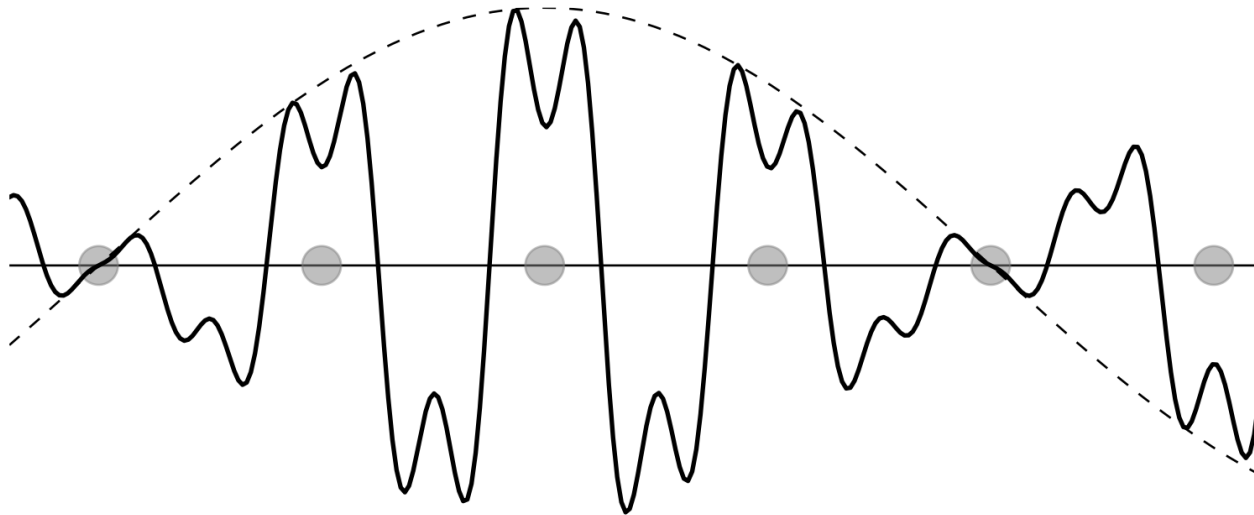
$$U(\mathbf{r} + \mathbf{T}) = U(\mathbf{r}) \quad \text{and} \quad \mathbf{T} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

Bloch showed that the solutions to the SE are the product of a plane wave and a function with the periodicity of the lattice:

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \quad \text{and} \quad u_{\mathbf{k}}(\mathbf{r} + \mathbf{T}) = u_{\mathbf{k}}(\mathbf{r})$$

# Bloch Wavefunctions

$$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}}$$



This result gives evidence to support the nearly-free electron approximation, in which the periodic potential is assumed to have a very small effect on the plane-wave character of a free electron wavefunction. It also explains why the free-electron gas model is so successful for the simple metals!

# Tight Binding Method

The tight binding approximation is also called the linear combination of atomic orbital (LCAO) approximation in which the one electron wavefunction  $\psi_{\mathbf{k}}(\mathbf{r})$  is built from the electron wavefunction of an isolated atom,  $\varphi(\mathbf{r})$ .

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_j C_{\mathbf{k}j} \varphi(\mathbf{r} - \mathbf{r}_j) ,$$

where the sum is over all lattice points.

This function is of the Bloch form if  $C_{\mathbf{k}j} = N^{-1/2} e^{i\mathbf{k} \cdot \mathbf{r}_j}$  for a crystal of  $N$  atoms:

$$\psi_{\mathbf{k}}(\mathbf{r}) = N^{-1/2} \sum_j \exp(i\mathbf{k} \cdot \mathbf{r}_j) \varphi(\mathbf{r} - \mathbf{r}_j) .$$

We find the first-order energy by calculating the diagonal matrix elements of the hamiltonian of the crystal:

$$\langle \mathbf{k} | H | \mathbf{k} \rangle = N^{-1} \sum_j \sum_m \exp[i\mathbf{k} \cdot (\mathbf{r}_j - \mathbf{r}_m)] \langle \varphi_m | H | \varphi_j \rangle ,$$

where  $\varphi_m \equiv \varphi(\mathbf{r} - \mathbf{r}_m)$ . Writing  $\boldsymbol{\rho}_m = \mathbf{r}_m - \mathbf{r}_j$ ,

$$\langle \mathbf{k} | H | \mathbf{k} \rangle = \sum_m \exp(-i\mathbf{k} \cdot \boldsymbol{\rho}_m) \int dV \varphi^*(\mathbf{r} - \boldsymbol{\rho}_m) H \varphi(\mathbf{r}) .$$

We consider the integrals over the same atom and the nearest neighbor atoms only, then

$$\int dV \varphi^*(\mathbf{r})H\varphi(\mathbf{r}) = -\alpha \quad ; \quad \int dV \varphi^*(\mathbf{r} - \boldsymbol{\rho})H\varphi(\mathbf{r}) = -\gamma \quad ;$$

and we have the first-order energy, provided  $\langle \mathbf{k} | \mathbf{k} \rangle = 1$ :

$$\langle \mathbf{k} | H | \mathbf{k} \rangle = -\alpha - \gamma \sum_m \exp(-i\mathbf{k} \cdot \boldsymbol{\rho}_m) = \epsilon_{\mathbf{k}} \quad .$$

For a simple cubic structure the nearest-neighbor atoms are at

$$\boldsymbol{\rho}_m = (\pm a, 0, 0) \quad ; \quad (0, \pm a, 0) \quad ; \quad (0, 0, \pm a) \quad ,$$

we have  $\epsilon_{\mathbf{k}} = -\alpha - 2\gamma(\cos k_x a + \cos k_y a + \cos k_z a)$  .

Thus the energies are confined to a band of width  $12\gamma$ . The weaker the overlap, the narrower is the energy band.

If  $ka \ll 1$ ,  $\epsilon_{\mathbf{k}} \simeq -\alpha - 6\gamma + \gamma k^2 a^2$ , the effective mass  $m^* = \hbar^2 / 2\gamma a^2$

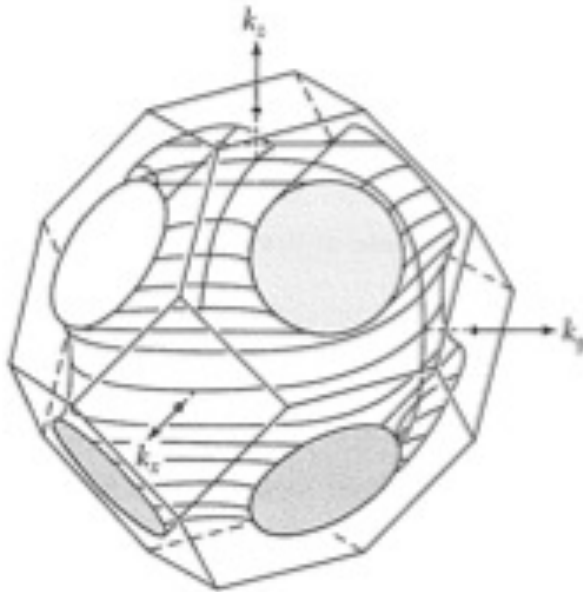
When the overlap integral  $\gamma$  is small, the band is narrow and the effective mass is high.

For the bcc structure with eight nearest neighbors,

$$\epsilon_{\mathbf{k}} = -\alpha - 8\gamma \cos \frac{1}{2} k_x a \cos \frac{1}{2} k_y a \cos \frac{1}{2} k_z a .$$

For the fcc structure with twelve nearest neighbors,

$$\epsilon_{\mathbf{k}} = -\alpha - 4\gamma(\cos \frac{1}{2} k_y a \cos \frac{1}{2} k_z a + \cos \frac{1}{2} k_z a \cos \frac{1}{2} k_x a + \cos \frac{1}{2} k_x a \cos \frac{1}{2} k_y a)$$



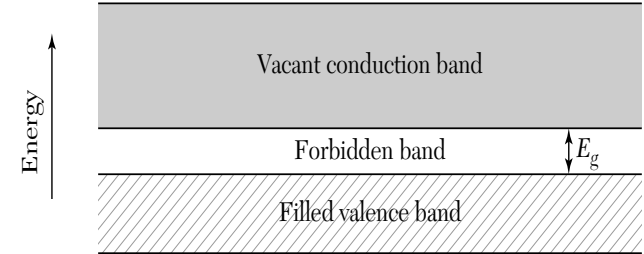
A constant energy surface of an fcc crystal structure in the nearest neighbor tight-binding approximation. The surface shown has  $\epsilon = -\alpha + 2|\gamma|$ .

