

Hot Electron Transport

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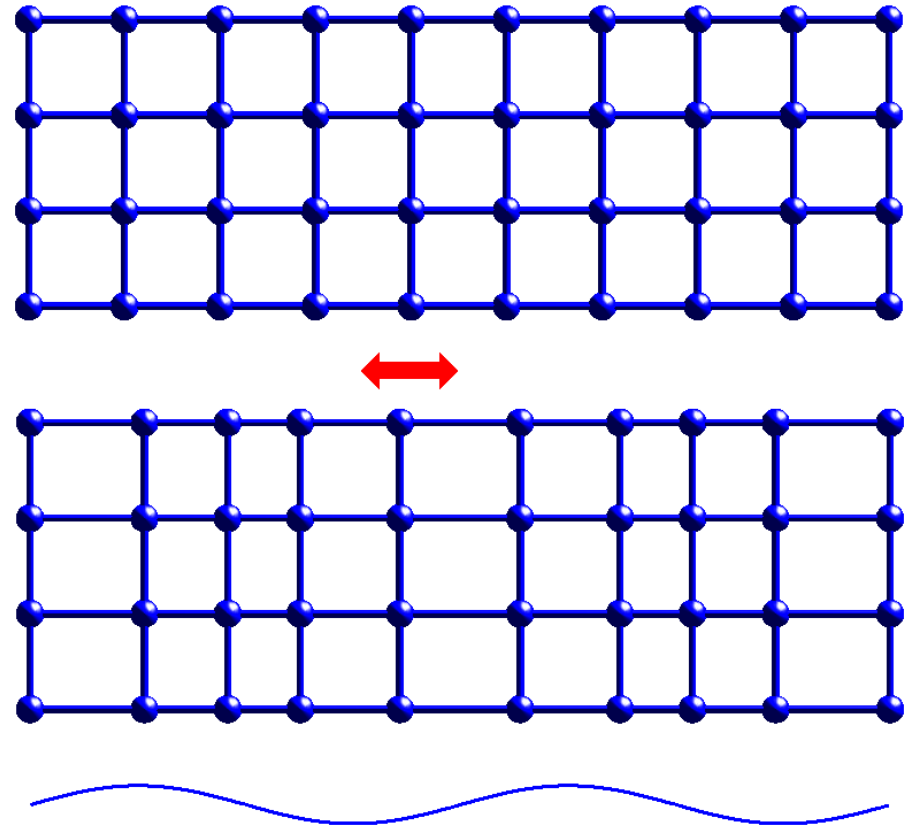
- Introduction
- Basic transport concepts
- High field phenomena
- Scattering mechanisms
- The Boltzmann transport equation

- **Introduction**
- Basic transport concepts
- High field phenomena
- Scattering mechanisms
- The Boltzmann transport equation

- The lattice temperature T_0
- Electrons in thermal equilibrium
- Hot electrons
- Scope of this talk

