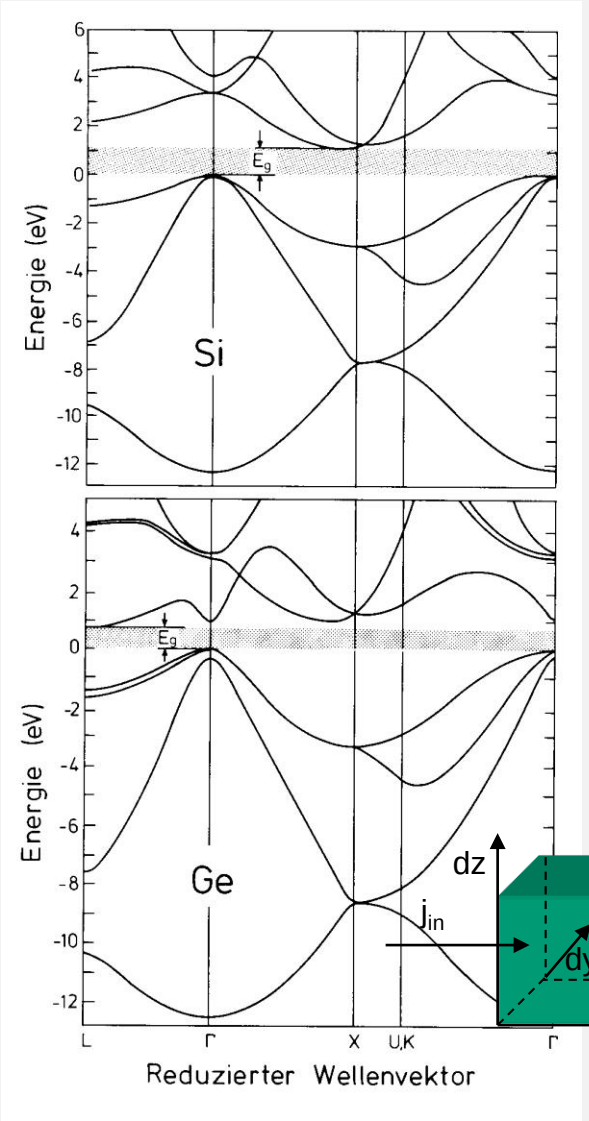
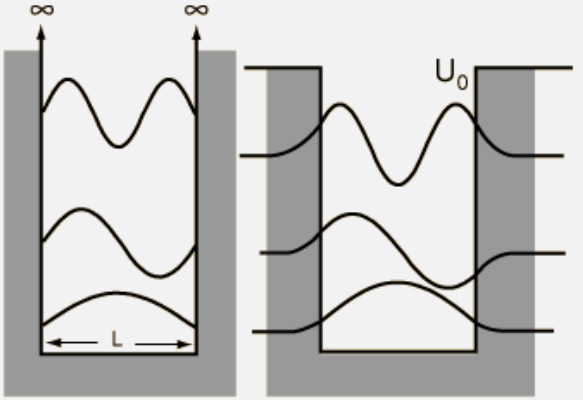
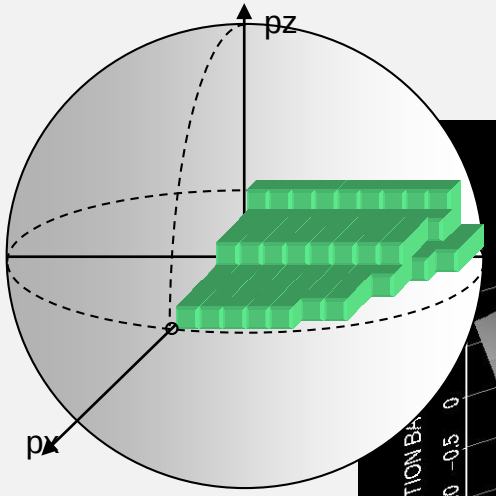
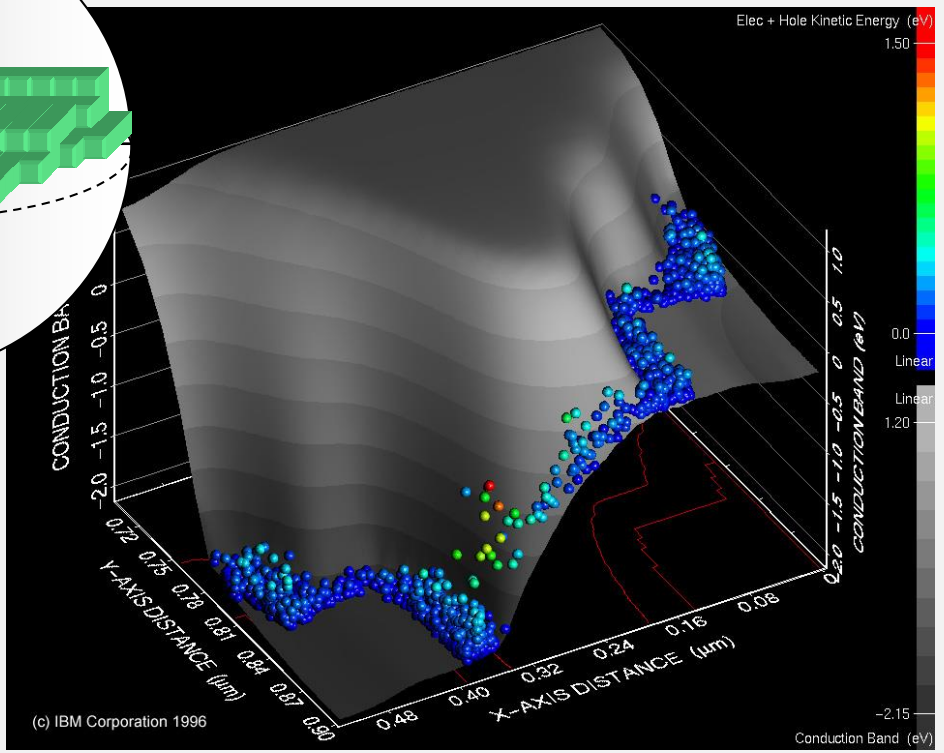


$$\frac{\partial f}{\partial t} = -\left[\frac{1}{\hbar}\nabla_k \varepsilon(k)\cdot\nabla_r f + \frac{q\vec{E}}{\hbar}\cdot\nabla_k f\right] + \left.\frac{\partial f}{\partial t}\right|_{coll}$$







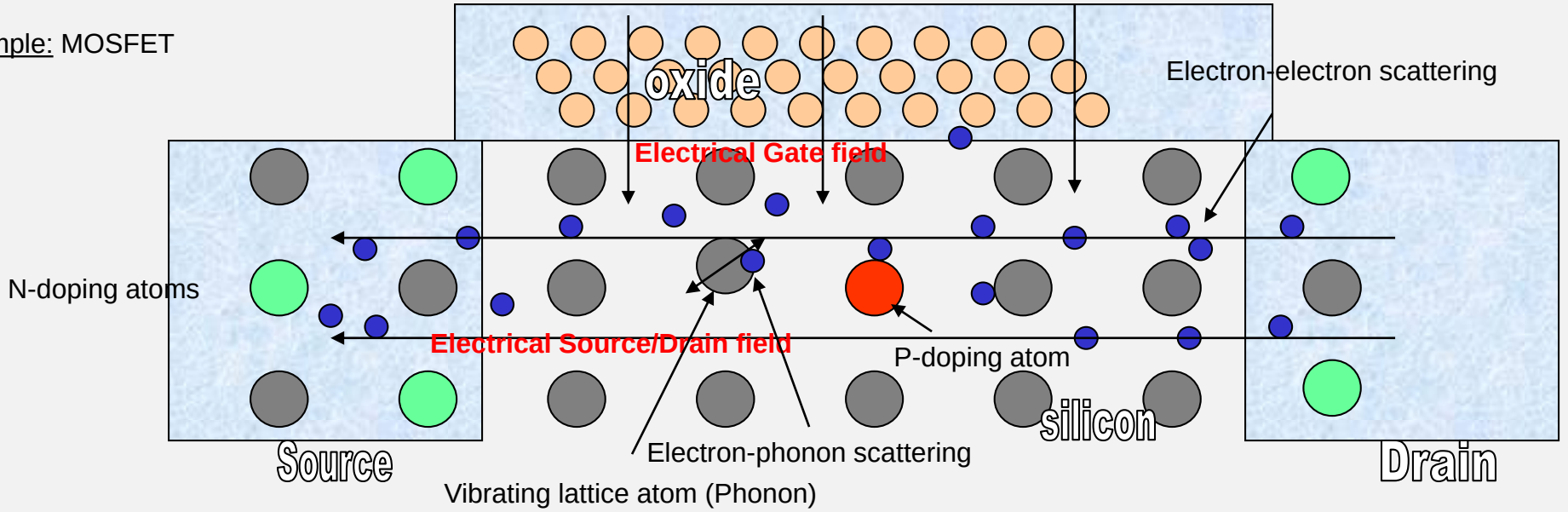
Transport Phenomena

Carrier transport in a spatially inhomogenous device, subjected to time-varying driving forces

will be

a nonlinear, nonstationary, nonequilibrium statistical, quantum mechanical problem

Example: MOSFET



1) all particles (electrons and atoms) are quantum mechanical particles (Fermi-statistics, Pauli-principle) — Nature of particles and statistics

2) different atoms (oxide, silicon, doping atoms) provide different intrinsic potentials and properties (electron density, scattering cross section,...)

3) Local distortions in space (defects,...) and time (phonon vibration) exist — environment

4) time and space varying external fields influence the motion of the charge carriers — Forces and motion -> transport

Basic Transport Phenomena

Transport describes how and how much of a physical quantity (mass, charge, heat,...) is moved from one location to another location. These quantities are always connected with a **carrier** (particle or wave).

.

We can look for transport on a very **microscopic view:**

1

Microscopic View ⇨ We observe **the carrier** which is characterized by several physical quantities.

There are external fields which interact with the physical quantities of the carrier by forces.
Because the physical quantity is tied to the carrier the forces usually will result in a movement of the carrier.
This movement in time and space by forces is described by **equations of motion**.

There is an environment which gives restrictions for the movement

But, in principle, transport is handled as a **macroscopic phenomenon**

2

Macroscopic View ⇨ We measure the **amount of a physical quantity** at a point in space and time.

We can measure the amount of this physical quantity:
- at the same location, but different time
- at an other location at different time

We try to find **phenomenological equations** of transport, based on some physical background

We try to use these equations for other transport phenomena

Transport is Current

A **current I** is defined as the (ex)change of a physical quantity Q with time:

$$I = \frac{dQ}{dt} = \dot{Q}$$

Note:
Q is just a quantity Q, not necessarily a charge
Current j is just a transported quantity, not necessarily an electrical current

If the current I is normalized to a cross-section A, a **current density j** can be defined:

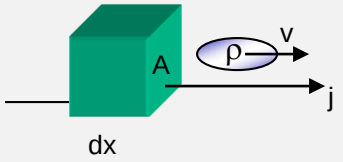
$$j = \frac{\dot{Q}}{A}$$

Note:
In physics a time derivate is noted with a point over the quantity,
a derivate to space (x,y,..) is noted by a bar

If the carrier of these quantities move with a common velocity v, the current density can be expressed as a moving density ρ :

$$\vec{j} = \frac{\dot{Q}}{A} = \frac{dQ}{dt \cdot A} \cdot \frac{dx}{dx} = \frac{dQ}{dV} \cdot \frac{dx}{dt} = \rho \cdot \vec{v}$$

V = Volume



$$\vec{j} = \rho \cdot \vec{v}$$ This we call the:

Stationary Continuity Equation

By this way the **density** ρ of the physical quantity is defined:

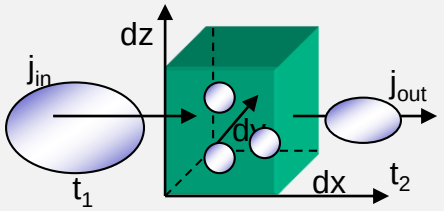
$$\rho_m = \frac{M_{ass}}{V_{olume}}$$ or $$\rho_q = \frac{Q}{V}$$ or .....

Conservation of current (**continuity equation**):

The density of a physical quantity changes in a volume with time, if current moves in or out

$$\vec{\nabla}_r \vec{j} = -\dot{\rho}$$

Continuity Equation



$$\vec{\nabla}_r \vec{j} = \frac{\partial}{\partial x} j_x + \frac{\partial}{\partial y} j_y + \frac{\partial}{\partial z} j_z$$

is called divergence of the vector field j and is a scalar. In the case that j = ρ*v than div j is called source density

Examples of Transport Equations

Transport	moving quantity	current density	observation	Transport equation
Mass (Diffusion)	mass = number of particles	$j_{mass} = \frac{1}{A} \cdot \frac{dN}{dt}$	$\vec{j} = -D \cdot \vec{\nabla} c$ gradient of particles	$\dot{\rho} = \frac{\partial c}{\partial t} = -\nabla j = -\nabla(-D \cdot \nabla c) = D \cdot \nabla^2 c = D \cdot \Delta c$ $\frac{\partial c}{\partial t} = D \cdot \Delta c$
Charge (el. conduction)	charge = number of electrons	$j = \frac{1}{A} \cdot \frac{dq}{dt}$	$\vec{j} = \sigma \vec{E} = -\sigma \cdot \vec{\nabla} \varphi$ gradient of potential	$\vec{\nabla} \vec{j} = -\dot{\rho}$ $\frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2} = \Delta \Psi$
Energy (Heat)	heat = number of particle collisions or number of photons (radiation)	$j = \frac{1}{A} \cdot \frac{dQ}{dt}$	$\vec{j} = -\lambda \cdot \vec{\nabla} T$ gradient of temperature	$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho \cdot c_v} \cdot \Delta T$
Particle (probability)	$particle = \Psi(r,t)$ *wave function*	$\vec{j} = \frac{i\hbar}{2m}(\Psi \cdot \nabla \Psi^* - \Psi^* \cdot \nabla \Psi)$ gradient of probability		$-\frac{\hbar^2}{2m} \cdot \Delta \Psi(r,t) + V(r) \cdot \Psi(r,t) = \frac{\hbar}{i} \cdot \frac{\partial}{dt} \Psi(r,t)$

wave equation, little more complicated because movement of charges causes electrical and magnetic fields

In each transport equation the timely change of one physical parameter $\frac{\partial X}{\partial t}$ results in a location change ΔY of an other parameter

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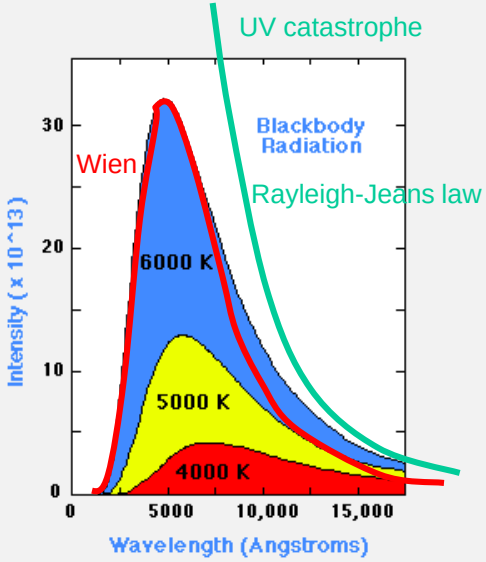
- Solving The Boltzmann-Bloch Equation

"Classical" Quantum Mechanics

Planck 1900:



Rayleigh-Jeans law: derived from classical physics:
(counting the oscillation modes of elmag waves in a box)

$$\rho\,df = \frac{8\pi k_B T}{c^3}\cdot f^2 df$$

Wien´s 2.Law 1896: derived empirically
(and already close to reality)

$$\rho\,df = \frac{8\pi\beta}{c^3}\cdot f^3 \cdot \exp\left[-\frac{\beta f}{k_B T}\right] df$$

In 1899 Plummer/Pringsheim made very carefull measurements of the experimental distribution.

Based on this results Planck was able to find the correct equation of the distribution
(first by determining ß in Wien´s law and after recognizing the consequence by light particle statistics):

$$\rho\,df = \frac{8\pi h f^3}{c^3}\cdot\frac{1}{\exp\left[\frac{hf}{k_B T}\right]-1}\,df$$

so this must be an energy as well

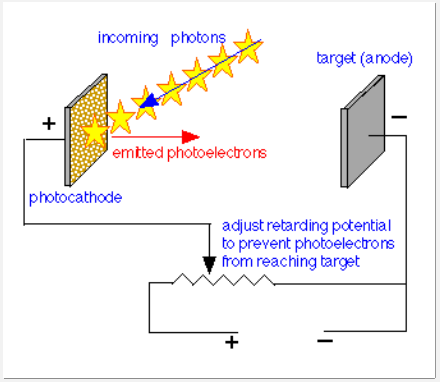
this is an energy

$k_B = 1.38*10^{-23}$ J/K = $8.617*10^{-5}$ eV/K

In contrast to classical wave theory it looked as the energy of a light **wave** with (any) **frequency f** can only have **portions (= quantums)** in steps of a constant h = $6.3*10^{-34}$ Jsec

Einstein 1905:

Photo effect



Hertz (1887) observed that light can induce the emission of electrons out of materials.
In classical electrodynamics the energy is delivered by the intensity of the light wave.
But the experiment showed that the frequency of light determines the emission:
very high intensity of red light does not cause emission, but very low intensity of blue light does.

Einstein used the "light quantum" of Planck to explain this effect:

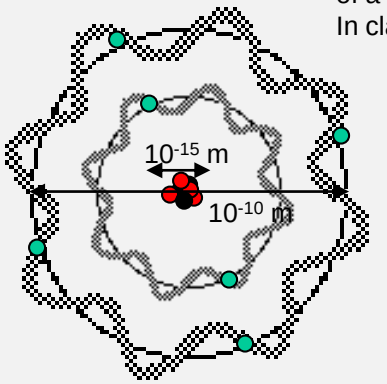
If a light quantum with an energy of E=hf hits an electron, it can transfer all it´s energy to the electron to leave the material.

$$E = h\cdot f$$

The "light particle", named **photon**, was discovered

"Classical" Quantum Mechanics

Bohr 1914:



Lenard (1903) shooted electrons, Rutherford (1911) alpha-particles at metals. Both found that the atom must consist of a heavy, but very small (~10^{-15} m) positively charged nucleus and an almost empty, but large (~10^{-10} m) electron shell.
In classical physics this atom can not be stable, because moving electrons will loose energy by radiation and should fall into the nucleus.

The assumptions of Bohr, stated in his original paper were simply:

* the electron is in a stationary energy state of which there exist a discrete set
* a quantisation condition is given by:

$$n \cdot \lambda = 2\pi \cdot r \quad \Rightarrow \quad L = mvr = n \cdot \hbar$$

where L is the angular momentum of the eletron, n is a positive integer and h is Planck's constant.

* transitions between these states are possible with frequency v, v given by:

$$\Delta E = h\nu = E_m - E_n$$

de Broglie 1923:

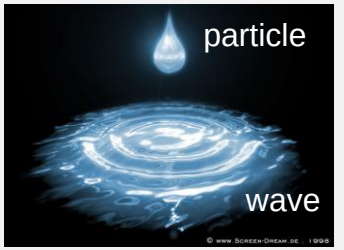
Based on the dualism of light, that light in some experiments behave like an electromagnetic wave in other experiments like a particle

wave: $c = \lambda \cdot f$

Photons: $E = h \cdot f = mc^2$

$$\lambda = \frac{h}{mc}$$

Dualism of wave (λ) and particle (m)



deBroglie postulated that in contradiction particles may be described as wave with a wavelength depending on velocity (momentum):

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

$$\lambda = \frac{1.23nm}{\sqrt{E_{kin}[eV]}}$$

for electrons with E=1eV the wave length λ ~ 1nm

Heisenberg 1927:

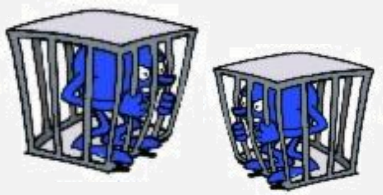
What Heisenberg discovered is that a wave packet confined to a very small region must be made up of a lot of different wavelengths, and therefore a lot of different momenta. In other words, if the uncertainty in the position of the particle is small, the uncertainty in the momentum is large. And similarly, a particle whose wave packet is made up of only a few wavelengths (and hence only a few momenta) will be spread out over a large region. That is, if the uncertainty in momentum is small, the uncertainty in position is large:

uncertainty principle $\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$ using the Planck constant: $\hbar \geq \frac{h}{2\pi}$

"Classical" Quantum Mechanics

Pauli 1925: Pauli exclusion:
quantum mechanical particles with the quantum number spin=1/2 only two can occupy the same energy state

Fermi 1926:



discovered the statistical laws for particles subject to the **Pauli exclusion principle**

$$f(E,T)=\frac{1}{\exp\left[\frac{E-E_F}{kT}\right]+1}$$

Schrödinger 1926: Based on deBroglie´s theory that qm particles in some situations can be described as waves
Schrödinger was looking for a wave equation to describe the movement of qm particles in position and momentum.

$$\vec{p}_{class} -> \vec{p}_{qm} = \frac{\hbar}{i}\cdot\frac{\partial}{\partial\vec{r}} = \frac{\hbar}{i}\cdot\nabla$$

Operator of momentum

$$E_{kin}=\frac{p^2}{2m} \longrightarrow E_{kin}=\frac{\hbar^2}{i^2 2m}\cdot\frac{\partial^2}{\partial r^2} = -\frac{\hbar^2}{2m}\cdot\Delta$$

Operator of kinetic energy

$$H = E_{kin}+E_{pot} = \frac{\hbar^2}{2m}\cdot\Delta + V(\vec{r})$$

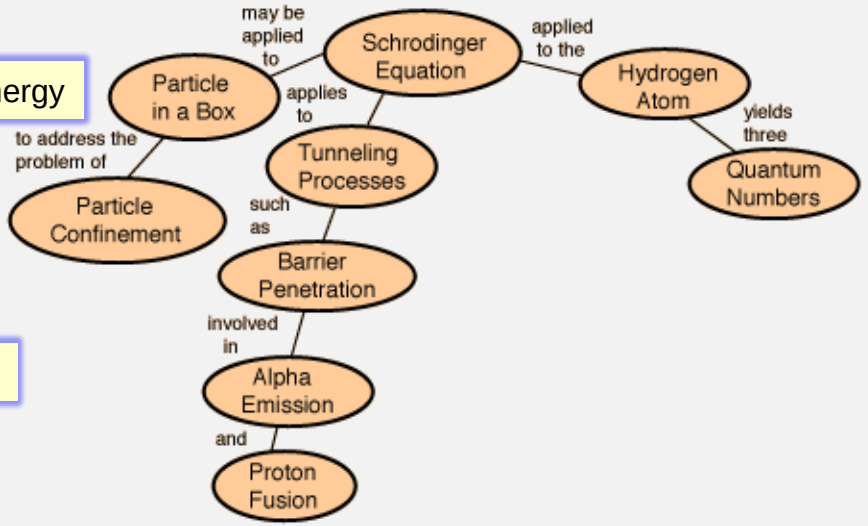
Hamilton-operator of energy

$$-\frac{\hbar^2}{2m}\cdot\Delta\Psi(r,t)+V(r)\cdot\Psi(r,t)=\frac{\hbar}{i}\cdot\frac{\partial}{dt}\Psi(r,t)$$

Schrödinger equation

$$H\Psi(r,t)=E\Psi(r,t)$$

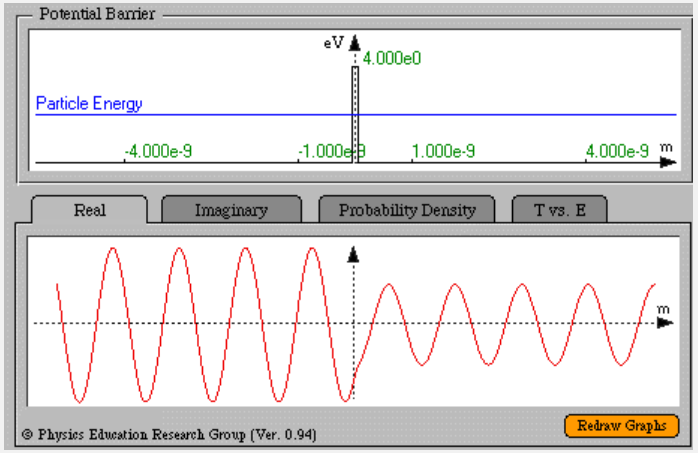
stationary Schrödinger equation



"Classical" Quantum Mechanics in Electronic Devices

Tunneling:

Quantum mechanical particles can penetrate a distance into barriers which corresponds to their wavelength



source: http://phys.educ.ksu.edu/vqm/html/qtunneling.html

For electrons in solids the wavelength is a few nanometer

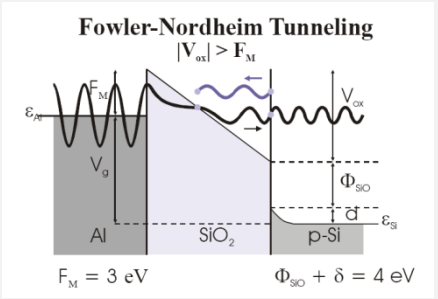
$$\lambda = \frac{h}{mv} = \frac{h}{p} \Rightarrow \lambda = \frac{1.23nm}{\sqrt{E_{kin}[eV]}}$$

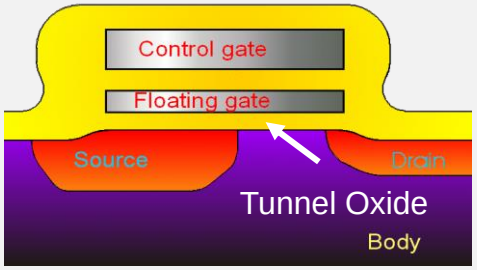
for electrons with thermal energy E=kT = 0.026eV
the wavelength is about λ ~ 8 nm !!

