Semiclassical Model of Electron Dynamics

The classical Drude’s theory suffered setbacks in explaining several anomalies in electron conduction. For example, measured hall coefficients were found to be field dependent, contrary to the prediction of the free electron theory. Further, they depend on temperature and sample purity and crystallinity. Although at very low temperatures and high magnetic fields measured Hall coefficients on highly pure, good single crystals, are consistent with the free electron model for some materials, drastic variations are observed in others. In some cases, measured Hall coefficients were found to be negative, which cannot be explained by the classical theory. Further, the magnetoresistance predicted by the classical theory is field independent (see Ch. 1 in A & M). However, careful measurements have demonstrated field dependence which can lead to divergence of the magnetoresistance at high fields. These anomalies, as well as others, are explained by the quantum theory of solids.

SEMICLASSICAL MECHANICS

Drude’s classical theory is concerned with the time evolution of the electronic classical state \((r, p)\) in the presence of applied fields, thus implying electron localization relative to the wavelength of the applied fields and the electron mean free path. In Sommerfeld theory, the classical approach to electron dynamics was applied to electrons obeying Fermi-Dirac statistics, where it was demonstrated that the classical description of electron dynamics is impossible (due to uncertainty principle) if electron localization on the scale of interatomic distances is to be assumed. The occurrence of mean free paths of the order of hundreds of angstroms is the reason for the success of Sommerfeld classical argument in resolving the thermal anomalies of the free electron model.

Sommerfeld approach can be generalized to electrons in a periodic potential, leading to a Semiclassical model, which provides explanation for several anomalous behaviors in electron dynamics. The electronic states in a solid with a periodic potential are described by Bloch levels. The motion of a Bloch electron can then be described by the evolution of mean position and wave vector of a wave packet of Bloch waves, provided that the spread of the wave packet in \(k\)-space is small on the scale of the Brillouin zone (so that the energy levels in the wave packet are nearly degenerate):

\[
\psi_n(r, t) = \sum_{k'} g(k') \psi_{nk'}(r) e^{-i\epsilon_n(k')t / \hbar}
\]

(1)

Using Bloch theory we obtain:

\[
\psi_n(r_0 + R, t) = \sum_{k'} [g(k') \psi_{nk'}(r_0, t)] e^{i(k' R - \epsilon_n(k')t / \hbar)}
\]

(2)
This is a wave packet of plane waves in which the wave function is appreciable within $\Delta R \approx 1/\Delta k$. If the spread in wave vector $\Delta k$ is small compared with the dimension of the Brillouin zone, which is of order $1/a_0$, then $\Delta R$ is large compared with the dimension of the direct space dimension, $a_0$, and the wave packet spreads in real space over many primitive cells. This suggests using equations of motion having the form of the classical equations. However, since the spatial spread of the wave packet is large compared with the characteristic length associated with the periodic crystal potential, the effect of this potential on determining electron dynamics have to be treated quantum mechanically. On the other hand, the externally applied fields in some experiments vary slowly on the scale of several primitive cells (Fig. 1). For example, the wavelength of visible light is of the order of a thousand lattice spacing. Thus, the wave packet is fairly localized on the scale of the distance over which the fields change appreciably. Consequently, these fields can be treated classically. If however the applied fields change appreciably on the scale of interionic separation (such as those of X-rays), we must use quantum mechanical approach to describe the effect of the fields on the electronic motion.

Hence, in the semiclassical model, the external fields are treated classically, but the interaction with ions is treated quantum mechanically. Since justifying the semiclassical model is a difficult task, we will focus on describing it within the limitations on its validity, and arrive at some major conclusions concerning the anomalous deviations of the observed electronic behavior from that predicted by the free electron model.