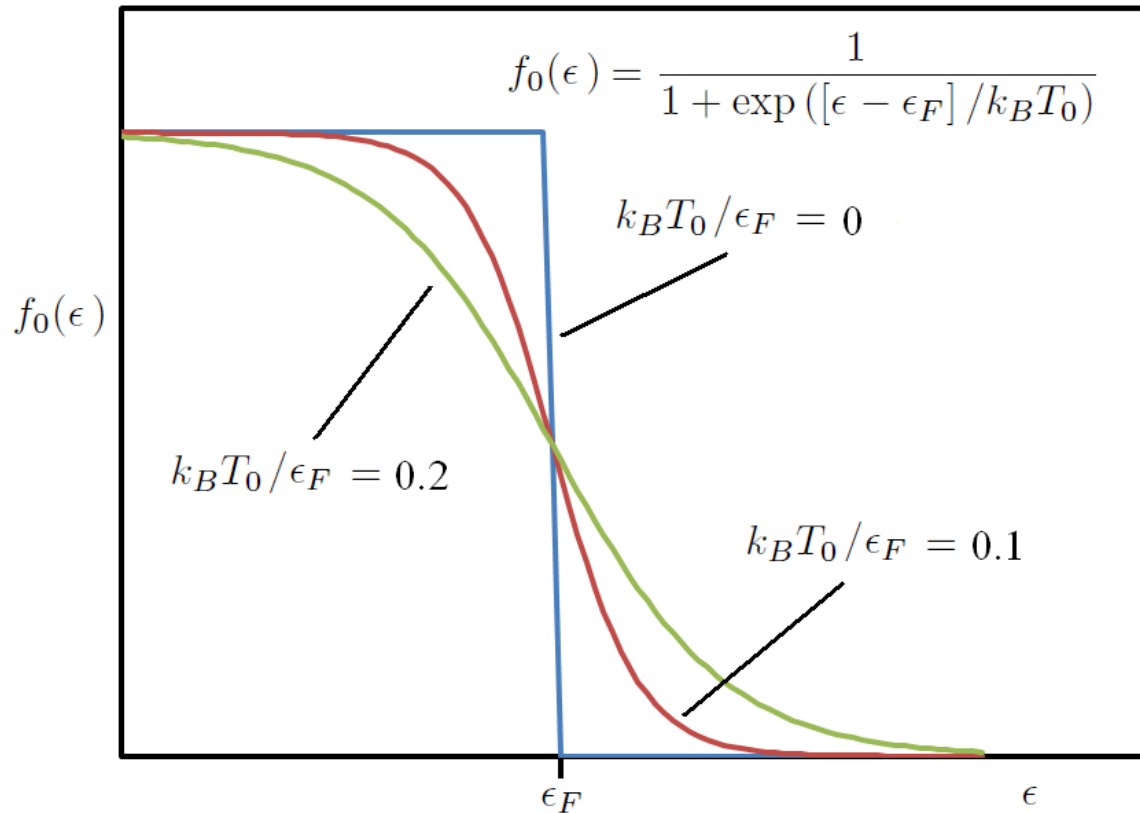
- Temperature is a measure of the average energy of a quantum of the system
- Lattice vibrations are quantised as *phonons*
- The average energy of a phonon determines the lattice temperature T_0

Schematic of a crystal lattice in its equilibrium configuration...



... and with a (longitudinal) phonon mode

The Fermi-Dirac distribution



Energetic distribution of electrons in thermal equilibrium with the crystal lattice

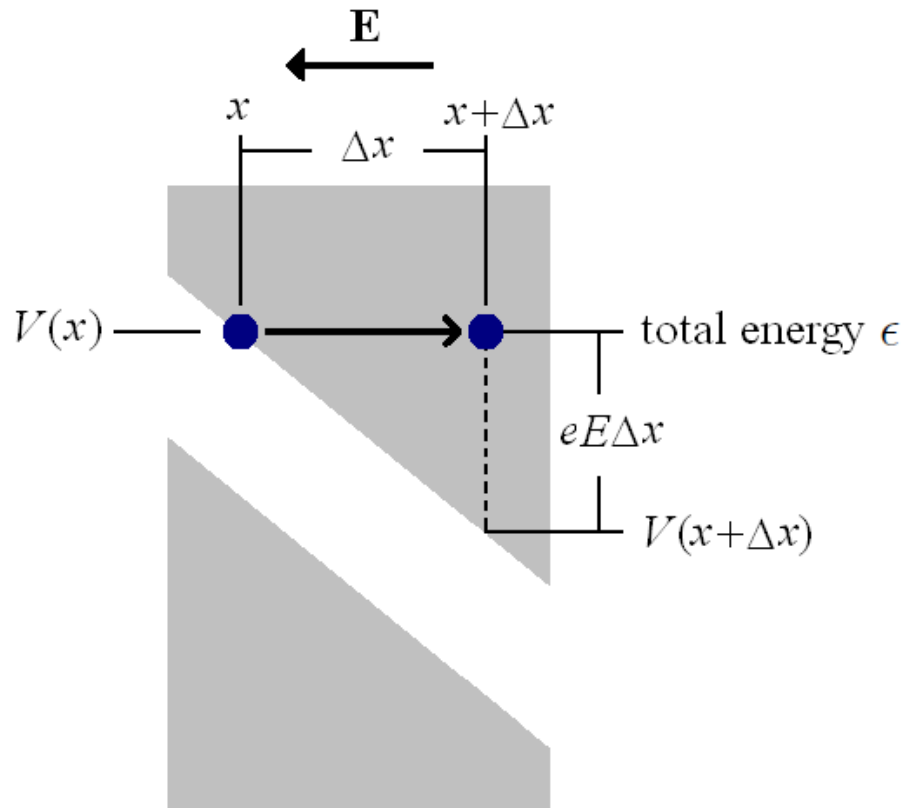
- The term **hot electrons** refers to a population of high-energy electrons out of thermal equilibrium with the crystal lattice
- Hot electrons may be sometimes be characterised by an electron temperature T_e , such that $T_e > T_0$.
- Hot electrons are typically produced by high electric fields, driving the electrons to higher energies
- Materials with a population of hot electrons may exhibit non-linear effects, such as
 - **Electrical breakdown**
 - **Negative differential resistance**

