Chapter 4: Summary

Solve lattice vibration equation of one atom/unit cell case.

Consider a set of ions M separated by a distance a,

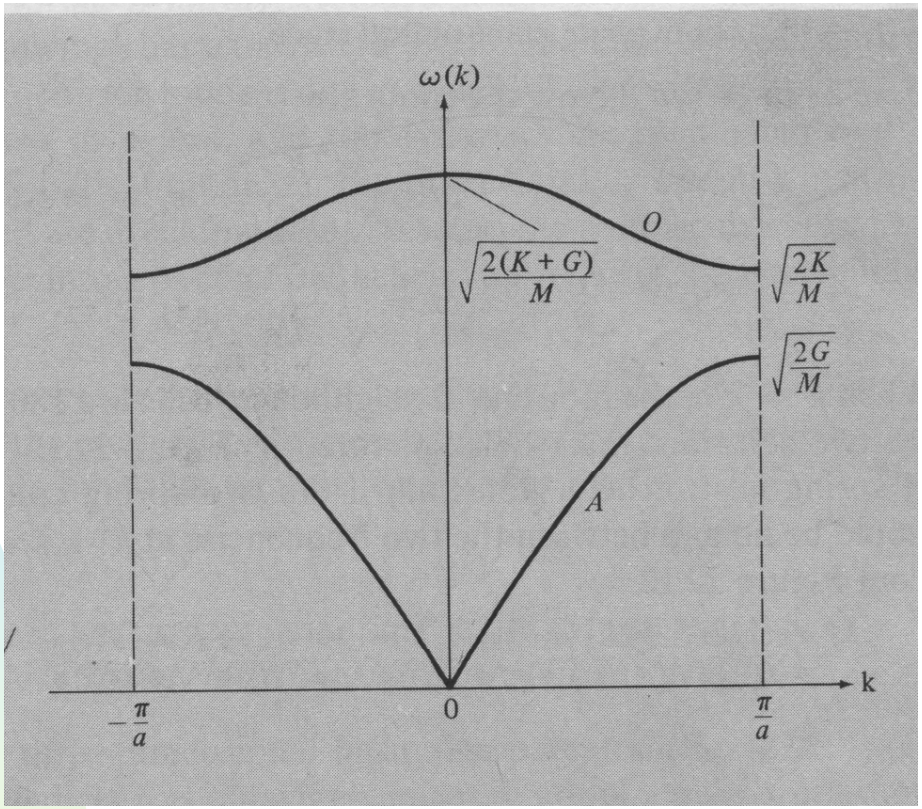
$\vec{R} = na$ for integral n. Let $u(na)$ be the displacement.

Assuming only neighboring ions interact, we have

$$U^{harm} = \frac{1}{2} C \sum_n \left[u(na) - u([n+1]a) \right]^2,$$

Newton's second law $F = Ma$ or

$$M \frac{du(na)}{dt^2} = -\frac{\partial U^{harm}}{\partial u(na)} = -C\left[2u(na) - u([n-1]a) - u([n+1]a) \right]$$



For each of the N values of k there are thus two solutions, leading to a total of $2N$ normal modes. The two ω vs k curves are two branches of the dispersion relation. Acoustic and optical branches.

Prob. 3, Consider a longitudinal wave $u_s = u\cos(\omega t - sKa)$ which propagates in a monatomic linear lattice of atoms of mass M, spacing a, and nearest neighbor interaction C.

a) show that the total energy of the wave is

$$E = \frac{1}{2}M\sum_s \left(du_s/dt\right)^2 + \frac{1}{2}C\sum_s \left(u_s - u_{s+1}\right)^2,$$

where s runs over all atoms.

b)By substitution of u_s in this expression, show that the time average total energy per atom is

$$\frac{1}{4}M\omega^2u^2 + \frac{1}{2}C\left(1-\cos Ka\right)u^2 = \frac{1}{2}M\omega^2u^2,$$

where the last step we have used the dispersion relation for this problem.

Chapter 5: Summary

Planck distribution function:

The average excitation quantum # of an oscillator is:

$$\langle n\rangle = \frac{\sum s\exp(-n\hbar\omega/\tau)}{\sum \exp(-s\hbar\omega/\tau)} = \frac{1}{\exp(\hbar\omega/\tau)-1}$$

At low temperatures,

$$\int_0^\infty dx\left(\frac{x}{e^x-1}\right) = \sum_{n=1}^{\infty}\int_0^\infty x^3 e^{-nx}dx = 6\sum_{n=1}^{\infty}\frac{1}{n^4} = \frac{\pi^4}{15},$$

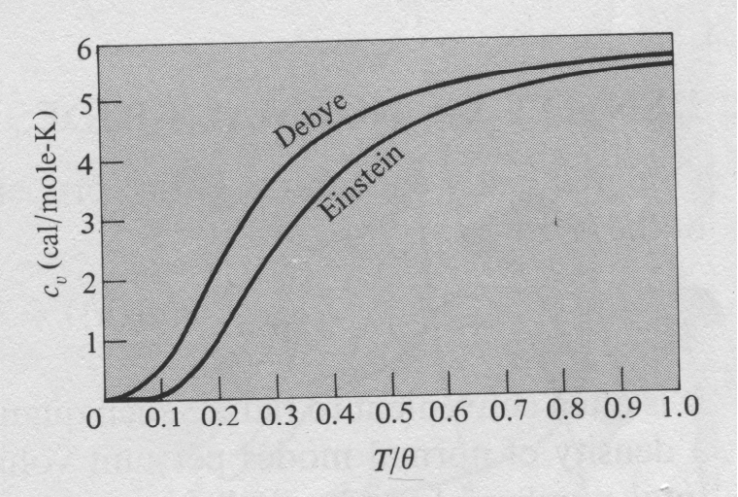
the heat capacity $C_V \cong \frac{12\pi^4}{5}Nk_B\left(\frac{T}{\theta}\right)^3$.