The semiclassical model is based on knowledge of $\mathcal{E}_n(k)$, and subsequently relates thermal and electric transport properties to band structure of the solid. The rules governing the model are:

1. Excluding interband transitions.
2. The semiclassical equations of motion are given by:

$$\dot{r} = v_n(k) = \frac{1}{\hbar} \frac{\partial \mathcal{E}_n(k)}{\partial k} \quad (3)$$

$$\hbar \dot{k} = -e \left[ E(r, t) + \frac{1}{c} v_n(k) \times H(r, t) \right] \quad (4)$$

Notice that equation (3) is just the group velocity of the wave packet representing the electron. Equation (4) can be justified by starting with a static field that conserves energy. Then we have:
Since we can add to the terms in the square bracket any vector perpendicular to the electron velocity without changing the identity, equation (5) can be rewritten as:

\[
0 = \frac{d[\varepsilon_n(k) - e\phi(r)]}{dt} = \frac{\partial \varepsilon_n}{\partial k} \cdot \dot{k} - e \nabla \phi \cdot \dot{r} = \mathbf{v}_n(k) \cdot [\hbar \dot{k} - e \nabla \phi] \tag{5}
\]

This immediately implies equation (4).

3. Since motion is considered within the same band, the energy is periodic in the reciprocal lattice, and thus translation of the wave vector by a reciprocal lattice vector \( \mathbf{K} \) corresponds to the same original state.

**COMMENTS**

1. Each band contains a fixed number of carriers of a given type. However, since at equilibrium only electrons in bands with energies within a few \( k_B T \) above or below the Fermi level contribute to transport, we only need to consider a few carrier types in these bands.

2. The rate of change of the crystal momentum in equation (4) is given by the forces of the externally applied only, excluding the forces due to the periodic field. Thus, the crystal momentum is not the Bloch electron momentum. Alternatively, since the wave packet of a Bloch electron spreads over many primitive cells, the periodic potential has to be included in Schrödinger equation in determining the electronic states. The Hamiltonian thus lacks full translational symmetry, in which case the momentum is not a good quantum number of the solutions. Consequently, the wave number appearing in the solutions is not proportional to the electron momentum.

3. Since interband transitions are not allowed in the semiclassical equations of motion, the validity of the equations requires a minimum value of the periodic potential (band gap) to confine the electronic energy within the limits of the band energies. The periodic potential thus acts to decelerate and reflect electrons with wave vectors approaching the zone boundary, in a direction opposing the effect of the applied fields. The conditions on the amplitudes of the applied fields are:

\[
eEa \ll \frac{\left[ \varepsilon_g(k) \right]^2}{\varepsilon_F} \tag{7}
\]

\[
h\omega_c \ll \frac{\left[ \varepsilon_g(k) \right]^2}{\varepsilon_F} \tag{8}
\]

In these equations \( \varepsilon_g(k) \) is just the difference between the energy of the electronic level and that of the level having the same wave number in the nearest band. Condition (7) is almost always applicable, since
even with a current density as large as 100 A/cm$^2$, and a resistivity as high as 100 $\mu\Omega$-cm, the field strength in such a metal is only $10^2$ volt/cm. With a of the order of an angstrom, the left-hand side of equation (7) is of order $10^{-10}$ eV. Considering the Fermi energy of the order of an electron volt, and the typical small band gap of order 0.1 eV, equation (7) is well satisfied. In occasions where it is possible to establish very high fields ($\sim 10^6$ volts/cm), *electric breakdown* could occur as a consequence of field driven interband transition.

The applicability of condition (8) on the magnetic field strength is not as straightforward.

$$\hbar \omega_c = H \frac{e \hbar}{mc} = \left( 2 \times \frac{9.27 \times 10^{-24}}{1.6 \times 10^{-19}} \right) \left( \frac{T}{e} \right) \left( \frac{\text{eV}}{T} \right) H = 1.16 \times 10^{-4} \left( \frac{\text{eV}}{T} \right) H$$

This last equation demonstrates that in magnetic fields as high as $10^4$ G ($= 1$ T), we have $\hbar \omega_c = 10^{-4}$ eV. Hence, condition (8) is not valid for band gaps of order $10^{-2}$ eV, which could arise from removal of degeneracy by spin-orbit coupling. In such cases, the electrons do not follow the orbits determined by the semiclassical equations of motion, a phenomenon known as *magnetic breakthrough*.