The tight-binding (or LCAO) approximation is quite good for inner electrons of atoms, but it is not often good description for the conduction electrons. It is used to describe approximately the *d* bands of transition metals and the valence bands of diamondlike and inert gas crystals.



# Band Gap

The **band gap** is the difference in energy between the lowest point of the conduction band and the highest point of the valence band. The lowest point in the conduction band is called the **conduction band edge**; the highest point in the valence band is called the **valence band edge**.



**Table 1 Energy gap between the valence and conduction bands**  
(*i* = indirect gap; *d* = direct gap)

Crystal	Gap	$E_g$ , eV		Crystal	Gap	$E_g$ , eV	
		0 K	300 K			0 K	300 K
Diamond	<i>i</i>	5.4		SiC(hex)	<i>i</i>	3.0	—
Si	<i>i</i>	1.17	1.11	Tc	<i>d</i>	0.33	—
Ge	<i>i</i>	0.744	0.66	HgTe <sup>a</sup>	<i>d</i>	−0.30	
$\alpha$ Sn	<i>d</i>	0.00	0.00	PbS	<i>d</i>	0.286	0.34–0.37
InSb	<i>d</i>	0.23	0.17	PbSe	<i>i</i>	0.165	0.27
InAs	<i>d</i>	0.43	0.36	PbTe	<i>i</i>	0.190	0.29
InP	<i>d</i>	1.42	1.27	CdS	<i>d</i>	2.582	2.42
GaP	<i>i</i>	2.32	2.25	CdSe	<i>d</i>	1.840	1.74
GaAs	<i>d</i>	1.52	1.43	CdTe	<i>d</i>	1.607	1.44
GaSb	<i>d</i>	0.81	0.68	SnTe	<i>d</i>	0.3	0.18
AlSb	<i>i</i>	1.65	1.6	Cu <sub>2</sub> O	<i>d</i>	2.172	—

<sup>a</sup>HgTe is a semimetal; the bands overlap.

# Equations of Motion

The propagation speed of an electron wavepacket in a periodic crystal can be calculated from the energy band along that direction in reciprocal space:

$$\text{electron velocity: (1-D)} \quad v_g = \frac{d\omega}{dk} = \frac{1}{\hbar} \frac{dE}{dk} \quad \text{(3-D)} \quad \mathbf{v}_g(\mathbf{k}) = \hbar^{-1} \nabla_{\mathbf{k}} \epsilon(\mathbf{k})$$

The work  $\delta\epsilon$  done on the electron by the electric field  $E$  in the time interval  $\delta t$  is

$$\delta\epsilon = -eEv_g \delta t, \quad \text{and since} \quad \delta\epsilon = (d\epsilon/dk)\delta k = \hbar v_g \delta k,$$

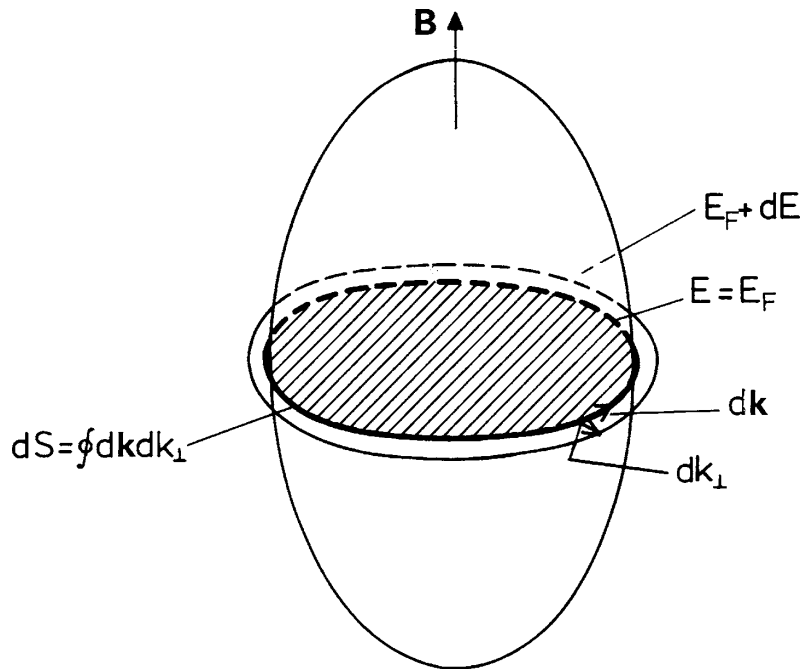
we have  $\delta k = -(eE/\hbar)\delta t$  and  $\hbar dk/dt = -eE = F$ , so we obtain

$$\hbar \frac{d\mathbf{k}}{dt} = \mathbf{F}$$

This is an important relation: in a crystal  $\hbar d\mathbf{k}/dt$  is equal to the external force on the electron. In free space  $d(m\mathbf{v})/dt$  is equal to the force. We have not overthrown Newton's second law of motion: the electron in the crystal is subject to forces from the crystal lattice as well as from external sources.

In a constant magnetic field  $\mathbf{B}$ , the equation of motion is

$$\hbar \frac{d\mathbf{k}}{dt} = -\frac{e}{c} \mathbf{v} \times \mathbf{B} \quad \text{or} \quad \frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar^2 c} \nabla_{\mathbf{k}} \epsilon \times \mathbf{B} \quad \text{with} \quad \mathbf{v} = \hbar^{-1} \nabla_{\mathbf{k}} \epsilon$$



an electron moves in  $\mathbf{k}$  space in a direction normal to the direction of the gradient of the energy  $\epsilon$ , so that **the electron moves on a surface of constant energy**. The value of the projection  $k_B$  of  $\mathbf{k}$  on  $\mathbf{B}$  is constant during the motion. The motion in  $\mathbf{k}$  space is on a plane normal to the direction of  $\mathbf{B}$ , and the orbit is defined by the intersection of this plane with a surface of constant energy.

# Physical Derivation of Equations of Motion

We consider the Bloch eigenfunction  $\psi_{\mathbf{k}}$  belonging to the energy eigenvalue  $\epsilon_{\mathbf{k}}$  and wavevector  $\mathbf{k}$ :

$$\psi_{\mathbf{k}} = \sum_{\mathbf{G}} C(\mathbf{k} + \mathbf{G}) \exp[i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}]$$

The expectation value of the momentum of an electron in the Bloch state  $\mathbf{k}$  is

$$\mathbf{P}_{\text{el}} = \langle \mathbf{k} | -i\hbar\nabla | \mathbf{k} \rangle = \sum_{\mathbf{G}} \hbar(\mathbf{k} + \mathbf{G}) |C(\mathbf{k} + \mathbf{G})|^2 = \hbar(\mathbf{k} + \sum_{\mathbf{G}} \mathbf{G} |C(\mathbf{k} + \mathbf{G})|^2) ,$$

using  $\sum |C(\mathbf{k} + \mathbf{G})|^2 = 1$ .

We suppose that a weak external force is applied to the crystal in a time interval such that the total impulse is  $\mathbf{J} = \int \mathbf{F} dt$ . We will have

$$\mathbf{J} = \Delta \mathbf{p}_{\text{tot}} = \Delta \mathbf{p}_{\text{lat}} + \Delta \mathbf{p}_{\text{el}}$$

The change of momentum of the electron will be

$$\Delta \mathbf{p}_{\text{el}} = \hbar \Delta \mathbf{k} + \sum_{\mathbf{G}} \hbar \mathbf{G} [(\nabla_{\mathbf{k}} |C(\mathbf{k} + \mathbf{G})|^2) \cdot \Delta \mathbf{k}]$$

The change  $\Delta \mathbf{p}_{\text{lat}}$  in the lattice momentum resulting from the change of state of the electron is

$$\Delta \mathbf{p}_{\text{lat}} = -\hbar \sum_{\mathbf{G}} \mathbf{G} [(\nabla_{\mathbf{k}} |C(\mathbf{k} + \mathbf{G})|^2) \cdot \Delta \mathbf{k}] ,$$

The total momentum change is therefore

$$\Delta \mathbf{p}_{\text{el}} + \Delta \mathbf{p}_{\text{lat}} = \mathbf{J} = \hbar \Delta \mathbf{k}$$