If the barrier is thinner than the wavelength the particles may pass the barrier:

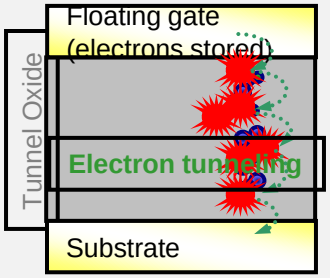
$$T \propto \exp\left[-2a \cdot \sqrt{\frac{2m \cdot (V_0 - E)}{\hbar^2}}\right]$$

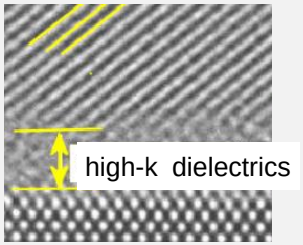
Tunneling through barriers is used in Flash-Memories:



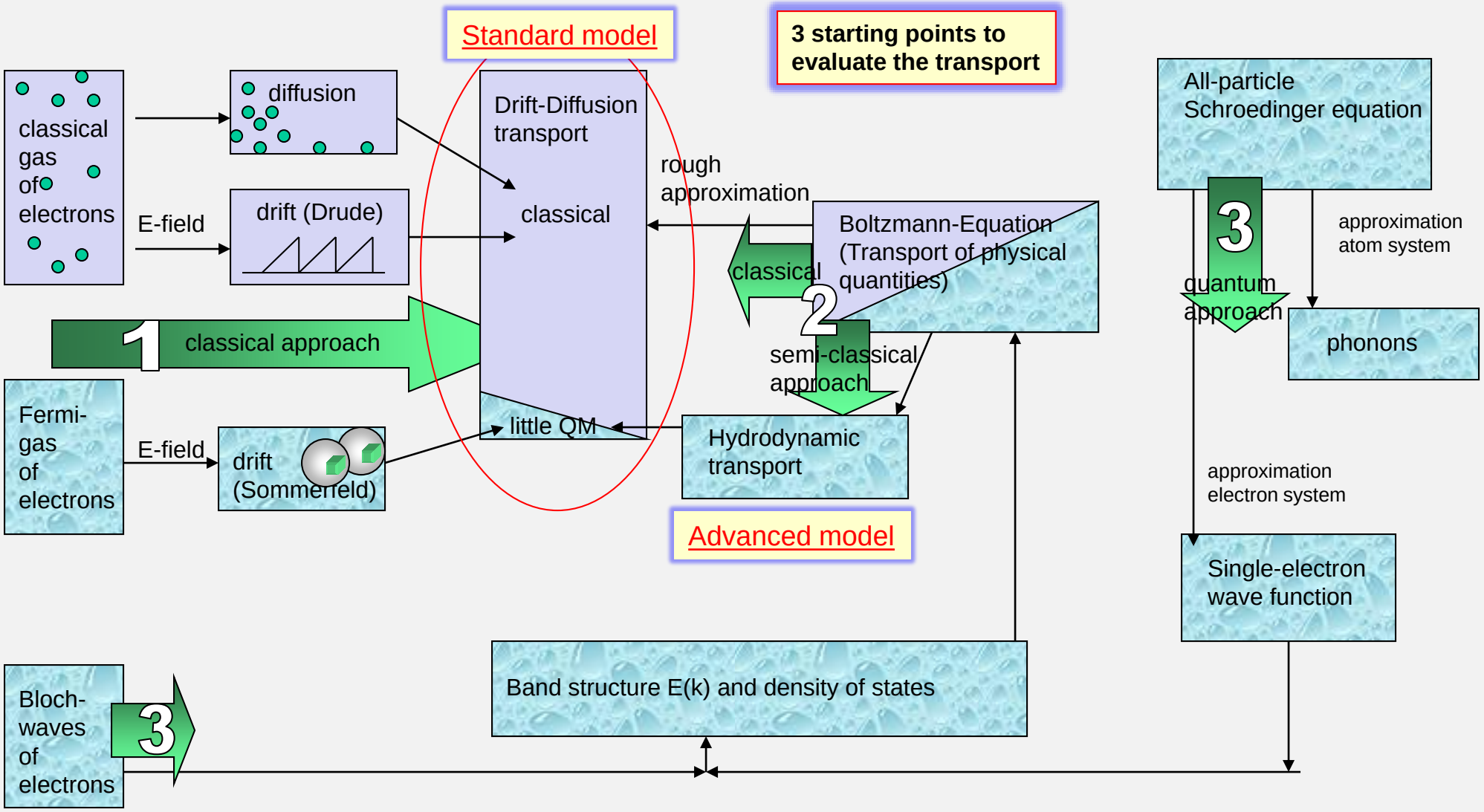


but hampers future MOSFET development
by gate leakage current for t_{ox} < 1nm:





Charge Transport Models - Overview



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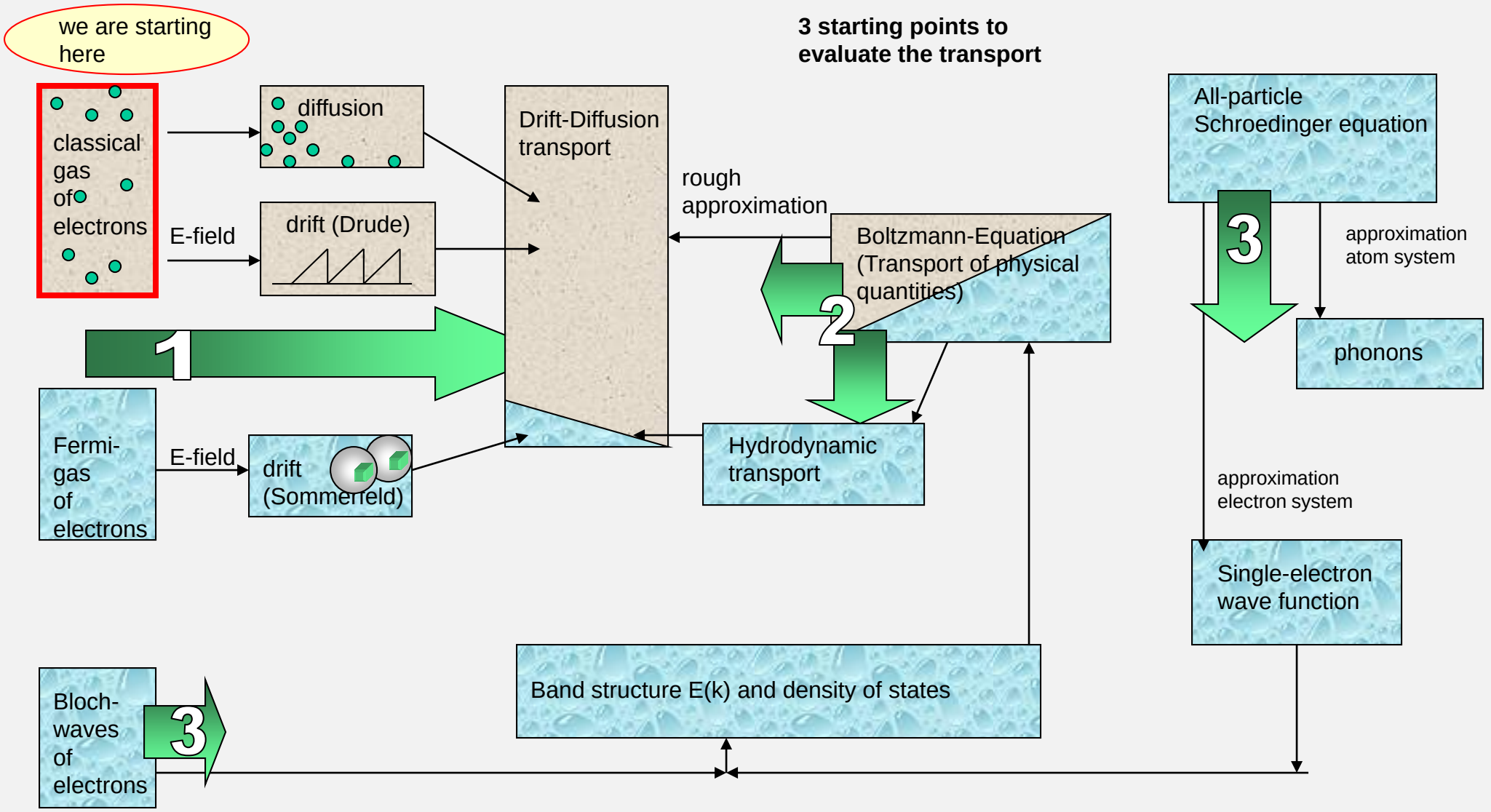
Charge Transport Models - Classical Start



Mechanics: Movement of particles

Mechanics:

1

If a **force F** acts on a free particle with **mass m** an **acceleration a** will be the result:

$$\vec{F} = m\vec{a}$$ **equation of motion**

If the acceleration a acts for a time interval dt a change dv in velocity v will be the result:

$$a \cdot dt = dv$$

If the mass m moves for a time interval dt with velocity v a change of location dx will be the result:

$$v \cdot dt = dx$$

2

The **momentum p** of a particle with mass m and velocity v is defined:

$$\vec{p} = m\vec{v}$$

Doing the time derivate:
(for m=constant)

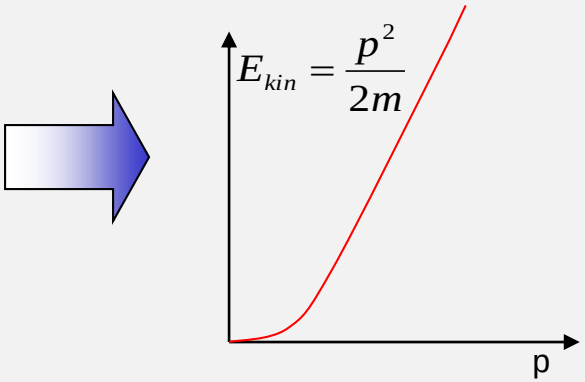
$$\frac{dp}{dt} = \frac{d(mv)}{dt} = m \cdot \frac{dv}{dt} = ma$$

$$F = \frac{dp}{dt} = \dot{p}$$

3

The **kinetic energy** of a particle with mass m can be followed:

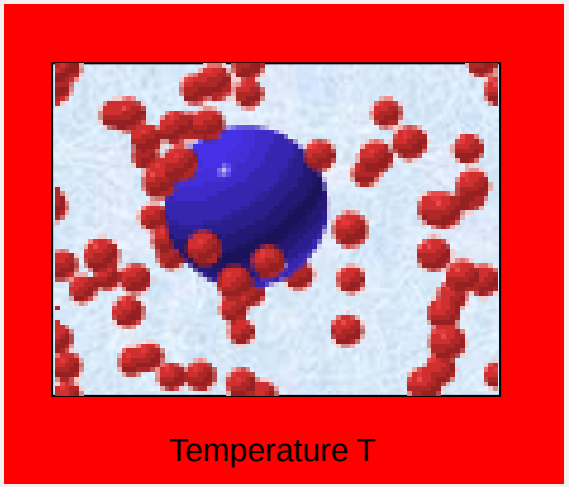
$$E_{kin} = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m}$$



The kinetic energy of a free particle is parabolic in momentum p

free: particle is not bonded (in potentials)

The Classical Gas Model: Energy distribution



Assumption:

1) All particles gain energy from temperature (e.g. collisions with the wall)

$$\Rightarrow E_{kin} = \frac{3}{2} k_B T = \frac{1}{2} m v^2 \Rightarrow$$

All particles should have the same velocity

2) collisions are short in time and space

3) collisions are independent

4) collisions change the direction of movement random

5) the movement of every particle is independent from other particles

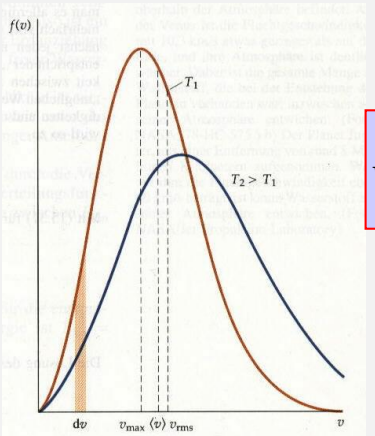
Maxwell: 6) the energy kT from the wall is supplied by swinging atoms, so the energy transfer is statistically -> #1 must be replaced

$\Rightarrow$ a velocity distribution is the result

Boltzmann: **the statistically probability:** $\frac{N}{N_0} = f(E) \propto \exp\left[-\frac{E}{kT}\right]$

$$f(v) = \sqrt{\frac{2}{\pi}} \cdot \left(\frac{m}{kT}\right)^{3/2} \cdot v^2 \cdot \exp\left[-\frac{\frac{1}{2}mv^2}{kT}\right]$$

Maxwell distribution



most probable velocity

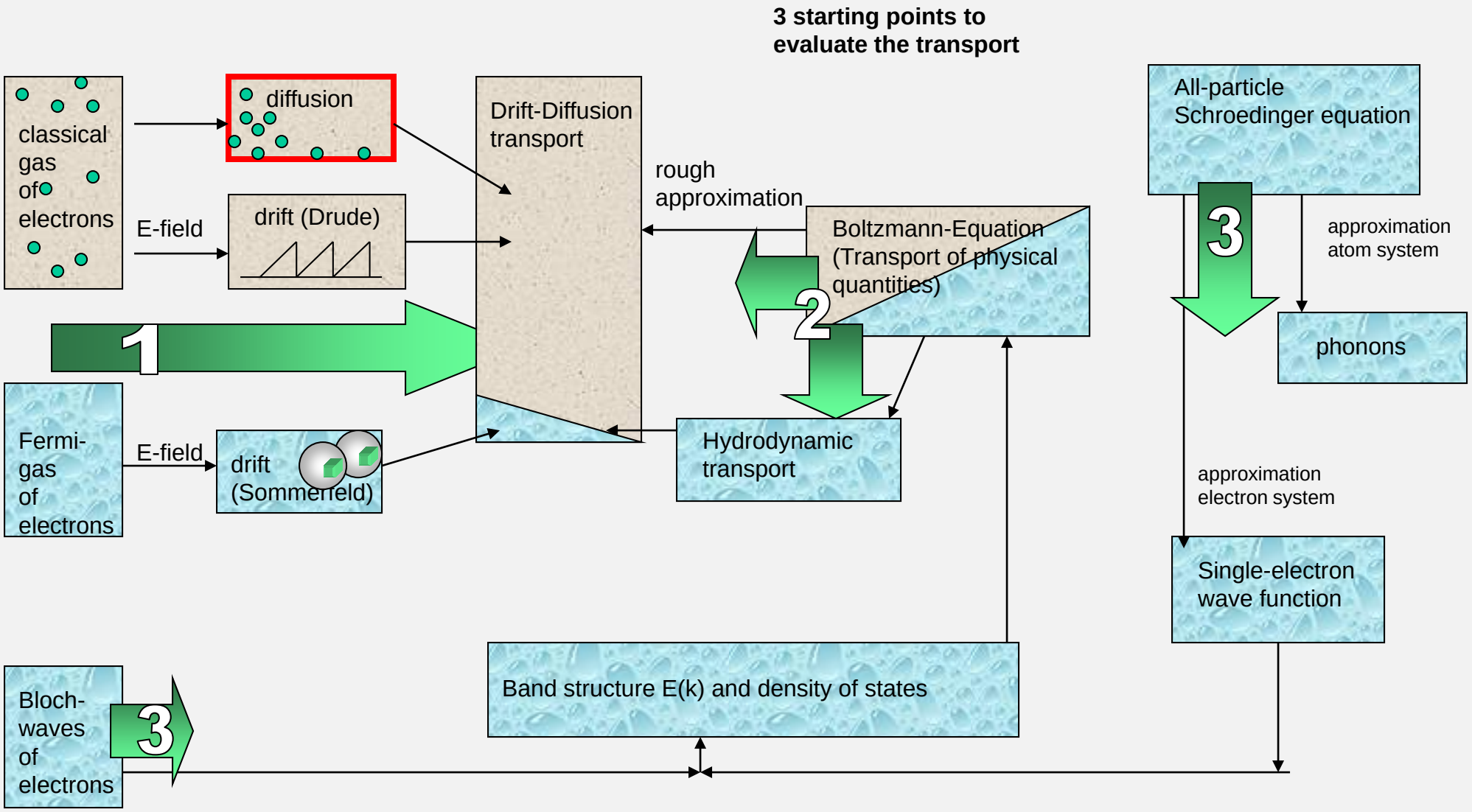
$$v_p = \sqrt{\frac{2kT}{m}} = 5.5 \cdot 10^5 \cdot \sqrt{T[K]} \quad [cm/sec]$$

average velocity

$$\bar{v} = \sqrt{\frac{8kT}{\pi m}} = 1.13 \cdot v_p$$

$\Rightarrow$ In a classical gas many particles may have the same energy

Charge Transport Models



The Classical Gas Model: Diffusion

Particles with thermal energy will distribute from points of high concentration to points of low concentration.
This movement is called **diffusion**.

$$j = -D \cdot \frac{dn}{dx}$$

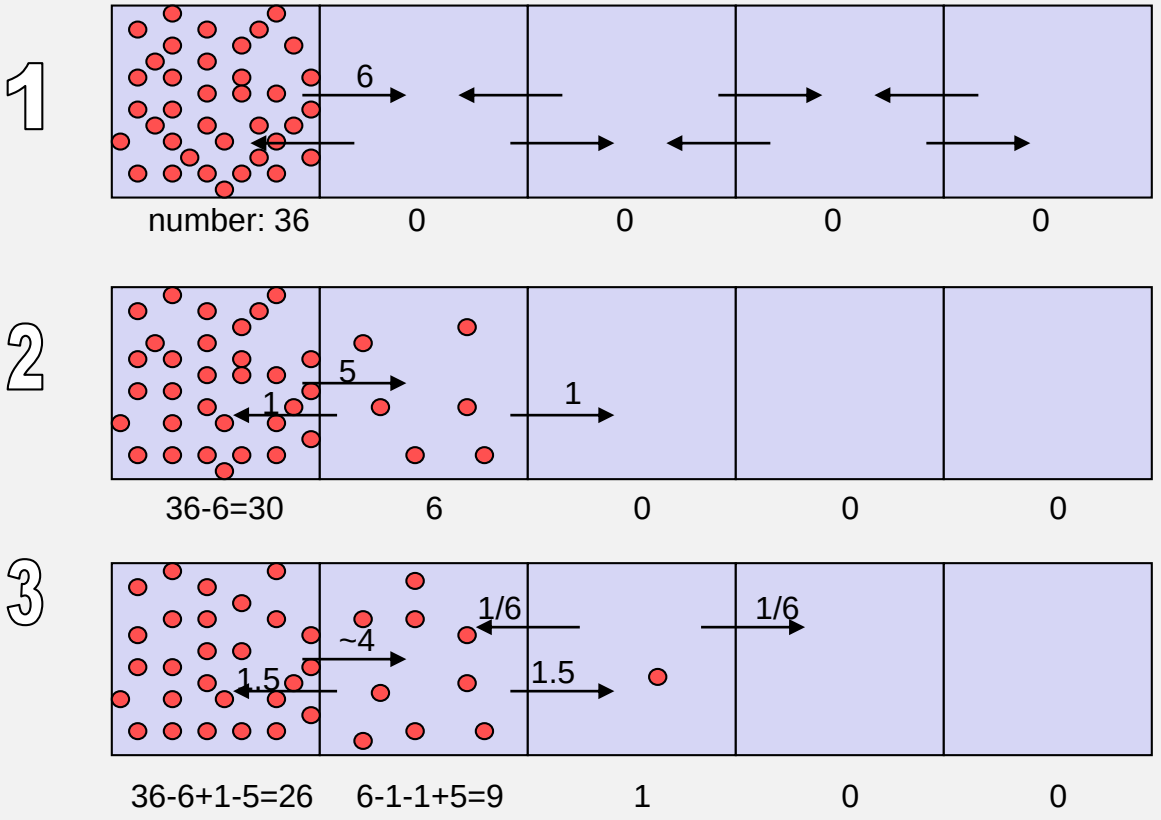
This is a **transport equation**, since it describes how a quantity (particles) is transported.