Einstein models of the density of states

In the case of N oscillators of the same frequency ω_0 in 1D, the Einstein density of states is $D(\omega) = N\delta(\omega - \omega_0)$

$$U = N\langle n\rangle \hbar\omega = \left(\frac{N\hbar\omega}{e^{\hbar\omega/\tau} - 1}\right).$$

The heat capacity $C_V = N\left(\frac{\partial U}{\partial T}\right)_V = Nk_B\left(\frac{\hbar\omega}{\tau}\right)^2 \frac{e^{\hbar\omega}}{(e^{\hbar\omega/\tau} - 1)^2}$



Thermal conductivity

The thermal conductivity coefficient K of a solid is defined as,

$j_U = -K\frac{dT}{dx}$, where j_U is the flux of thermal energy, and

x is distance. From the kinetic theory of gases we find

$K = \frac{1}{3}Cvl = \frac{1}{3}Cv^2\tau$, where C is the heat capacity per volume,

v is the average particle velocity, and l is the mean free path of a particle between collisions, τ^{-1} is the phonon collision rate.

1. ***Singularity in density of states.*** (a) From the dispersion relation derived in Chapter 4 for a monatomic linear lattice of N atoms with nearest-neighbor interactions, show that the density of modes is

$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{(\omega_m^2 - \omega^2)^{1/2}} \ ,$$

where ω_m is the maximum frequency. (b) Suppose that an optical phonon branch has the form $\omega(K) = \omega_0 - AK^2$, near $K = 0$ in three dimensions. Show that $D(\omega) = (L/2\pi)^3(2\pi/A^{3/2})(\omega_0 - \omega)^{1/2}$ for $\omega < \omega_0$ and $D(\omega) = 0$ for $\omega > \omega_0$. Here the density of modes is discontinuous.

Chapter 6: Free electron Fermi gas

Under quantum theory and the Pauli exclusion principle, we consider N noninteracting electrons confined to a volume $V(L^3)$. If the wave function of single electron is $\psi(\vec{r})$, then

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(\vec{r})=-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})=\varepsilon\psi(\vec{r}).$$

Applying boundary condition

$\psi(x,y,z+L)=\psi(x,y,z);\psi(x,y+L,z)=\psi(x,y,z);$

$\psi(x+L,y,z+L)=\psi(x,y,z)$. The solutions are

$\psi_K(\vec{r})=\frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}}, \varepsilon(k)=\frac{\hbar^2k^2}{2m}$. Note the probability of finding the electron somewhere in the volume is $1=\int d\vec{r}\left|\psi(\vec{r})\right|^2$.

Note that $\psi_K(\vec{r})$ is an eigenstate of the momentum operator,

$$\vec{\mathrm{p}} = \frac{\hbar}{i}\frac{\partial}{\partial \vec{r}} = \frac{\hbar}{i}\nabla, \frac{\hbar}{i}\frac{\partial}{\partial \vec{r}} e^{i\vec{k}\cdot\vec{r}} = \hbar\vec{k}e^{i\vec{k}\cdot\vec{r}}$$

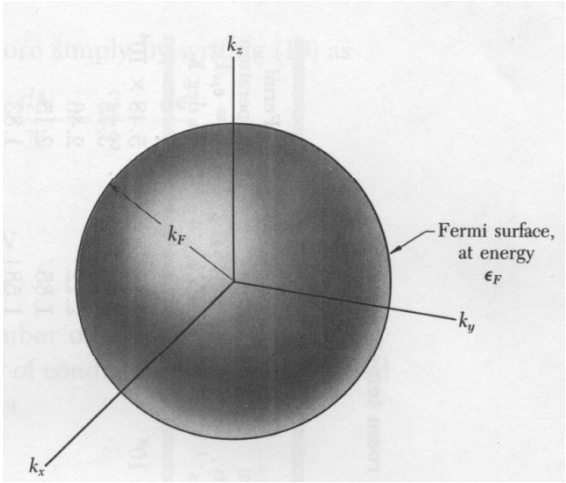
an electron in the level $\psi_K(\vec{r})$ has a momentum $\vec{\mathrm{p}} = \hbar\vec{k}$ and a velocity $\vec{v} = \vec{\mathrm{p}}/m = \hbar\vec{k}/m,$ where $\lambda = 2\pi/k.$

Periodic boundary condition requires

$$e^{ik_x L} = e^{ik_y L} = e^{ik_z L} = 1 \text{ or } k_x = \frac{2\pi n_x}{L}, k_y = \frac{2\pi n_y}{L}, k_z = \frac{2\pi n_z}{L}$$

Thus in a 3-D k-space, the allowed wavevectors are those along the three axes given integer mutiples of $\frac{2\pi}{L}$.

To calculate the allowed states in a region of k-space volume Ω, $\frac{\Omega}{(2\pi/L)^3} = \frac{\Omega V}{(2\pi)^3}$ or the number of allowed k-values per unit volume of k-space (known as the k-space density of levels) is $\frac{V}{(2\pi)^3}$. Because the electrons are noninteracting we can built up the N-electron ground state by placing electrons into the allowed one-electron levels. Pauli exclusion principle allows each wavevector to have 2 electronic levels with spins up and down.



Since the energy of a one-electron level is directly proportional to k^2, when N is enormous the occupied region will be indistinguishable from a sphere. The radius of this sphere is called k_F (F for Fermi), and its volume Ω is $4\pi k_F^3/3$. The # of allowed $\vec{k}$ within the sphere is: $\left(\frac{4\pi k_F^3}{3}\right)\left(\frac{V}{8\pi^3}\right)=\frac{k_F^3}{6\pi^2}V$. Since each allowed k-value leads to two one-electron levels, we must have $N=2\frac{k_F^3}{6\pi^2}V=\frac{k_F^3}{3\pi^2}V$.

If electron density is $n=N/V$, then we have $n=k_F^3/3\pi^2$.

The sphere of radius k_F containing the occupied one eletron levels is called the Fermi sphere.

The Surface of the Fermi sphere, which separate the occupied form the unoccupied levels is called the Fermi surface.

The momentum $p_F = \hbar k_F = \hbar \left(\frac{3\pi^2 N}{V} \right)^{1/3}$ of the occupied one-electron levels of highest energy is the Fermi momentum.