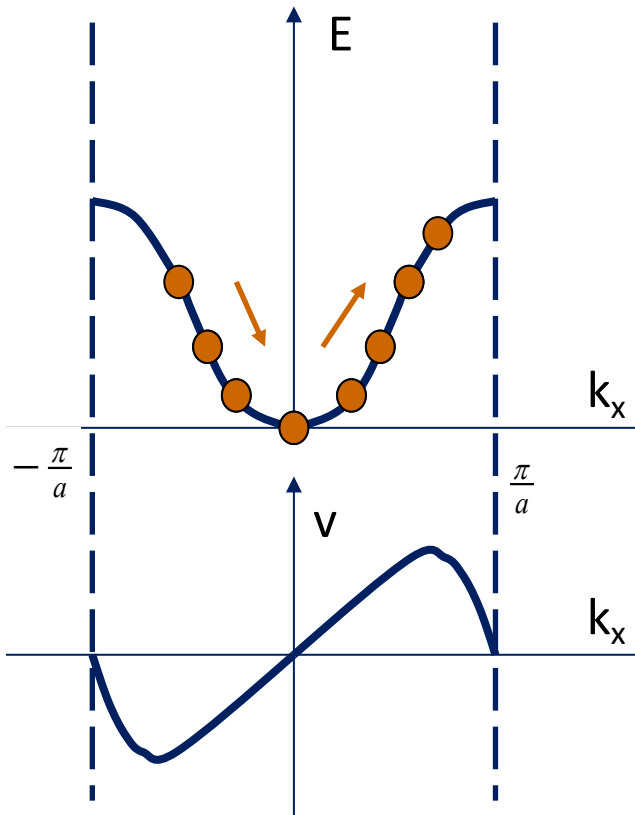
Since  $d\mathbf{J}/dt = \mathbf{F}$ , we thus have

$$\hbar d\mathbf{k} / dt = \mathbf{F}$$

# Band Electron in E Field

Now we see that the external electric field causes a change in the  $k$  vectors of all electrons:

$$\vec{F} = \hbar \frac{d\vec{k}}{dt} = -e\vec{E} \quad \longrightarrow \quad \frac{d\vec{k}}{dt} = \frac{-e\vec{E}}{\hbar}$$



If the electrons are in a partially filled band, this will break the symmetry of electron states in the 1<sup>st</sup> BZ and produce a net current. But if they are in a filled band, even though all electrons change  $k$  vectors, the symmetry remains, so  $J = 0$ .

When an electron reaches the 1<sup>st</sup> BZ edge (at  $k = \pi/a$ ) it immediately reappears at the opposite edge ( $k = -\pi/a$ ) and continues to increase its  $k$ .

As an electron's  $k$  value increases, its velocity increases, then decreases to zero and then becomes negative when it reemerges at  $k = -\pi/a$ .

Thus, an AC current is predicted to result from a DC field (Bloch oscillations).

# Band Effective Mass of an Electron

We can write the equation of motion of a Bloch electron in 1-D:

$$a_x = \frac{dv_x}{dt} = \frac{dv_x}{dk_x} \frac{dk_x}{dt} \quad \text{and} \quad \frac{dv_x}{dk_x} = \frac{dv_g}{dk_x} = \frac{d}{dk_x} \left( \frac{1}{\hbar} \frac{dE}{dk_x} \right) = \frac{1}{\hbar} \frac{d^2 E}{dk_x^2}$$

Also, from the acceleration theorem:  $\frac{dk_x}{dt} = \frac{F_x}{\hbar}$

This gives:

$$a_x = \frac{1}{\hbar} \frac{d^2 E}{dk_x^2} \left( \frac{F_x}{\hbar} \right) \quad \text{or} \quad F_x = \frac{\hbar^2}{d^2 E / dk_x^2} a_x$$

With the analogy of  $F = ma$ , the band effective mass is defined as:

$$m^* \equiv \frac{\hbar^2}{d^2 E / dk_x^2} \quad \text{or} \quad \boxed{\frac{1}{m^*} \equiv \frac{1}{\hbar^2} \frac{d^2 E}{dk_x^2}}$$

The effective mass depends on the electron's energy and thus its location in the band.

# Physical Meaning of Effective Mass

For a free electron:

$$E = \frac{\hbar^2 k_x^2}{2m} \quad \text{and} \quad m^* \equiv \frac{\hbar^2}{\left(\frac{\hbar^2}{m}\right)} = m$$

It is easy to generalize this to a 3-D solid to take account of an anisotropic electron energy surface. We would find that  $m^*$  is a second-order tensor with 9 components:

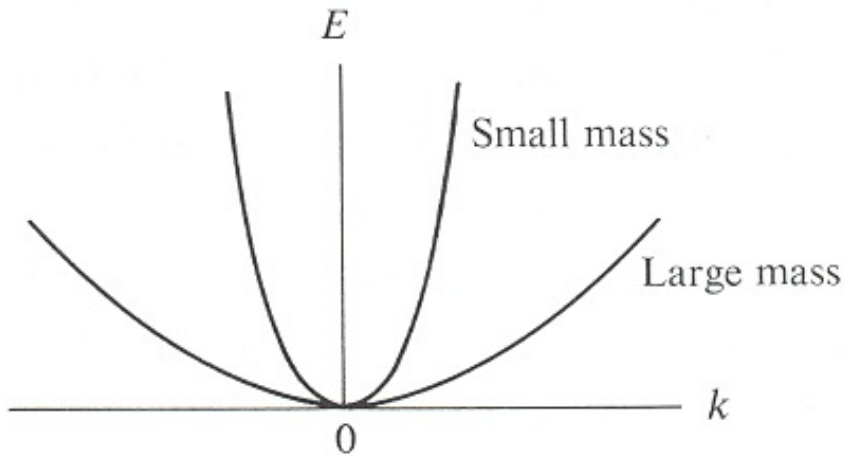
$$\left(\frac{1}{m^*}\right)_{\mu\nu} = \frac{1}{\hbar^2} \frac{d^2 \epsilon_k}{dk_\mu dk_\nu} ; \quad \frac{dv_\mu}{dt} = \left(\frac{1}{m^*}\right)_{\mu\nu} F_\nu ,$$

where  $\mu, \nu$  are Cartesian coordinates.

The effective mass concept is useful because it allows us to retain the notion of a free-electron even when we have a periodic potential, as long as we use  $m^*$  to account for the effect of the lattice on the acceleration of the electron.

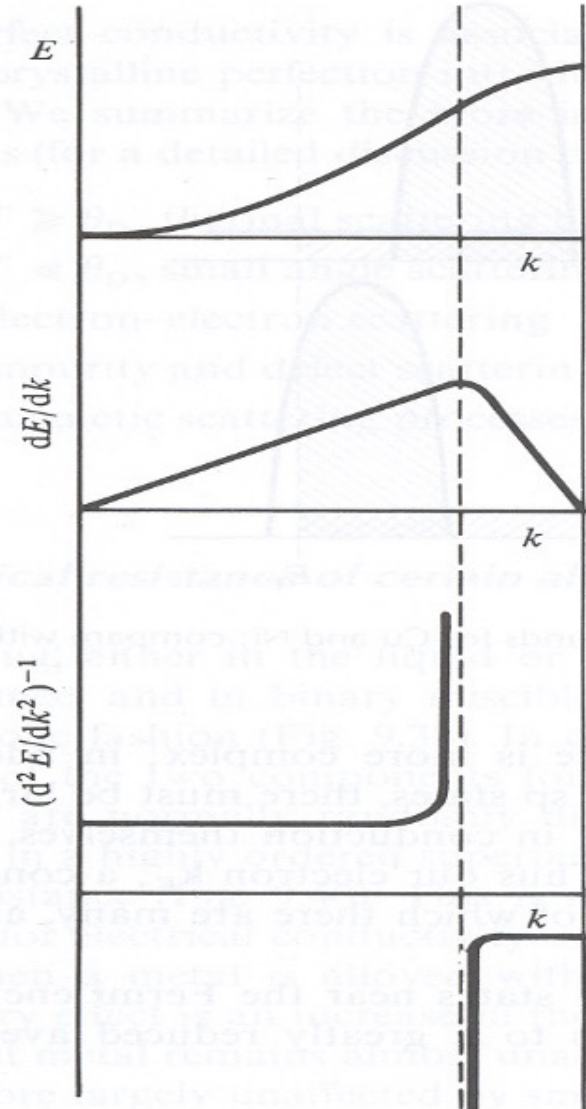


# Physical Meaning of Effective Mass

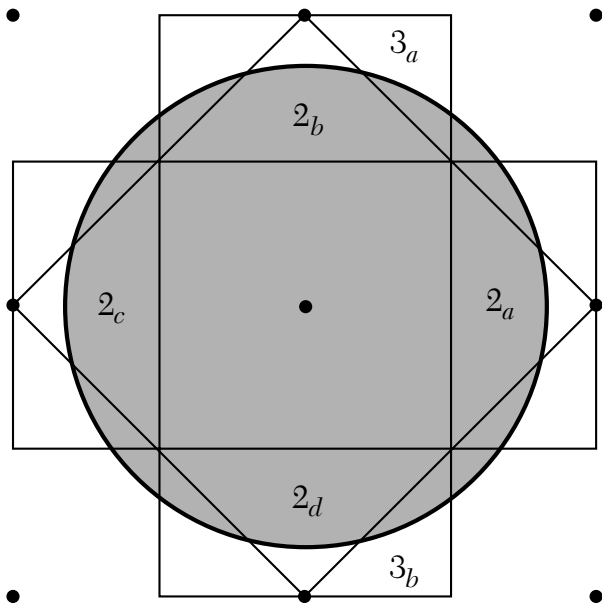


The effective mass is inversely proportional to the curvature of the energy band.