The Classical Gas Model: Diffusion

Diffusion is a fundamental equalization process driven by temperature

Process:

With each step about 1/6. of the atoms try to escape out of the units cubes in the axis directions (± x, ± y, ± z)



□□□□□□ and so on

Description

$$j = -D \cdot \frac{dn}{dx}$$

1st law
(in one dimension)

The particle current j is proportional to the particle gradient dn/dx with the **diffusion coefficient D**

$$\frac{dN}{dt} = -\frac{dj}{dx}$$

2nd law
(in one dimension)

The change of number N of particles with time dt is due to the change of flux dj with location dx

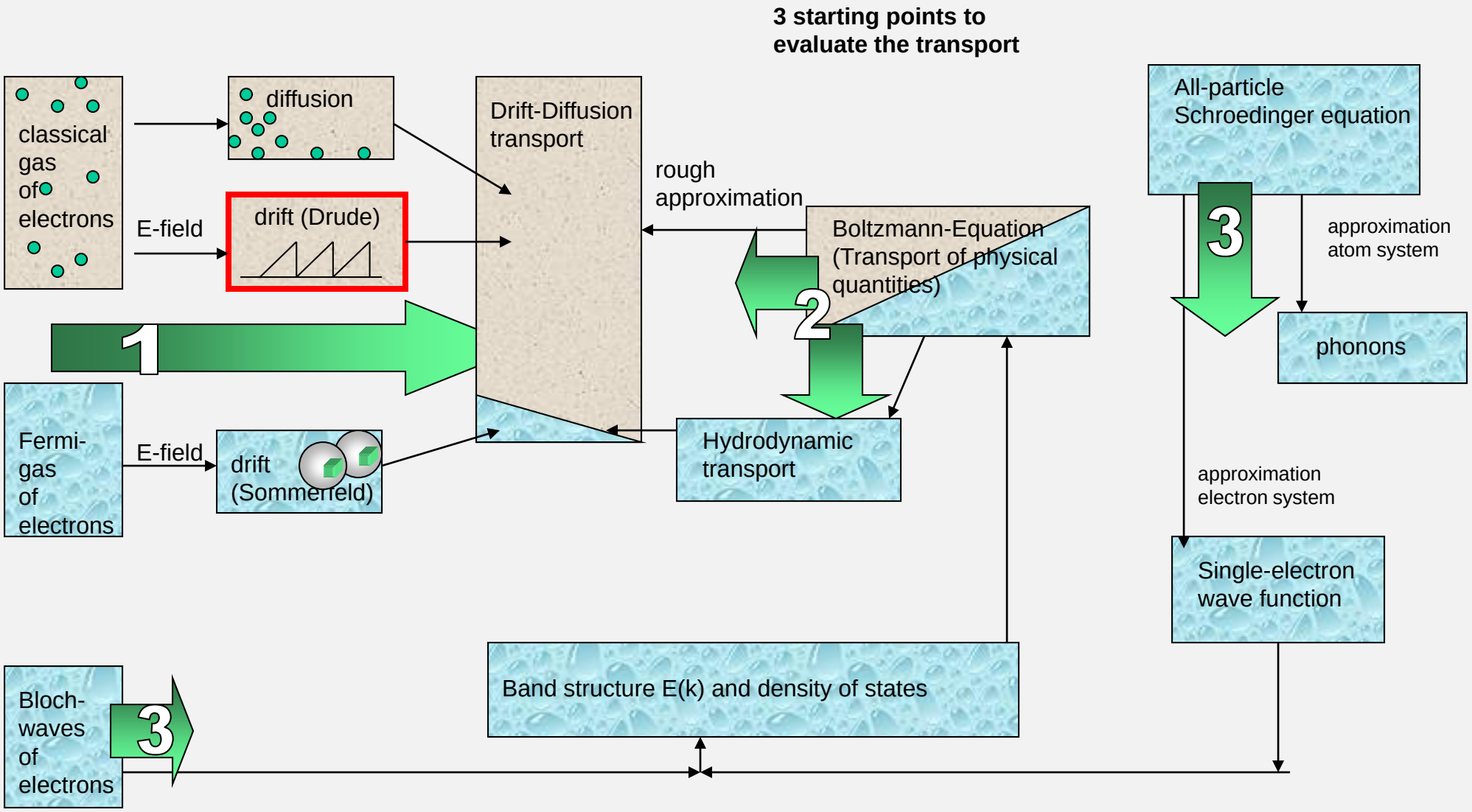
$$\frac{dN}{dt} = D \cdot \frac{d^2N}{dx^2}$$

see page 5.6

Equation of diffusion

$$D = D_0 \cdot \exp\left[-\frac{Q}{kT}\right]$$

Charge Transport Models



The Drude Model of Drift Conduction

~1800: Volta realizes a first electrochemical battery

1826: Ohm discovers that the voltage drop in a metallic wire is proportional the flowing current: $\vec{E} = \rho_R \cdot \vec{j}$ or: $\vec{j} = \sigma \cdot \vec{E}$

1865: Maxwell equations for electromagnetic current transport

current density $\vec{j} = \rho_n \cdot \vec{v}$ continuity equation: $div\ j = -\dot{\rho}_n$

or stationary: $\vec{j} = q \cdot n \cdot \vec{v}$

1895: discovery of the electron as charge carrier

1900: Drude-Model of current transport in a solid:

Assumption: 1) Electrons are treated as charged, classical particles

2) Movement according a classical gas

"classical" electron gas

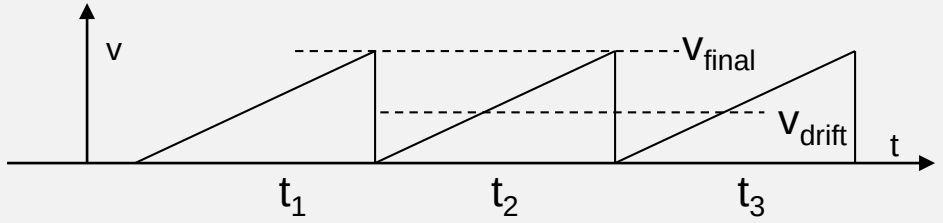
3) Electrons are accelerated by an Electric Field

$$\vec{F} = m \cdot \vec{a} = m \cdot \frac{d\vec{v}}{dt} = -e \cdot \vec{E} \Rightarrow \vec{v}_{final} = -\frac{e \cdot \vec{E} \cdot t}{m}$$

the final velocity after acceleration in the field E for a time t

Drude: 4) the accelearation time corresponds to the meanfree path time τ_λ between two collisions

5) in collisions the field-induced velocity is destroyed



a constant, average speed is the result

$$\vec{v}_{drift} = -\frac{e \cdot \tau_\lambda}{2m} \cdot \vec{E} = \mu \cdot \vec{E}$$

If a particle loses in a collision all its energy gained from an accelerating field, the resulting macroscopic movement is called **drift**. Drift results in a linear dependence of velocity from the electric field. The proportional constant is called **mobility μ.**

The Drude Model of Drift Conduction

Some numbers from Drude Model:

1) from Hall measurements

⇒ every atom in a metal contributes with approximately one free electron per atom for electric transport

$$n_e \approx 10^{22}\,cm^{-3}$$

2) from continuity equation a theoretical value for the **conductivity σ** can be derived:

$$\vec{j} = \rho_q \cdot \vec{v} = e \cdot n \cdot \frac{e\tau_\lambda}{m} \cdot \vec{E} = \sigma \cdot \vec{E}$$

3) from electrical measurements the **specific electrical resistance** of metals is around:

$$\rho_R \approx 5\mu\Omega \cdot cm$$

Using: $\sigma = \frac{1}{\rho_R}$ the mean **inter-collision time τ_λ** can be calculated to around:
(because all other numbers like n, e, m and σ are known)

$$\tau_\lambda \approx 10^{-13}\,\text{sec}$$

4) the **thermal velocity** was calculated in the Gas Model to

$$v_p = \sqrt{\frac{2kT}{m}} = 5.5 \cdot 10^5 \cdot \sqrt{T[K]} \quad [cm/\text{sec}]$$

at 300 K room temperature:

$$v_{th} = \sqrt{\frac{2kT}{m}} = 5.5 \cdot 10^5 \cdot \sqrt{300[K]} = 9.5 \cdot 10^6 \ [\text{cm/sec}] \approx 10^7\,\text{cm/sec}$$

$$v_{th} \approx 10^7\,cm/\text{sec}$$

5) Estimating: $v_{th} \approx \frac{\lambda}{\tau_\lambda}$ **mean free path λ** can be calculated:

$$\lambda \approx 10^{-6}\,\text{cm} \approx 10\text{nm}$$

6) with common current densities of ~A/mm² the resulting **drift velocity** can be calculated with the help of the continuity equation to

$$v_{drift} \approx 10^{-2}\,\text{cm/sec}$$

It is reasonable, that this small v_{drift} will be lost in a collision compared to $v_{th} \sim 10^7$ cm/sec

The Drude Model

Some values for various materials:

Metals

Metall	T [K]	σ [10^{-5} / (Ωcm)]	τ [10^{-14} sec]	λ [nm]	μ [cm²/(Vsec)]
Li	273	1.18	0.85	11	15
Na	273	2.34	3.1	35	55
Al	273	4.0	0.80	17	14
Ag	273	6.6	4.1	57	72
Au	273	4.9	2.9	41	51
Cu	273	6.5	2.7	42	48

from: Hellwege: Einführung in die Festkörperphysik", Springer, 3.Auflage, 1988

Semiconductors

	Ge	Si	GaAs	InSb	InP
Band gap E_g (eV)	**0.66**	1.12	1.42	0.17	1.35
Hole mobility μ_h (cm²/Vs)	**1900**	450	400	1250	150
Electron mobility μ_e (cm²/Vs)	**3900**	1500	8500	80000	4600

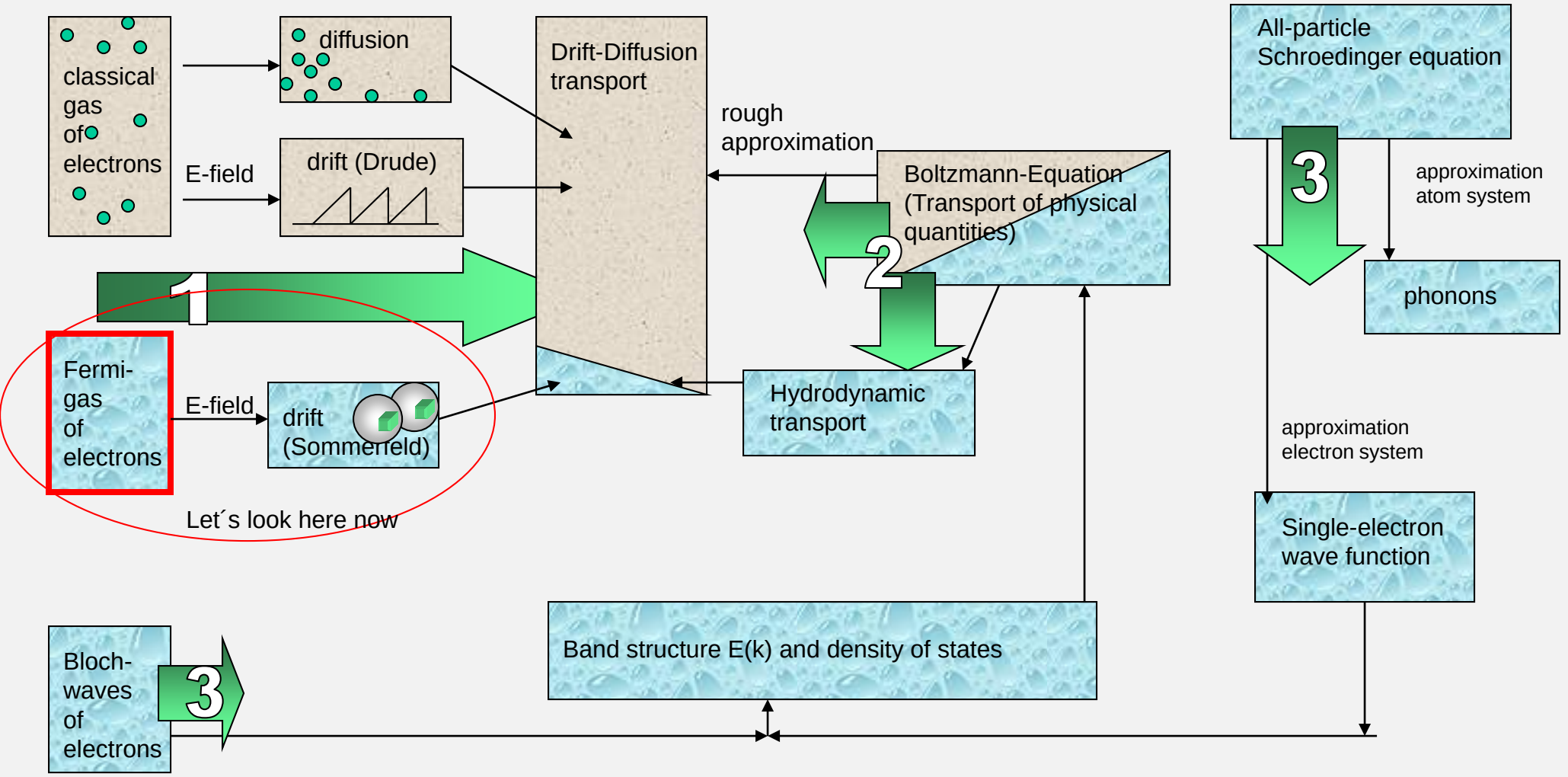
very low mobilities 10-100 cm²/(Vsec)
compared to
semiconductors 1000 - 100´000 cm²/(Vsec)

Remember:

we need number n of electrons and their velocity v to calculate the current in a semiconductor device:

$$\vec{j} = n \cdot e \cdot \vec{v}$$

Charge Transport Models



The Fermi Gas Model

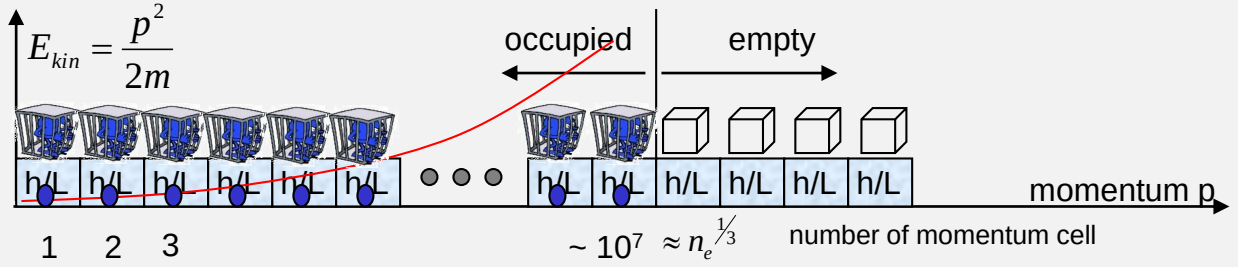
1 From mechanics we know: Free electrons will move according: $\vec{F} = \frac{d\vec{p}}{dt}$ and with energy $E_{kin} = \frac{p^2}{2m}$

2 **Classical particles** never can be on the same location, but may have identical energies (momentum) -> see Maxwell distribution
Quantum-mechanical particles (as superposition of planar waves) are in principle on every location present, but can never have the same energy (momentum)

If qm-electrons are localized in a crystal with dimension $\Delta x = L$, then every single electron must have:
- a different value of energy (momentum p)
- and a uncertainty of momentum Δp: $\Delta p = \frac{h}{\Delta x} = \frac{h}{L}$ which is the same for all electrons

3 All these different values of momentum p and size Δp create the **momentum space**:

-> in one coordinate:



Without any external energy (temperature, electric fields) the electrons must occupy the states of minimum energy.
But because every electron must have a different momentum, the momentum cells are filled from zero to the last electron.

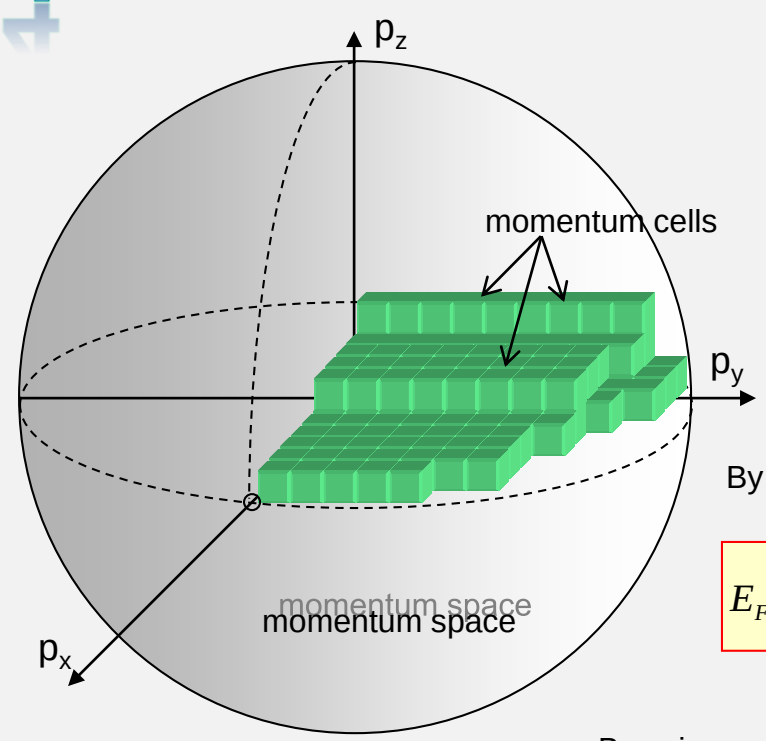
The highest occupied momentum value is called **Fermi-momentum** p_F or k_F
the corresponding energy is called **Fermi-energy** E_F

for the next relations we will use the transformation of particle momentum p to wavevector k : $\vec{p} = \hbar\vec{k}$ $\hbar = \frac{h}{2\pi}$

The Fermi Gas Model

4

-> in 3 coordinates p_x, p_y, p_z, the energy represents a sphere of radius p:



N electrons can occupy N/2 momentum cells 2, because of electron spin

The volume of all these cells is: $V_p = \frac{N}{2} \cdot \frac{h^3}{L^3} = \frac{h^3}{2} \cdot n_e$ just summed up

All these cells fill the Fermi sphere: $V_p = \frac{4}{3}\pi\, p_F^3$ geometry of a sphere

From both we can calculate: $k_F = \left(3\pi^2 \cdot n\right)^{1/3} \rightarrow k_F[cm] \approx 3.1 \cdot n^{1/3}[cm^{-3}]$

Fermi momentum

By using free electron energy $E=p^2/2m$ $\quad E_F = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

$$E_F = \frac{\hbar^2}{2m} \cdot \left(3\pi^2 \cdot n\right)^{2/3} \longrightarrow E_F[eV] \approx 3.65 \cdot 10^{-15} \cdot n^{2/3}[cm^{-3}]$$

Fermi energy

By using v=p/m we can calculate the velocity of the particle with highest momentum: $v_F = \frac{\hbar k_F}{m}$

To get a feeling for temperatures we do analogous to a classical gas: $1/2mv^2=3/2kT$

a **Fermi temperature T_F** in a qm-gas: $E_F = k_B T_F \longrightarrow T[eV] = \frac{T[K]}{11600}$

The material dependence of all Fermi values is only in electron density n

calculations can be done easy by using: hc = 1240 eV*nm and electron mass mc^2= 511 keV

The Fermi Gas Model

Assumptions from classical mechanics:

1) electrons are very small particles

2) collisions are short in time and space

3) collisions are independent

4) collisions change the direction of movement random

5) the movement of every particle is independent from other particles

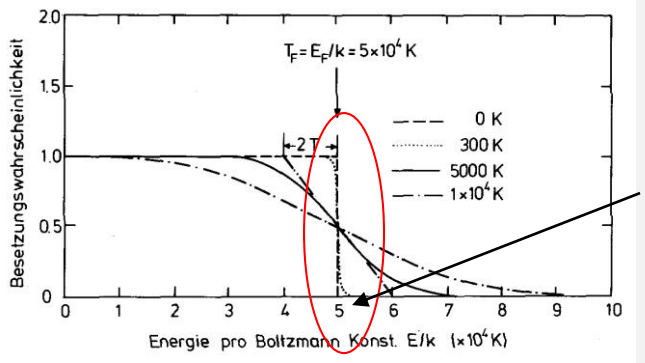
but now quantum mechanics:

6) electrons are Fermi particles -> the Pauli principle must be observed :

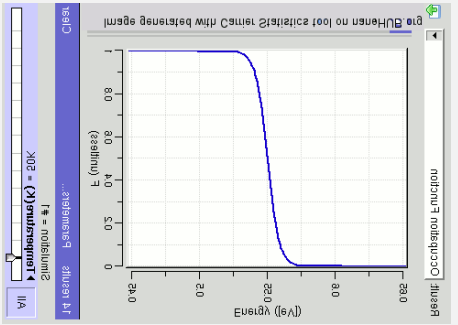
only two electrons (with different spin quantum number) are allowed to have the same energy

the energy distribution function must be modified:

Boltzmann statistics: $f(E) = N(E)/N_0 \propto \exp[-\frac{E}{kT}]$ changes to: **Fermi statistics** $f(E,T) = \frac{1}{\exp\left[\frac{E-E_F}{kT}\right]+1}$



the average energy of
Fermi electrons is about
5 times higher as calculated
by classical Maxwell distribution

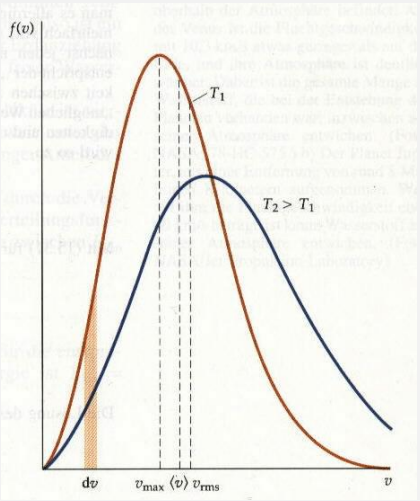


The Fermi Gas Model

1) velocity of electrons in a Maxwell-Boltzmann gas

$$f(v) = \sqrt{\frac{2}{\pi}} \cdot \left(\frac{m}{kT}\right)^{3/2} \cdot v^2 \cdot \exp\left[-\frac{\frac{1}{2}mv^2}{kT}\right]$$

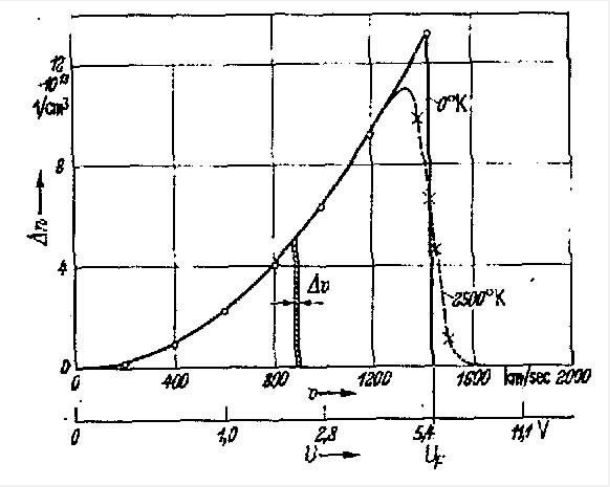
electrons are handled as **classical** particles



2) velocity of electrons in a Fermi gas

$$f(v) = 3\left(\frac{kT}{E_F}\right)^{3/2} \cdot \frac{v^2 / v_{p,\max\ well}^3}{1 + \exp\left[\left(\frac{v}{v_{p,\max\ well}}\right)^2 - \frac{E_F}{kT}\right]}$$