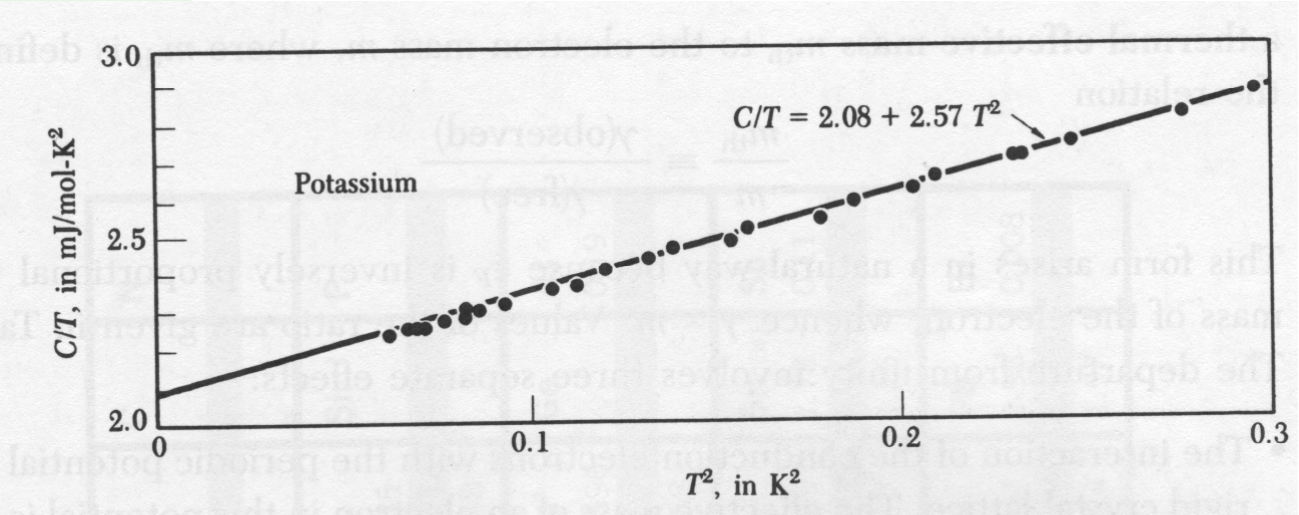
$\varepsilon_F = \hbar^2 k_F^2 / 2m = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$ is the Fermi energy;

$v_F = p_F / m = (\frac{\hbar}{m}) \left(\frac{3\pi^2 N}{V} \right)^{1/3}$ is the Fermi velocity.

Experimental heat capacity of metals

At sufficient low temperatures, $C_V = \gamma T + AT^3$. Where γ is the Sommerfeld parameter. The ratio of the observed to the free electron values of the electronic heat capacity is related to thermal effective mass as:

$$\frac{m_{th}}{m} \equiv \frac{\gamma(\text{observed})}{\gamma(\text{free})}$$



Electrical conductivity and Ohm's law

Considering Newton's second law, we have

$$\vec{F} = m\frac{d\vec{v}}{dt} = \hbar\frac{d\vec{k}}{dt} = -e(\vec{E} + \frac{1}{c}\vec{v} \times \vec{B})$$

The displacement of the Fermi sphere, $\delta\vec{k} = -e\vec{E}t / \hbar$.

If collision time is τ, the incremental velocity is $\vec{v} = -e\vec{E}\tau / m$.

In a constant electric field $\vec{E}$ and n electrons per volume, the electric current density is $\vec{j} = nq\vec{v} = ne^2\vec{E}\tau / m = \sigma\vec{E}$.

The electrical conductivity $\sigma = ne^2\tau / m$.

Thermal conductivity of metals
Wiedemann-Franz law

Thermal conductivity for a Fermi gas

$$K_{el} = \frac{1}{3} Cvl = \frac{\pi^2}{3} \cdot \frac{nk_B^2 T}{mv_F^2} \cdot v_F \cdot l = \frac{\pi^2 nk_B^2 T\tau}{3m}$$

The Wiedemann-Franz law states that for metals at not too low temperatures the ratio of the thermal conductivity to the electrical conductivity is directly proportional to the temperature, independent of the particular metal.

$$\frac{K_{el}}{\sigma} = \frac{\pi^2 nk_B^2 T\tau / 3m}{ne^2\tau / m} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 T \equiv LT.$$

Lorenz number $L = 2.45 \times 10^{-8}$ watt-ohm/deg^2

Chapter 7: Summary

Bloch's theorem

The eigenstates ψ of the one-electron Hamiltonian

$H = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) \right)$, where $U(\vec{r}+\vec{R}) = U(\vec{r})$ for all $\vec{R}$ in a Bravias lattice, can be chosen to have the form of a plane wave times a function with the periodicity of the Bravias lattice:

$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(\vec{r})$, where $u_{n\vec{k}}(\vec{r}+\vec{R}) = u_{n\vec{k}}(\vec{r})$ for all $\vec{R}$ in the Bravias lattice. or

$$\boxed{\psi(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\psi(\vec{r})}$$

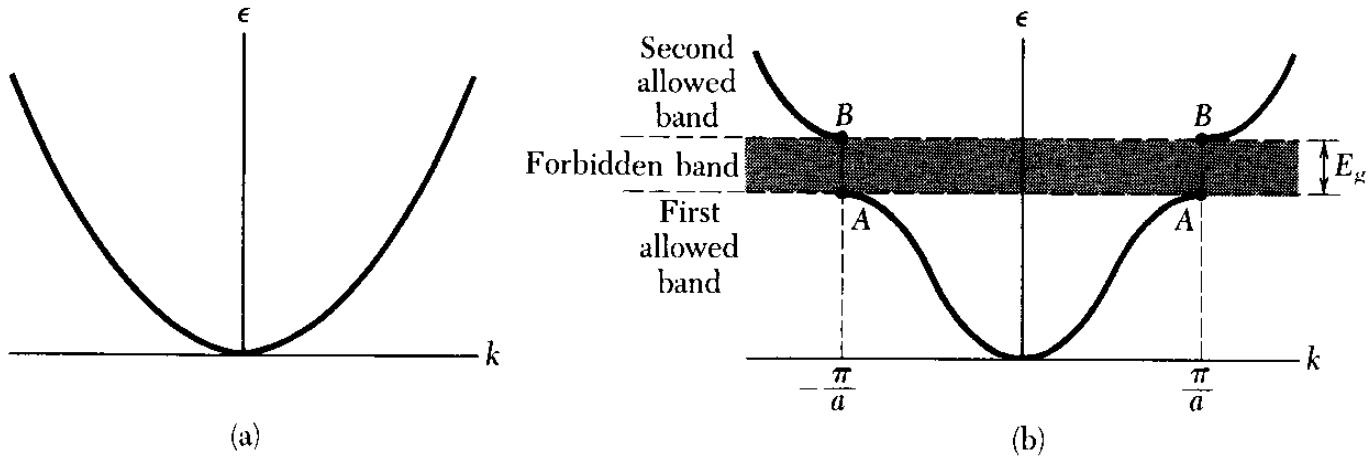
The effect of a periodic potential

The periodic potential has form:

$U = U_0 + U_1 \cos\frac{2\pi x}{a}$, where a is lattice parameter

and $U_1 \ll U_0$. If $U_1 = 0$ then we have the free

electron gas case where $\varepsilon = \frac{\hbar^2 k^2}{2m}$



Wave equation of electron in periodic potential

$$U(x)=\sum_G U_G e^{iGx}=\sum_{G>0} U_G(e^{iGx}+e^{-iGx})=2\sum_{G>0} U_G\cos Gx$$

$$H\psi=\varepsilon\psi=(\frac{1}{2m}p^2+\sum_G U_G e^{iGx})\psi(x)=\varepsilon\psi(x)$$

$$\psi(x)=\sum_k C(k)e^{ikx}, k=2\pi n/L.$$

$$\frac{1}{2m}p^2\psi(x)=\frac{\hbar^2}{2m}\sum_k k^2 C(k)e^{ikx},$$

$$(\sum_G U_G e^{iGx})\psi(x)=\sum_G\sum_k U_G e^{iGx}C(k)e^{ikx},$$

$$\sum_k\frac{\hbar^2}{2m}k^2C(k)e^{ikx}+\sum_G\sum_k U_G e^{iGx}C(k)e^{ikx}=\varepsilon\sum_k C(k)e^{ikx}$$

$$(\frac{\hbar^2k^2}{2m}-\varepsilon)C(k)+\sum_G U_G C(k-G)=0.\ \ \lambda_k=\hbar^2k^2/2m.$$

Crystal momentum of an electron

Under a crystal lattice translation we have

$$\psi_k(\vec{r}+\vec{T}) = e^{i\vec{k}\cdot\vec{T}} e^{i\vec{k}\cdot\vec{r}} u_k(\vec{r}+\vec{T}) = e^{i\vec{k}\cdot\vec{T}} \psi_k(\vec{r}).$$

If the lattice potential vanishes, the result recovers to that of free electron gas.

$\hbar\vec{k}$ is called the crystal momentum of an electron.

If an electron $\vec{k}$ absorbs in a collision a phonon of wavevector $\vec{q}$, the selection rule is $\vec{k}+\vec{q} = \vec{k}'+\vec{G}$.

Approximate solution near a zone boundary

At the zone boundary the kinetic energy of the waves $k = \pm\frac{1}{2}G$ are equal. $(\lambda - \varepsilon)C(k) + \sum_G U_G C(k-G) = 0.$

$$(\lambda - \varepsilon)C(G/2) + UC(-G/2) = 0$$

$$(\lambda - \varepsilon)C(-G/2) + UC(G/2) = 0$$

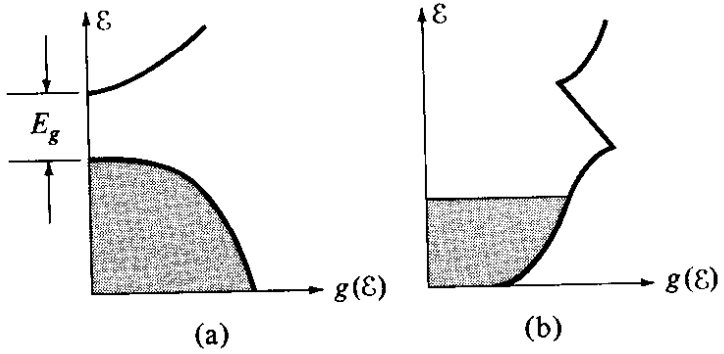
$$(\lambda - \varepsilon)^2 = U^2; \quad \varepsilon = \lambda \pm U = \frac{\hbar^2}{2m}(\frac{1}{2}G)^2 \pm U.$$

Thus the potential energy has created an energy gap $2U$ at the zone boundary.

Chapter 8: Summary

A solid with an energy gap will be nonconducting at $T = 0$ unless electric breakdown occurs or unless the AC field is of such high frequency that $\hbar\omega$ exceeds the energy gap. However, when $T \neq 0$ some electrons will be thermally excited to unoccupied bands (conduction bands).

If the enegy gap $E_g \approx 0.25$ eV, the fraction of electrons across the gap is of order $e^{-E_g/2k_BT} \approx 10^{-2}$, and observable conductivity will occur. These materials are semiconductors.