In addition, two conditions on the frequency and wavelength of the applied fields must be satisfied:

$$\hbar \omega \ll \hbar \omega_c$$

(10)

This condition is necessary to exclude interband transition by photon absorption processes.

$$\lambda \gg a$$

(11)

This condition is necessary to guarantee the validity of semiclassical equations of motion.

**TRANSPORT PROPERTIES OF METALS**

In discussing transport in metals, we will always consider the electronic equilibrium distribution function to be that at zero temperature:

$$\frac{d k / 4\pi^3}{e^{(\varepsilon - \varepsilon_F) / k_B T} + 1} = \frac{d k}{4\pi^3}$$

(12)

This is a sound assumption since the Fermi temperature in metals is higher than $10^4$ K (equation 2.33 A & M). Further, we will disregard the question concerning the nature of collisions, and describe them in terms of relaxation time approximation. Then we shall use the semiclassical equations to determine the motion of electrons between collisions.

**Conduction by Electrons in Filled Bands**

All energy levels in a filled band lie below Fermi level. Using the electronic density (12) in volume $d k$, the number of such electrons in direct space volume $d r$ is simply $d r \ d k / 4\pi^3$. Since integrating over the six-dimensional $rk$-space gives twice the number of $k$-points, we conclude that the number of $k$-points in
the volume is half the number of electrons, which is characteristic of a filled band. The phase space density of electrons in a filled band is thus a constant = \(1/4\pi^3\). The electric and thermal currents due to electrons in a filled band are:

\[
j = (-e) \int \frac{d\mathbf{k}}{4\pi^3} \frac{\partial\mathcal{E}}{\hbar \partial \mathbf{k}} = 0
\]

\[
j_T = \int \frac{d\mathbf{k}}{4\pi^3} \mathcal{E} \frac{1}{\hbar} \partial \mathbf{k} = 1/2 \int \frac{d\mathbf{k}}{4\pi^3} \frac{1}{\hbar} \frac{\partial (\mathcal{E})^2}{\partial \mathbf{k}} = 0
\]

Both of the above integrals vanish for a filled band, since the integral of the gradient of a periodic function over a primitive cell is zero. Thus, a solid in which all bands are either full or empty is an insulator. Since the number of levels in a given band is twice the number of primitive cells in the solid, all insulators should have an even number of valence electrons per primitive cell. But not all solids with even number of electrons per primitive cell are insulators. This is a consequence of band overlap which results in more than one partially filled bands rather than a single filled band.

**Semiclassical Motion in a DC electric Field**

The solutions to the semiclassical equations in this case are:

\[
k(t) = k(0) - \frac{eEt}{\hbar}
\]

\[
v(k(t)) = v(k(0) - \frac{eEt}{\hbar})
\]

Equation (15) implies that at time \(t\) every wave vector is shifted uniformly by the same amount. This is consistent with the previous discussion that filled bands do not contribute to conduction in solids since a uniform shift in wave vector does not change the constant phase space electronic density in the case of a filled band. Notice that while the wave vector grows linearly with time, the velocity does not, since it is not proportional to the wave vector. Since the velocity is periodic in the reciprocal lattice, it must be

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Fig. 2: Band structure and Fermi surface for a divalent metal in a square lattice
bounded in time and oscillatory when the applied field is in
the direction of a reciprocal lattice vector (Fig. 3).

If changes in the wave vector larger than the zone dimension
could be established, the DC field will induce AC current. This
could not be observed due to degradation of the growth of
the wave number by collisions. For typical values of electric
field and relaxation time the change in wave vector is only
about 0.1 cm⁻¹, which is negligible in comparison with the zone
dimension of 10⁸ cm⁻¹. However, effects dominated by electrons with wave number close to the zone
boundary to accelerate in opposite direction to the applied field are observable through conduction by
“holes”.