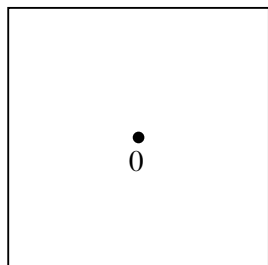
Near the bottom of a nearly-free electron band  $m^*$  is approximately constant, but it increases dramatically near the inflection point and even becomes negative near the zone edge.



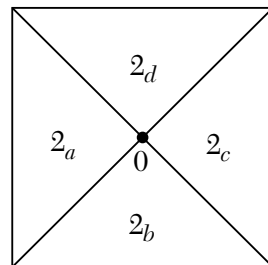
# Construction of Fermi Surfaces for Free Electrons



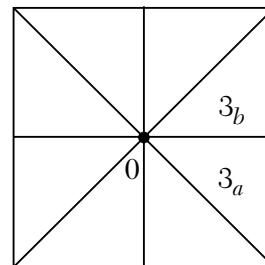
Brillouin zones of a square lattice in two dimensions. The circle shown is a surface of constant energy for free electrons; it will be the Fermi surface for some particular value of the electron concentration. The total area of the filled region in  $\mathbf{k}$  space depends only on the electron concentration 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.



1st zone



2nd zone



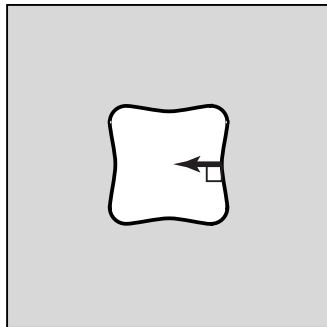
3rd zone

Fermi circle viewed in the reduced zone scheme

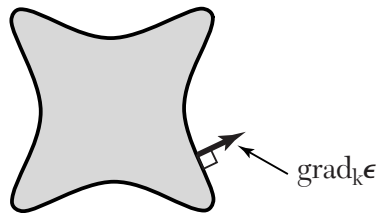
# Nearly Free Electrons Fermi Surfaces

From free electrons Fermi surfaces to nearly free electrons Fermi surfaces:

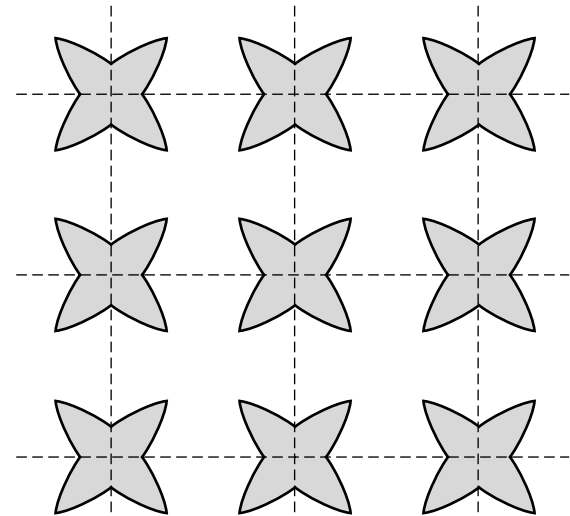
- The interaction of the electron with the periodic potential of the crystal creates energy gaps at the zone boundaries.
- Almost always the Fermi surface will intersect zone boundaries perpendicularly.
- The crystal potential will round out sharp corners in the Fermi surfaces.
- The total volume enclosed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



2nd zone



3rd zone



Free electron Fermi circle in the third zone drawn in the periodic zone scheme



# Quantization of Orbits in Magnetic Field

The momentum  $\mathbf{p}$  of a particle (with charge  $q$ ) in a magnetic field  $\mathbf{B}$  is the sum of two parts:  $\mathbf{p} = \mathbf{p}_{\text{kin}} + \mathbf{p}_{\text{field}} = \hbar\mathbf{k} + q\mathbf{A}/c$  and  $\mathbf{B} = \nabla \times \mathbf{A}$

The orbits in a magnetic field are quantized by the Bohr-Sommerfeld relation

$$\oint \mathbf{p} \cdot d\mathbf{r} = (n + \gamma)2\pi\hbar ,$$

when  $n$  is an integer and  $\gamma$  is a phase correction that for free electrons has the value  $1/2$ . The equation of motion of a particle of charge  $q$  in a magnetic field is

$$\hbar \frac{d\mathbf{k}}{dt} = \frac{q}{c} \frac{d\mathbf{r}}{dt} \times \mathbf{B} \quad \longrightarrow \quad \hbar\mathbf{k} = \frac{q}{c} \mathbf{r} \times \mathbf{B}$$

Thus,

$$\begin{aligned} \oint \mathbf{p} \cdot d\mathbf{r} &= \oint \hbar\mathbf{k} \cdot d\mathbf{r} + \frac{q}{c} \oint \mathbf{A} \cdot d\mathbf{r} \\ &= \frac{q}{c} \oint \mathbf{r} \times \mathbf{B} \cdot d\mathbf{r} + \frac{q}{c} \int \mathbf{curl} \mathbf{A} \cdot d\boldsymbol{\sigma} \\ &= -\frac{q}{c} \mathbf{B} \cdot \oint \mathbf{r} \times d\mathbf{r} + \frac{q}{c} \int \mathbf{B} \cdot d\boldsymbol{\sigma} \\ &= -\frac{2q}{c} \Phi + \frac{q}{c} \Phi = -\frac{q}{c} \Phi = (n + \gamma)2\pi\hbar \end{aligned}$$

It follows that the orbit of an electron is quantized in such a way that the flux through it is

$$\Phi_n = (n + \gamma)(2\pi\hbar c/e)$$

The flux unit  $2\pi\hbar c/e = 4.14 \times 10^{-7}$  gauss cm<sup>2</sup> or T m<sup>2</sup>.

$\therefore \hbar\mathbf{k} = \frac{q}{c} \mathbf{r} \times \mathbf{B}$ , a line element  $\Delta r$  in the plane normal to  $\mathbf{B}$  is related to  $\Delta k$  by  $\Delta r = (\hbar c/eB)\Delta k$ , so that the area  $S_n$  in  $\mathbf{k}$  space is related to the area  $A_n$  of the orbit in  $\mathbf{r}$  space by

$$A_n = (\hbar c/eB)^2 S_n .$$

Thus,

$$\Phi_n = BA_n = \left(\frac{\hbar c}{e}\right)^2 \frac{1}{B} S_n = (n + \gamma) \frac{2\pi\hbar c}{e}$$



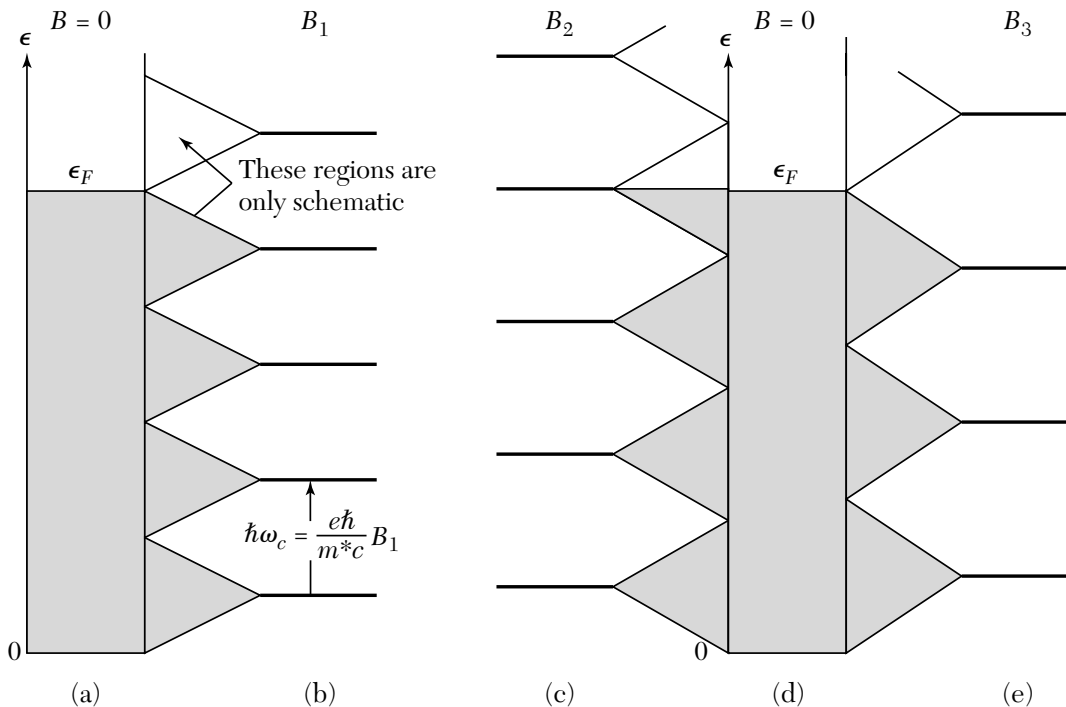
$$S_n = (n + \gamma) \frac{2\pi e}{\hbar c} B$$

# De Haas-van Alphen Effect

The de Haas-van Alphen effect is the oscillation of the magnetic moment of a metal as a function of the static magnetic field intensity. The effect can be observed in pure specimens at low temperatures in strong magnetic fields.