Effective Mass

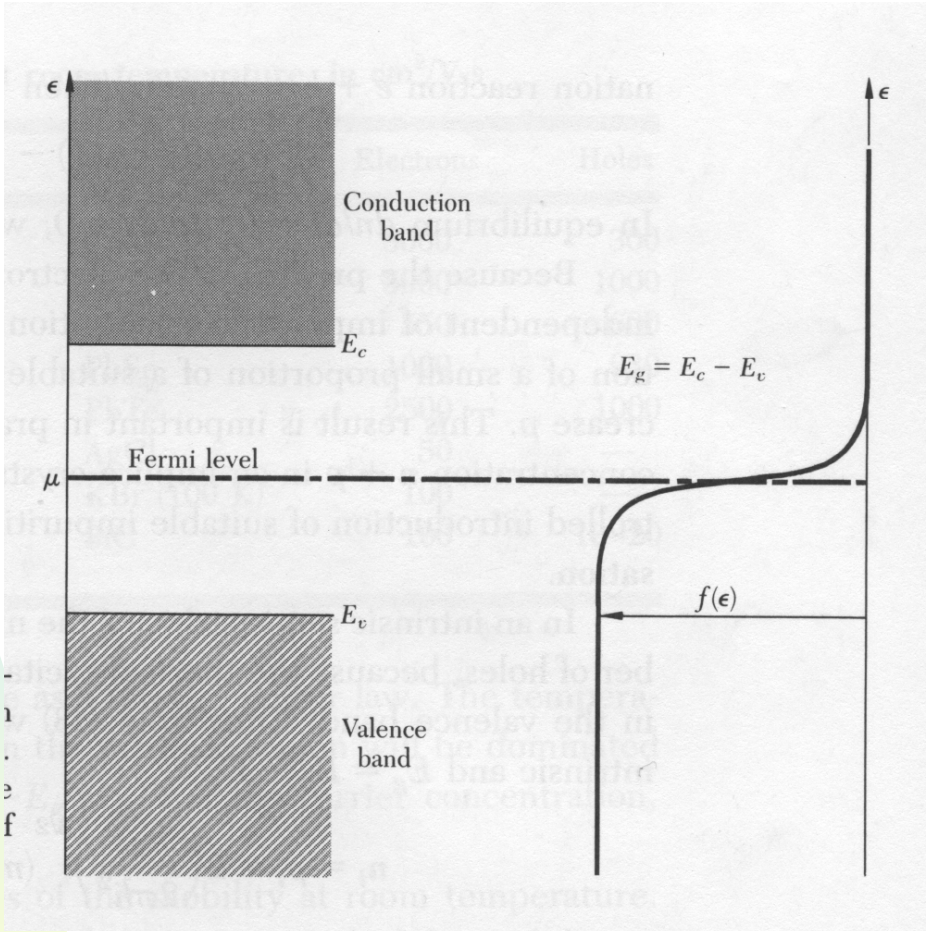
The group velocity $v_g = d\omega / dk, \omega = \varepsilon / \hbar,$ so $v_g = \hbar^{-1} d\varepsilon / dk.$

$$\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d^2\varepsilon}{dkdt} = \frac{1}{\hbar}\left(\frac{d^2\varepsilon}{dk^2}\frac{dk}{dt}\right) = \frac{1}{\hbar}\left(\frac{d^2\varepsilon}{dk^2}\right)\left(\frac{dk}{dt}\right) = \frac{1}{\hbar}\left(\frac{d^2\varepsilon}{dk^2}\right)\left(\frac{F}{\hbar}\right)$$

$F = ma,$ then we have $\frac{1}{m^*} = \frac{1}{\hbar^2}\left(\frac{d^2\varepsilon}{dk^2}\right).$

Effective Mass in Semiconductors

The angular rotation frequency ω_c of the current carriers is: $\omega_c = \frac{eB}{m^* c},$ where m^* is the effective mass.



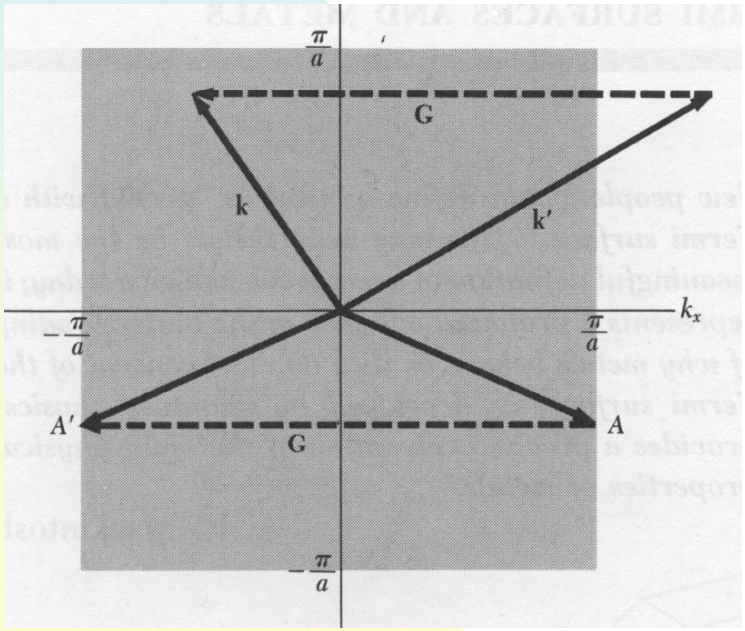
In an intrinsic semiconductor, $n = p, E_g = E_c - E_v$,

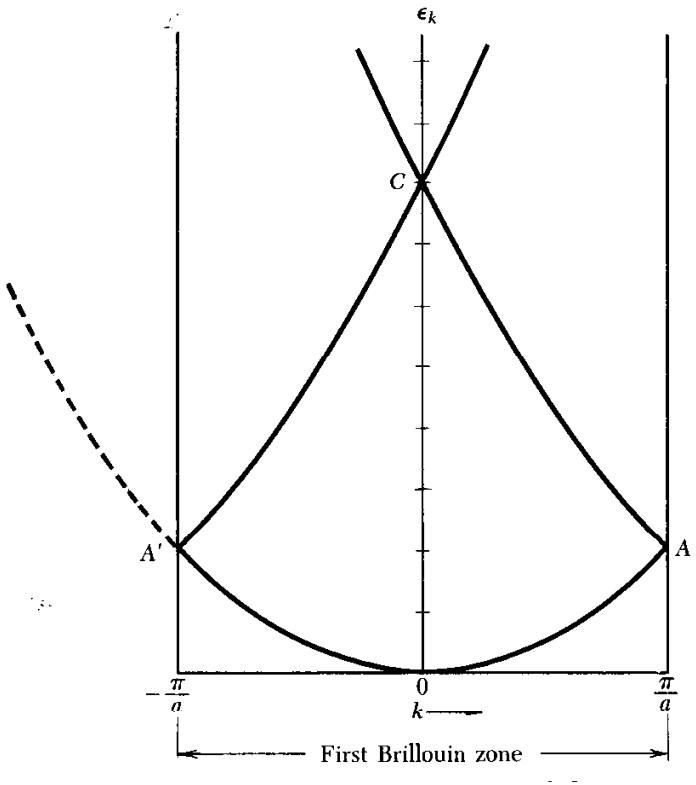
$$n = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} \left(m_e m_h\right)^{3/4} \exp[(E_g / 2k_B T].$$