- The purpose of this talk is
 - To introduce the audience to the concept of hot electrons and some high-field phenomena
 - To give the audience an introduction into the theoretical approaches used to understand the details of hot electron transport
- Limitations of the talk
 - We shall only be looking at the semi-classical approach, so there will be no discussion of quantum transport or non-equilibrium Green's functions
 - Due to time constraints, we shall only consider the solution of Boltzmann's transport equation
 - Although hot electrons are particularly important in nano-devices, there will be no specialisation to low dimensional structures

- Introduction
- **Basic transport concepts**
- High field phenomena
- Scattering mechanisms
- The Boltzmann transport equation

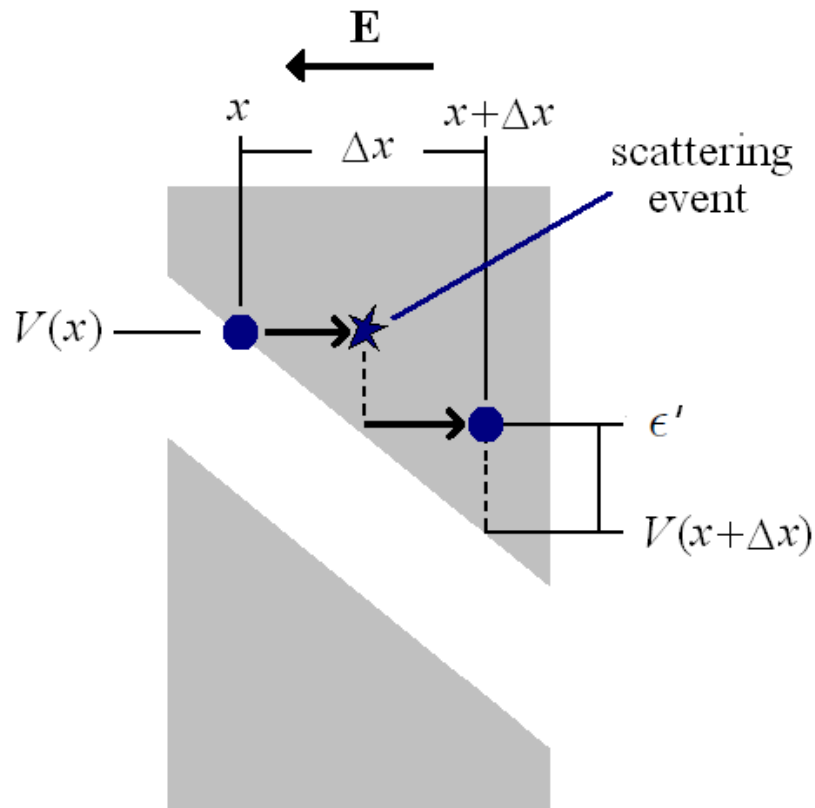
- **Ballistic transport**
- **Energy and momentum relaxation**
- **Describing energy bands**
- **Group velocity and density of states**
- **The non-equilibrium distribution function**
- **Transport properties**
- **The conservation equations**

Ballistic transport describes a regime of transport in which no scattering (and hence no energy or momentum relaxation) takes place.

