2 Basic Classical Concepts

2.1 Eigenstates, Dispersion

Most mesoscopic phenomena can be understood using the free-electron approximation of independent electrons. One assumes parabolic bands with an effective electron (hole) mass m. Hence, bandstructure effects are taken into account only via the effective mass, which we assume to be a scalar. Notable examples, for which the picture of independent electrons (quasi-particles) is not correct, are the fractional quantum Hall-effect and superconductivity. Model systems that are often used for basic mesoscopic experiments are either semiconductors (systems with very few defects) and simple metals like Au, Ag, Cu. In the former, very high electron mobilities can be realized.

As a reminder to solid-sate physics, the following figures show some band structures for important model systems. Although all electric phenomena will be treated using a *single* parabolic-band in 3-dimensions (3d) in the following, it is important to emphasize, that this is just an (the simplest) approximation. For example, a single isotropic band does not result in a magnetoresistance (change in resistance if a magnetic field B is applied), a phenomenon experimentally well established. Similarly, a single electron band cannot explain the 'wrong' sign in the Hall resistance which is often observed, even for very good metals, e.g. Aluminium.

Finally, we note, that an electron state in a crystal is described by a Bloch wave characterized by the band index n and a wavevector $\vec{k}$. An electron that occupies such a state has a (group-) velocity given by:

$$\vec{v} = \frac{1}{\hbar}\frac{\partial E_n(\vec{k})}{\partial \vec{k}}$$

Hence, in a crystal (in zero magnetic field) the relevant *quantum numbers* are: n (*bandindex*), $\vec{k}$ (*wavevector or wavenumber*), $q = -e$ (*charge*, $e > 0$), and $m_z = \pm 1/2$ (*spin*). The discrete set of independent wavevectors define the *1st Brillouin zone* in reciprocical space.

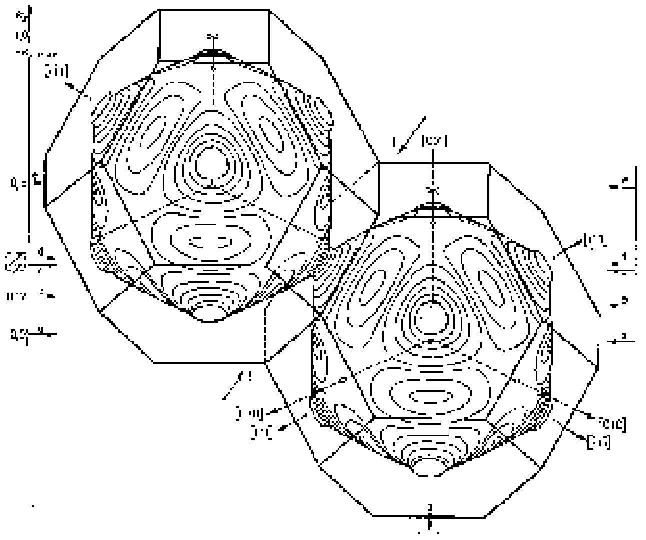


Fig 2.1 Fermi surface of Cu. This surface is nearly spherical, so that the free-electron approximation is quite good here.

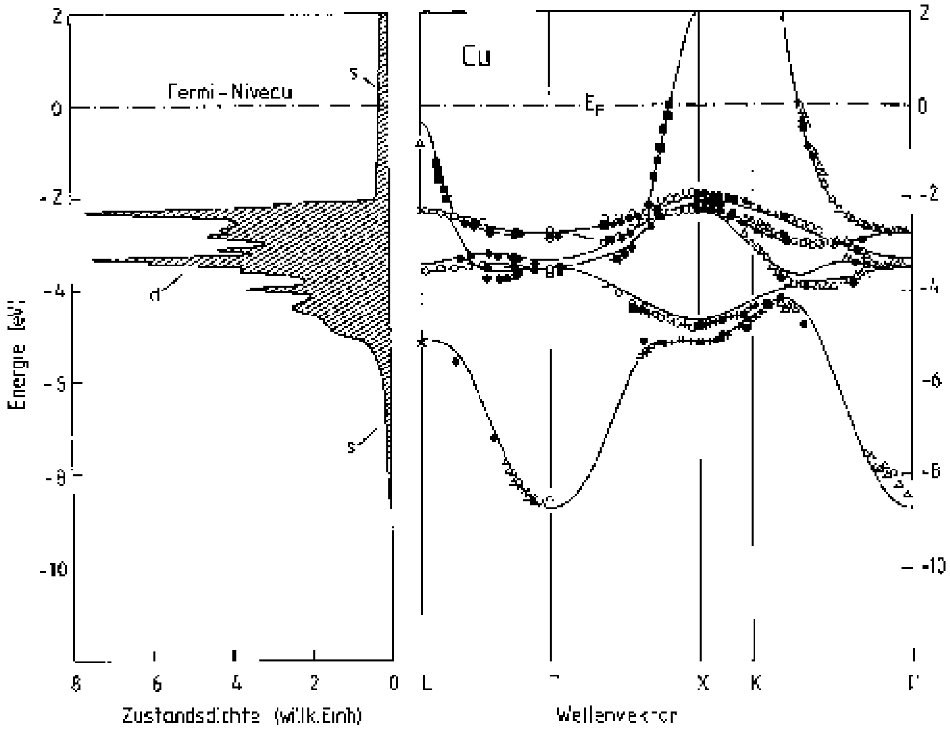


Fig 2.2 Bandstructure of cooper.