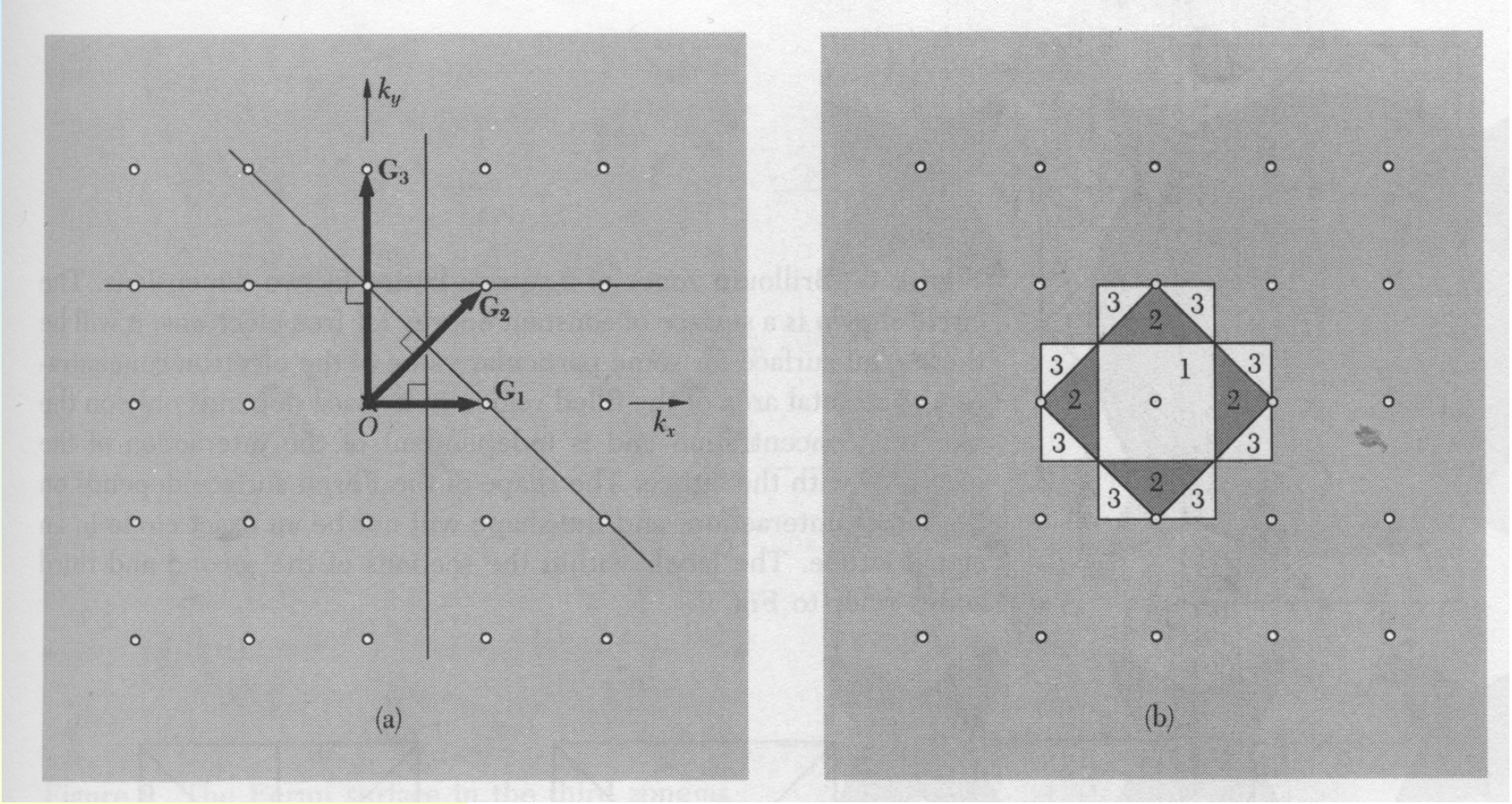
Chapter 9: Reduced zone scheme

For a Bloch function written as $\psi_{k'}(\vec{r}) = e^{i\vec{k}'\cdot\vec{r}} u_{k'}(\vec{r})$, with $\vec{k}'$ outside the first Brillouin zone, we have $\vec{k} = \vec{k}' + \vec{G}$.

$$\psi_{k'}(\vec{r}) = e^{i\vec{k}'\cdot\vec{r}} u_{k'}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \left(e^{-i\vec{G}\cdot\vec{r}} u_{k'}(\vec{r}) \right) \equiv e^{i\vec{k}\cdot\vec{r}} u_k(\vec{r}) = \psi_k(\vec{r})$$