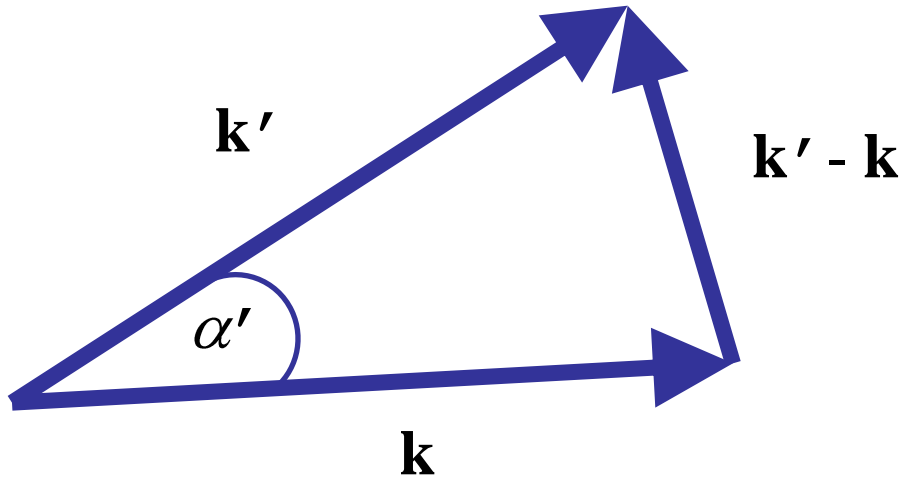


- The application of an electric field E gives rise to a spatially varying potential $V(r)$
- If the electron travels ballistically for a distance Δx , it gains a kinetic energy $eE\Delta x$ above the conduction band edge
- If $eE\Delta x$ is significantly greater than the thermal energy $k_B T_0$, then we may describe the electron as being *hot*

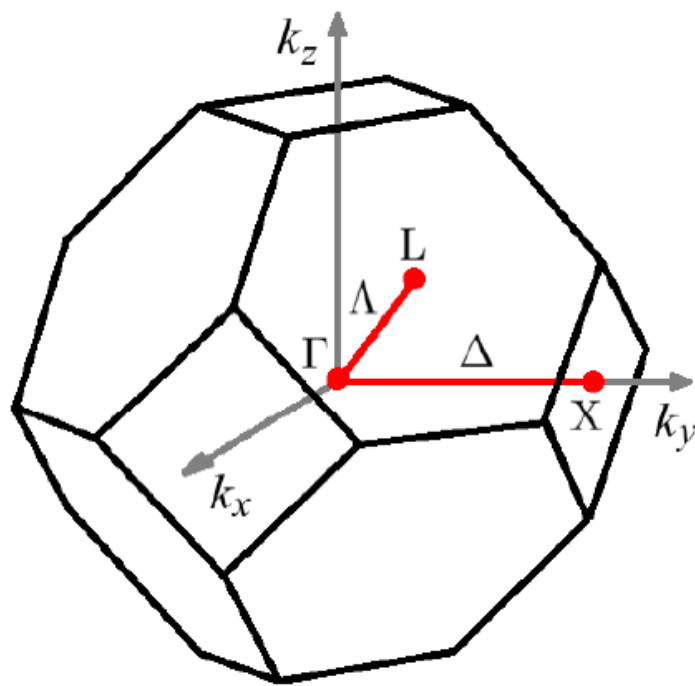
An electron will not continue to travel ballistically indefinitely. At some point it is likely to scatter, which will change its momentum and, sometimes, its energy.



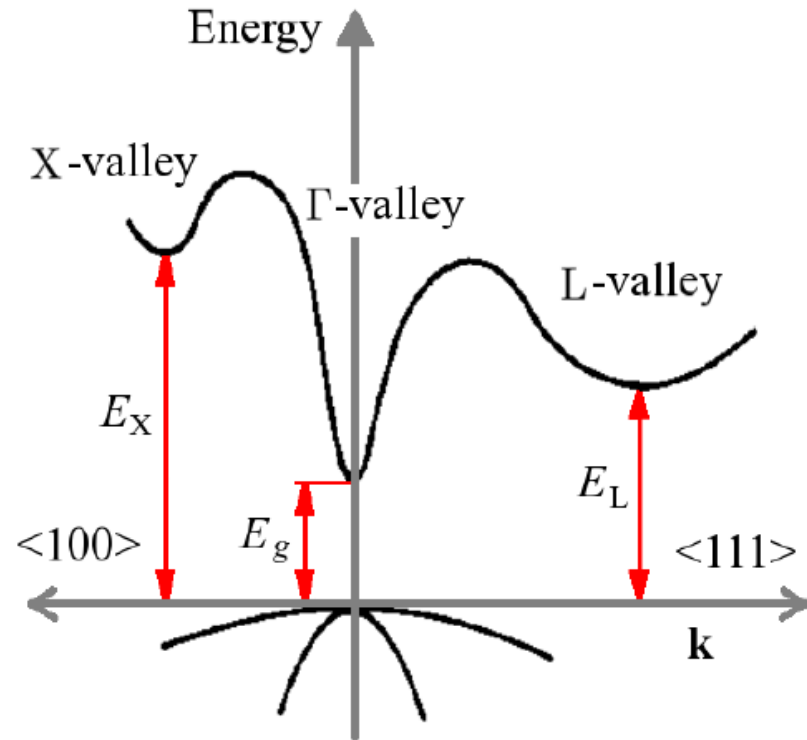
- The electron undergoes an energy relaxing (inelastic) scattering event, changing to a state with energy ϵ'
- We may define an energy relaxation time $\tau_{\epsilon}(\epsilon)$, which is the average time an electron of energy ϵ will travel before undergoing an inelastic scattering event
- Note that since $e = \hbar\omega$, $\tau_{\epsilon}(\epsilon)$ may also be thought of as a coherence time