**Holes**

In a partially filled band, some levels are occupied by electrons and the remaining levels are not
occupied. The current produced by all electrons in the band is given by:

\[ j = -e \int \frac{d\mathbf{k}}{4\pi^3} v(\mathbf{k}) \]  

(17)

Since equation (13) for a filled band can be rewritten as:

\[ 0 = -e \int \frac{d\mathbf{k}}{4\pi^3} v(\mathbf{k}) + (-e) \int \frac{d\mathbf{k}}{4\pi^3} v(\mathbf{k}) \]  

(18)

Then the current produced by electrons in occupied levels is given by:

\[ j = +e \int \frac{d\mathbf{k}}{4\pi^3} v(\mathbf{k}) \]  

(19)

This is a statement that conduction by electrons in occupied levels of a partially filled band can be
viewed as conduction by *positively charged* electrons occupying the empty states of the band. Thus we
can regard the contribution of a given band to current as being due to real electrons (in the electron
picture) or to holes (in the hole picture). One can chose any picture for a given band, but the pictures
cannot be mixed for the same band. For example, in calculating the contribution of the bands in Fig. 2
to current, one may adopt the “electron picture” to determine the current produced by electrons in the
higher band along the \( \Gamma X \) direction, and the “hole picture” to determine the current produced by
electrons in the lower band along the \( \Gamma M \) direction.

Further, the unoccupied levels evolve in time in the same manner as they would if they were occupied
by real electros, since the semiclassical equations and the initial conditions completely determine the
electron orbit regardless of the orbit itself. Therefore, understanding the response of electrons to
applied fields is sufficient to understand conduction.
The semiclassical motion of an electron is determined by the equation (4). If in equilibrium the unoccupied levels are close to the band maximum at \( \mathbf{k}_0 \), a point which assumed for the time being to be with high (cubic) symmetry, then the semiclassical equations (3) and (4) are reduced to:

\[
\mathbf{a} = \frac{\mathbf{d} \mathbf{v}}{\mathbf{d}t} = \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial \mathbf{k}^2} (\hbar \dot{\mathbf{k}})
\]

This indicates that the acceleration of an electron in a level near the band maximum is in opposite direction to the rate of change of the wave vector. Accordingly, such an electron responds to the applied fields as if it has a negative effective mass defined by:

\[
\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial \mathbf{k}^2}
\]

Notice that an electron in levels near the band minimum accelerates parallel to the rate of change of the wave vector and thus responds as a real electron with positive effective mass.

Substituting equation (20) into the semiclassical equation (4) we obtain:

\[
\hbar \dot{\mathbf{k}} = \left[ \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial \mathbf{k}^2} \right] \mathbf{a} = -e \left[ E + \frac{1}{c} \mathbf{v} \times \mathbf{H} \right]
\]

By changing the sign of both sides, equation (22) for levels near the band maximum can be regarded as describing the motion of a positively charged electron with positive effective mass. This last picture can be understood if we consider one missing electron from an otherwise filled band. If the electron is missing from the level at \( \mathbf{k}_0 \), the total wavenumber of the electrons in occupied levels is then \( -\mathbf{k}_0 \), which is associated with the wave number of the hole. Therefore, a hole responds to the fields like a positively charged electron in the unoccupied levels.

**Effective Mass**

Equation (21) indicates that the curvature of the energy versus wave vector is a measure of the reciprocal of the effective mass. Near the zone boundary, the curvature is increases by a factor of \( \mathcal{E}_b / \mathcal{E}_g \) where \( \mathcal{E}_b \) is the energy at the zone boundary and \( \mathcal{E}_g \) is the energy gap (see homework). For typical values of the electron energy in levels at the zone boundary and energy gaps the curvature could enhance by one or two orders of magnitude, resulting in an effective of the order of 0.1 to 0.01 of the free electron value.