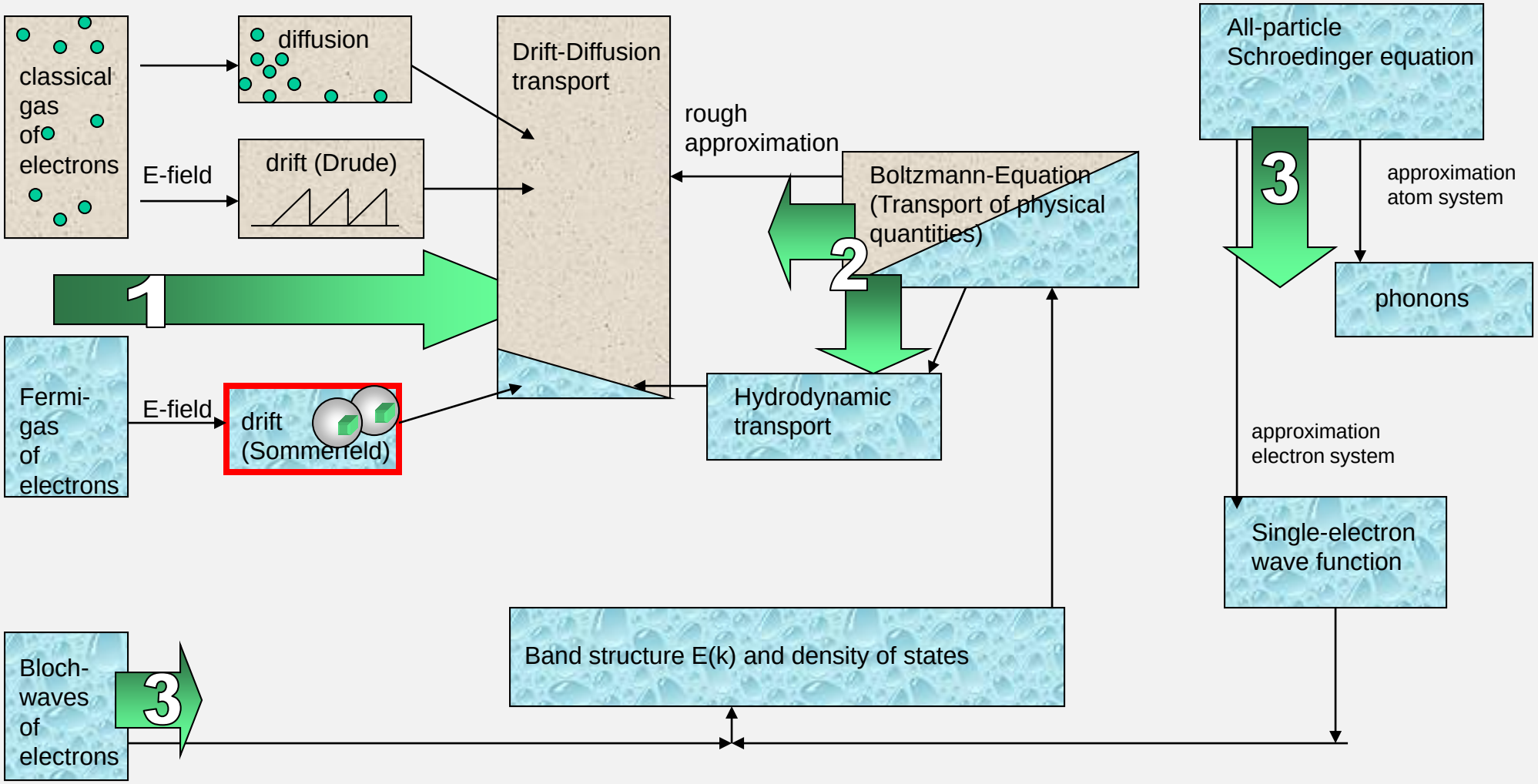
electrons are handled as **quantum-mechanical** particles



Remember:

we need number n of electrons and their velocity v to calculate the current in a semiconductor device: $\vec{j} = n \cdot e \cdot \vec{v}$

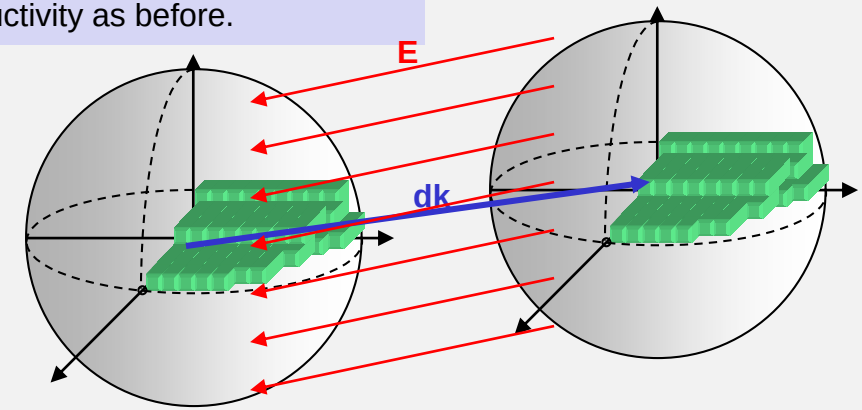
Charge Transport Models



The Sommerfeld Conduction Model

When deriving the Drude conductivity of metals we noted that the derivation is inappropriate for metals, because it does not take the Pauli principle and the Fermi energy into account.
Sommerfeld recognized this early on and proposed a different model which does take account of the quantum mechanics and the Pauli principle.
Surprisingly enough, we we obtain finally the same expression for the conductivity as before.

Starting point: All electrons are sited in the Fermi sphere

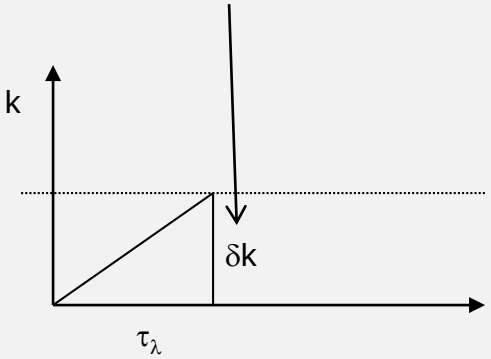


An external electric field E will act a force F to all electrons: $\vec{F} = q\vec{E}$

which will change the momentum k of all electrons: $F = p = \frac{dp}{dt} = \frac{\hbar dk}{dt}$

In the electric field the whole Fermi sphere will move away by dk in the time dt

If we assume, that after a time τ_λ a scattering event to all electrons will completely throw back the Fremi sphere, a maximum change in momentum δk is reachable:



$$\vec{F} = \frac{\hbar d\vec{k}}{dt} = q\vec{E} \longrightarrow \delta\vec{k} = \frac{q\vec{E}}{\hbar}\cdot\tau$$

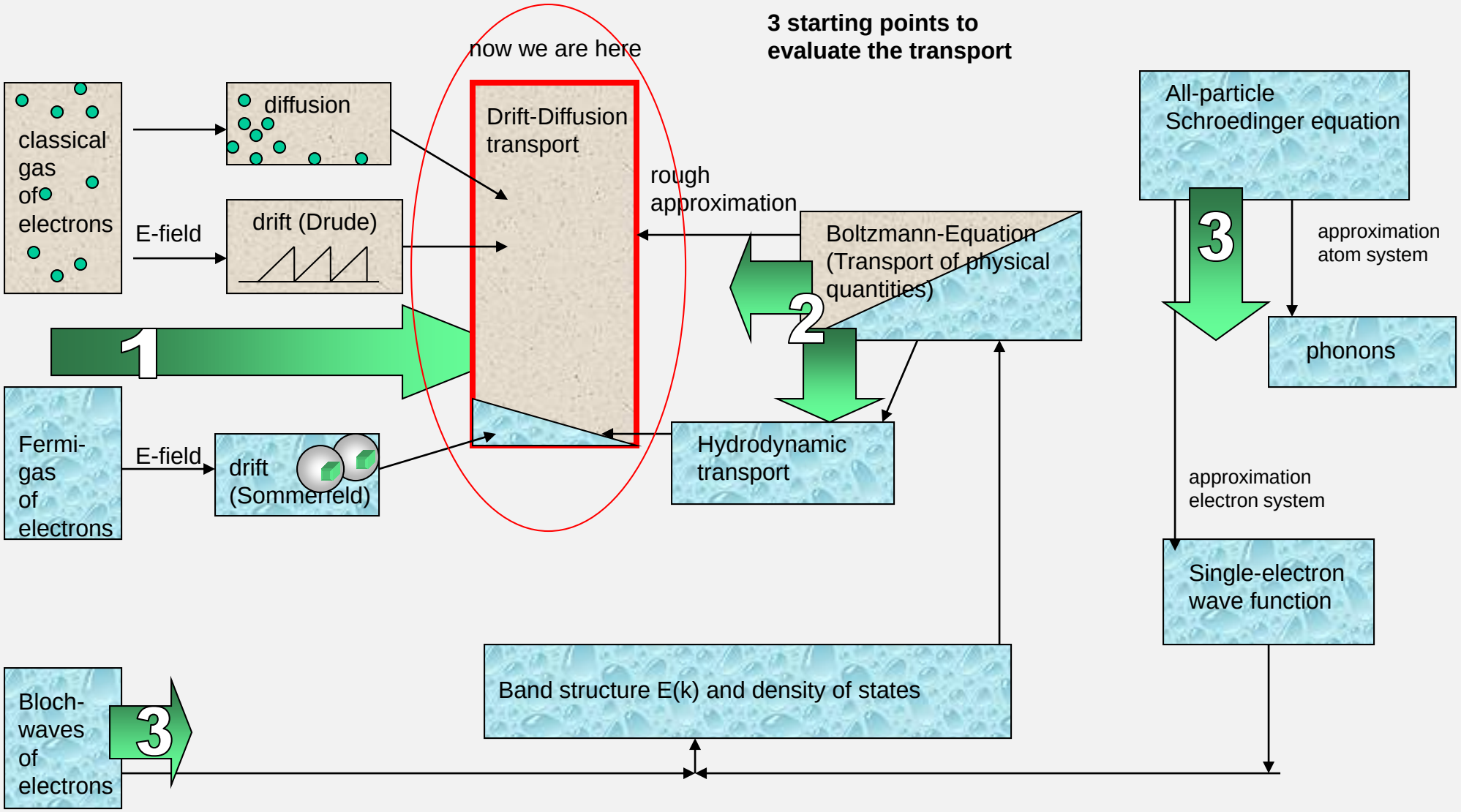
But this back momentum can only be carried by a fraction N_{FS} of electrons at the Fermi surface moving with Fermi velocity/momentum:

$$\frac{N_{FS}}{N} = \frac{\delta k}{k_F}$$

$$j = N_{FS}\cdot q\cdot v_F = N\cdot\frac{\delta k}{k_F}\cdot q v_F = Nq^2\tau\frac{v_F}{\hbar k_F}\vec{E} \xrightarrow{mv_F=\hbar k_F} \frac{Nq^2\tau}{m}\vec{E}$$

Finally the same conductivity as derived by the Drude model results

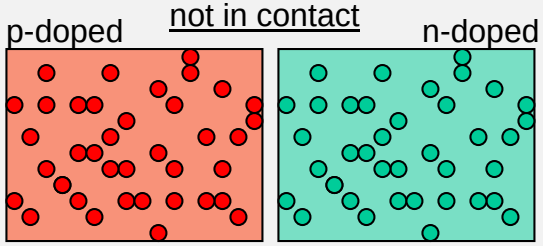
Charge Transport Models

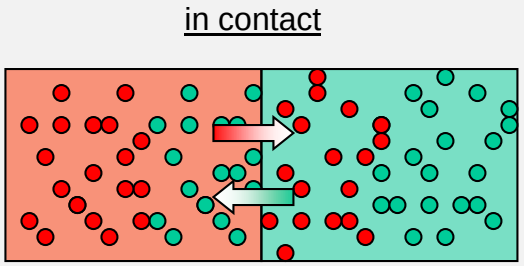


The Drift-Diffusion Model

In semiconductors we can observe: for example a pn-junction

1 Diffusion:





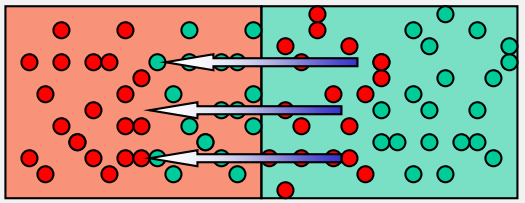
electrons diffuse into electron free p-region

holes diffuse into hole free n-region

density n_p of electrons in p-region: $n_p = \frac{n_i^2}{N_A}$

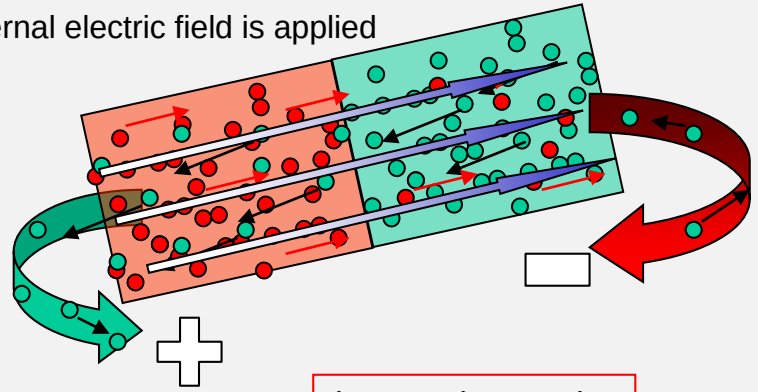
density p_n of holes in n-region: $p_n = \frac{n_i^2}{N_D}$

2 Drift:



Diffusion is stopped, because an internal electric field is created, which moves back the diffused carriers

if an external electric field is applied



The sum of all currents (averaged in time) will be:

$$j_{total} = j_{drift} + j_{diff} = 0$$

$$j_{total} = j_{drift} + j_{diff}$$

The Drift-Diffusion Model

We introduce the:

Drift-Diffusion-Equation DDE

$$\vec{j}_{total} = \vec{j}_{drift} + \vec{j}_{diff} = q\mu \cdot n(x)\vec{E}(x) + qD \cdot \frac{\partial n(x)}{\partial x}$$

$$\vec{j}_{total} = \vec{j}_{drift} + \vec{j}_{diff} = q\mu \cdot n(x)\vec{E}(x) + q\mu \cdot \frac{kT}{q} \cdot \frac{\partial n(x)}{\partial x}$$

using the Einstein Relationship:

$$D = \mu \cdot \frac{kT}{q}$$

For the calculation of the current j in a device, we need:

charge of carrier: q= ± e
mobility μ: in first approximation taken as a constant, but also dependent on the electric field E

locally varying number of charge carriers: n(x)
locally varying Electric Field: E(x)

This DDE has been solved analytically in many 1-dim problems (pn-junctions in diodes, bipolar transistors, MOSFETs,..), if the various regions in the device and the boundary conditions are described correctly.

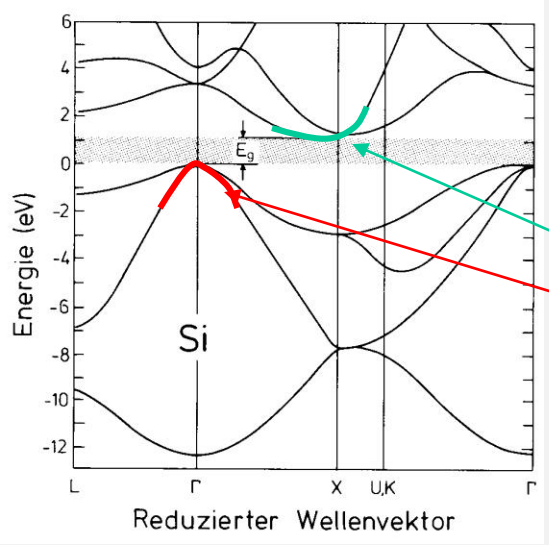
With increased computational power the DDE is solved numerically, especially for 2-dim or 3-dim structures

! If problems can be solved by analytical methods an insight in physical effects and an "universal" solution is the result
! A numerical solution will always give a result, but the solution is restricted to the special problem and physics is covered.

Solving the Drift-Diffusion Model

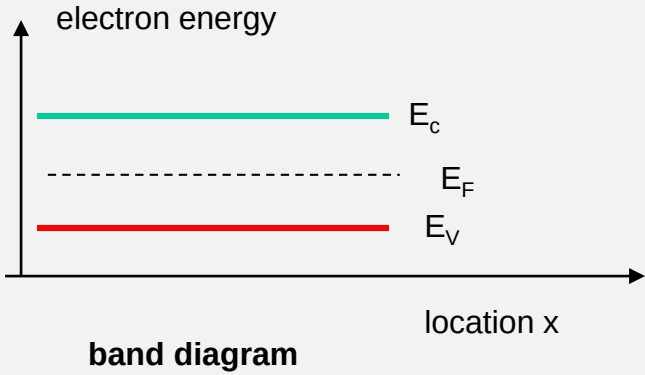
In a semiconductor (silicon) the **bandstructure** looks:

1



transformation
from momentum to space

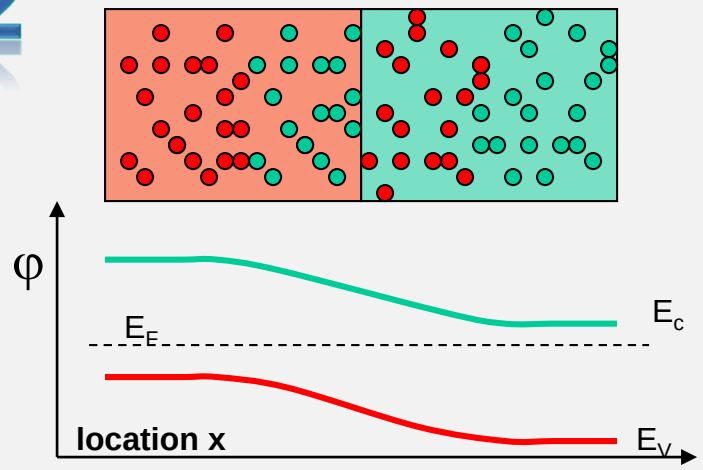
simplified, because electrons and holes are localized
within the minimum of conduction band
or maximum of valence band



band diagram

2

By doping the Fermi-level will be locally changed, in contact the Fermi-level must be equalized (see chap.3)



The local variation of the bands and potentials is calculated by the:

Poisson equation

$$\nabla\vec{E} = -\nabla^2\varphi = \frac{\rho_{charges}}{\varepsilon_0\varepsilon_{Si}} = \frac{q}{\varepsilon_0\varepsilon_{Si}}\cdot\left[p(x) - n(x) + N_D^+(x) - N_A^-(x)\right]$$

mobile charges

fixed and charged doping atoms

Example: Simple Calculation for *p-n* Junction

Mother of all band calculations:

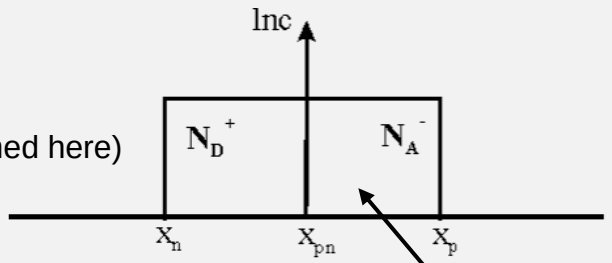
Solve the **Poisson-Equation**

$$\frac{d^2\Phi}{dx^2} = -\frac{\rho_c(x)}{\varepsilon_0 \varepsilon_r}$$

the local bending of potential is dependent on local charge distribution

Charge Density

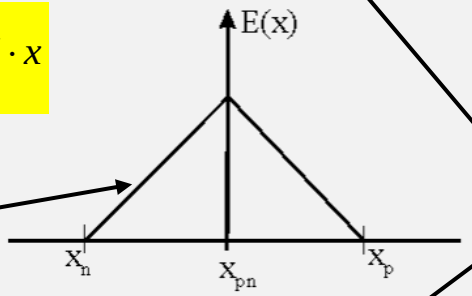
(abrupt, constant doping assumed here)



Electric Field

1. integration: $\frac{d\Phi}{dx} = \int -\frac{N_x}{\varepsilon_0 \varepsilon_{Si}} dx \propto N \cdot x$

Because: $\frac{d\Phi}{dx} = \vec{E}$

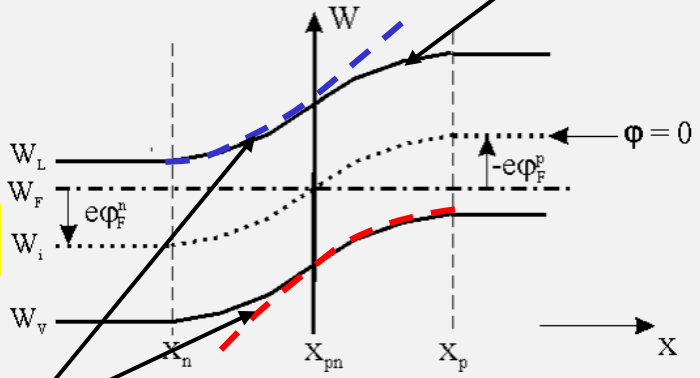


$$\rightarrow \quad \vec{E} \propto N \cdot \vec{x}$$

Potential

2. integration: $\frac{d\Phi}{dx} \propto N \cdot x$

$$\Phi = \int \vec{E} dx = \int (N \cdot x) dx \propto N \cdot x^2$$



$$\Phi \propto N \cdot x^2$$

$$\Rightarrow \quad W = q\Phi \propto N \cdot x^2$$ parabolic

Depletion Approximation:

no free carriers n,p => depletion,
the charge distribution is determined by doping atoms N_D^+ and N_A^-

Solving the Drift-Diffusion Model

3

From solving the Poisson equation we get the local variation of the electric Field E, the potential φ and the local mobile carrier distribution n(x), p(x)

This we introduce into the **drift-diffusion equation (DDE)**:

$$\vec{j}_{total} = \vec{j}_{drift} + \vec{j}_{diff} = q\mu\left(n(x)\vec{E}(x) + \frac{kT}{q}\frac{\partial n(x)}{\partial x} \right)$$

4A

This DDE has been solved **analytically** in many 1-dim problems (pn-junctions in diodes, bipolar transistors, MOSFETs,..), if the various regions in the device and the boundary conditions are described correctly.

4B

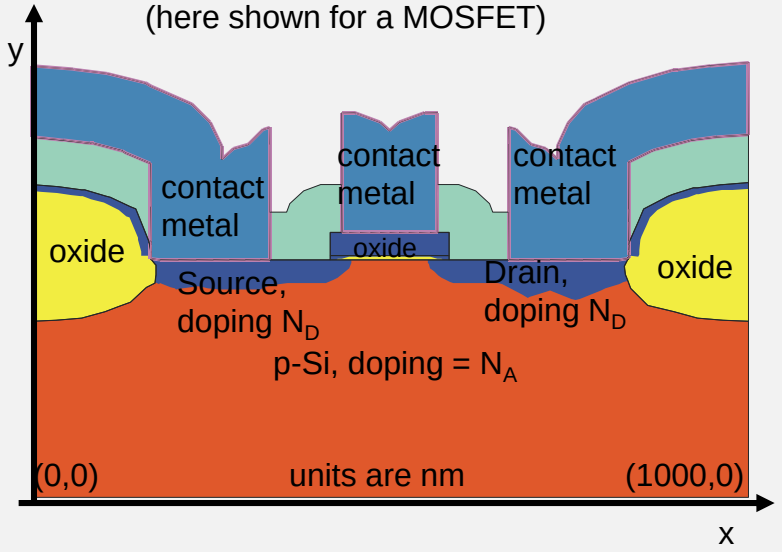
With increased computational power the DDE is solved **numerically**, especially for 2-dim or 3-dim structures

! If problems can be solved by analytical methods an insight in physical effects and an "universal" solution is the result
! A numerical solution will always give a result, but the solution is restricted to the special problem and physics is covered.