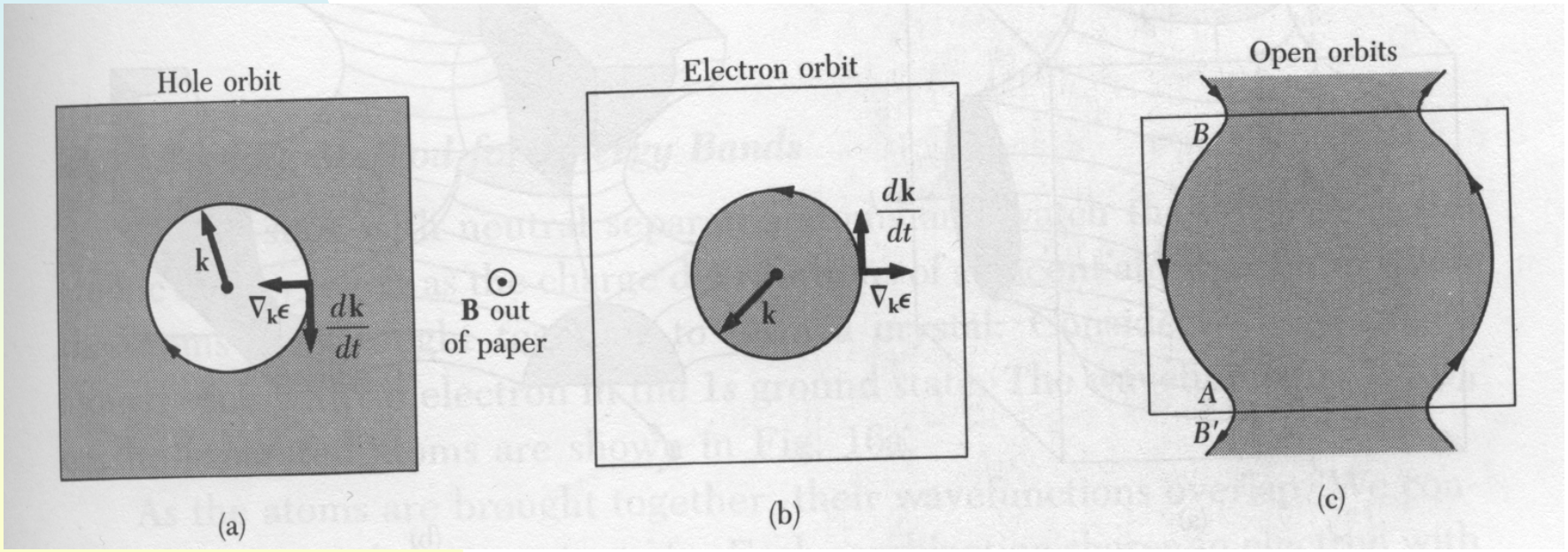





k_y
G_3
G_2
G_1
O
k_x
(a)
3
2
3
3
1
3
2
2
3
3
2
3
(b)

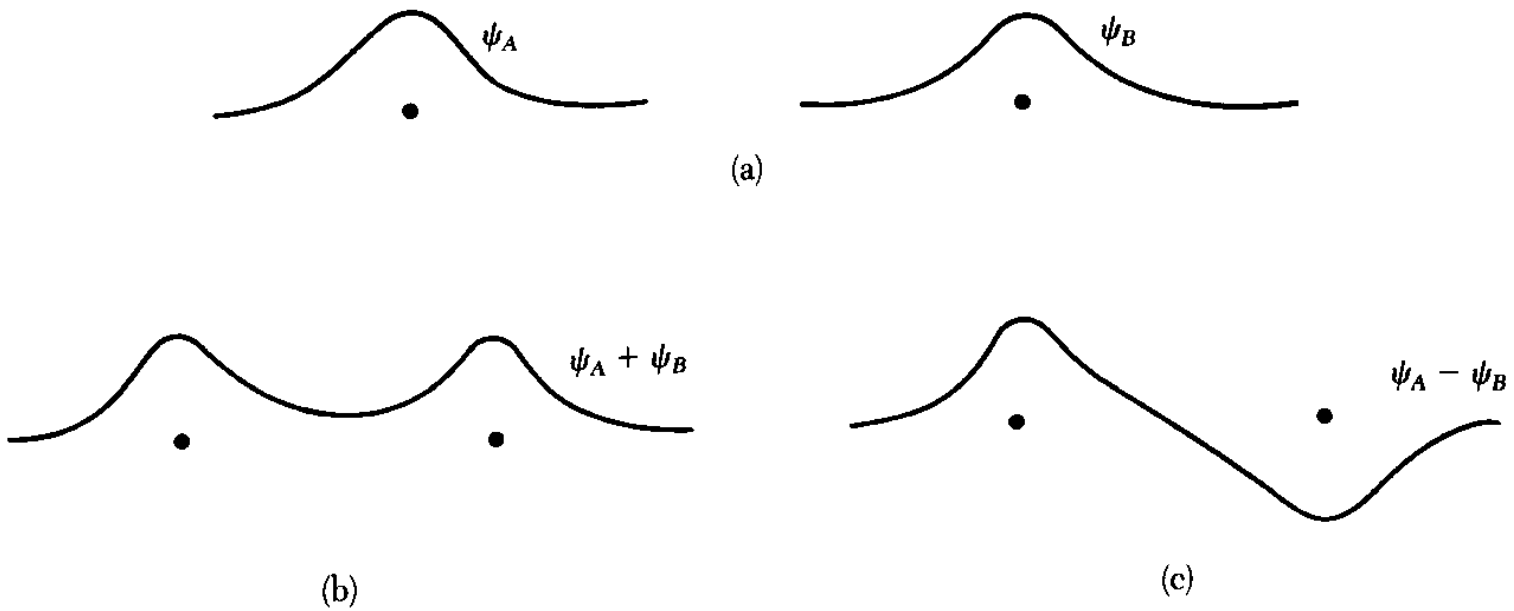
Electron orbits, hole orbits, and open orbits

An electron on the Fermi surface will move in a curve on the Fermi surface, because it is a surface of constant energy.



Tight banding method for energy bands

Tight banding approximation deals with the case in which the ovelap of atomic wave functions is enough to require corrections to the picture of isolated atoms, but not so much as to render the atomic description irrelevant.



Free electrons in a uniform magnetic field

The orbital energy levels of an electron in a cubic box with sides of length L parallel to the x-, y-, and z-axes are determined in the presence of a uniform magnetic field H along the z-direction by two quantum numbers, ν and k_z :