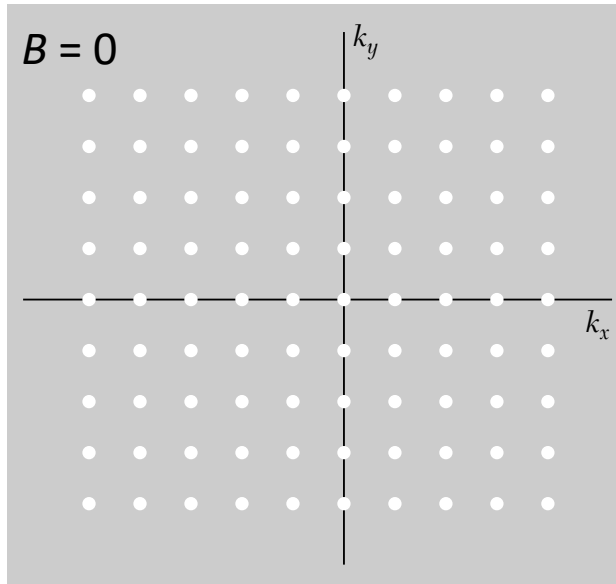
Assume the magnetic field is applied along the  $z$  axis, the area of an orbit in  $k_x, k_y$  plane is quantized and the area between successive orbits is

$$\Delta S = S_n - S_{n-1} = 2\pi eB/\hbar c$$

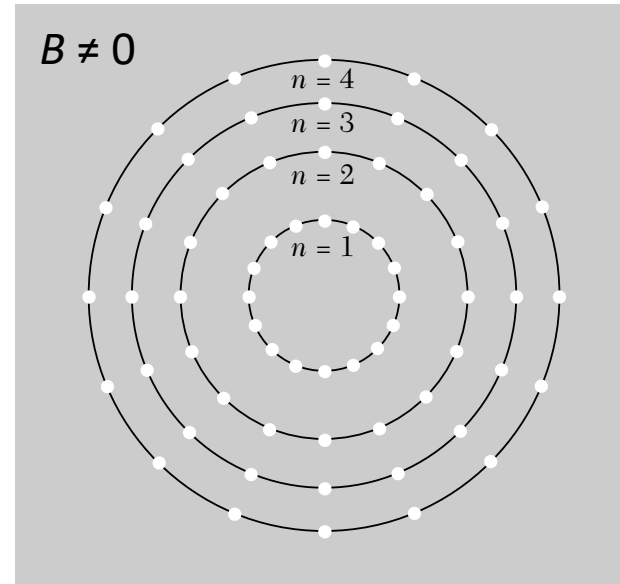


Explanation of the de Haas-van Alphen effect for a free electron gas in two dimensions in a magnetic field with  $B_1 < B_2 < B_3$ .

# Degeneracy of Orbits in Magnetic Field



(a)



(b)

allowed electron orbitals in two dimensions

The area between successive circles is

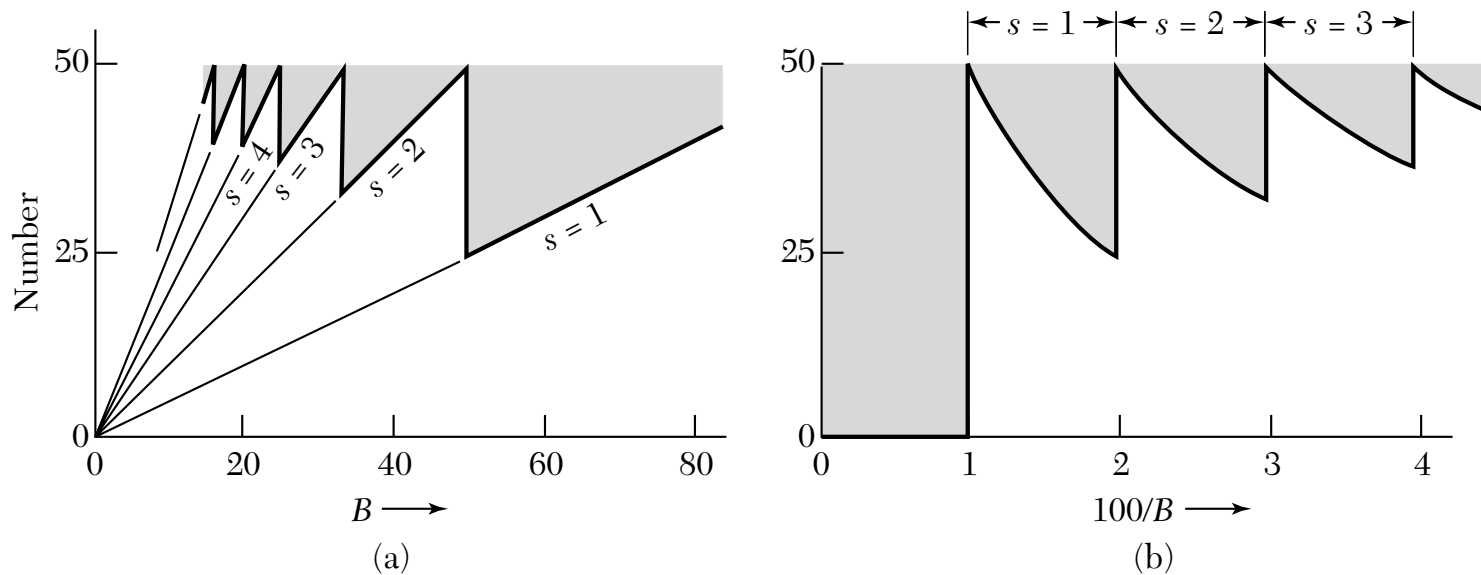
$$\pi\Delta(k^2) = 2\pi k(\Delta k) = (2\pi m/\hbar^2) \Delta\epsilon = 2\pi m\omega_c/\hbar - 2\pi eB/\hbar c$$

The number of free electron orbits collapsed into a **Landau level** is

$$D = (2\pi eB/\hbar c)(L/2\pi)^2 = \rho B \quad , \quad \text{and} \quad \rho = eL^2/2\pi\hbar c$$



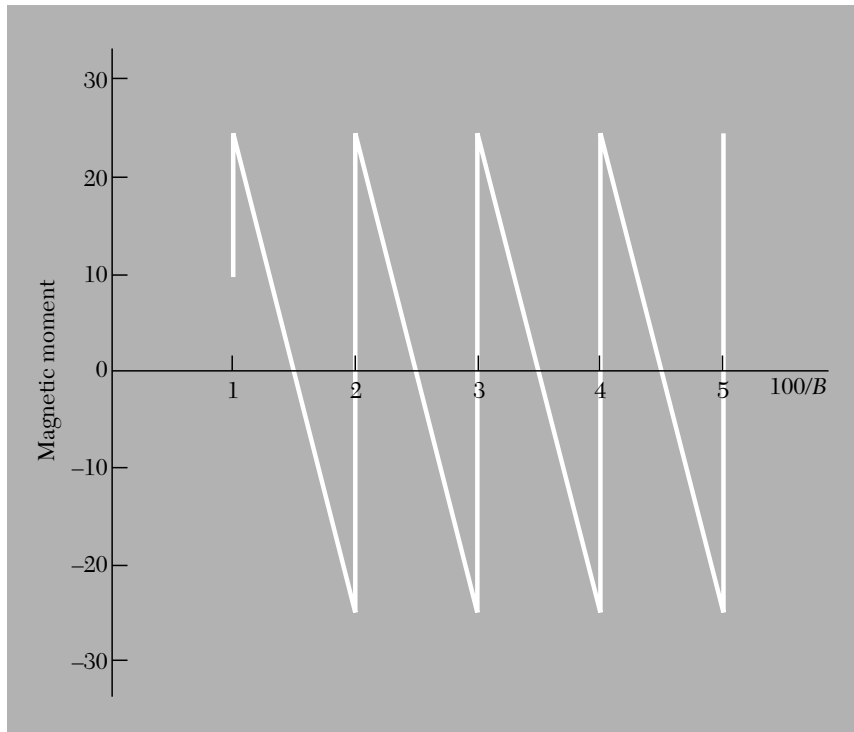
# Orbital Degeneracy Increases with $B$



**Figure 25** (a) The heavy line gives the number of particles in levels which are completely occupied in a magnetic field  $B$ , for a two-dimensional system with  $N = 50$  and  $\rho = 0.50$ . The shaded area gives the number of particles in levels partially occupied. The value of  $s$  denotes the quantum number of the highest level which is completely filled. Thus at  $B = 40$  we have  $s = 2$ ; the levels  $n = 1$  and  $n = 2$  are filled and there are 10 particles in the level  $n = 3$ . At  $B = 50$  the level  $n = 3$  is empty. (b) The periodicity in  $1/B$  is evident when the same points are plotted against  $1/B$ .