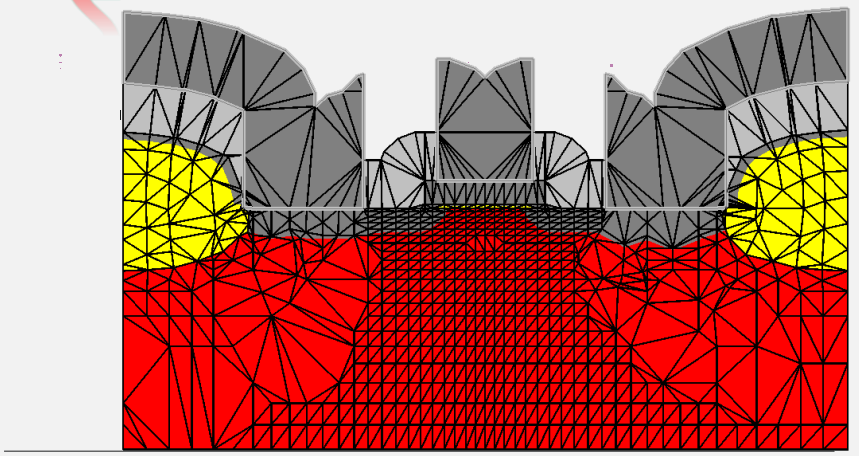
Drift-Diffusion Equation: - Numerical Solution

On computers several "simulation" software was developed. The procedure is always the same:

1 Put in geometry with materials and doping (here shown for a MOSFET)



2 Put a mesh on the structure



3 Solve Poisson equation numerically

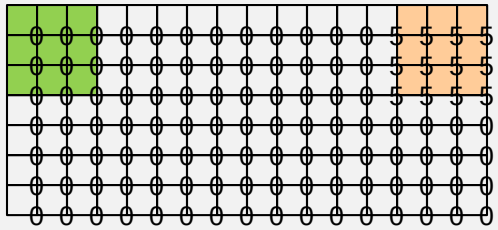
Here we use a trick:

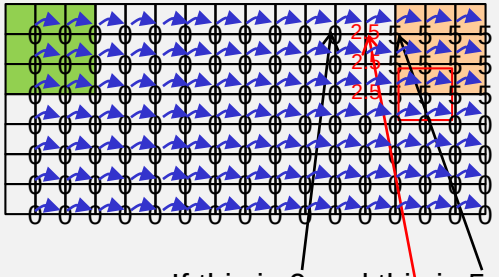
1. Put on every mesh point the information of doping N(x) and potential $\varphi(x)$ (=zero, with exception of contacts)
2. Then we investigate every mesh point for its potential value: we are looking one mesh point behind and one mesh point ahead and then put the mesh point potential value just in the middle of both.
   Then we step ahead for one mesh point, doing the same procedure. We proceed until we have set every mesh point on a new potential value. This is the first iteration.
3. Then we start again on the first mesh point, repeating the whole procedure is given above. All values will change a little. This is the second iteration
4. Do so many iterations until nothing changes anymore.

Drift-Diffusion Equation: - Numerical Solution

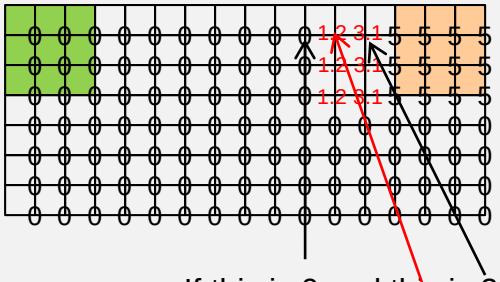
Source
(grounded)

Drain
(at +5V)



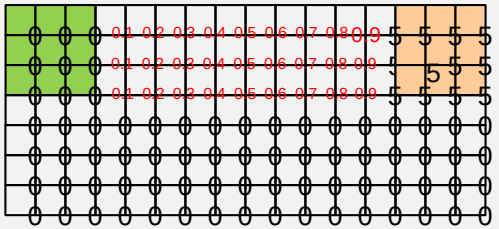


If this is 0 and this is 5,
then this must be 2.5



If this is 0 and this is 2.5,
then this must be 1.25

after many iterations:



we have a potential value on every mesh point x

Hey

we have solved the Poisson equation

In addition:
at every mesh point we have the local potential, so taking two mesh points with their potential value and their coordinates:

Hey

we can calculate the Electric Field E at every mesh point

Drift-Diffusion Equation: - Numerical Solution

4 Next step:
in the simulator physical models must be switched on, what the charge carriers can do at every meshpoint

Basics: movement by drift due to an electric field -> check, if the values of the parameters (e.g. mobility) in the simulator model are ok
(in addition, depending on the physical possibilities usually various mobility models can be chosen, with various parameters)

movement by diffusion due to carrier concentration gradients -> check models, check parameters

additional effects may be: hot electrons, impact ionization, tunneling, ... -> check models and parameters

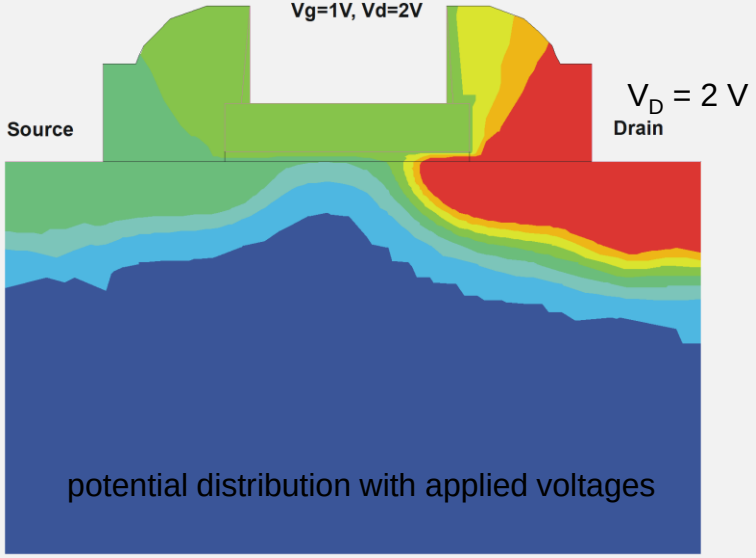
Without any physical background, what may happen in the charge carrier transport, the simulated result may be completely wrong !

5 Next step:
Choose an other external voltages and repeat step 3 and 4

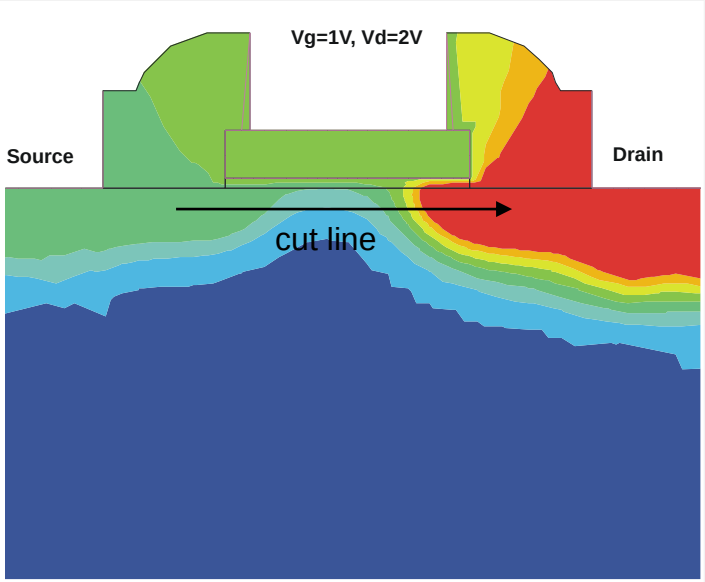
1. repeat step (3) = again solving Poisson-equation,
   using equilibrium solution as a start, with applied voltages

It is always a good idea to change voltages not in large steps
-> convergence problems may occure

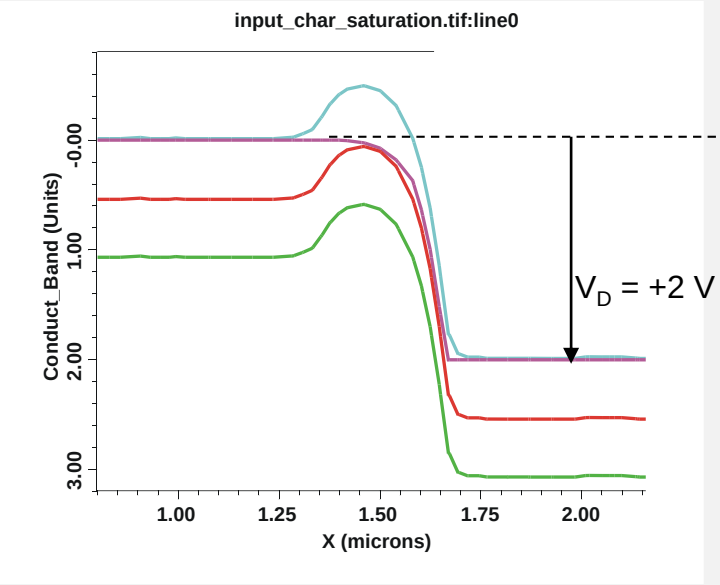
2. Using electric fields and charge distribution the transport equation is solved iterative at each mesh point, again and again,
until nothing changes anymore



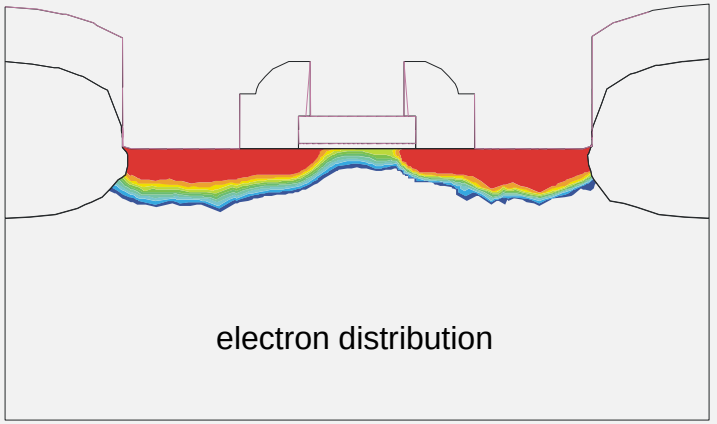
Drift-Diffusion Equation: - Numerical Solution

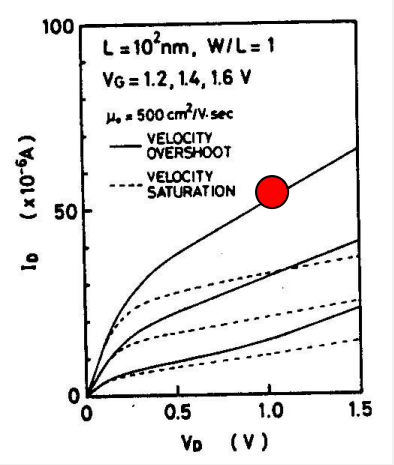


potential distribution with applied voltages



cut line of band diagram under the gate





with each set of applied voltages
one point of IV-characteristics
is found.

6 repeat step (5) with next set of voltages

complete IV-characteristics

Summary of the Drift-Diffusion Model

Drift-diffusion assumptions

* electrons are classical particles
* electrons move like free gas particles
  -> Boltzmann statistics is used -> Maxwell distribution of energy
* equations used are:
  - Maxwell equations, especially Poisson equation
  - continuity equation
  - transport equation = drift + diffusion
    (-> restriction on two phenomenological laws !)

We have to solve:
5 partial differential equations (Maxwell 4 + continuity equation)
+ 1 algebraic transport equation
with 6 field-dependent parameters

Drift diffusion results

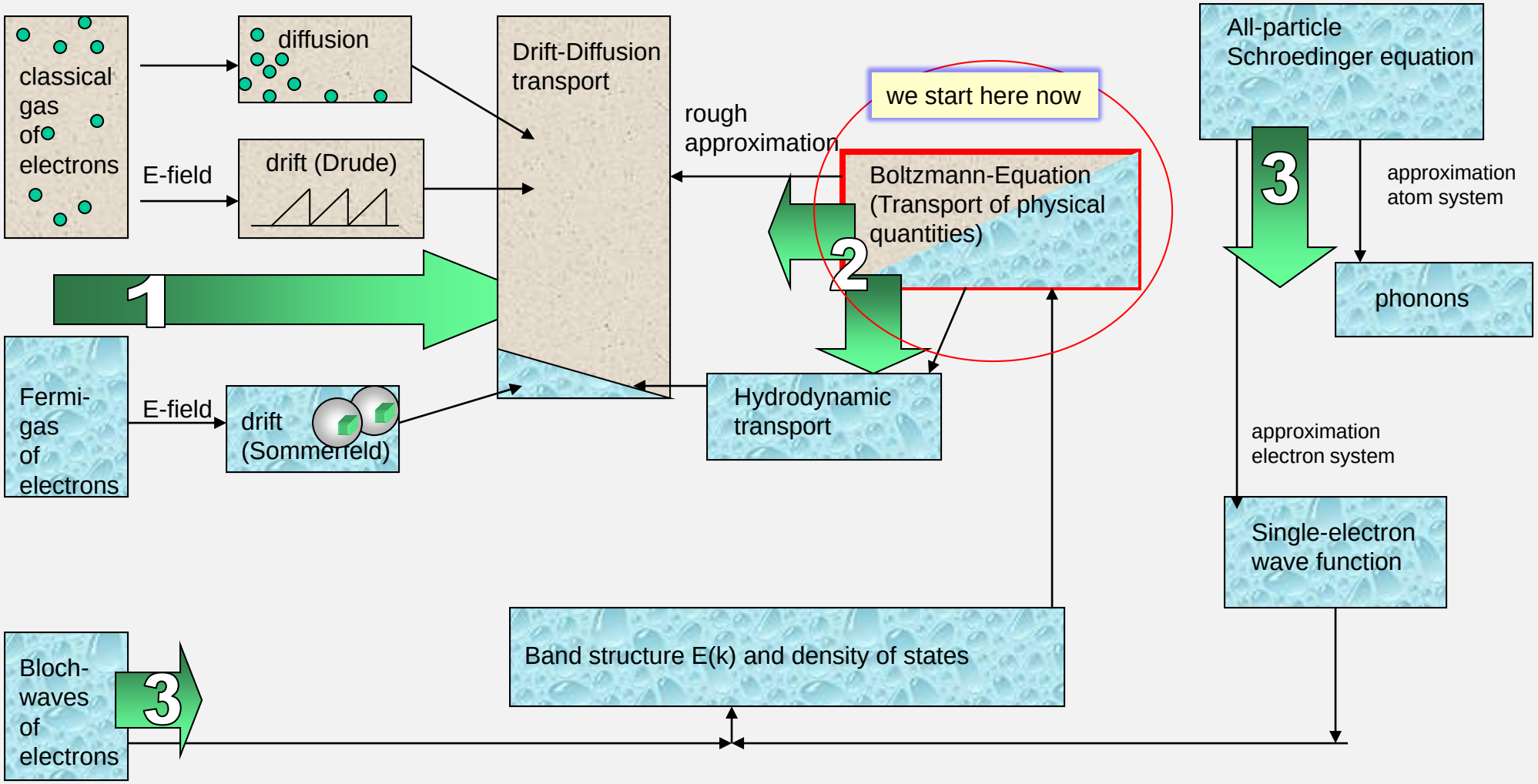
* electrons are always at equilibrium
  -> unchanged Maxwell distribution all the time
  -> velocity saturation
  -> no description of transport, when changes of potentials or electric fields are large between collisions
* no interaction of electrons, no interaction with lattice
  -> no **heating of electrons and lattice**
  -> no **impact ionization**
  -> no **tunneling**

Although these not-included effects can be described by phenomenological equations, a general description of transport (= calculating IV-characteristics) is not possible.

→ other approach:
Try to find a general description of transport

→ Boltzmann Equation

Charge Transport Models



The Boltzmann Transport Equation (BTE)

In the model of the classical gas two phenomena (particle transport by diffusion and drift) could be described by phenomenological laws.
But transportation of heat or other quantities was missing.
In 1867 Boltzmann derivated a unique theoretical equation to describe transport phenomena (based on several assumptions) on a statistical basis.

Transport is a macroscopic phenomena, where many particles are involved

way 1: describe the movement of every single particle, then do statistics to find distributions

but: the problem of movement of more than 2 particles can not be solved analytically

→ in days of high performance computers this way is used by so-called "**Monte-Carlo**" methods

way 2: We first assume a statistics and a connected distribution

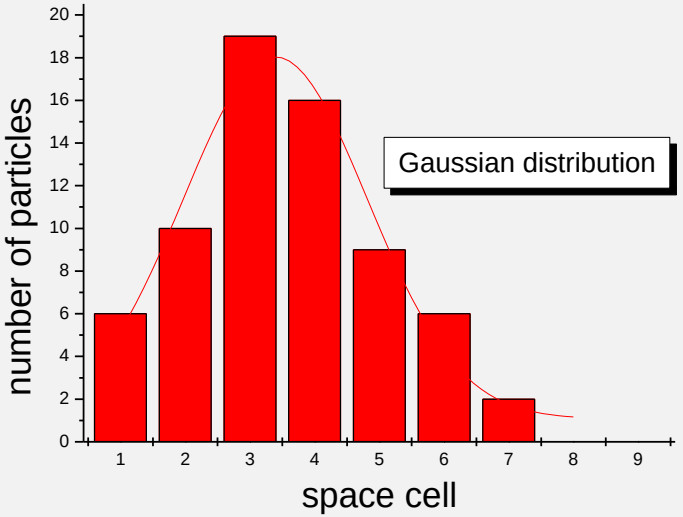
we describe the change of the distribution

→ historical and analytically approach -> **Boltzmann Transport Equation (BTE)**

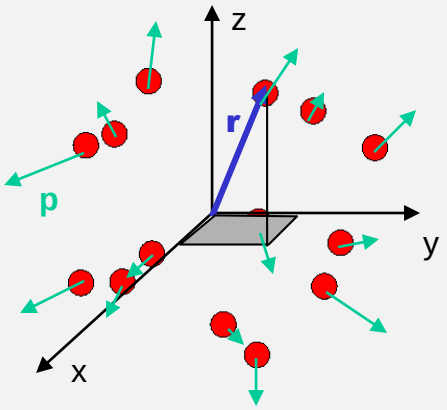
Several ways exist to derivate the BTE.

⟶ We will do a heuristic derivation for classical particles and then modify it for electrons in band structures

Replacement of Particles by Distributions

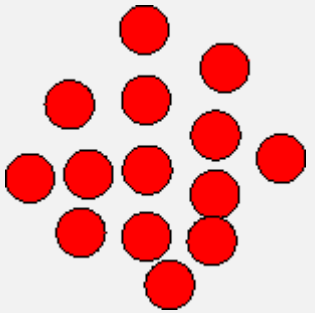


Every particle has a space coordinate r
and a velocity or momentum p



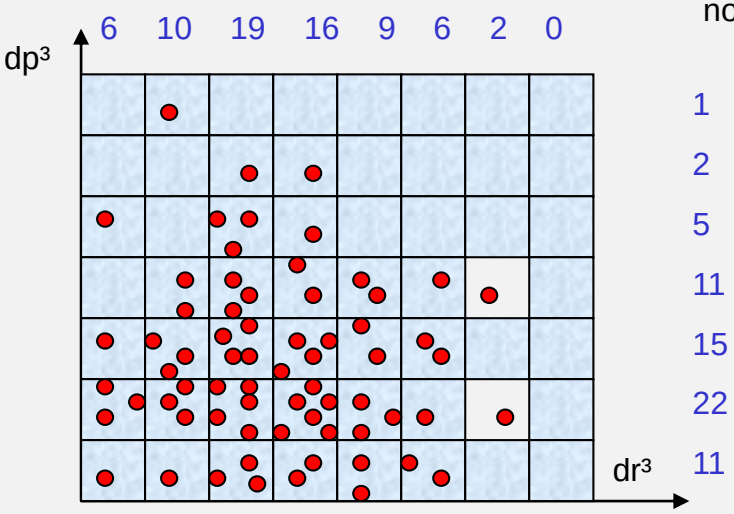
1

we start here



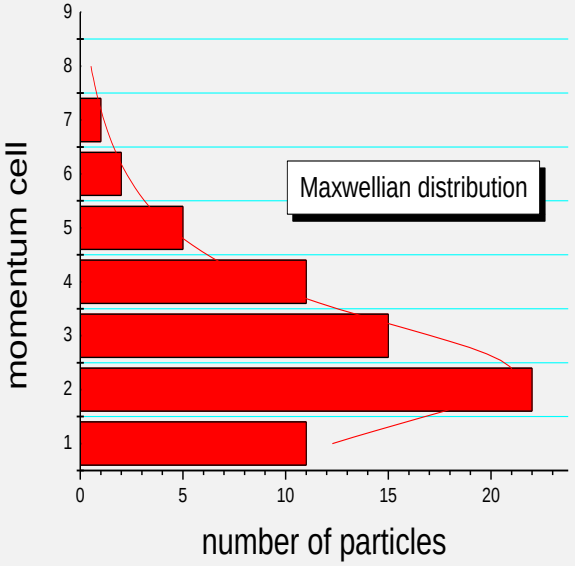
with some given particles

3 projection on space



2 now we sort

3 projection on momentum



Now we can replace the knowledge of all particles by their distributions in space and momentum

Of course we lose single particle information

Finding the Boltzmann Transport Equation (BTE)

Basic mechanics:

A change in location dr = v*dt is the result, if the particle moves with velocity v:

$$r' = r + dr = r + v \cdot dt = r + \frac{p}{m} \cdot dt$$

A change in momentum dp = F*dt is the result, if an external force F acts on the particle:

$$p' = p + dp = p + \vec{F} \cdot dt$$

Basic statistics:

At a time t the actual values of location r and momentum p (=velocity) of all particles are determined and described by a distribution f(r,p,t)

Because the external forces act on all particles also the distribution will change:

As a result the change df of the distribution is:

$$df = f(r', p', t+dt) - f(r, p, t)$$

change = new function - old function

Ansatz:

$$f(r', p', t+dt) = f(r + v \cdot dt,\ p + F \cdot dt,\ t+dt) - \left.\frac{\partial f}{\partial t}\right|_{coll} \cdot dt$$

time of changing

change during time of collision

new function

change of old function due to external forces

we add a collision term, because the final states f(r´,p´) will be emptied by collisions

For small changes dr and dp a series development can be done and for small change of df in dt we receive: (see next page)

$$v \cdot \nabla_r f + F \cdot \nabla_p f + \frac{\partial f}{\partial t} = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

the time-dependent Boltzmann-Transport Equation

in detail: series development of the distribution change

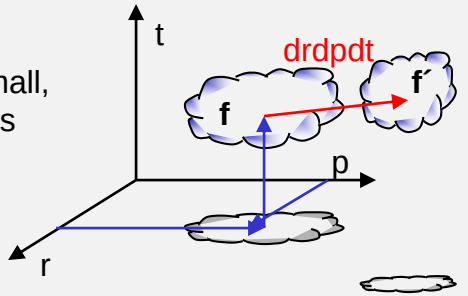
$$f(r',p',t+dt) = f(r+v\cdot dt, p+F\cdot dt, t+dt) - \left.\frac{\partial f}{\partial t}\right|_{coll}\cdot dt$$

$$\approx \left(f(r) + \frac{\partial f}{\partial r}\cdot v dt + \frac{\partial^2 f}{\partial r^2}\cdot (v dt)^2 + ...,\right.$$

$$f(p) + \frac{\partial f}{\partial p}\cdot F dt + \frac{\partial^2 f}{\partial p^2}\cdot (F dt)^2 + ...,$$

$$\left. f(t) + \frac{\partial f}{\partial t}\cdot dt + \frac{\partial^2 f}{\partial t^2}\cdot (dt)^2 + ...\right) \quad - \left.\frac{\partial f}{\partial t}\right|_{coll} dt$$

series development, if df is small, we neglect second order terms



Because v is not dependent on the particles location r and F not dependent on the particles momentum p we can separate starting distribution and development:

$$\approx f(r,p,t) + \frac{\partial f}{\partial r}\cdot v dt + \frac{\partial f}{\partial p}\cdot F dt + \frac{\partial f}{\partial t}\cdot dt - \left.\frac{\partial f}{\partial t}\right|_{coll} dt = f(r,p,t) + \left(v\cdot\frac{\partial f}{\partial r} + F\cdot\frac{\partial f}{\partial p} + \frac{\partial f}{\partial t}\right)dt - \left.\frac{\partial f}{\partial t}\right|_{coll} dt$$

This introduced in:

$$df = f(r',p',t+dt) - f(r,p,t) = f(r,p,t) + \left(\frac{\partial}{\partial r}(f\cdot v) + \frac{\partial}{\partial p}(f\cdot F) + \frac{\partial f}{\partial t}\right)dt - \left.\frac{\partial f}{\partial t}\right|_{coll} dt - f(r,p,t)$$

+f(r,p,t) cancels out with -f(r,p,t), and we do the derivative to dt

$$\frac{df}{dt} = v\cdot\frac{\partial f}{\partial r} + F\cdot\frac{\partial f}{\partial p} + \frac{\partial f}{\partial t} - \left.\frac{\partial f}{\partial t}\right|_{coll} = v\cdot\nabla_r f + F\cdot\nabla_p f + \frac{\partial f}{\partial t} - \left.\frac{\partial f}{\partial t}\right|_{coll} \overset{!}{=} 0$$

if we assume, that the change df is very,very small in dt

$$v\cdot\nabla_r f + F\cdot\nabla_p f + \frac{\partial f}{\partial t} = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

the time-dependent Boltzmann-Transport Equation

see previous page

Finding the Boltzmann Transport Equation

$$\frac{\partial f}{\partial t} = -\left[\vec{v}\cdot\nabla_r f + \vec{F}\cdot\nabla_p f\right] + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

The Boltzmann equation shows:

The particle distribution f changes (= particles change their cell in phase space) due to:

local dependent forces

time-varying forces

internal forces

Depending on the physical problem the forces must be specified

For a stationary problem the change of the distribution is zero:
(this means, the influence of external forces v, F is cancelled out by internal collisions df/dt_{coll}, so with time nothing changes, it is a stationary behavior.)

$$\frac{\partial f}{\partial t} = 0$$

$$\vec{v}\cdot\nabla_r f + \vec{F}\cdot\nabla_p f = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

stationary Boltzmann equation

Although we tried to find a general equation, we did some heavy restrictions:

the change of the distribution (not defined yet) should be very small

How we can handle the BTE ?