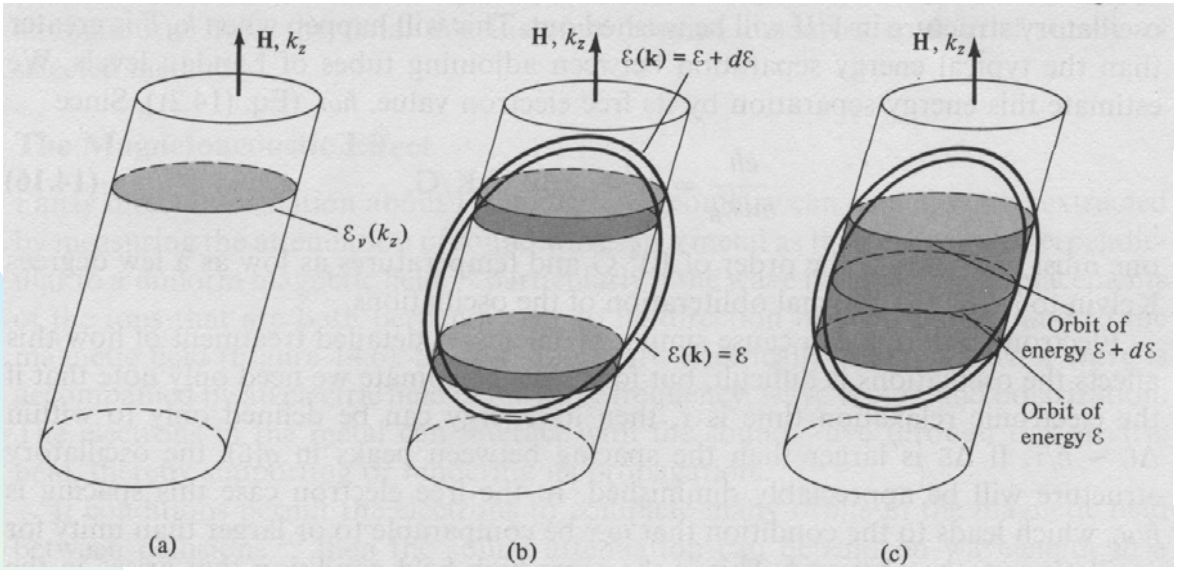
$$\varepsilon_\nu(k_z) = \frac{\hbar^2}{2m}k_z^2 + (\nu + \frac{1}{2})\hbar\omega_c, \quad \omega_c = \frac{eH}{mc}.$$

ν runs through all nonmagnetic integers, and k_z takes on the same values as in the absence of a magnetic field:

$k_z = 2\pi n_z / L$ for any integral n_z.

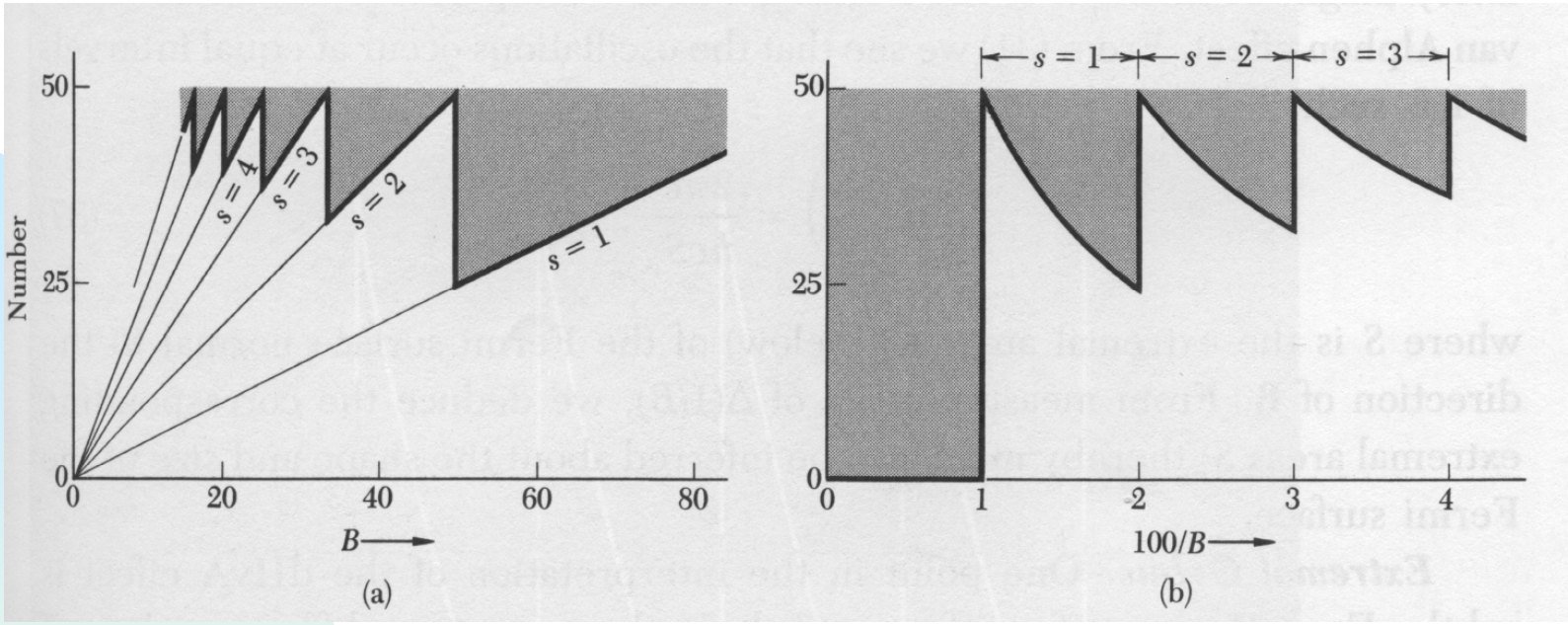
The energy of motion perpendicular to the field, which would be $\hbar^2(k_x^2 + k_y^2)/2m$ if no field were present, is quantized in steps of $\hbar\omega_c$ ($\omega_c = eH/mc$). This is orbit quantization.

Origin of the oscillatory phenomena



Most electronic properties of metals depend on the density of levels at the Fermi energy, $g(\varepsilon_F)$. It follows that $g(\varepsilon_F)$ will be singular whenever the value of H causes an extramal orbit on the Fermi surface to satisfy the quantization condition $(\nu+\lambda)\Delta A = A_e(\varepsilon_F)$.

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e}{\hbar c}\frac{1}{A_e(\varepsilon_F)}. \quad \frac{e\hbar}{mck_B} = 1.34\times10^{-4}\,K/G.$$



For a system of N electrons at absolute zero the Landau levels are filled to s. Orbitals at the next higher level $s+1$ will be partially filled. The Fermi level will lie between s and $s+1$. As the magnetic field is increased the electrons move to lower levels because the area between successive circles are increased

$$\pi\Delta(k^2) = (2\pi k)(\Delta k) = 2\pi eB/\hbar c.$$