# dHvA Oscillation

The magnetic moment  $\mu$  of a system at absolute zero is given by  $\mu = -\partial U/\partial B$ . The moment here is an oscillatory function of  $1/B$ . This oscillatory magnetic moment of the Fermi gas at low temperatures is the de Haas-van Alphen effect.



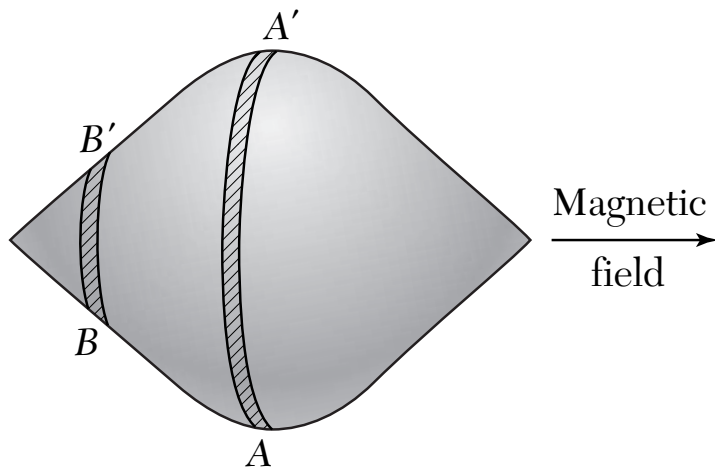
The oscillations occur at equal interval of  $1/B$  so that

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar c S}$$

where  $S$  is the extremal area of the Fermi surface normal to the direction of  $\mathbf{B}$ .

# Extremal Orbits in Magnetic Field

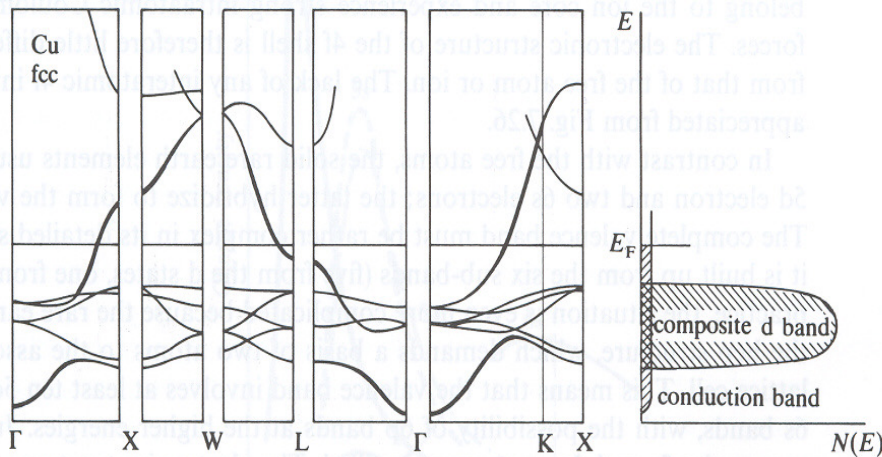
For a Fermi surface of general shape the sections at different values of  $kB$  will have different periods. Here  $kB$  is the component of  $k$  along the direction of the magnetic field. The response will be the sum of contributions from all sections or all orbits. *But the dominant response of the system comes from orbits whose periods are stationary with respect to small changes in  $kB$ .* Such orbits are called extremal orbits. Thus, in the figure, the section  $AA'$  dominates the observed cyclotron period.



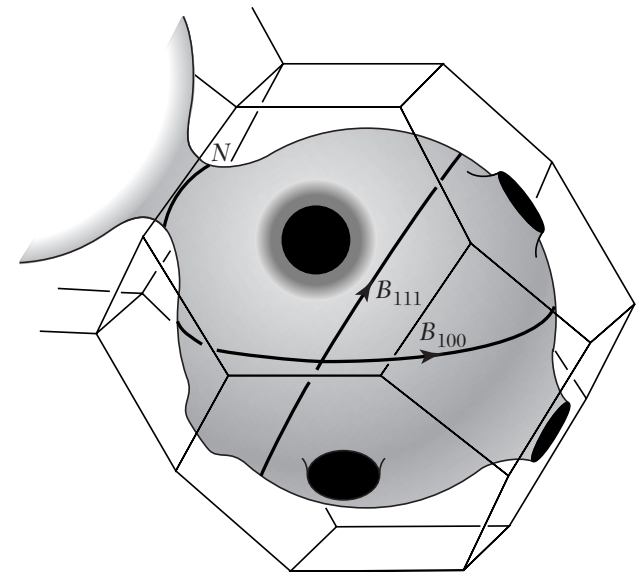
The orbits in the section  $AA'$  are extremal orbits: the cyclotron period is roughly constant over a reasonable section of the Fermi surface. Other sections such as  $BB'$  have orbits that vary in period along the section.

# Fermi Surface of Copper

Even if the free-electron Fermi sphere does not intersect a BZ boundary, its shape can still be affected at points close to the boundary where the energy bands begin to deviate from the free-electron parabolic shape. This is the case with Cu.



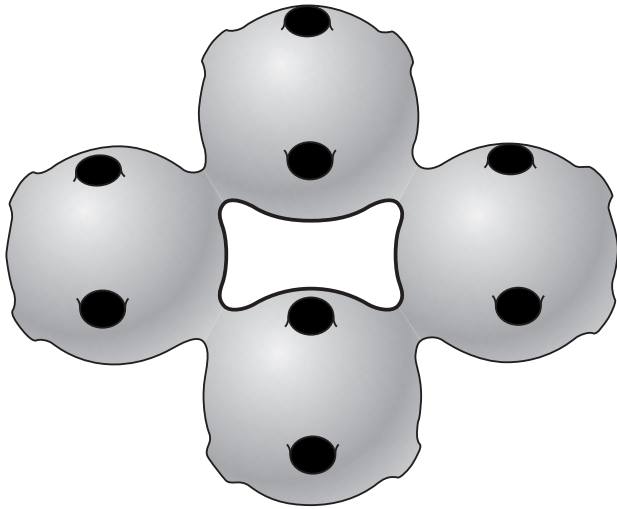
**Figure 7.25** The complete band structure diagram for Cu along the major symmetry directions (compare with the Brillouin zone of Fig. 7.15b). The diagram to the right is a simple schematic representation of the integrated density of levels and is convenient as a basis for the discussion of many physical properties of the later 'd' metals. We shall soon find that the sp valence electrons are responsible for the electrical conductivity of these metals; one therefore speaks of the 'conduction band'. (After Segall 1962.)



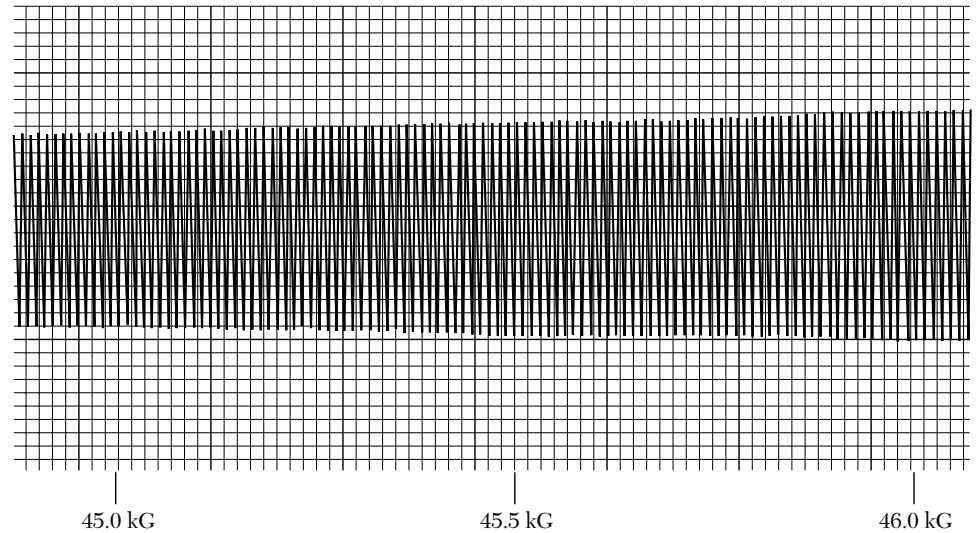
Fermi surface of copper

Just a slightly perturbed free-electron sphere!