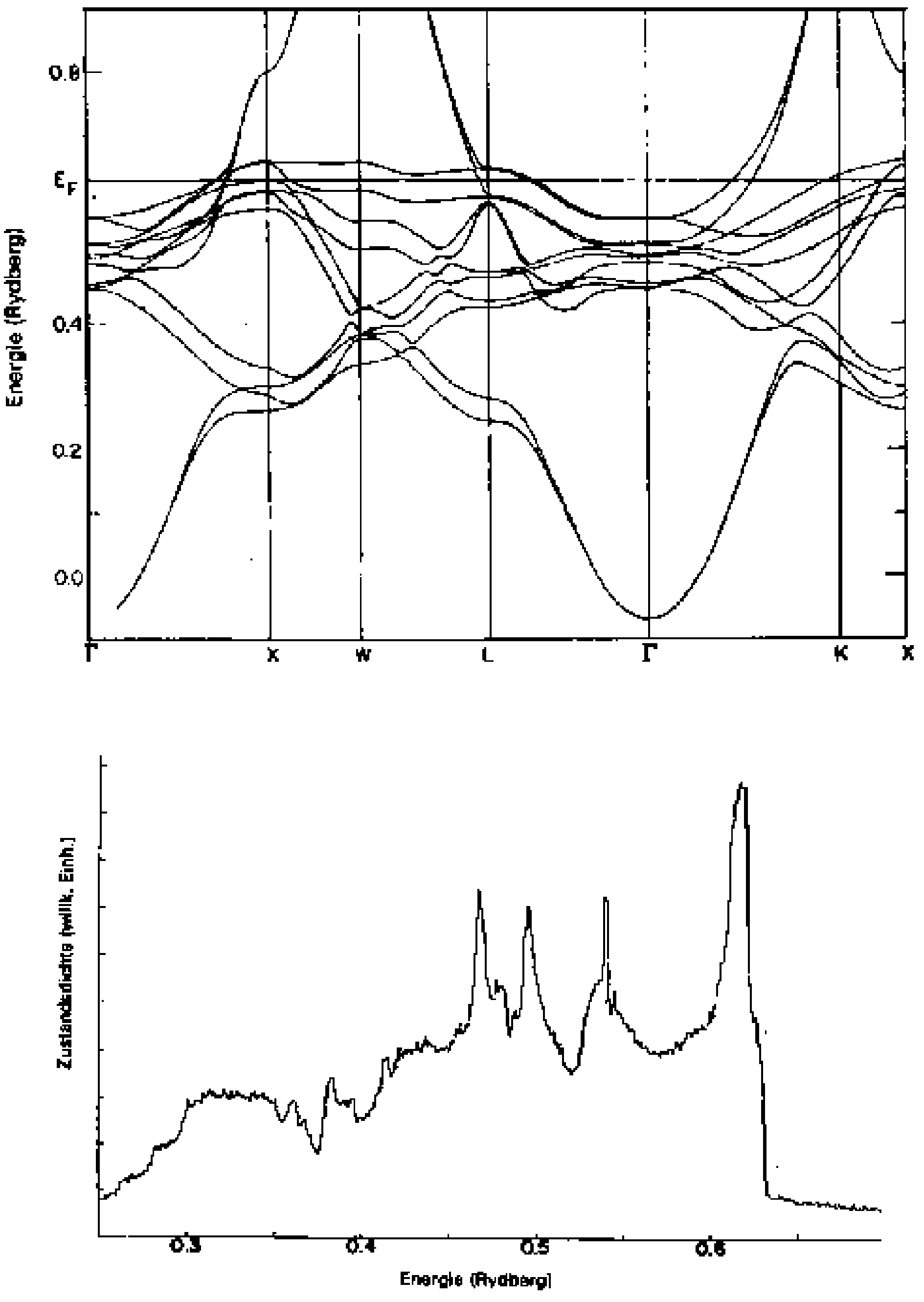


Fig 2.3 Bandstructure of Nickel (top) and the density-of-states (bottom). Compare with Cu.

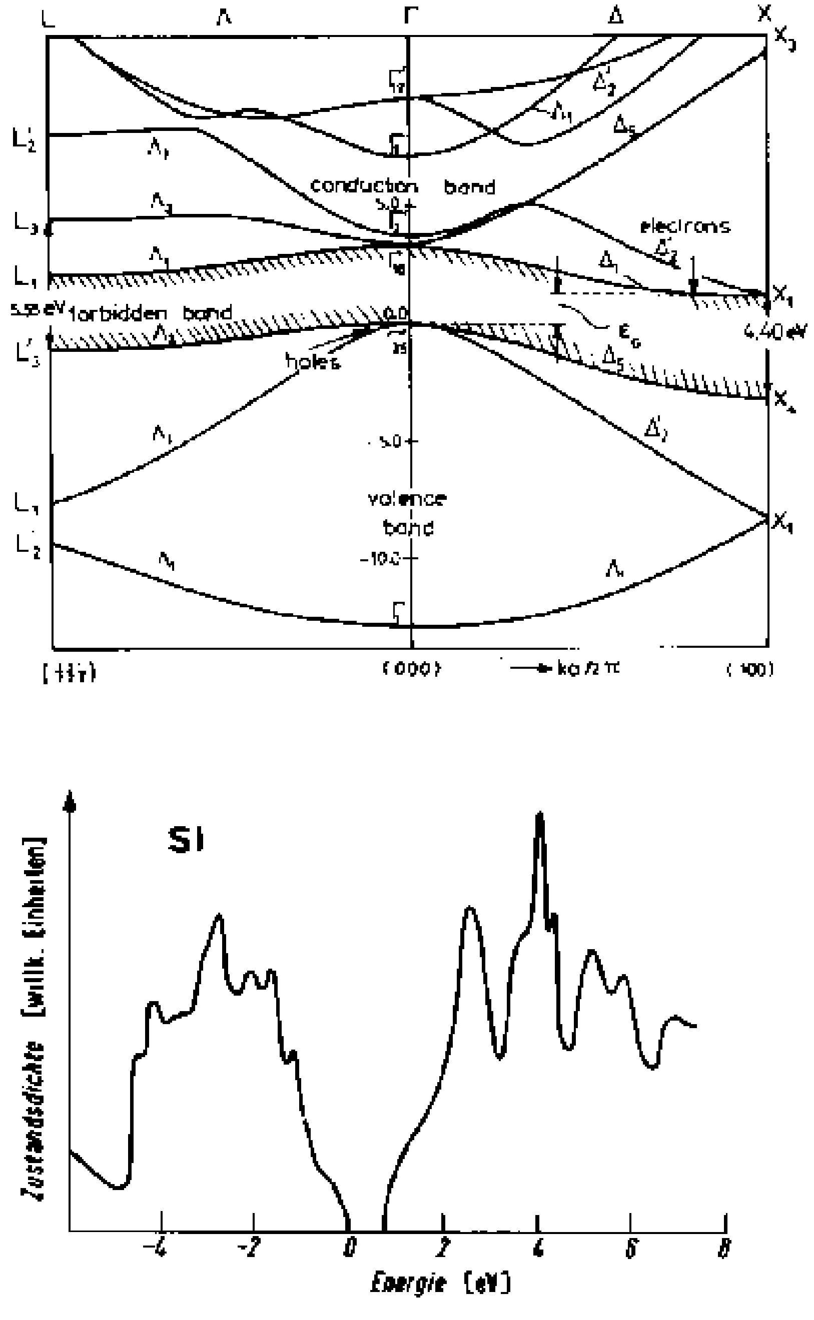


Fig. 2.4 Bandstructure of silicon (top) and the density-of-states (bottom).