Simplification: Boltzmann Transport Equation -> Drift-Diffusion

$$\vec{v}\cdot\nabla_r f + \vec{F}\cdot\nabla_p f = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

we use: $\vec{F} = q\vec{E}$ (only assuming electric forces, no heat, nothing else) and transform p to v using: $\vec{p} = m\vec{v} \rightarrow \frac{1}{p} = \frac{1}{mv} \rightarrow \frac{\partial}{\partial p} = \frac{1}{m}\cdot\frac{\partial}{\partial v}$

$$\vec{v}\cdot\nabla_r f + \frac{qE}{m}\cdot\nabla_v f = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

we use a **relaxation time approach**: $\left.\frac{\partial f}{\partial t}\right|_{coll} = \frac{f_{eq} - f(r,v,t)}{\tau}$ (so we don´t have to integrate over time)

$$\vec{v}\cdot\nabla_r f + \frac{qE}{m}\cdot\nabla_v f = \frac{f_{eq} - f(r,v,t)}{\tau}$$

we multiply both sides with v and integrate over all velocities (which we need to calculate current!)

$$\int v^2\cdot\nabla_r f\,dv + \frac{qE}{m}\cdot\int_{-\infty}^{+\infty} v\cdot\nabla_v f\,dv = \frac{1}{\tau}\cdot\left[\int_{-\infty}^{+\infty} v f_{eq}\,dv - \int_{-\infty}^{+\infty} v f(r,v,t)\,dv\right]$$

$\int_{-\infty}^{+\infty} v f_{eq}\,dv = 0$ because the equilibrium function f_{eq} is symmetric in v this integral is zero

$\int_{-\infty}^{+\infty} v f(r,v,t)\,dv$: we use the general definition of the current density: $j(r) = q\int_{-\infty}^{+\infty} v\cdot f(r,v)\,dv$

$$\int v^2\cdot\nabla_r f\,dv + \frac{qE}{m}\cdot\int_{-\infty}^{+\infty} v\cdot\nabla_v f\,dv = -\frac{j}{q\tau}$$

We use partial integration

$$\int v^2\cdot\nabla_r f\,dv + \frac{qE}{m}\cdot\left(\left[v\cdot f\right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} f\,dv\right) = -\frac{j}{q\tau}$$

$[v\cdot f]_{-\infty}^{+\infty} = 0$ because the equilibrium function f_{eq} is symmetric in v this integral is zero

$\int_{-\infty}^{+\infty} f\,dv$: we use the general definition of the particle conservation: $n(r) = \int_{-\infty}^{+\infty} f(r,v)\,dv$

$$\int v^2\cdot\nabla_r f\,dv - \frac{qE}{m}\cdot n(r) = -\frac{j}{q\tau}$$

we replace v^2 by the mean value $v^2 = kT/m$ of the **Maxwell-Boltzmann distribution**

$$\frac{kT}{m}\nabla_r\int f\,dv + \frac{qE}{m}\cdot n(r) = -\frac{j}{q\tau}$$

we rearrange and use again $n(r) = \int_{-\infty}^{+\infty} f(r,v)\,dv$

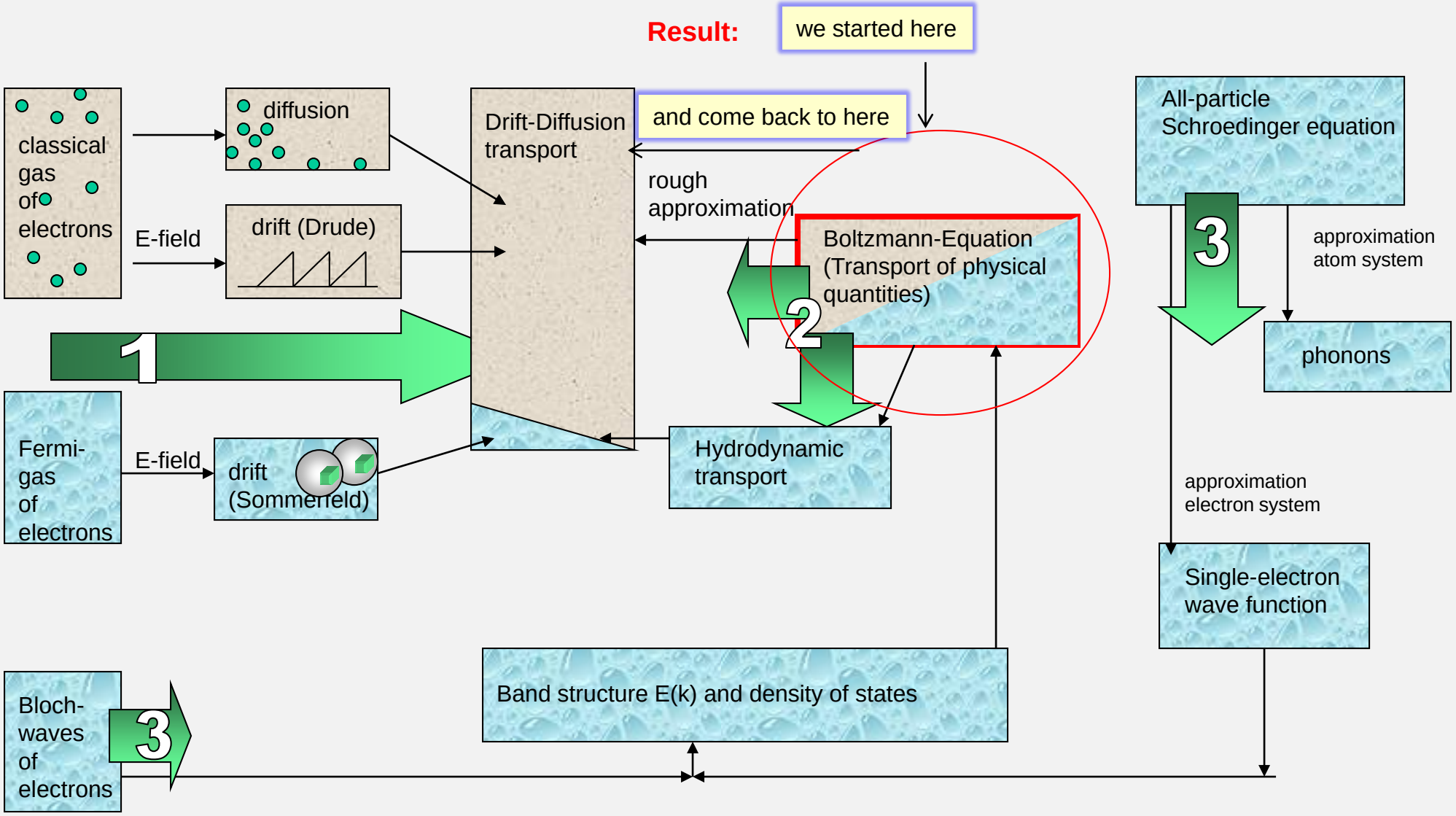
$$q\tau\cdot\frac{kT}{m}\nabla_r n - q\tau\cdot\frac{qE}{m}\cdot n(r) = -j$$

we use: $\mu = \frac{\tau q}{m}$ for mobility and: $D = \frac{\mu kT}{m}$

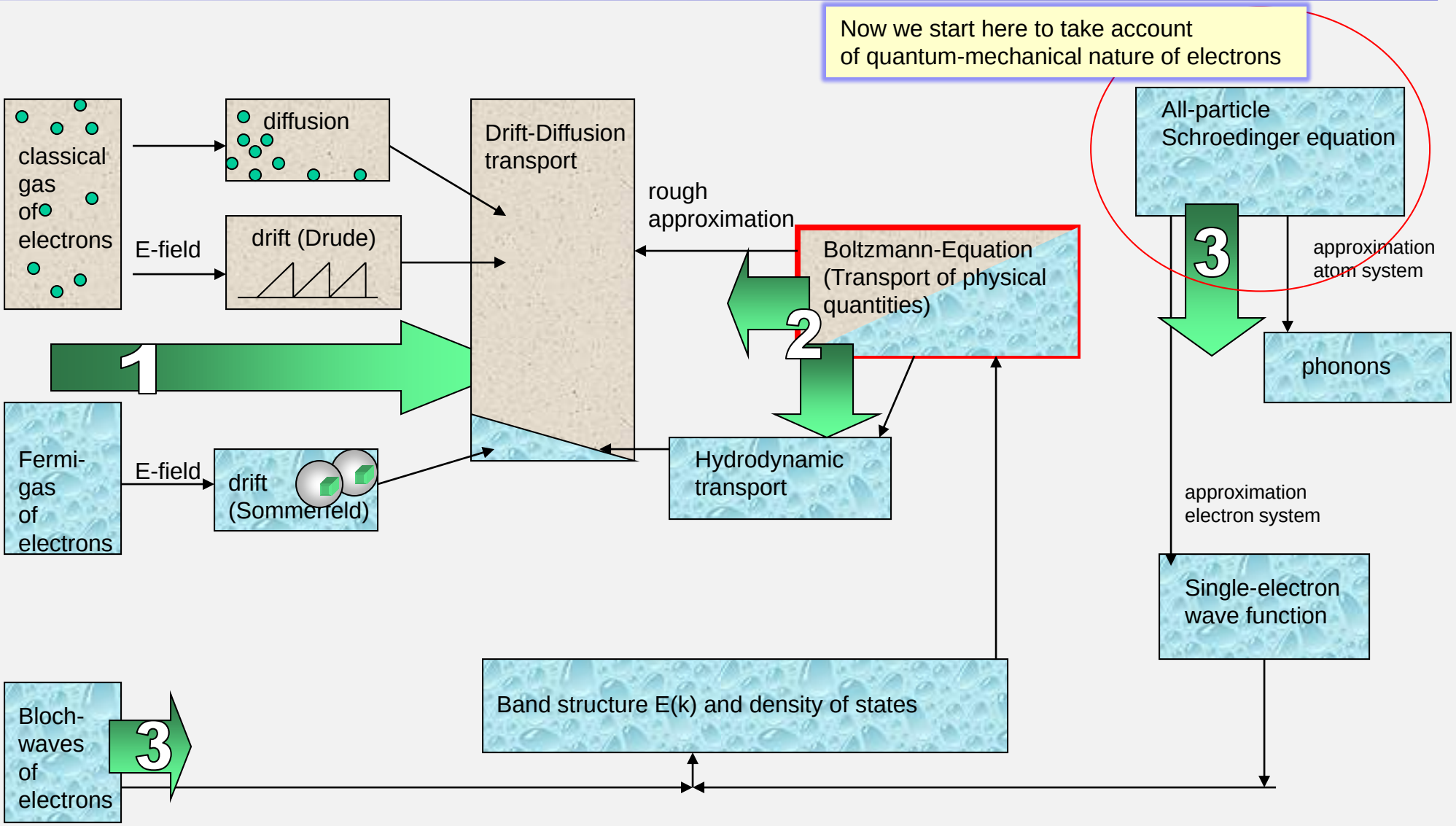
$$qD\nabla_r n(r) - q\mu E n(r) = -j \rightarrow \boxed{j = q\mu E n(r) - qD\nabla_r n(r)}$$

Drift-Diffusion Equation

Charge Transport Models



Charge Transport Models



The BTE for Electrons in Bandstructures

All-particles Schroedinger Equation S-E

reduce number of particles

Reduction of particles in 2 classes:
-> free moving electrons + localized moving core lattice ions

movement of 10^{22} electrons per cm^3

adiabatic approach: ion masses >> electron masses
-> for movement of ions the electrons do not exist
-> for movement of electrons the ions are in rest

phonon calculations

1 electron moves, no interaction between electrons

1 electron moves in a common background Coulomb potential of all other electrons

1 electron moves, realizing other electrons as qm particles

simplifications:
try to find a single-electron wave function

S-E without ee-interaction

Hartree-equation

Hartree-Fock equation

These 3 are:

Single-electron Schroedinger equation

for the potential we use: periodic lattice ion potentials
for the wave function we use: Bloch-waves exp(ikr)

solve single electron equation

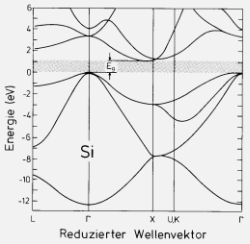
various methods:

orthogonal plane waves

pseudopotentials

k*p method

Single-electron band structure ε(k) + density of states N(ε)



fill in electrons

electron system in rest

-> basic properties: E_{Fermi}, ...

we recognize in the bandstructure: maxima and minima are parabolic shaped -> movement of carriers "quasi-free" (no wonder, it was a starting condidtion)

we introduce "quasi-free" terms $v=1/h*\nabla\varepsilon(k)$ and $\nabla p=1/h\nabla k$ in:

Boltzmann equation

Electron Boltzmann-(Bloch) equation

* external fields
* internal fields (=collisions)

Try to find a solution

The Bloch waves

$$H\Psi = -\frac{\hbar^2}{2m}\cdot\nabla^2\Psi(r,t)+V(r)\cdot\Psi(r,t)=E\Psi(r,t)$$

We start with the one-electron stationary Schrödinger equation

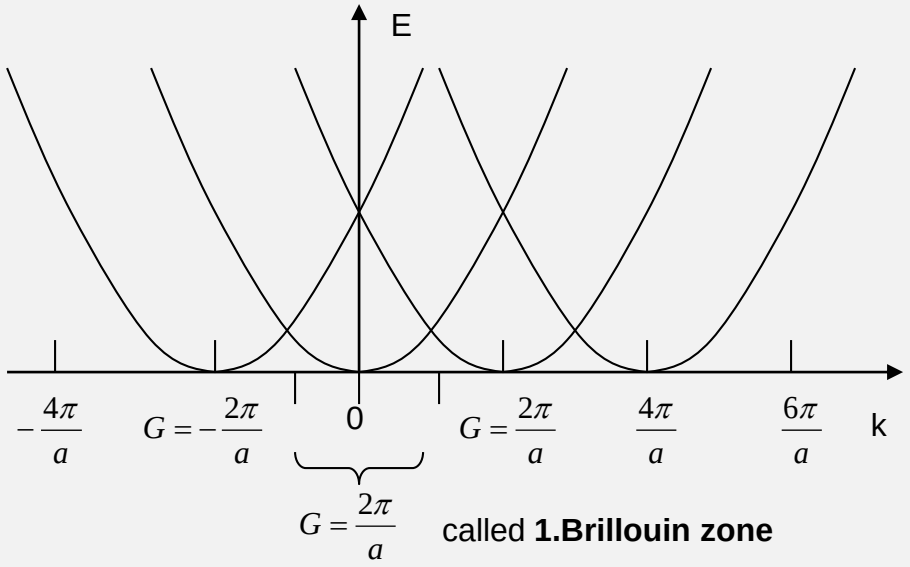
We use a periodic potential: $V(r)=V(r+a)$ a: lattice vector of real lattice

We can show, that a solution is a modulated, planar wave: $\Psi(r)=u(r)\cdot\exp[ikr]$ called **Bloch-waves**

As a solution for the energy states E(k) we find, that they are also periodically in the reciprocal lattice: $E(k)=E(k+G)$

If we use "free" electrons, we set the value of the potential to zero,
but keeping the periodicity as a boundary condition

$$V(r)=V(r+R)$$



called **1.Brillouin zone**

1. Because we used "zero potential", which means "free" electrons the energy states are parabolic as for free electrons:

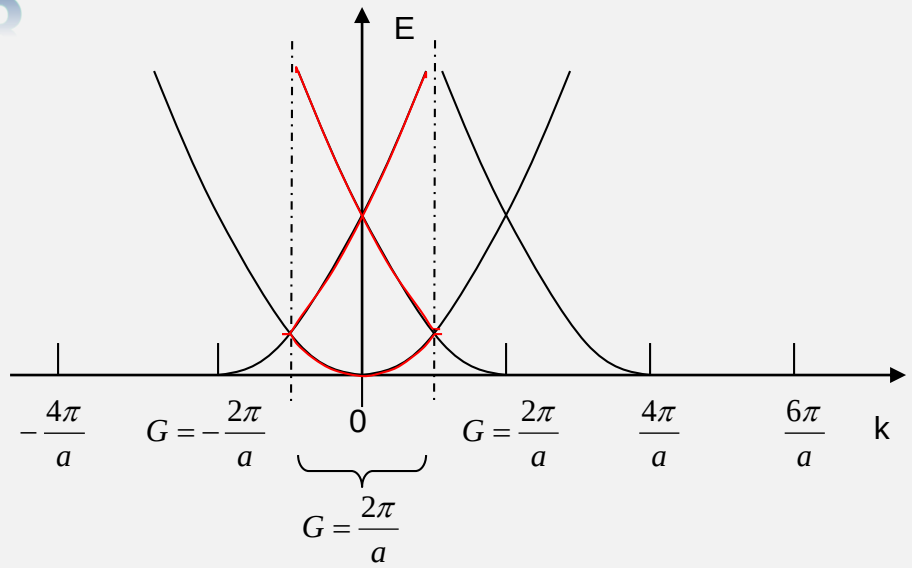
$$E(k)=\frac{\hbar^2k^2}{2m}$$

2. Because of periodicity the 1.Brillouin zone contains all possible k-states of the crystal. All other zones are only periodic repetitions.