# Fermi Surface of Gold



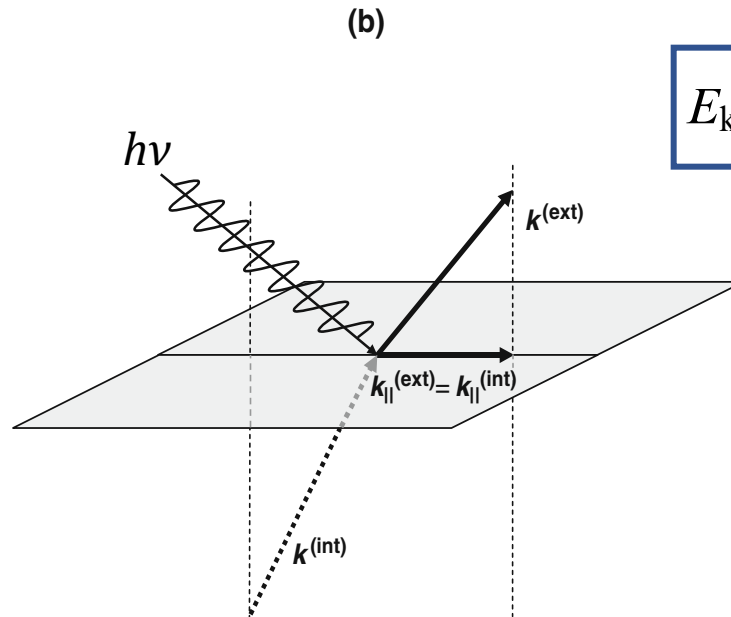
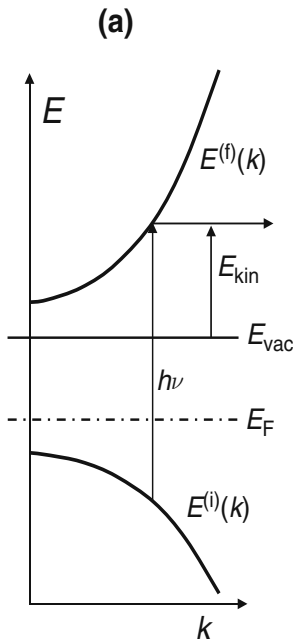
Dog's bone orbit of an electron on the Fermi surface of copper or gold in a magnetic field.



De Haas-van Alphen effect in gold with  $\mathbf{B} // [110]$ . The oscillation is from the dog's bone orbit of the left figure.

# Photoemission Process

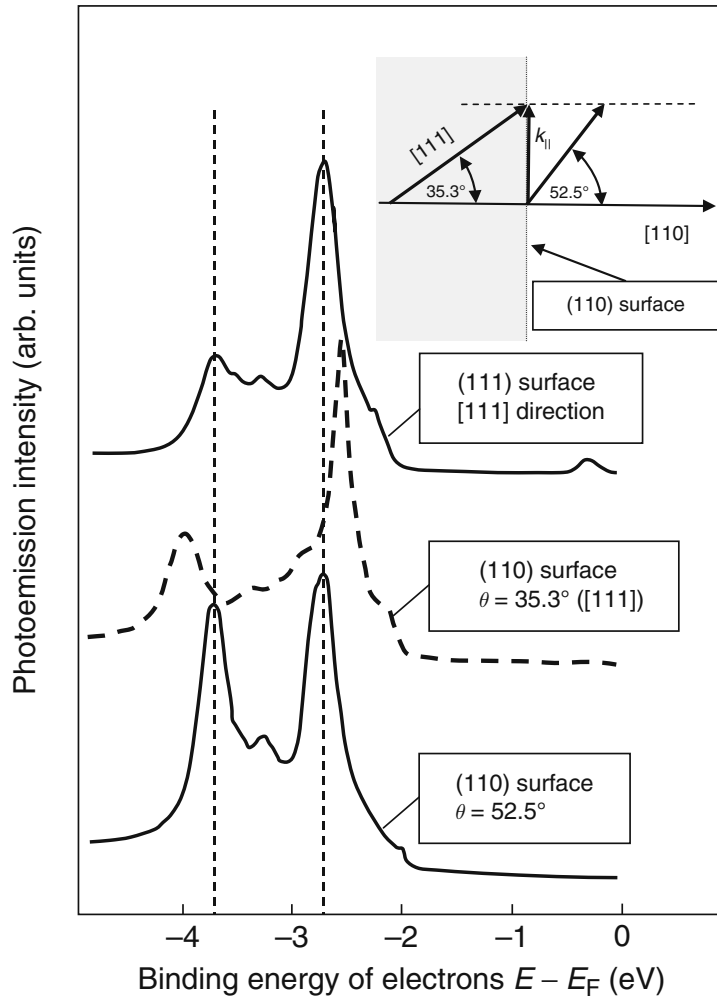
$$I_{\text{ph}}(\mathbf{k}_{\parallel}^{(\text{el})}, E_{\text{kin}}) \propto \sum_{i,j} \sum_{k_z} \left| \langle j, \mathbf{k}_{\parallel}, k_z | \mathbf{x} | i, \mathbf{k}_{\parallel}, k_z \rangle \right|^2 \\ \times \delta(E_{\text{kin}} + E_{\text{vac}} - E^{(i)}(\mathbf{k}_{\parallel}, k_z) - h\nu) \delta(\mathbf{k}_{\parallel} - \mathbf{k}_{\parallel}^{(\text{el})})$$



$$E_{\text{kin}} = -E_{\text{vac}} + E^{(i)}(\mathbf{k}_{\parallel}, k_z) + h\nu$$

Here,  $i, j$  denote the initial and final bands,  $\mathbf{k}_{\parallel}, k_z$  are the components of the wave vector in the initial and the final state, and  $E^{(i)}, E_{\text{vac}}$  are the energies of the initial state and the vacuum level.

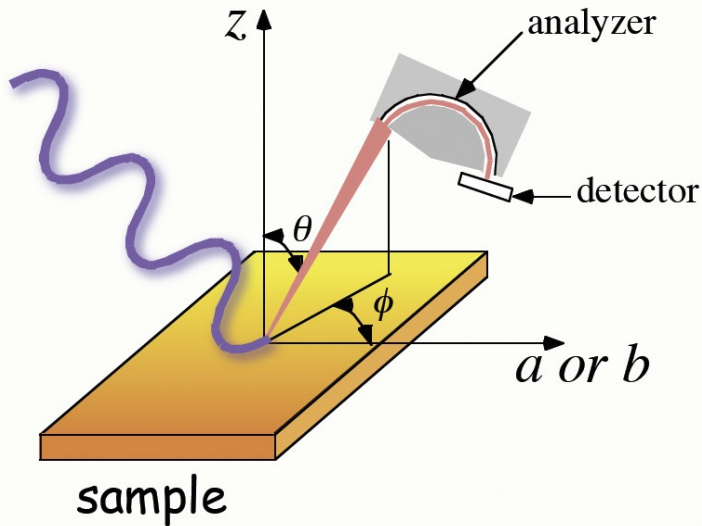
# Photoemission Spectra of Cu(111) and Cu(110)



Photoemission spectra of Cu(111) and Cu(110) surfaces serving to establish the wave vector  $k_{111}$  for bulk electronic states: the two prominent peaks appearing in the spectra along [111] on Cu(111) are found at an angle of  $\theta = 52.5^\circ$  in the [110] zone on Cu(110). The magnitude of  $k_{111}$  is determined by considering  $k_{\parallel}$  conservation.

$$k_{\parallel}^{(\text{int})} = k_{\parallel}^{(\text{ext})} \Rightarrow k_{111}^{(\text{int})} \sin 35^\circ = k^{(\text{ext})} \sin 52.5^\circ$$

# Angle-Resolved PhotoEmission Spectroscopy (ARPES)



We need:

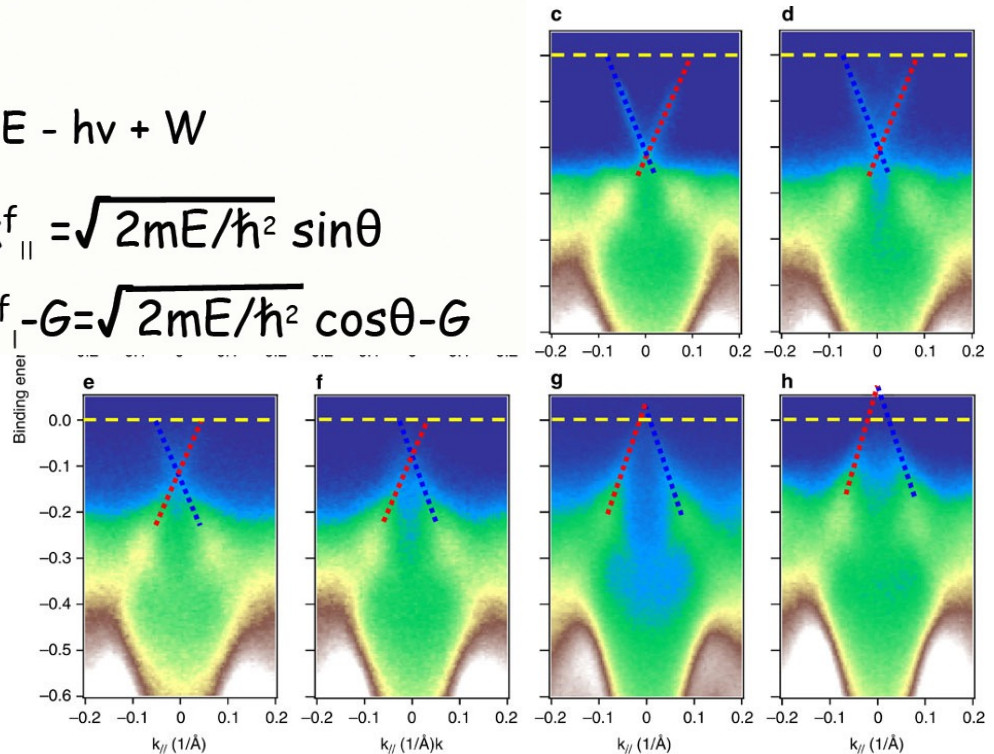
binding energy -  $E_b$

initial momentum -  $k^i$

$$E_b = E - h\nu + W$$

$$k_{||}^i = k_{||}^f = \sqrt{2mE/h^2} \sin\theta$$

$$k_{\perp}^i = k_{\perp}^f - G = \sqrt{2mE/h^2} \cos\theta - G$$



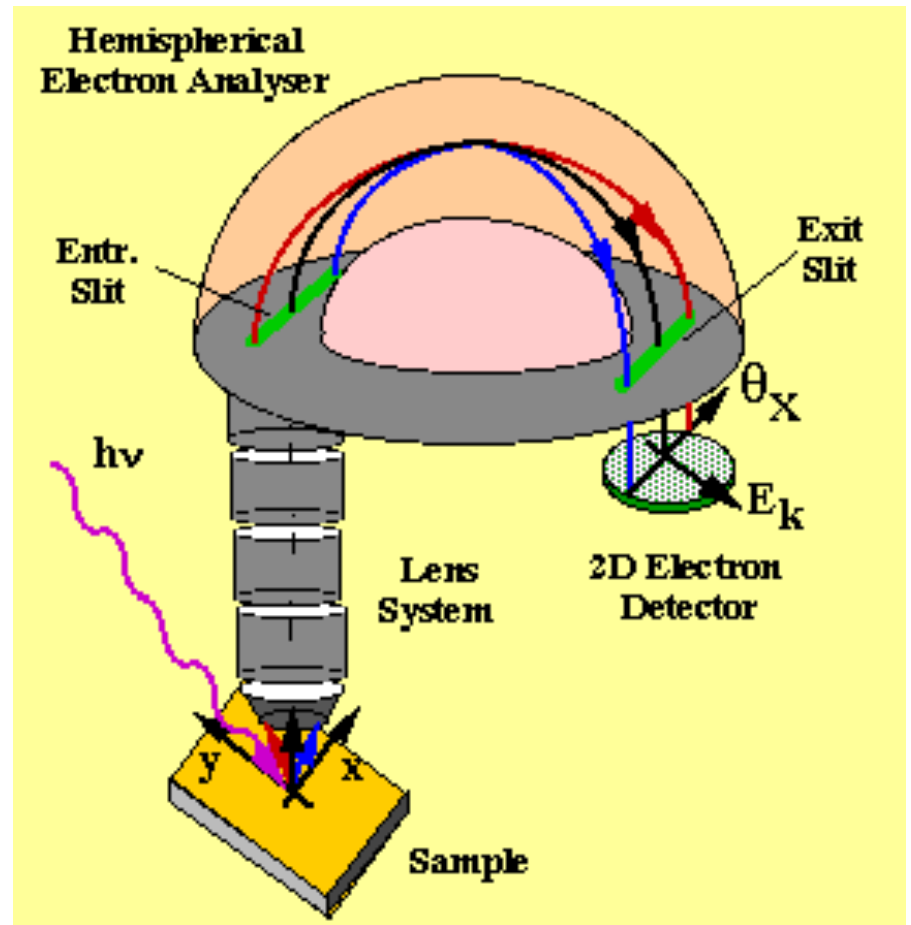


# Concentric Hemispherical Analyzer (CHA)



$$\Delta E/E_0 = s/R_0$$

s: mean slit width;  $R_0$ : mean radius



# Bloch oscillations

The one-dimensional equation of motion for an electron with wave vector  $k$  in a constant electric field  $E$  is:

$$\frac{dp}{dt} = \hbar \frac{dk}{dt} = -eE, \quad \longrightarrow \quad k(t) = k(0) - \frac{eE}{\hbar}t.$$

Suppose the dispersion relation for a given band  $\mathcal{E}(k) = A \cos ak$ ,

The group velocity  $v$  of the electron is given by

$$v(k) = \frac{1}{\hbar} \frac{d\mathcal{E}}{dk} = -\frac{Aa}{\hbar} \sin ak,$$

and the electron position  $x$  can be computed as a function of time:

$$x(t) = \int_0^t v(k(t')) dt' = x(0) + \frac{A}{eE} \cos\left(\frac{aeE}{\hbar}t\right).$$

This shows that the electron oscillates in real space. The angular frequency of the oscillations is given by

$$\omega_B = ae|E|/\hbar.$$

Bloch oscillations are not routinely observed because the electrons in a periodic system undergo collisions with ions in the lattice much too frequently, on the time scale of  $\tau$  ( $\approx 10^{-14}$  s).

# Problems

- 1. Impurity orbits.** Indium antimonide has  $E_g = 0.23$  eV; dielectric constant  $\epsilon = 18$ ; electron effective mass  $m_e = 0.015 m$ . Calculate (a) the donor ionization energy; (b) the radius of the ground state orbit. (c) At what minimum donor concentration will appreciable overlap effects between the orbits of adjacent impurity atoms occur? This overlap tends to produce an impurity band—a band of energy levels which permit conductivity presumably by a hopping mechanism in which electrons move from one impurity site to a neighboring ionized impurity site.
- 2. Hall effect with two carrier types.** Assuming concentration  $n, p$ ; relaxation times  $\tau_e, \tau_h$ ; and masses  $m_e, m_h$ , show that the Hall coefficient in the drift velocity approximation is

$$R_H = \frac{1}{ec} \cdot \frac{p - nb^2}{(p + nb)^2},$$

where  $b = \mu_e/\mu_h$  is the mobility ratio. In the derivation neglect terms of order  $B^2$ . In SI we drop the  $c$ . Hint: In the presence of a longitudinal electric field, find the transverse electric field such that the transverse current vanishes. The algebra may seem tedious, but the result is worth the trouble. Neglect  $(\omega_c\tau)^2$  in comparison with  $\omega_c\tau$ .

3. A semiconductor with a band gap energy  $E_g$  of 1eV and equal hole and electron effective masses  $m_e^* = m_h^* = m_0$  ( $m_0$  is free electron mass) is p-doped with an acceptor concentration of  $p = 10^{-18} \text{ cm}^{-3}$ . The acceptor energy level is located 0.2 eV above the valence band edge of the material.
- Show that intrinsic conduction in this material is negligible at 300 K.
  - Calculate the conductivity  $\sigma$  of the material at room temperature (300 K), given a hole mobility of  $\mu_p = 100 \text{ cm}^2/\text{Vs}$  at 300 K.
  - Plot the logarithm of the hole concentration,  $\ln p$ , versus reciprocal temperature  $1/T$  for the temperature range 100 to 1000 K.