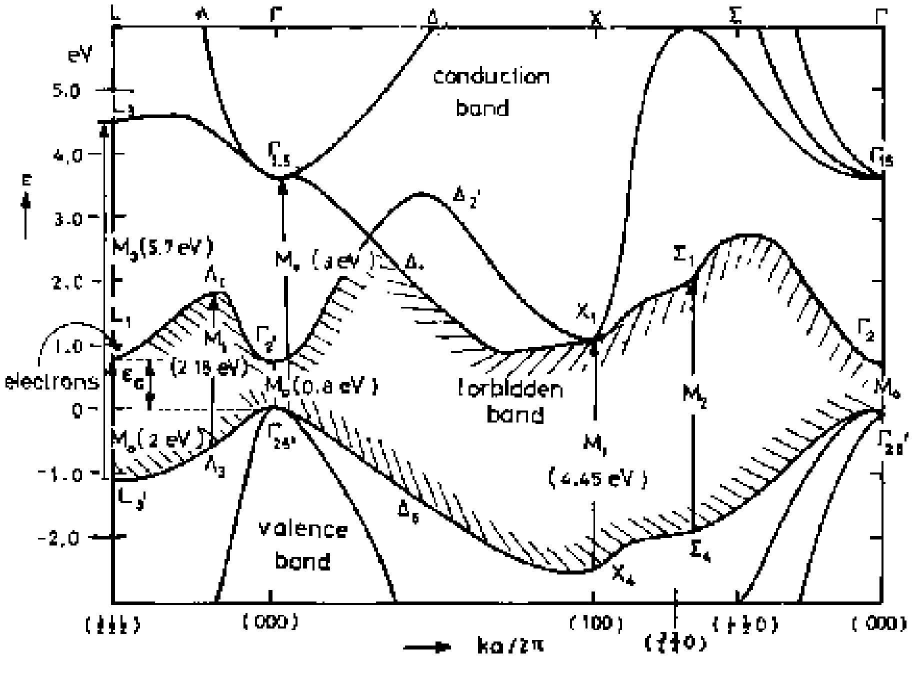


Fig. 2.5 Bandstructure of Ge. Note, the valence-band maximum is located at the Γ-point, while there are several minima in the conduction band located at the Brillouin-zone boundary.

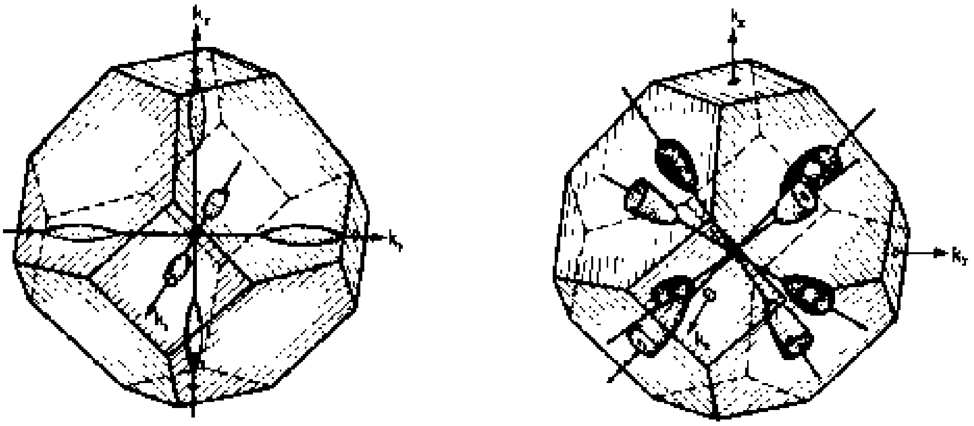


Fig. 2.6 Fermi surface for conduction electrons for Si (left) and Ge (right).

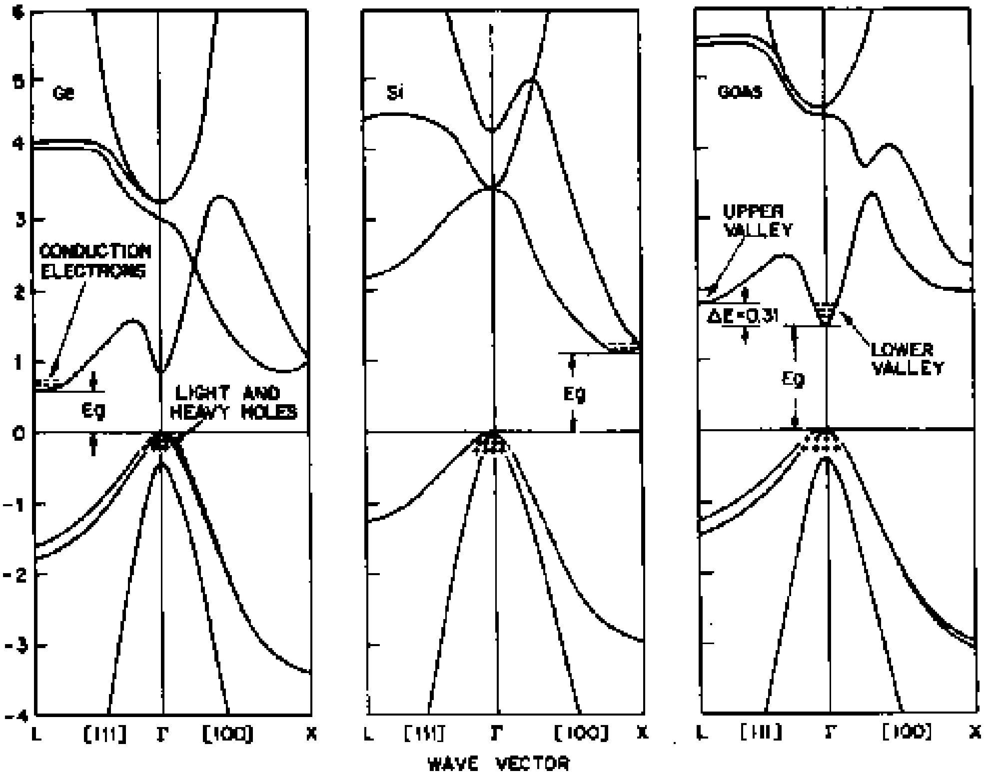


Fig. 2.7 Bandstructure for GaAs (right), which is a direct band-gap material as compared to Ge and Si that are indirect.

The wavefunction for electrons in a confining potential $U(\vec{x})$ is an eigenfunction of the Schrödinger equation:

$$\left\{\frac{1}{2m}(\vec{p}-q\vec{A})^2+U(\vec{x})\right\}\Psi(\vec{x}) \;=\; E\Psi(\vec{x})$$

Here, $\vec{p}=\frac{\hbar}{i}\vec{\nabla}$ is the momentum operator, $q=-e$ the charge of an electron, and $\vec{A}$ the vector-potential, i.e. $\vec{\nabla}\wedge\vec{A}=\vec{B}$. In the following, we will have a look to a few simple cases for zero magnetic field.