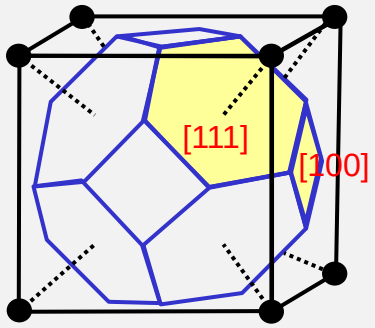
3. Because of periodicity the diagram usually is reduced to the 1.BZ

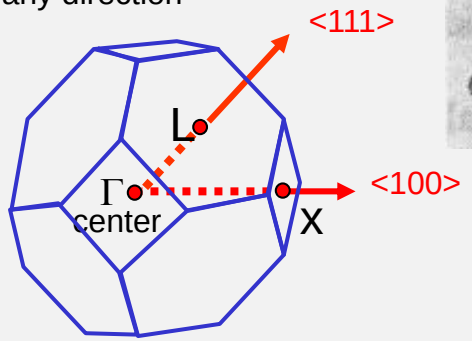
Empty Bandstructures

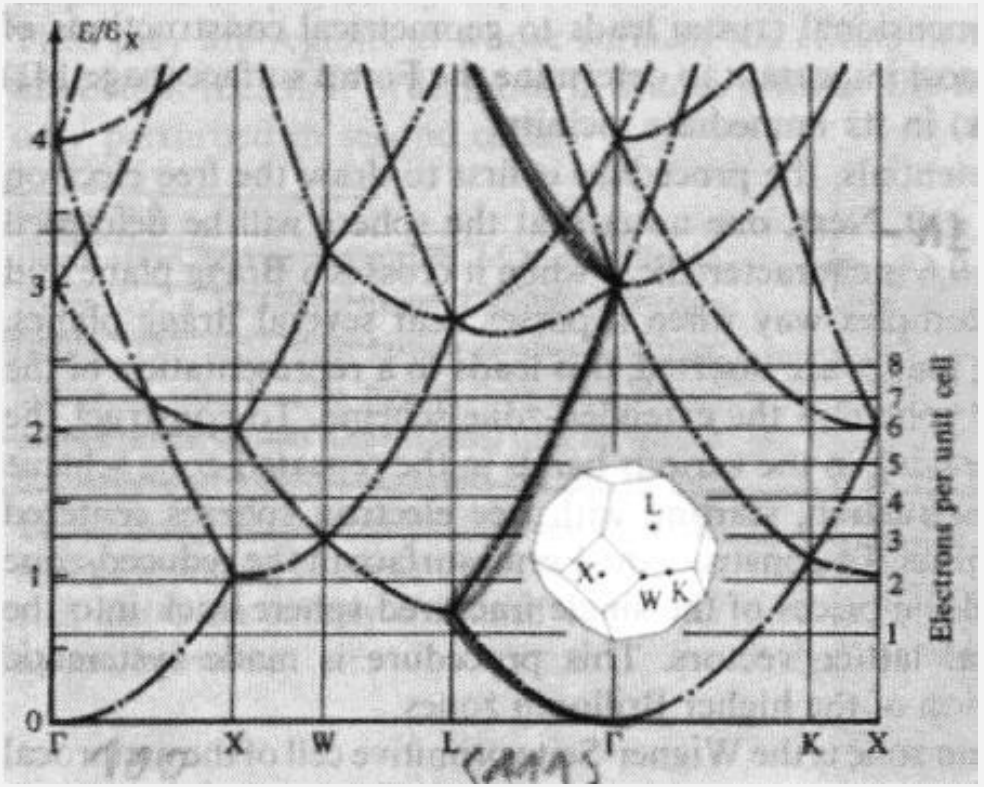
3 Because of periodicity the diagram usually is reduced to the 1.BZ



4 Because the periodicity (of location and potential) in any crystal depends on the direction in the crystal, the banddiagram is different in any direction







band structure of an "empty" fcc-lattice

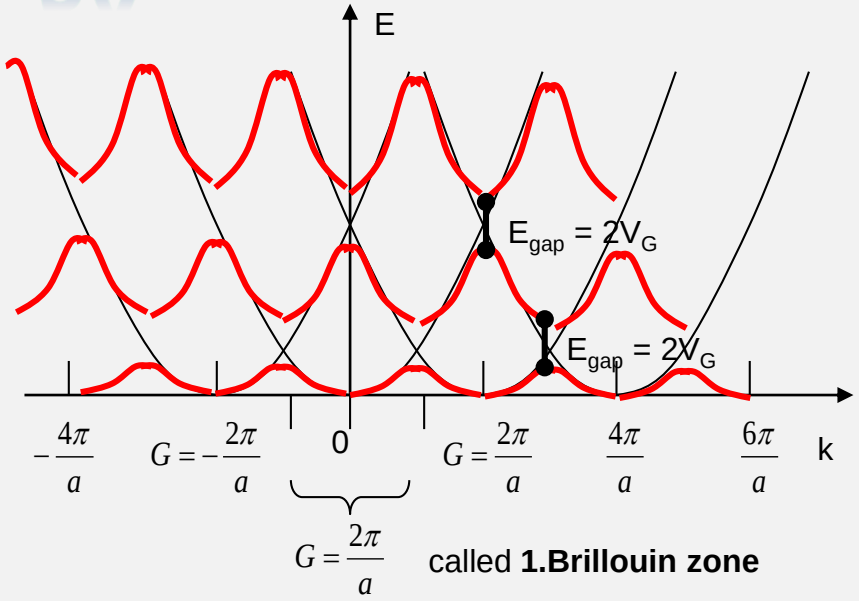
Ashcroft, Solid State Physics, CBS Publishing, 1976

Bandstructures

In reality the potential is not zero, there exist several approaches of calculating a "real" band structure

5A

In the "free"-electron model we switch on a weak potential

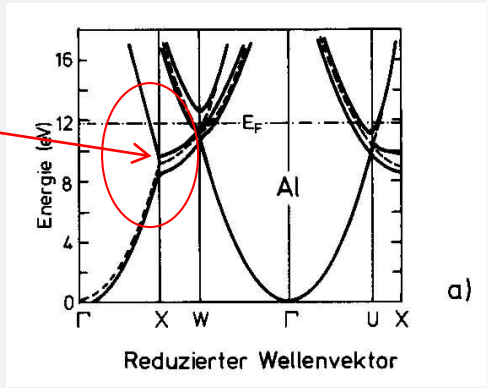


called **1.Brillouin zone**

As a result bandgaps appear

in theory the gap is twice the potential at G

band structure of Al:
---- calculated without potential
__ calculated with potential



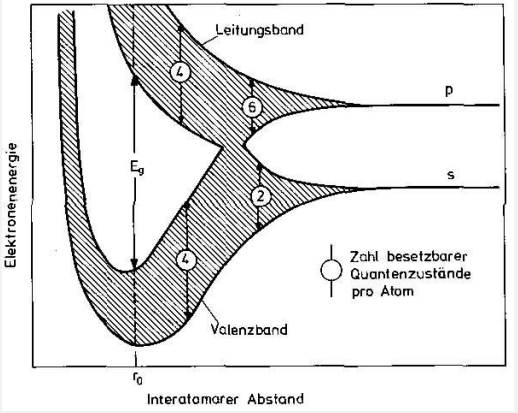
two of them are:

5B

The tight-binding of electrons
(LCAO, linear combination of atomic orbitals)

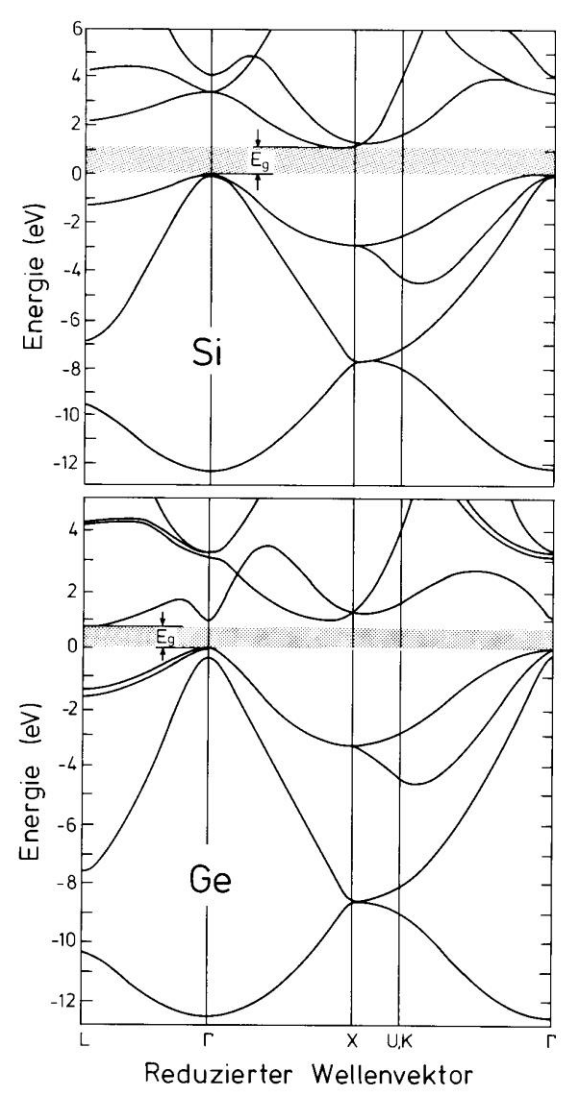
1. We solve the one-electron Schrödinger equation for a single atom potential and calculate the energy levels and wave functions:

2. Then we shift the atoms together and calculate new wave functions from the superposition of the atomic wave functions:



Bandstructures

Examples of band structures:



From the bandstructures we can see:

The maxima and minima of the bands are almost parabolic.

Electrons (or holes) with energies close to the minima (or maxima) (~kT) can only occupy k-states like "free" particles.

$$E(k) = \frac{\hbar^2 k^2}{2m}$$

Because the electrons are now handled as quantum mechanical particles (= wave packets) the group velocity is described by:

$$\vec{v} = \nabla_k \omega(\vec{k}) = \frac{1}{\hbar} \nabla_k \varepsilon(\vec{k})$$

and

$$m^* = \frac{\hbar^2}{d^2\varepsilon(k) / dk^2}$$

m* is called a "quasi-free" mass and depends from the curvation of the energy ε(k)

The Boltzmann-Bloch Equation

If we use the classical BTE:

$$\frac{\partial f}{\partial t} = -\left[\vec{v}\cdot\nabla_r f + \vec{F}\cdot\nabla_p f\right] + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

and replace:

$$\vec{v} = \frac{1}{\hbar}\nabla_k \varepsilon(\vec{k})$$

and using:

$$\nabla_p = \frac{1}{\hbar}\nabla_k$$

and:

$$\vec{F} = q\vec{E}$$

the electric field E as driving force

we achieve:

the **Boltzmann-Bloch equation** for electrons in semiconductors

$$\frac{\partial f}{\partial t} = -\left[\frac{1}{\hbar}\nabla_k \varepsilon(k)\cdot\nabla_r f + \frac{q\vec{E}}{\hbar}\cdot\nabla_k f\right] + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

We introduce some basic quantum mechanics in a classical transport equation

Solving the Boltzmann-Bloch Equation

Solving the Boltzmann-Bloch equation

Analytical solutions:

Linearization	separate distribution function f in equilibrium distribution f_0 (well-known) and unknown, small perturbation $f_1(\mathbf{k},\mathbf{r})$	small perturbation -> no abrupt, high field effects but which are common in submicron MOSFETs
method of moments	multiply BBE by powers of k^n	* collision integral -> relaxation time approximation (no linearization)

Formal Solution

Numerical solutions

iterative	use a test function f, calculate the differences f - f_0 , try to find a better f
Monte-Carlo	use single particles (electrons), estimate the influence of external fields, estimate the probability and effect of scattering events -> sum up all particles

The Hydrodynamic Approach

Approach: First simplify the collision integral by relaxation times, second handle the remaining terms

Developing the set of momentum equations: multiply the BTE by k^n and then integrate over k

$$\int \vec{k} \cdot \left\{ \frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f + \frac{\vec{E}}{\hbar} \cdot \nabla_k f = \left(\frac{\partial f}{\partial t} \right)_{coll} \right\} d\vec{k}$$

Generally the m+1 moment appears in the equation for the m-th moment

0th moment equation:

$$\frac{\partial n}{\partial t} + \nabla(nv) = \left(\frac{\partial}{\partial t} n \right)_{coll}$$

carrier conservation

1th moment equation:

$$\frac{\partial v}{\partial t} = -\frac{1}{2}\nabla_x v^2 + \frac{qE}{m^*} - \frac{2}{3m^* n} \cdot \nabla_x \left[n\left(\varepsilon(k) - \frac{1}{2} m^* v^2 \right) \right] + \left. \frac{\partial v}{\partial t} \right|_{coll}$$

momentum conservation

2nd moment equation:

$$\frac{\partial \varepsilon}{\partial t} = -v\nabla_x \varepsilon + qEv - \frac{2}{3m^* n} \cdot \nabla_x \left[nv\left(\varepsilon(k) - \frac{1}{2} m^* v^2 \right) \right] - \frac{1}{n}\nabla_x h + \left. \frac{\partial v}{\partial t} \right|_{coll}$$

energy conservation

3rd moment

$$\frac{\partial h}{\partial t} = ...$$

heat flow

heat generation, usually neglected

Drift-Diffusion

Hydrodynamic Transport

and so on ... getting more and more complicated and long-winding simulations

In detail: multiplying by powers of k

Phase space

We know: $n(r,t) = \frac{1}{4\pi^3}\int f(r,k,t)dk$ the local carrier distribution, which could be used in Poisson equation (Input equation)

$$j(r,t) = -\frac{e}{4\pi^3}\int f(r,k,t)\cdot v(k)dk \xrightarrow{\text{classical}} qnv$$ the current flow in a device (output information)

Now calculating the zero moment $k^0 = 1$:

$$\int \vec{k}\cdot\left\{\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla f + \frac{\vec{E}}{\hbar}\cdot\nabla_k f = \left(\frac{\partial f}{\partial t}\right)_{coll}\right\}d\vec{k}$$

$$\int 1\cdot\left\{\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla f + \frac{\vec{E}}{\hbar}\cdot\nabla_k f = \left(\frac{\partial f}{\partial t}\right)_{coll}\right\}d\vec{k}$$

$$\rightarrow \int\frac{\partial f}{\partial t}d\vec{k} + \int\vec{v}\cdot\nabla f d\vec{k} + \int\frac{\vec{E}}{\hbar}\cdot\nabla_k f d\vec{k} = \int\left(\frac{\partial f}{\partial t}\right)_{coll}d\vec{k}$$

$$\rightarrow \frac{\partial}{\partial t}\cdot\int f d\vec{k} + \frac{\partial}{\partial r}\int f v d\vec{k} + 0 = \frac{\partial}{\partial t}\int f d\vec{k}$$

$$\rightarrow \frac{\partial}{\partial t}n + \frac{\partial}{\partial r}j = \left(\frac{\partial}{\partial t}n\right)_{coll}$$

$$\rightarrow \frac{\partial n}{\partial t} + \nabla(nv) = \left(\frac{\partial}{\partial t}n\right)_{coll}$$

Now calculating the 1-st moment $k^1 = k$: $\int \vec{k}\cdot\left\{\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla f + \frac{\vec{E}}{\hbar}\cdot\nabla_k f = \left(\frac{\partial f}{\partial t}\right)_{coll}\right\}d\vec{k}$ $\longrightarrow$ we will not do here

Now calculating the 2nd moment $k^2 = k$: $\longrightarrow$ we will not do here

... and so on

Results

1) Drift-Diffusion

Everything is in thermal equilibrium, carriers themselves, carriers with lattice, carriers with external fields
collisions are point effects in space and time.
-> in equilibrium the energy distribution is always a Maxwellian distribution with mean energy kT.
This equilibrium process results in a mean maximum velocity of particles -> velocity saturation of drift at kT ?
From Maxwellian distribution it is clear that some electrons have higher energies than kT, they are "hot".
Their existence is stationary, the amount is always the same.
Non-equilibrium processes, like additional generation of "hot electrons" can not be described.

2) Hydrodynamic Equations

Using hydrodynamic equations uses the description of non-stationary (=dynamic) processes which may change the Maxwell equilibrium distribution a little bit in space and time.
This is usually the case for abrupt high electric fields (in space or time).

Example: heterojunction or emission or tunneling

Results of analytical hydrodynamic solutions

velocity overshoot

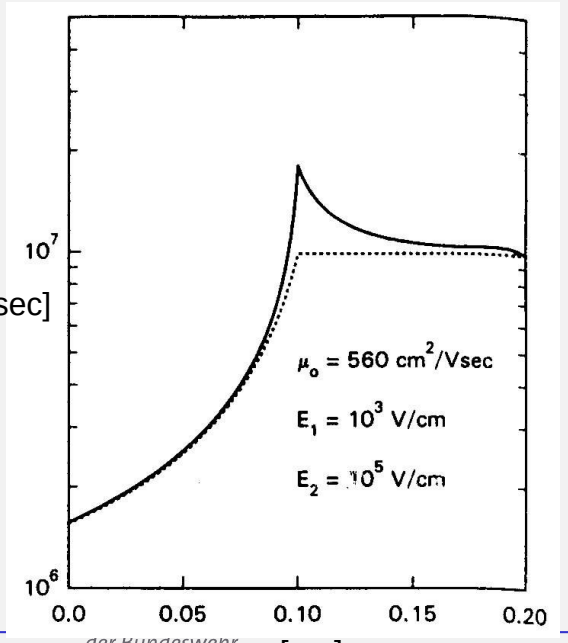
In drift-diffusion approximation the electron energy distribution is always a Maxwell-Boltzmann distribution with a mean value of

$$v_p = \sqrt{\frac{8kT}{\pi m}}$$

This is, because we assumed that the electrons are always in thermal equilibrium with the lattice.

If we shrink the time and space scales, that geometries are in the range of mean free path of scattering or electric fields change rapidly in time or space during the mean free path, the electron energy distribution will shift away from Maxwellian.
We need to solve the Boltzmann-Bloch equation.

velocity overshoot describes the phenomenum, that the velocity of electrons exceeds the saturation velocity.



Overshoot-predictions from Baccarani/Wordeman

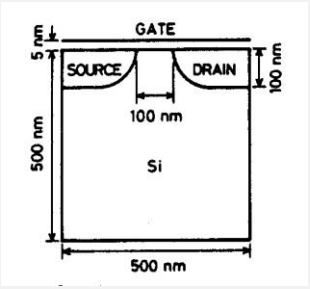
"An investigation of steady-state velocity overshoot in silicon"
Solid-State Electronics, *Volume 28, Issue 4, April 1985, Pages 407-416*

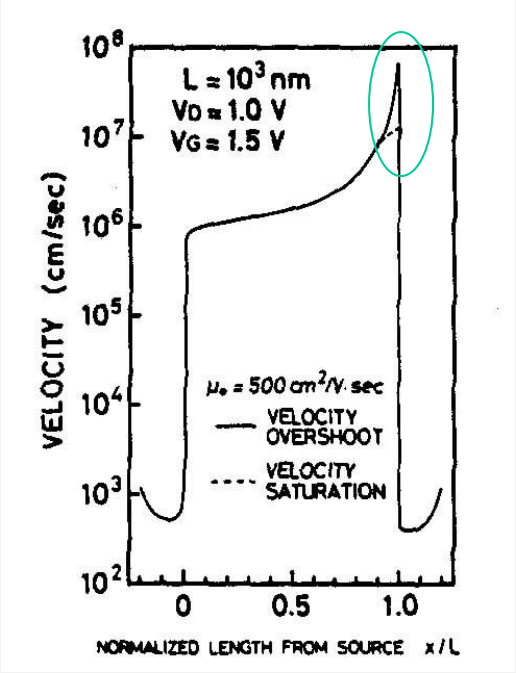
Results of analytical hydrodynamic solutions

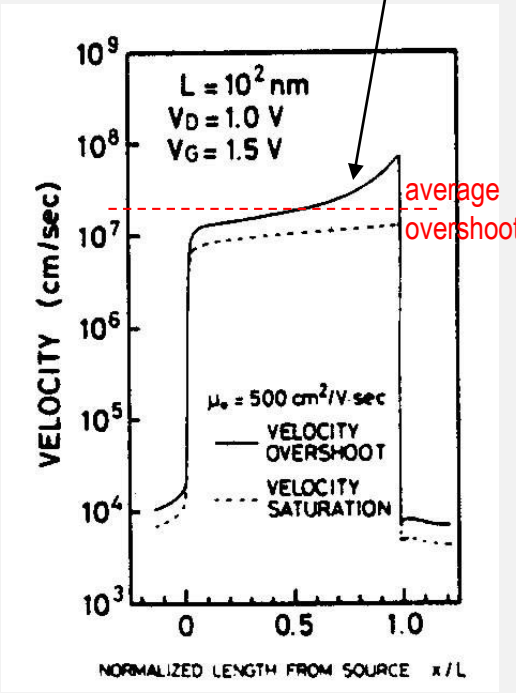
At low voltages and long channel (1µm) the overshoot is merely existing -> DD is ok

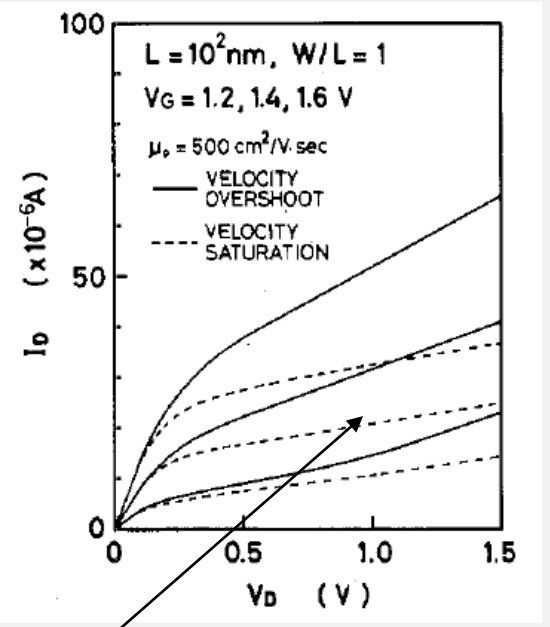
In a short channel MOSFET (0.1µm) the overshoot is clearly visible

Kobayashi, Saito, ED-32 (1985)788





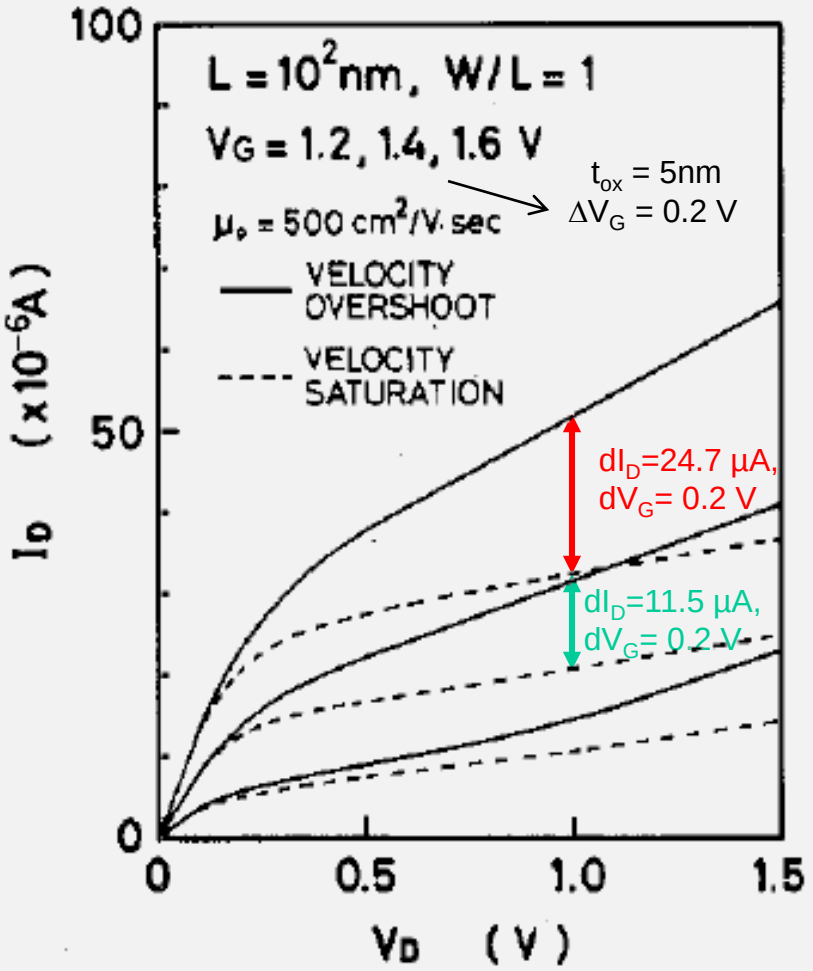




Velocity overshoot increases the device current by the same factor compared for drift-diffusion current

For proper circuit design the device current must be adjusted to ±10%.
-> Not taking into account hydrodynamics will result in non working ICs

Quantitative Proof from IV-characteristics



Kobayashi, Saito, ED-32 (1985)788

From MOSFET characteristics:

if a maximum velocity (~10^7 cm/sec) limits transport:

$$I_D = w \cdot C'' \cdot (V_G - V_T) \cdot v_{sat} \qquad g_m^{max} = \frac{\partial I_D}{\partial V_G} = w \cdot C'' \cdot v_{sat}$$

$$\frac{g_m^{max}}{w[mm]} = \frac{\varepsilon_0 \varepsilon_{Ox}}{t_{ox}} \cdot v_{sat} = \frac{8.85 \cdot 10^{-14}\, Asec/Vm \cdot 3.9 \cdot v[10^7\, cm/sec] \cdot 10^7}{t_{ox}[nm] \cdot 10^{-7}} = \frac{3450\, mS/mm}{t_{ox}[nm]}$$

$$\frac{v_{over}}{v_{sat}} = \frac{g_m^{meas} \cdot t_{ox}[nm]}{3450\, mS/mm}$$

Drift-Diffusion:

$$\frac{g_m^{meas}}{w[mm]} = \frac{dI_D/dV_G}{w} = \frac{11.5\mu A/0.2V}{100nm} = 570\, mS/mm$$

$$\frac{v_{over}}{v_{sat}} = \frac{g_m^{meas} \cdot t_{ox}[nm]}{3450\, mS/mm} = \frac{570\, mS/mm \cdot 5[nm]}{3450\, mS/mm} = 0.83$$