If now we abandon the assumption that the maximum is at a point of high symmetry, then it suffices to consider that the dynamical behavior of the electrons is suggestive of positively charged particles if:

\[
\dot{\mathbf{k}} \cdot \mathbf{a} < 0
\]

Thus we have for condition (23):
\[ \mathbf{k}. \frac{d}{dt} \mathbf{v} = \mathbf{k}. \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial \mathbf{k}} = \frac{1}{\hbar} \sum_{ij} k_i \frac{\partial^2 \mathcal{E}}{\partial k_i \partial k_j} k_j < 0 \] (24)

The effective mass for a general anisotropic solid is defined by:

\[ [M^{-1}]_{ij} = \pm \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial k_i \partial k_j} = \pm \frac{1}{\hbar} \frac{\partial v_i}{\partial k_j} \] (25)

Here the sign is chosen according to whether \( k \) is an electron or a hole level. Notice that the second-rank tensor in (25) becomes diagonal when the energy is quadratic in wave number, in which case the three principal components are:

\[ [M^{-1}]_i = \pm \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial k_i^2} \] (26)

Equation (26) reduces to equation (21) in the case of cubic symmetry (the isotropic case). The effective mass for the free electron and the nearly free electron models is shown schematically in Fig. 4.

 Fig. 4: (a) free electron, and (b) nearly free electron
Semiclassical Motion in a Uniform Magnetic Field

The semiclassical equations in the presence of a uniform field read:

\[ \dot{\mathbf{r}} = \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial \mathbf{k}} \quad (27) \]

\[ \hbar \dot{\mathbf{k}} = -e \frac{\mathbf{\hat{r}} \times \mathbf{H}}{c} \quad (28) \]

There are two constants of the motion in this case. The first is the component \( k \) in the direction of the field. The second constant of the motion is the energy, since:

\[ \frac{d\mathcal{E}}{dt} = \frac{\partial \mathcal{E}}{\partial \mathbf{k}} \cdot \dot{\mathbf{k}} = \hbar \dot{\mathbf{r}} \cdot \dot{\mathbf{k}} = 0 \quad (29) \]

Therefore the electron orbits in \( k \)-space are the curves determined by the intersection of constant energy surfaces with planes perpendicular to the magnetic field. Notice that the direction of the velocity is perpendicular to the constant energy surface along the direction of increasing energy. Thus if the field is in the \( z \)-direction and \( k \) increases along the \( x \)-direction then electron’s velocity will be in the negative \( y \)-direction, while hole’s velocity will be in the positive \( y \)-direction. This indicates that electron orbit surrounds levels with lower energy, while hole orbit surrounds levels with higher energy (Fig. 5).

Equation (28) is used to find the electron orbit in real space, where:

\[ \hat{\mathbf{H}} \times \hbar \dot{\mathbf{k}} = -eH \frac{\mathbf{\hat{r}} \times \mathbf{H}}{c} = -eH \frac{\mathbf{\hat{r}}}{c} \quad (29) \]

Fig. 5: (a) Electron orbit, and (b) hole orbit.
Notice that since the k-space velocity is perpendicular to the magnetic field and real space velocity, then the real space velocity in the plane of the orbit is always perpendicular to the k-space orbit (this follows from combination of equations (28) and (29)). Integrating this last equation we obtain:

\[
\mathbf{r}_\perp(t) - \mathbf{r}_\perp(0) = -\frac{\hbar c}{eH} \hat{\mathbf{H}} \times [\mathbf{k}(t) - \mathbf{k}(0)]
\]  

Equation (30) indicates that the projection of the real space orbit in a plane perpendicular to the field is the k-space orbit rotated by 90° about the field direction, and scaled by a factor (Fig. 6).

![Fig. 6: (a) k-space orbit, and (b) real space orbit. The field is pointing out of the paper plane. The real space velocity is indicated by an arrow at a given point.](image)

This result explains the circular projection of free electron real-space orbit in a plane normal to the field, since the k-space orbit of a free electron system is circular, which maintains its shape upon rotation about the field direction.