Case A), no confinement:

Hence, $U(\vec{x})=0$ and

$$\Psi(\vec{x}) \;=\; e^{i\vec{k}\cdot\vec{x}} \quad \text{and} \quad E(\vec{k}) \;=\; \frac{(\hbar k)^2}{2m}$$

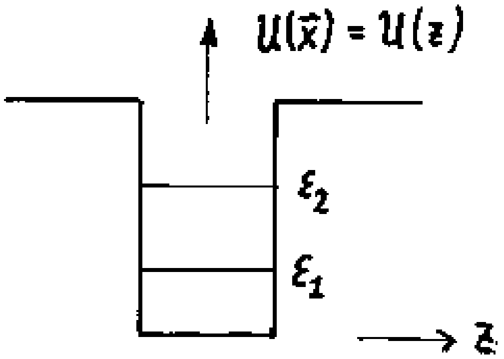
The plane-wave solution can be regarded an approximation for real Bloch electrons of a crystal, for which

$$\Psi_{\vec{k}}(\vec{x}) \;=\; u_{\vec{k}}(\vec{x})e^{i\vec{k}\cdot\vec{x}}$$

It is important to note that the (quasi-) plane-wave solution is a consequence of translation invariance in all three directions.

Case B), confinement in one dimension (2d case):

For a confining potential $U(\vec{x}) = U(z)$ translation invariance in the z-direction is broken.



For this reason, free propagation in z-direction is no longer possible and only two components of the wavevector remain, i.e. the components in the x-y-plane. The wavefunction is given by:

$$\Psi_{n,\vec{k}_\parallel} = \phi_n(z) e^{i(\vec{k}_\parallel \cdot \vec{x}_\parallel)} \quad , \quad \vec{k}_\parallel = k_x \vec{e}_x + k_y \vec{e}_y ,$$

and $\phi(z)$ has to obey the equation:

$$\left\{ \frac{1}{2m} \left(\frac{\hbar}{i} \partial_z \right)^2 + U(z) \right\} \phi_n(z) = \epsilon_n \phi_n(z)$$

Ther different eigenfunctions are distinguished by the index n. The total energy is now:

$$E_n(\vec{k}) = \epsilon_n + \frac{(\hbar \vec{k}_\parallel)^2}{2m}$$

This dispersion relation is shown in Fig. 2.9. If the Fermi energy E_F is larger than ϵ_j, it is said that j two-dimensional subbands are occupied. The energy ϵ_n is the cut-off energy for the subband n. Note, that a system is truly two-dimensional only if $\epsilon_1 < E_F < \epsilon_2$.

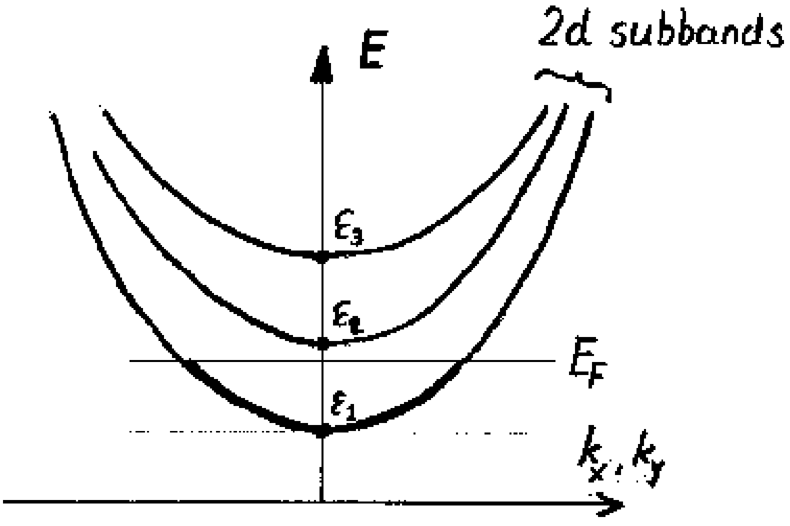


Fig. 2.9 Dispersion for 2d-subbands. A system is truly 2-dimensional if the lowest subband is the only one occupied, i.e. $\epsilon_1 < E_F < \epsilon_2$.

For electrons in an n-type semiconductor, the zero of energy in Fig. 2.9 corresponds to E_c, the minimum of the conduction band.

CASE C), CONFINEMENT IN TWO DIMENSION (1D CASE):

In addition to the z-direction, electrons are now also confined within e.g. the y-direction. Then,

$$E_n(k) = \epsilon_n + \frac{(\hbar k)^2}{2m} \quad \text{, where} \quad k = k_x$$

Here, one refers to the energy bands as one-dimensional subbands. Since translation invariance is not broken along the x-axis, the solutions of the Schrödinger equation correspond to plane waves that match the boundary condition. This is analogous to an optical waveguide, so that we can speak of an *electron waveguide* here, though often the term *quantum wire* is prefered.

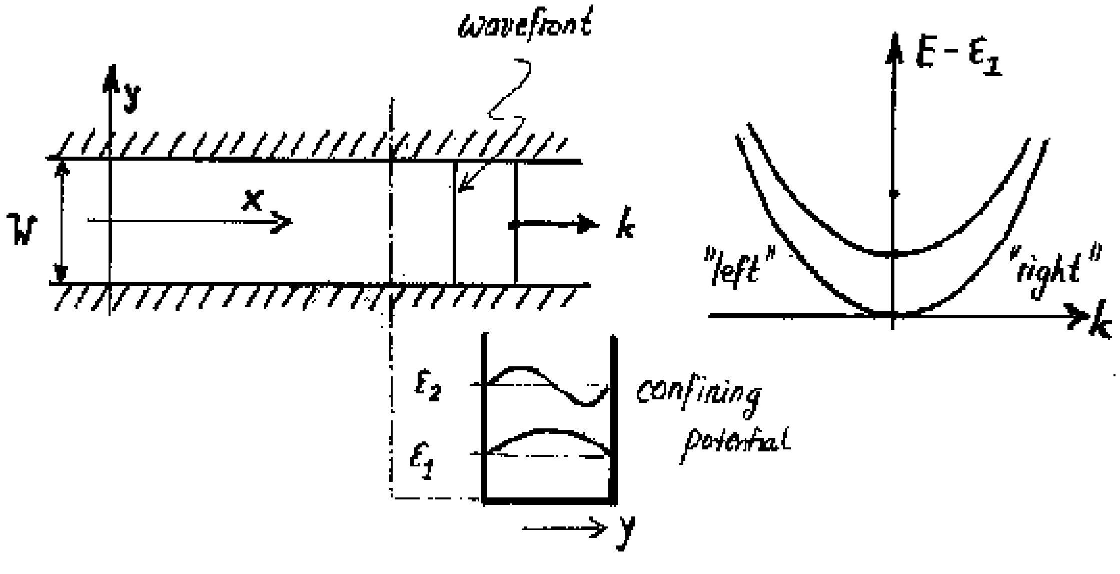


Fig. 2.10 Schetch of a 1d-waveguide for electrons and the corresponding dispersion relation.