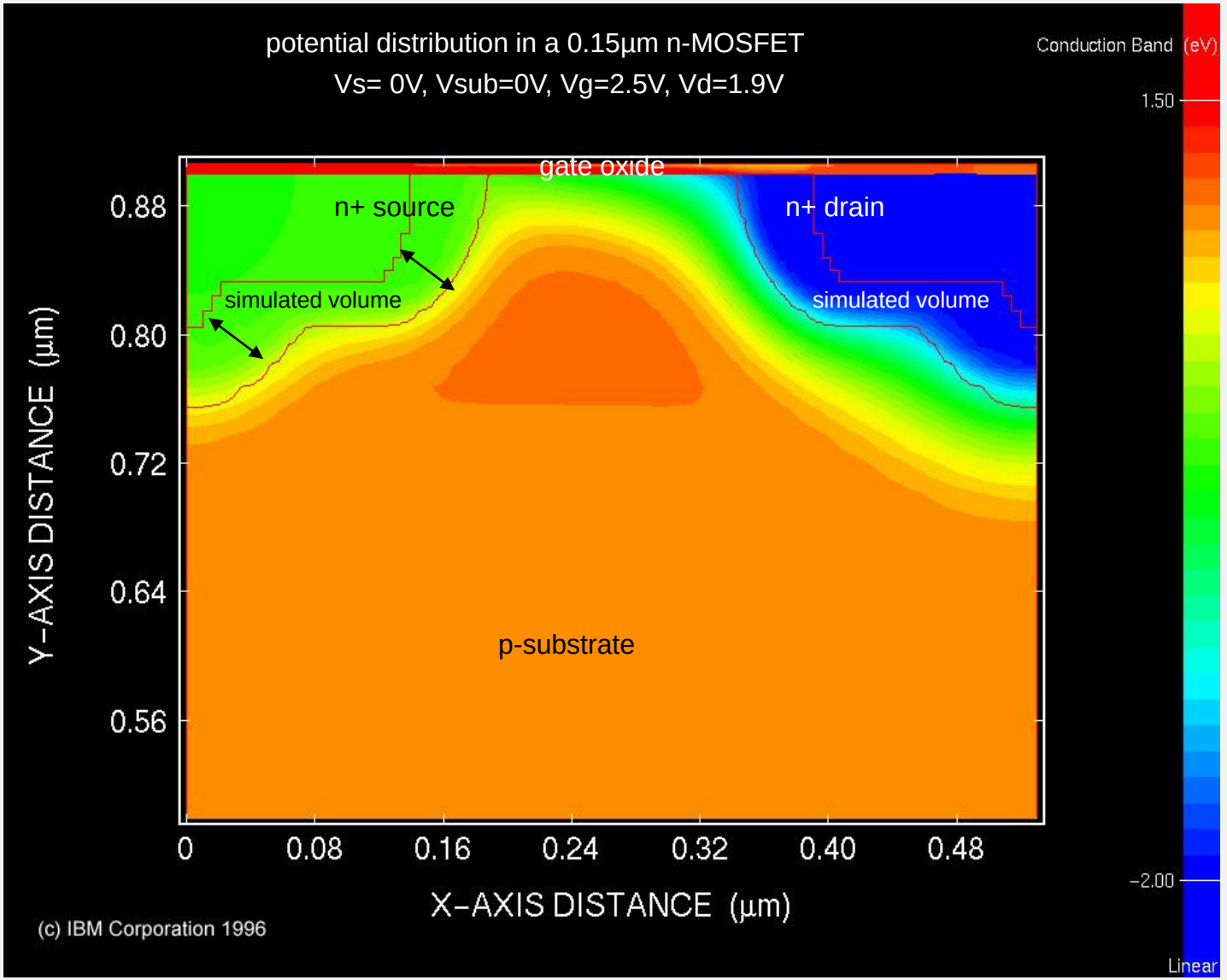
Hydrodynamic:

$$\frac{g_m^{meas}}{w[mm]} = \frac{dI_D/dV_G}{w} = \frac{24.7\mu A/0.2V}{100nm} = 1235\, mS/mm$$

$$\frac{v_{over}}{v_{sat}} = \frac{g_m^{meas} \cdot t_{ox}[nm]}{3450\, mS/mm} = \frac{1235\, mS/mm \cdot 5[nm]}{3450\, mS/mm} = 1.8$$

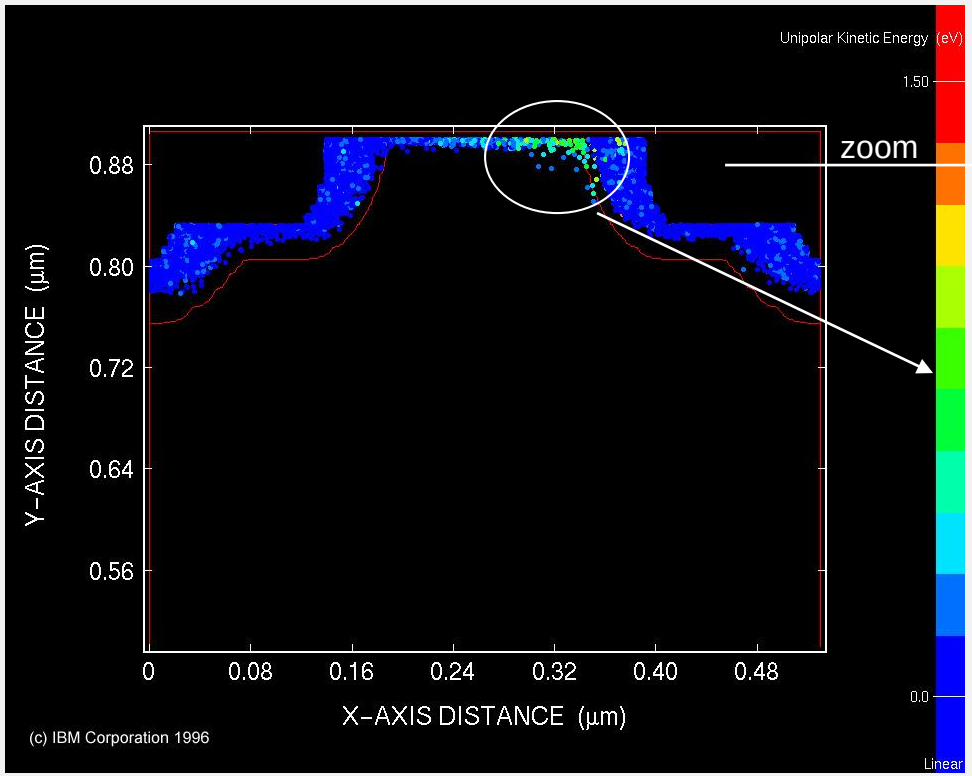
see picture last page

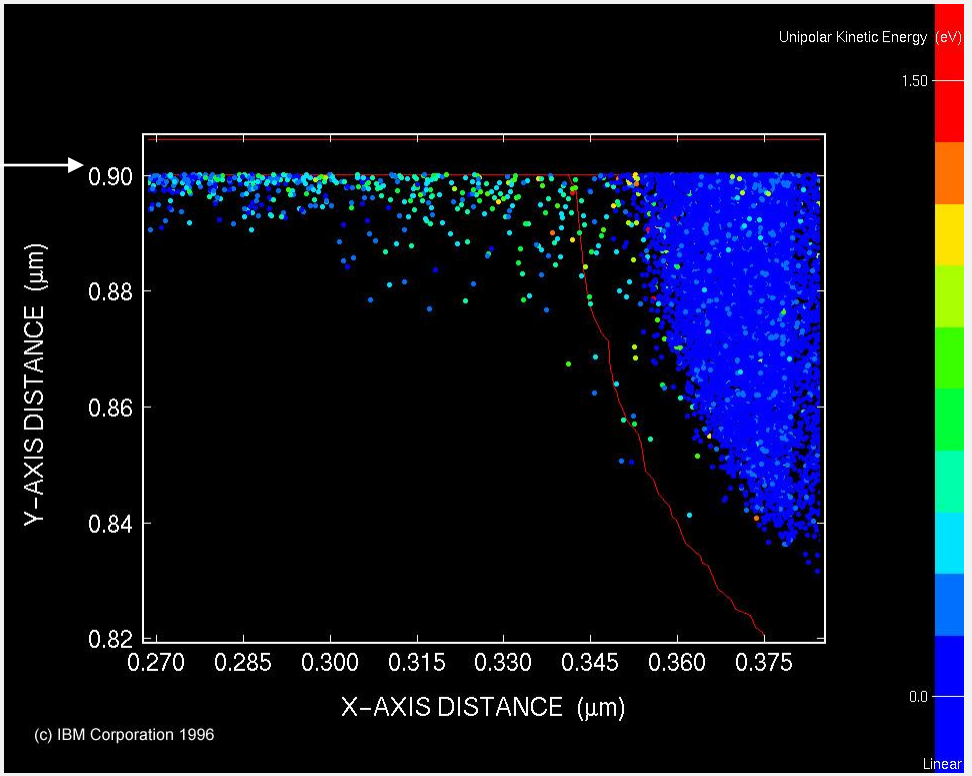
Results: Monte-Carlo-Simulations by DAMOCLES



Results: Monte-Carlo-Simulations by DAMOCLES

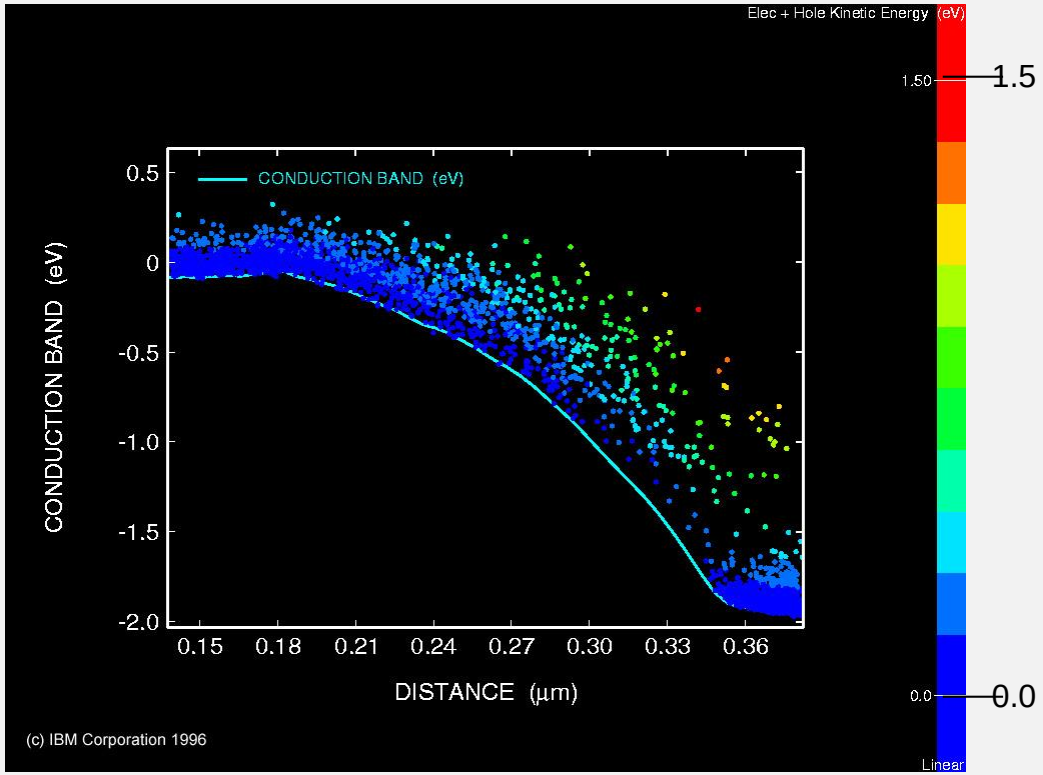
Energy of electrons at various positions within the MOSFET:

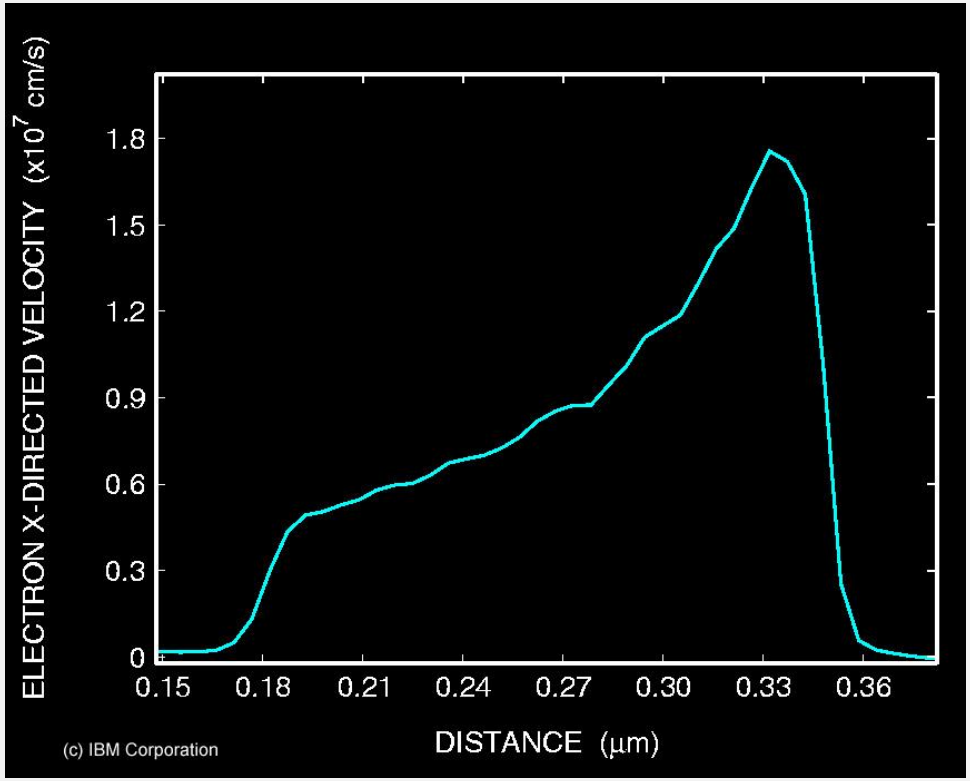




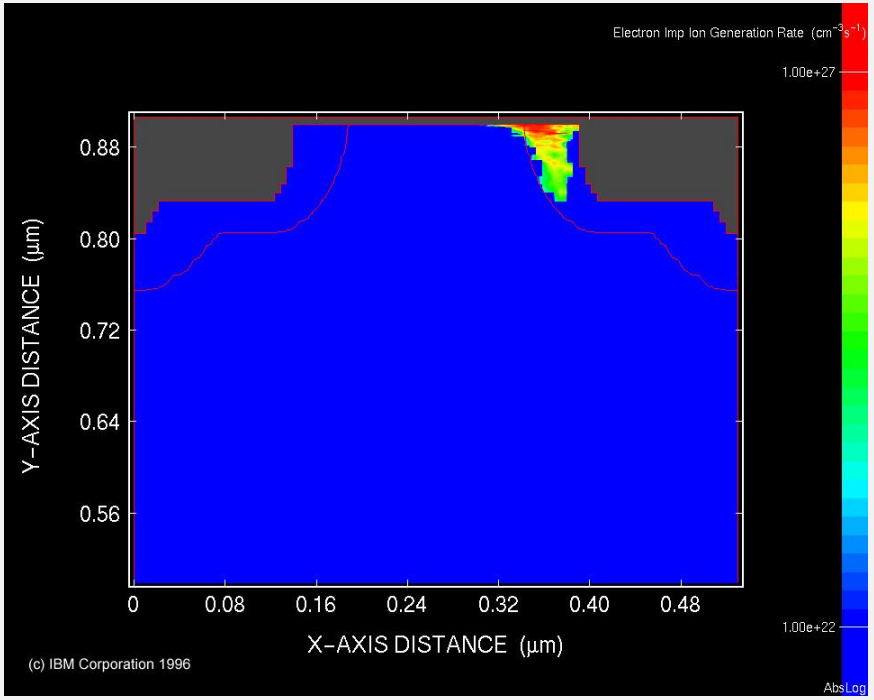
Near drain, electron energies well above the thermal limit (kT= 0.026 eV) are realistic

Results: Monte-Carlo-Simulations by DAMOCLES

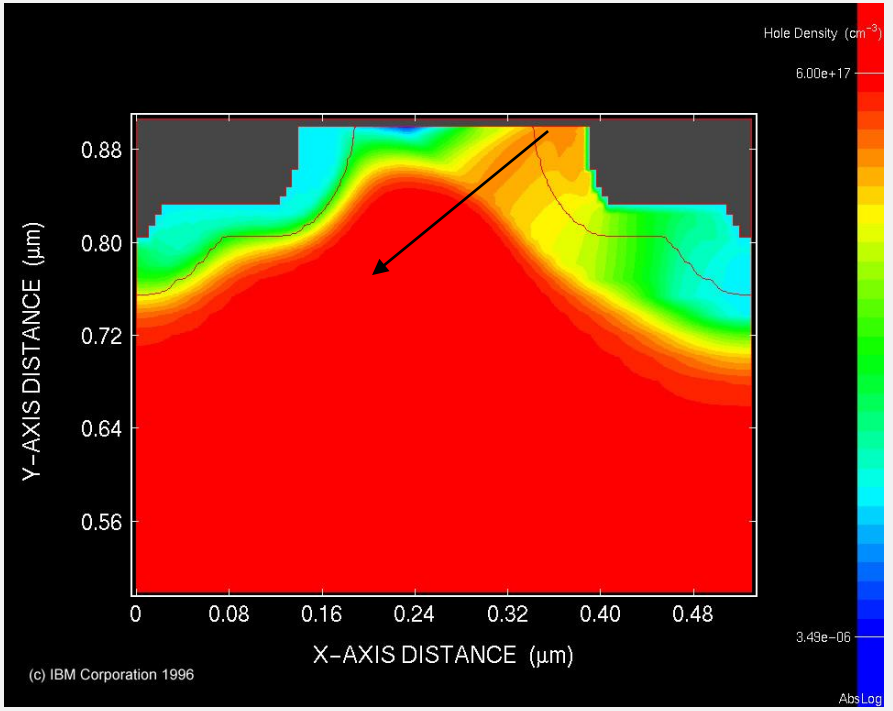




Results: Monte-Carlo-Simulations by DAMOCLES

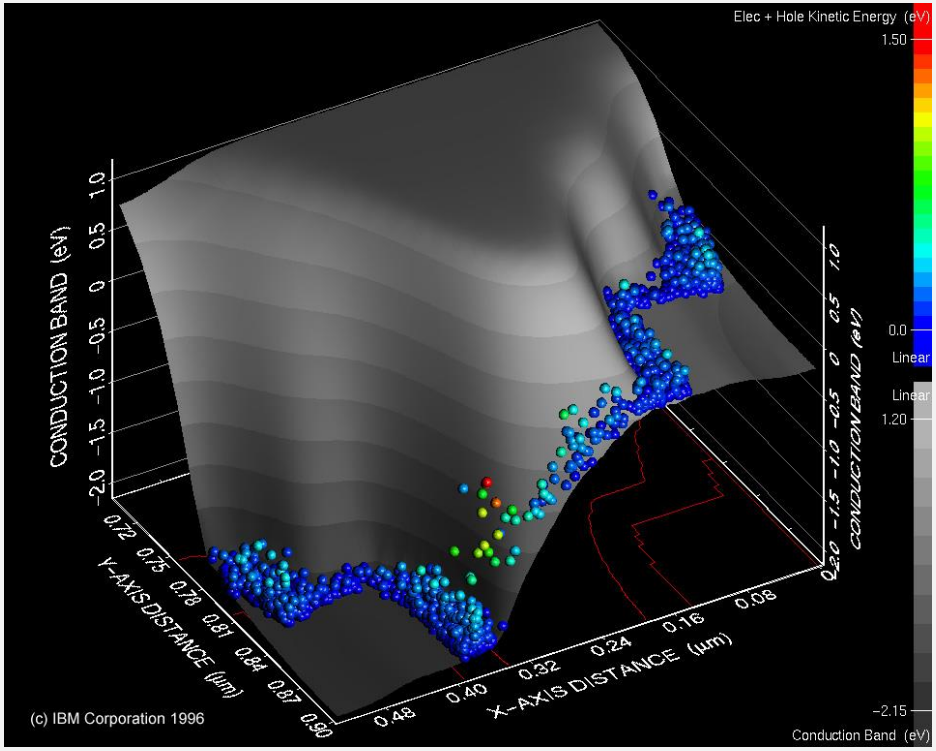


region of impact ionization

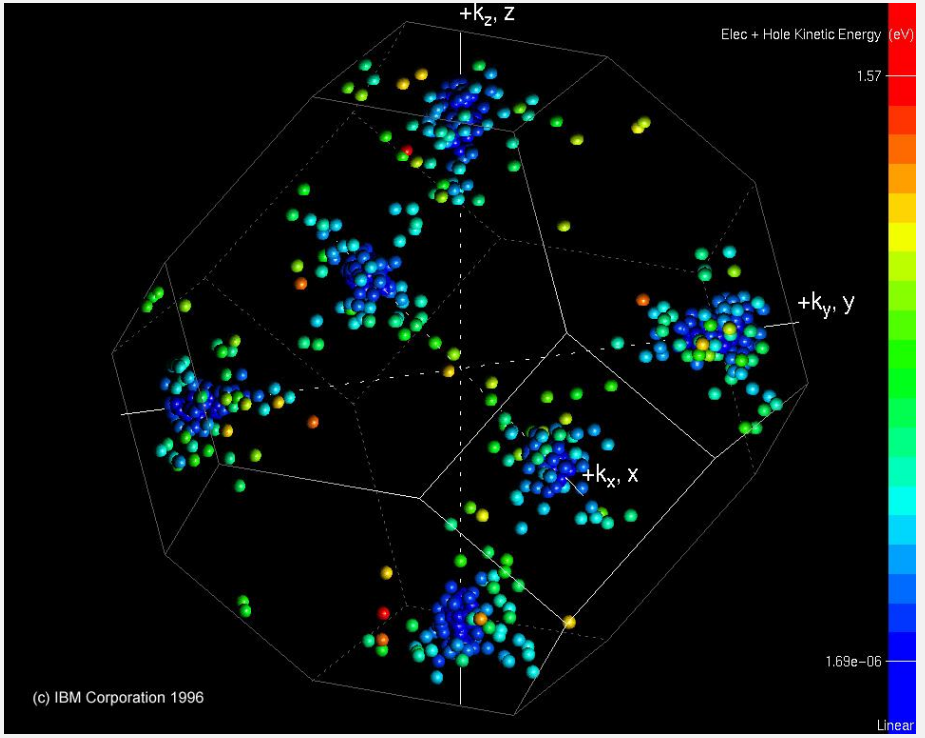


flow of generated holes into the substrate

Results: Monte-Carlo-Simulations by DAMOCLES



3-dim energy picture in real space



3-dim energy picture in k-space

5.1 Fundamental Transport
- Basic Definitions and Equations

5.2 Basic Quantum Mechanics
- Particles and Waves

5.3 Classical Electron Transport
- Classical Gas, Diffusion, Drude Drift Modell
- Fermi Gas, Sommerfeld Drift Model
- Classical Drift-Diffusion Model (DDE)

5.4 Boltzmann Transport Equation (BTE)
- Classical Boltzmann Transport Equation
- Quantum Mechanical Transport, Electrons in Bandstructures
- Quantum Mechanical Boltzmann-Bloch Equation
- Solving The Boltzmann-Bloch Equation

End of Chapter 5