The time taken between two points in k-space is given by:

\[
t_2 - t_1 = \int_{k_1}^{k_2} \frac{dk}{|k|} = \frac{\hbar^2 c}{eH} \int_{k_1}^{k_2} \frac{dk}{|\partial \mathbf{E}/\partial \mathbf{k} \times \hat{\mathbf{H}}|}
\]  

(31)

Notice that \(\frac{\partial \mathbf{E}}{\partial \mathbf{k}} \times \hat{\mathbf{H}}\) is the projection of the gradient of the energy in the plane perpendicular to the field. This component is also perpendicular to the orbit in k-space as pointed out in the above discussion. Thus in moving between two orbits on adjacent energy surfaces in a direction perpendicular to the orbit the projection of the energy gradient in the plane is parallel to the change in wave vector (Fig. 7). Consequently, the energy change encountered is given by:

\[
\Delta \mathbf{E} = \left|\left(\frac{\partial \mathbf{E}}{\partial \mathbf{k}}\right)_\perp\right| \Delta \mathbf{k}
\]  

(32)

Hence we obtain from equation (31):

![Fig. 7](image)
The integral is simply the area (shaded) between the two orbits from the initial to the final wave vector. If the difference in energy between the two surfaces is infinitesimally small, equation (33) reduces to the form:

\[ t_2 - t_1 = \frac{\hbar^2 c}{eH} \int_{k_1}^{k_2} \Delta(k)\,dk \]  

(33)

When the orbit is closed, the period of the orbit is then related to the area of the \( k \)-space orbit by:

\[ T(E, k_z) = \frac{\hbar^2 c}{eH} \frac{\partial A(E, k_z)}{\partial E} \]  

(35)

The period of the orbit is related to the cyclotron frequency and effective mass by:

\[ T = \frac{2\pi}{\omega_c} = \frac{2\pi m^* c}{eH} \]  

(36)

This last equation defines the cyclotron effective mass:

\[ m^*(E, k_z) = \frac{\hbar^2}{2\pi} \frac{\partial A(E, k_z)}{\partial E} \]  

(37)

Notice that this equation gives the expected result for the free electron case (problem 12.1), where the area of the orbit is given by:

\[ A = \pi k_\perp^2 = \pi \left[ \frac{2mE}{\hbar^2} - k_z^2 \right] \]  

(38)

**Semiclassical Motion in Crossed Uniform Electric and Magnetic**

A slight modification of the semiclassical motion of electron in a uniform magnetic field is introduced if a uniform electric field is applied perpendicular to the magnetic field.

\[ \vec{H} \times \hbar \vec{k} = eE(\vec{E} \times \vec{H}) - \frac{eH}{c} \vec{H} \times (\vec{r} \times \vec{H}) = -\frac{eH}{c} \vec{r}_\perp + \frac{eH}{c} \vec{w} \]  

(39)

Thus a uniform drift with velocity \( \vec{w} = c \frac{E}{H} (\vec{E} \times \vec{H}) \) is superimposed on the motion under the influence of only uniform magnetic field. Then by integration we obtain:
\[ r_\perp(t) - r_\perp(0) = -\frac{\hbar c}{eH} \hat{H} \times [k(t) - k(0)] + wt \]  

(40)

Notice that:

\[ \hbar \dot{k} = -e \left[ E + \frac{1}{c} \dot{r} \times H \right] = -e \left[ - (E \times \hat{H}) \times \hat{H} + \frac{1}{c} \dot{r} \times H \right] = -\frac{e}{c} \left[ -c \frac{E}{H} (\hat{E} \times \hat{H}) \times H + \frac{1}{c} \dot{r} \times H \right] \]

\[ = -\frac{e}{c} \left[ -c \frac{E}{H} (\hat{E} \times \hat{H}) + \dot{r} \right] \times H = -\frac{e}{c} [v - w] \times H \]  

(41)

Thus that the equation of motion in the presence of an electric field perpendicular to the magnetic field is the same as that without electric field but the velocity is now modified by the drift velocity term \( w \).