CASE D), CONFINEMENT IN ALL THREE DIMENSION (0D CASE):

Now an *artificial atom* has been generated. There are no propagating states anymore. Such systems are often refered to as *quantum dots*.

One may wonder, why not any real crystal is a quantum dot, since it is finite in size. As a Gedankenexperiment take a piece of metal 1 μm in size. Then, the average energy-level spacing is of order $\Delta E \approx E_F/N \approx 5\,\mathrm{peV}$. $N \approx 10^{12}$ is the number of atoms and $E_F \sim 5\,\mathrm{eV}$ the Fermi energy. Since the level-spacing corresponds to a temperature of $\approx 60\,\mathrm{nK}$, which is far lower than everything accessible in a real experiment, the states are sufficiently broadened and overlap. Hence, a continuous energy-band is formed. From this we learn, that one may talk of a quantum dot only if the condition $\Delta E << kT$ is met.

2.2 Density of States

Assume a crystal in 3-d of size $L \times L \times L$. Periodic boundary conditions restrict allowed wavevectors to:

$$k_j \;=\; n_j \frac{2\pi}{L} \quad ; \quad j = 1, 2, 3 \; ; \quad n_j \in \mathbf{Z}$$

Therefore, there is one state (not counting the spin degeneracy) per k-state volume of $(2\pi)^d/V$, so that the density of states is given by:

$$\rho = \mathcal{D}(k,x) \;=\; \frac{1}{(2\pi)^d} \quad , \quad (k,x) := (\vec{k},\vec{x})$$

Note, this state-density is per unit volume in k- and x-space. Hence, the total number of states is given by

$$Z \;=\; \int_V d^d x \int_{1.\mathrm{BZ}} d^d k \; \mathcal{D}(k,x)$$

Most often we are interested in the density-of-states per unit energy.

Case A), Three Dimensions

The total number of states $Z(E)$ with energies $\leq E$ is (now including a factor 2 for spin degeneracy):

$$Z(E) \;=\; 2 \sum_{\{\vec{k}_j | E(\vec{k}_j) <= E\}} 1 \;=\; 2 \frac{V}{(2\pi)^3} \int_{E(\vec{k}) \leq E} d^3 k$$

Defining $z(E) := Z(E)/V$ and $\mathcal{D}(E,x) := \partial z(E)/\partial E$, one obtains:

$$\boxed{\mathcal{D}_{3d}(E,x) \;=\; \frac{2}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}} \qquad (\mathbf{2}.1)$$

Case B), Two Dimensions

For one 2-d subband with energy cutoff ϵ_n:

$$z_n(E) \;=\; \frac{2}{(2\pi)^2}\pi\left\{\frac{(E-\epsilon_n)2m}{\hbar^2}\right\} \quad , \quad E \geq \epsilon_n$$

It follows that the density-of-state $\mathcal{D}(E)$ is *constant* and for each 2-d subband *equal*:

$$\boxed{\mathcal{D}_{2d}(E,x) \;=\; \frac{m}{\pi\hbar^2}\sum_{n=1}^{\infty}\Theta(E-\epsilon_n)} \qquad (\mathbf{2}.2)$$

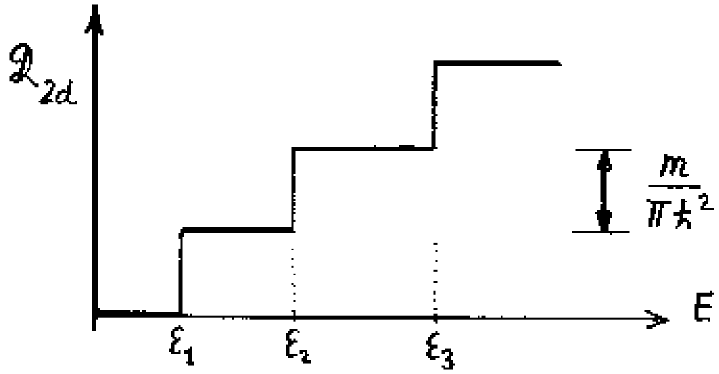


Fig. 2.11 Density-of-states per unit energy for a set of 2-d subbands

CASE C), ONE DIMENSION

For a 1-d subband with energy cutoff ϵ_n:

$$z_n(E) = \frac{2}{2\pi} 2 \sqrt{\frac{(E-\epsilon_n)2m}{\hbar^2}} \quad , \quad E \geq \epsilon_n$$

Density-of-state $\mathcal{D}(E) := \partial z_n(E)/\partial E$ per volume and unit energy:

$$\boxed{\mathcal{D}_{1d}(E,x) = \frac{1}{\pi}\sqrt{\frac{2m}{\hbar^2}} \sum_{n=1}^{\infty} \frac{\Theta(E-\epsilon_n)}{\sqrt{E-\epsilon_n}}} \qquad (\mathbf{2}.3)$$

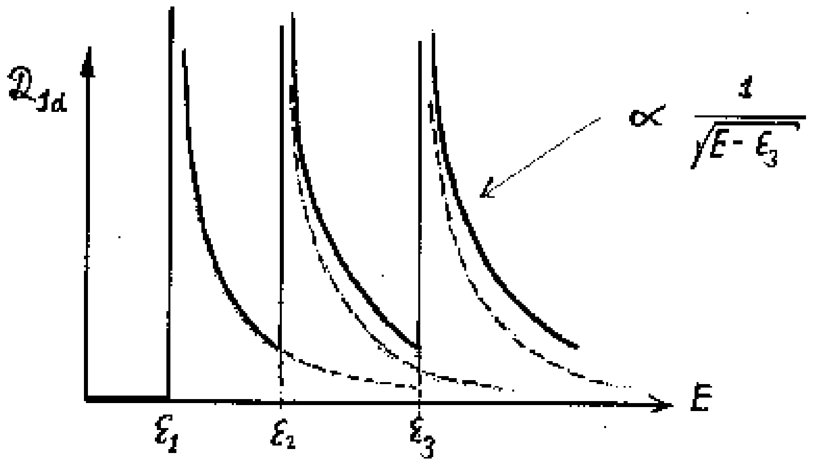


Fig. 2.12 Density-of-states per unit energy for a set of 1-d subbands

GENERAL CASE APPLICABLE TO ANY ENERGY SURFACE

$$z(E) = \frac{2}{V} \sum_{\{k|E(\vec{k})<=E\}} 1 = \frac{2}{(2\pi)^d} \int_{E(\vec{k})<=E} d^d k$$

$$z(E) = \frac{2}{(2\pi)^d} \int_0^{\tilde{E}} d\tilde{E} \int_{E(\vec{k})=\tilde{E}} d^{d-1} S(\vec{k}) \frac{1}{|\partial E(\vec{k})/\partial \vec{k}|}$$

$$\boxed{\mathcal{D}(E,x) \;=\; \frac{2}{(2\pi)^d}\int_{E(\vec{k})=E} d^{d-1}S(\vec{k})\frac{1}{|\partial E(\vec{k})/\partial\vec{k}|} \qquad (\mathbf{2}.4)}$$

The electron density-of-states can be probed with the very elegant method of *capacitance spectroscopy.* The basic principle is explained with reference to Fig. 2.13.

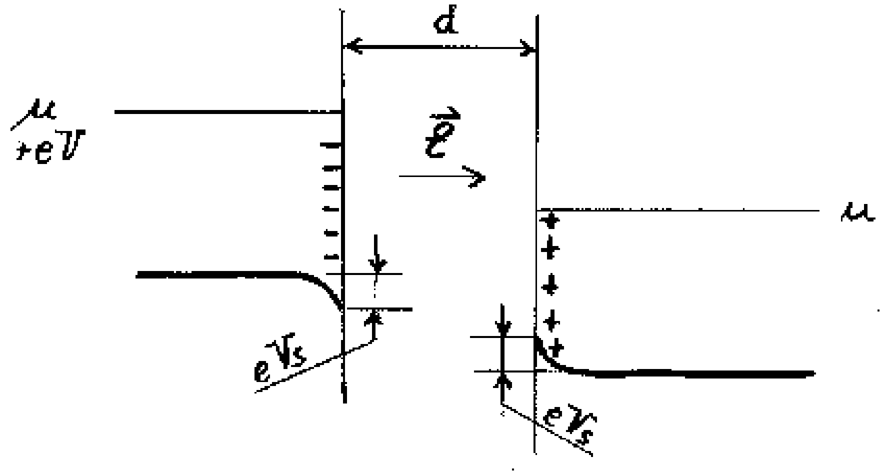


Fig. 2.13 Schematics for electron states of two identical metal electrodes separated by an insulator of thickness d to form a capacitor. The voltage drops partially over the insulator, but in part also at the surface of the electrodes.

Having applied the voltage V, the electrode to the left is charged negatively and the one to right positively. Focusing on the left electrode, we see that the number of electrons is increased near the surface by δn_s (the index s refers to a density per surface area). As a consequence, a fraction of the voltage drops near the surface of the electrode (within the screening length). Hence, $\delta n_s = \mathcal{D}_s(E_F)eV_s$, where $\mathcal{D}_s(E_F)$ is the state density per surface area (integrated over the screening length). The surface-charge density σ is now given by

$$\sigma \;=\; e^2\mathcal{D}_s(E_F)V_s$$

Using $\mathcal{E} = \sigma/\epsilon_0$ for the electric field one obtains for the total voltage drop:

$$V = \sigma \left\{ \frac{d}{\epsilon_0} + \frac{2}{e^2 \mathcal{D}_s(E_F)} \right\}$$

The part within the brackets is the inverse of the total capacitance per unit area. There are three contributions: a geometrical capacitance $C_{geom} = \epsilon_0/d$ and two (equal) electrode capacitances $C_s = e^2\mathcal{D}_s(E_F)$ for each electrode. In good metals like gold, the electrode surface-capacitance is large of order $1\,\mathrm{Fm}^{-2}$. Therefore, the total capacitance is in most situations very well approximated by the geometrical capacitance. In semiconductors, on the contrary, the capacitance intrinsic to the depletion or population of e.g. the conduction band may even dominate the total capacitance.

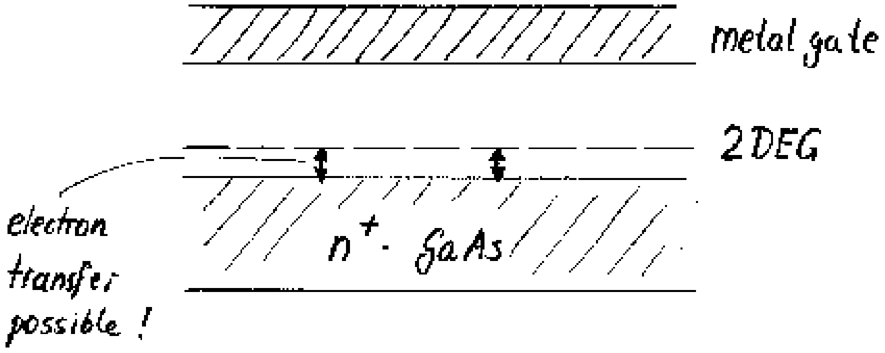


Fig. 2.14 One measures the capacitance between the top gate and a conducting back electrode, which in this GaAs-based heterostructure is n^+ doped. The dashed line indicate the 2DEG. This 2-dimensional electron gas is so close to the bottom layer that electron transfer (by tunneling) is possible within a reasonable time scale. One can now adjust the electron density in the 2DEG by applying the corresponding dc-voltage. Next, the capacitance is measured dynamically by applying in addition a small ac-voltage.

A particular simple situation arises in measurements of a 2-dimensional electron gas (2-DEG) sandwiched in between a top metal gate and a bottom highly doped layer, see Fig. 2.14. Here, the capacitance is given by

$$C = e^2 \mathcal{D}_2(E_F) \ ,$$

with $\mathcal{D}_2(E_F)$ being the $2d$-density-of-states of the 2DEG.

A measurement example is shown in Fig. 2.15 for arrays of one-dimensional wires of different widths formed by a corrugated gate ontop of the 2DEG (scheme d of Fig 1.9). The visible oscillations are due to a modulation of the density-of-states.