Further, since the velocity is given by the energy gradient with respect to \( k \), and observing that:

\[ w = \frac{1}{\hbar} \frac{\partial}{\partial k} \hbar \dot{k} \cdot \dot{w} \]  

(42)

The semiclassical equation can be rewritten as:

\[ \hbar \dot{k} = -\frac{e}{\hbar c} \frac{\partial}{\partial k} [\mathcal{E} - \hbar k \cdot \dot{w}] \times H = -\frac{e}{\hbar c} \frac{\partial \mathcal{E}}{\partial k} \times H \]  

(43)

The modified energy is given in the square parentheses. Then the k-space orbit is determined by the intersection of planes perpendicular to the magnetic field with surfaces of constant modified energy.

**High-Field Hall Effect and Magnetoresistance**

The contribution to the energy from the drift velocity is:

\[ \hbar \dot{k}, w < \frac{\hbar c E}{a_0 H} (\frac{a_0}{\hbar^2/me^2}) = \frac{\hbar}{a_0} (\frac{cE}{\omega_c mc/e}) (\frac{a_0}{\hbar^2/me^2}) = \frac{e^2}{a_0} (\frac{E a_0}{\hbar \omega_c}) \]  

(44)

In the limit of high magnetic field this contribution is of the order of \( 10^{-5} \) eV, which indicates that the modified energy by the drift term is negligibly small, and the criteria satisfied by the orbits determined from the energy in the absence of electric field are also satisfied by orbits determined from the modified energy function. To account for the observed anomalous behavior of Hall coefficient and magnetoresistance we must examine the limiting behavior of the current induced by the electric field at high magnetic fields in two different cases: (a) when all electron or hole orbits are closed, and (b) when some of the orbits are open.

a. When all levels lie on closed orbits, the high field condition means that the orbit is traversed many times between collisions, which requires \( \omega_c \tau \gg 1 \). This in turn requires long mean free times, and hence very pure single crystals at very low temperature.

The current density at a given time \( t = 0 \) is \( j = -nev \), where \( v \) is the mean velocity acquired by an electron since its last collision, averaged over all electrons in occupied levels (or \( j = +n_e ev \) where \( v \) is averaged over all electrons in unoccupied levels for holes). The mean time taken by an electron picked
at random back to its last collision, averaged over all electrons is $\tau$. Hence equation (40) can be rewritten as:

$$\frac{\mathbf{r}_\perp(0) - \mathbf{r}_\perp(-\tau)}{\tau} = -\frac{\hbar c}{eH} \mathbf{\hat{H}} \times \frac{[\mathbf{k}(0) - \mathbf{k}(-\tau)]}{\tau} + \mathbf{w}$$

(45)

Thus for sufficiently large relaxation time, the dominant term in the average velocity is the drift term (as in the free electron case). This can be further observed by noting that the modified energy surface is displaced in the same general direction in $k$-space (Fig. 7).

The last statement can be easily justified for free electrons, from which we can conclude an estimate for the contribution of $\Delta \mathbf{k}$ to the mean velocity for a general band structure. In the free electron model we have:

$$\bar{\mathbf{E}} = [\mathcal{E} - \hbar \mathbf{k} \cdot \mathbf{w}] = \frac{\hbar^2}{2m} \left( \frac{\mathbf{k} - \frac{m\mathbf{w}}{\hbar}}{\mathbf{w}} \right)^2 - \frac{m\mathbf{w}^2}{2}$$

(46)

Thus equation (43) becomes:

$$\frac{\mathbf{r}_\perp(0) - \mathbf{r}_\perp(-\tau)}{\tau} = -\frac{\hbar c}{eH} \mathbf{\hat{H}} \times \frac{m\mathbf{w}}{\hbar \tau} + \mathbf{w} = \mathbf{w} - \frac{\mathbf{\hat{H}} \times \mathbf{w}}{\omega_c \tau}$$

(47)

The high field condition leads to the conclusion that the mean velocity is dominated by the drift velocity. From equation (45) we find:

$$\lim_{\tau/T \rightarrow \infty} \mathbf{j}_\perp = -ne\mathbf{w} = -\frac{ne}{H} (\mathbf{E} \times \mathbf{\hat{H}}) = -\frac{ne}{H} (-E_x \mathbf{\hat{y}} + E_y \mathbf{\hat{x}})$$