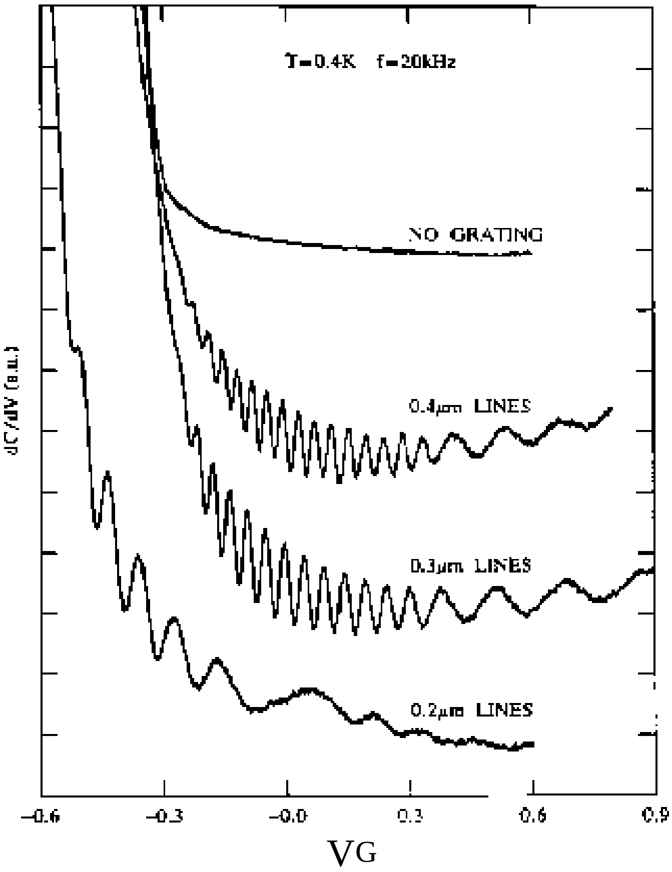


Fig. 2.15 The derivate of the capacitance recorded as a function of the gate voltage on 1d-electron channels with different widths in an GaAs-Al$_x$Ga$_{1-x}$As heterojunction with corrugated gates. The line widths denoted are the lithographic widths defining the channels.

The following figures highlight recent developments (by R. Ashoori 1993) allowing to analyze the energy-level spectrum in quntum-dot structures.

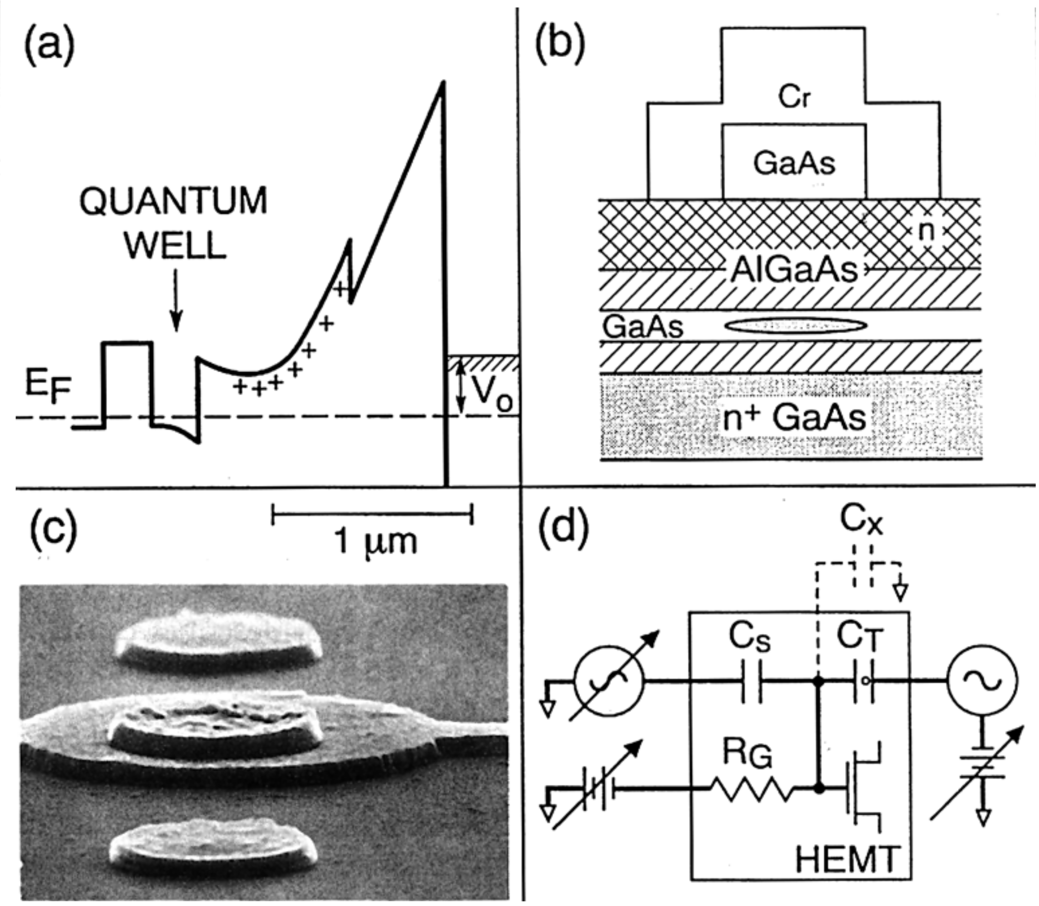


Fig. 2.16 (a) Conduction band profile of the multilayer sample. E_F is the Fermi level in the n^+ doped bottom layer and V_0 is the voltage applied to the gate. (b) Schematic cross-section through the tunnel capacitor. (c) SEM image of the tunnel capacitor showing the top gate.

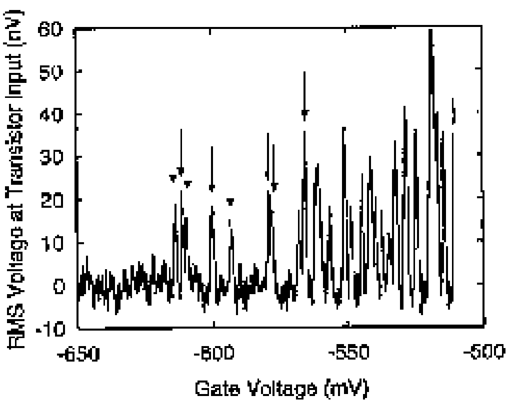


Fig. 2.17 Measured signal proportional to the capacitance for a voltage sweep starting at negative voltages. Each visible peak corresponds to the opening of a new quantum-dot state at which instant the dot is populated. The first peak occurs at −620 mV and there exist no such feature at lower voltages. This technique allows to study single elctron states in a quantum dot.

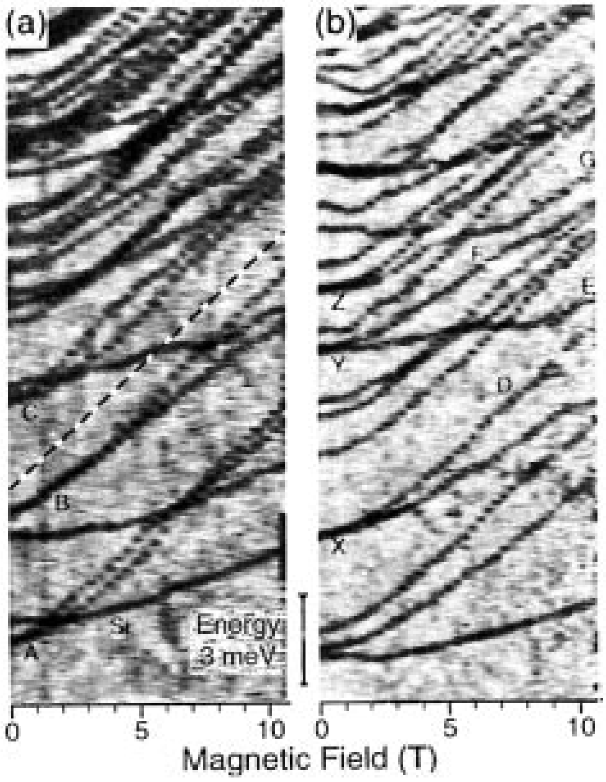


Fig. 2.18 Gray scale images of the capacitance of one sample (thermally cycled in between) as a function of energy and magnetic field.

2.3 Thermodynamics

Since electrons are fermions, the state occupancy in thermodynamical equilibrium is determined by the Fermi-Dirac distribution function f_0. This function depends on temperature and on the energy E of the respective state:

$$\boxed{f_0(E) = \frac{1}{e^{(E-\mu)/kT} + 1} \qquad (\mathbf{2}.5)}$$

Herein, $\mu = \mu(T)$ is the chemical potential. Some authors exclusively use the assignment $\mu(T \rightarrow 0) \equiv E_F$ for the Fermi-energy E_F, while for others $\mu = E_F$ for any temperatures. The latter definition is widely used in the semiconductor literature.

The Fermi-energy (or chemical potential) has to be determined selfconsistently via the following equation that determines the electron density:

$$n = \int_0^\infty \mathcal{D}(E) f_0(E) dE$$

We sometimes will use the abreviation $f_0(\epsilon)$ for

$$f_0(\epsilon) = \frac{1}{1 + exp(\epsilon)} \quad \text{with} \quad \epsilon := (E-\mu)/kT$$

There are the following useful relation for the Fermi-Dirac function, see also Fig. 2.19:

$$f_0(E)(1 - f_0(E)) = -kT \left(\frac{\partial f_0}{\partial E}\right) \qquad (\mathbf{2}.6)$$

$$\frac{\partial f_0(E)}{\partial E} = -\frac{1}{4kT}\left(cosh\left(\frac{E-\mu}{2kT}\right)\right)^{-2} \qquad (\mathbf{2}.7)$$

$$lim_{T\rightarrow 0}\left(\frac{\partial f_0(E)}{\partial E}\right) = -\delta(E-\mu) \qquad (\mathbf{2}.8)$$

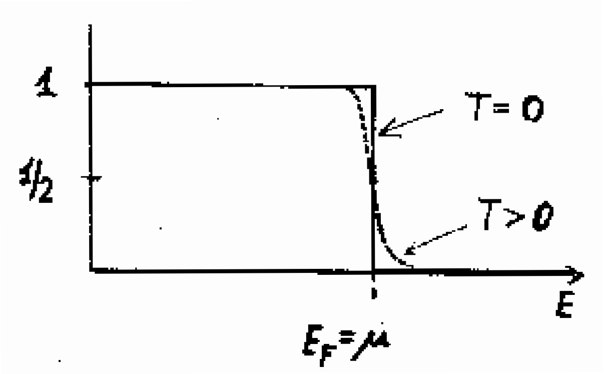


Fig. 2.19 The Fermi-Dirac distribution function.

While the equilibrium distribution does depend on energy only, in situations where transport takes place the *non-equilibrium distribution function* f differs from f_0:

$$f \;=\; f(\vec{k},\vec{x},t)$$

In general, one would also have to include the spin in order to describe a non-equilibrium spin distribution (in e.g. a magnet). In many situation a *local equilibrium* is formed. The stationary distribution function is then of the form:

$$f(\vec{k},\vec{x}) \;=\; f_0(E(\vec{k})) \;\; \text{with} \;\; \mu := \mu(\vec{x}),\; T := T(\vec{x})$$

How to caclulate a current ?

The current density is $\vec{\jmath}$ = charge-density × velocity. In a volume of size L^3 each electron in an extended state contributes the charge density by q/L^3. Since the velocity $\vec{v}$ equals $\frac{1}{\hbar}\partial E/\partial\vec{k}$, which amounts to $\hbar\vec{k}/m$ for 'free' electrons, we obtain for zero temperature:

$$\vec{\jmath} \;=\; -\frac{2e}{L^3}\sum_{occupied}\hbar\vec{k}/m \;=\; -\frac{2e}{(2\pi)^3}\int_{E(\vec{k})\le E_F} d^3k\,(\hbar\vec{k})/m$$

This is obviously zero in equilibrium, since $E(-\vec{k}) = E(\vec{k})$. Using the distribution function we now write:

$$\vec{\jmath} \;=\; -\frac{2e}{(2\pi)^3}\int d^3k\, f(\vec{k},\vec{x})(\hbar\vec{k})/m$$

If $f(-\vec{k},\vec{x}) = f(\vec{k},\vec{x})$, then $\vec{j} = 0$, which is obviously the case in equilibrium.

2.4 Classical Transport

The electron gas is viewed as a classical fluid and described by a simple Newton-like equation for the mean particle momentum $\langle\vec{p}\rangle$. Scattering among the particles allows the exchange of momentum and is taken into account by a friction term proportional to $\langle\vec{p}\rangle$. In an electric field $\vec{\mathcal{E}}$ we have:

$$\left\{\frac{d}{dt} + \frac{1}{\tau_m}\right\}\langle\vec{p}\rangle = q\vec{\mathcal{E}} \qquad (\mathbf{2}.9)$$

The parameter τ_m is called the *momentum relaxation time*, since it determines the time scale with which the (non-equilibrium) momentum relaxes after turning off the external force. Since in equilibrium $\langle\vec{p}\rangle_0 = 0$, the relaxation follows the law $\propto exp(-t/\tau_m)$.

The stationary solution of **2**.9 is given by $\langle\vec{p}\rangle = q\tau_m\vec{\mathcal{E}}$. The mean velocity, which is called the *drift velocity* $\vec{v}_D$ follows by divinding through m. Since the current density is given by

$$\vec{j} = qn\vec{v}_D = \sigma_D\vec{\mathcal{E}}$$

the so called Drude-conductivity σ_D is obtained:

$$\sigma_D = \frac{e^2 n}{m}\tau_m \quad (n = \text{density of electrons}) \qquad (\mathbf{2}.10)$$

It appears from this equation that σ is determined by all electrons (since the total density of electrons enter). We will show below, however, that σ is soley determined by properties of the electrons at (or close to) the Fermi energy in degenerate electron gases. It is said that σ is a *Fermi-level property.*