(48)

Similarly, for holes we have:

$$\lim_{\tau/T \rightarrow \infty} \mathbf{j}_\perp = -ne\mathbf{w} = -\frac{ne}{H} (\mathbf{E} \times \mathbf{\hat{H}})$$

(49)

This indicates that the current in the plane perpendicular to the magnetic field is also perpendicular to the electric field, and thus the magnetic field prevents the electrons from accelerating along the direction of the electric field and acquiring energy. If only a single band contributes to current carriers, equations (48) and (49) yield a Hall coefficient of:

$$R_\infty = \frac{E_y}{j_x H} = -\frac{1}{ne} \quad \text{(electrons)}; \quad R_\infty = +\frac{1}{n_h ec} \quad \text{(holes)}$$

(50)
If several bands with only closed orbits contribute to the current density, equation (50) gives a Hall coefficient of:

$$R_{\infty} = -\frac{1}{n_{\text{eff}} c}$$

(51)

For compensated materials (in which the density of electrons is equal to the density of holes) this last result should be modified (Problem 12.4 A & M). In such a material the magnetoresistance diverges quadratically with magnetic field strength.

b. If some orbits at the Fermi level are open, electrons do not undergo periodic motion along the electric field, and the magnetic field does not quench the acceleration in the direction of the applied electric field. The change in wave vector on an open orbit is unbounded, leading to its growth at a rate proportional to $H$ (equation (34)). Thus the mean velocity in (45) is not dominated by the drift term, and the contribution of the change in wave vector is field independent. If the open orbit runs in the direction $\hat{n}$ in real space, one would expect in the high magnetic field limit to have a non-vanishing current density along the open orbit as a result of acceleration produced by the electric field along that direction. Thus we may write in general:

$$\mathbf{j} = \sigma_0 \hat{n} (\hat{n} \cdot \mathbf{E}) + \sigma_1 \cdot \mathbf{E}$$

(52)

Here in the high field limit $\sigma_0$ is a constant and $\sigma_1$ vanishes. The Hall coefficient no longer has the simple high-field value derived above. To investigate the magnetoresistance we consider an experiment in which the current does not flow along the open orbit. The high field limit then requires that $\hat{n} \cdot \mathbf{E} = 0$, and the electric field is in the direction $\hat{n}'$ perpendicular to the direction of the open orbit (Fig. 8). Accordingly, we can express the electric field in terms of the two alternative components:

$$\mathbf{E} = E_0 \hat{n}' + E_1 \hat{n}$$

(53)

Again in the high field limit $E_0$ is a constant and $E_1$ vanishes. The current (52) in the high field limit is therefore rather small, and the leading terms are obtained from combining equations (52) and (53) to obtain:

$$\mathbf{j} = \sigma_0 \hat{n} E_1 + \sigma_1 \cdot \hat{n}' E_0$$

(54)

The magnetoresistance in the high field limit is given by:

$$\rho = \frac{\mathbf{E} \cdot \mathbf{j}}{\mathbf{j} \cdot (\hat{n}' \cdot \mathbf{j})} = \frac{E_0}{j} (\hat{n}' \cdot \mathbf{j})$$

(55)
From equation (54) we have:

\[ \hat{n}' \cdot \hat{j} = \hat{n}' \cdot \sigma_1 \cdot \hat{n}' \left( \frac{E_0}{j} \right) \]  

(56)

Then from (55) and (56) we obtain:

\[ \rho = \frac{(\hat{n}' \cdot \hat{j})^2}{\hat{n}' \cdot \sigma_1 \cdot \hat{n}'} \]  

(57)

The magnetoresistance is proportional to the square of the sine of the angle between the current and the real-space direction. Further, as the magnetic field intensity increases, the denominator of equation (57) vanishes, leading to divergence of the magnetoresistance.

Thus far, the semiclassical model has provided two mechanisms to explain the anomalous field dependence of the magnetoresistance at high applied magnetic fields, namely: compensation and open orbits.

Fig. 8