- The electron undergoes a momentum scattering event, changing its momentum from $\hbar\mathbf{k}$ to $\hbar\mathbf{k}'$
- If $|\mathbf{k}| = |\mathbf{k}'|$, then energy is conserved and the interaction is elastic
- We may define an energy relaxation time $\tau_m(\epsilon_k)$, which is the average time an electron of energy ϵ_k and momentum $\hbar\mathbf{k}$ will travel before undergoing a momentum changing scattering event
- Note that, particularly at low T_0 , we usually have $\tau_\epsilon(\epsilon) \gg \tau_m(\epsilon_k)$, meaning an electron may change momentum many times before losing coherence



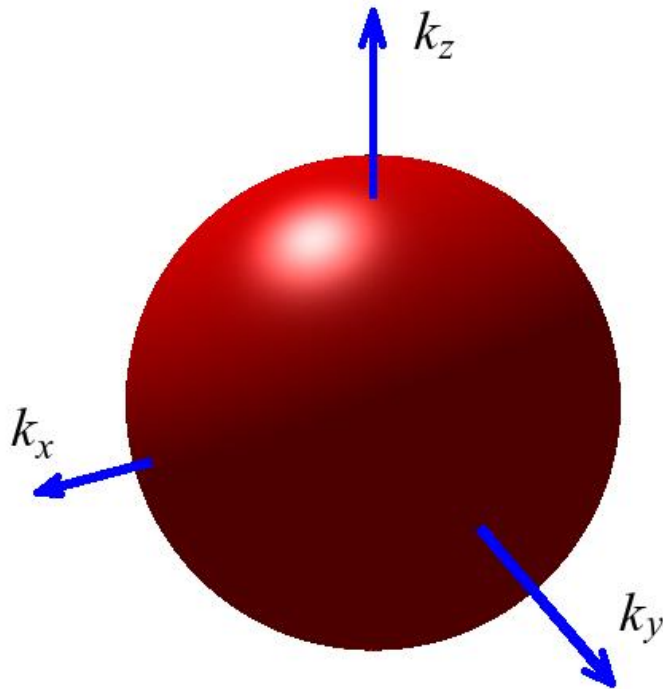
(a)



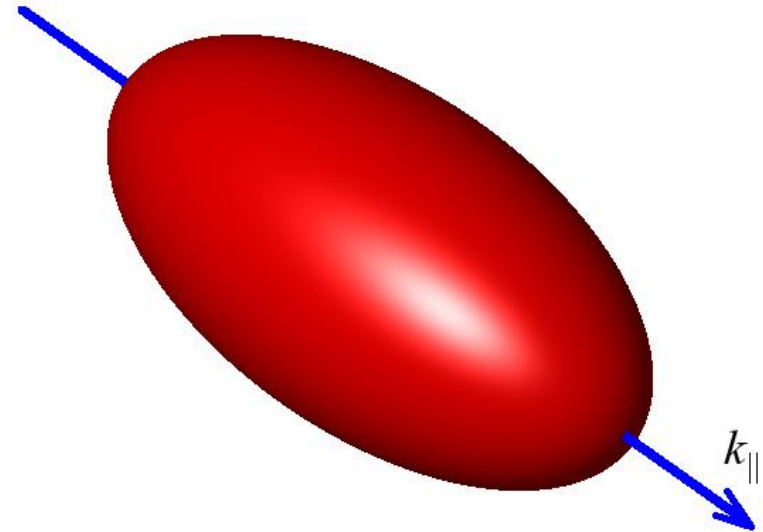
(b)

Fig. 1 (a) The Brillouin zone of a face-centred cubic crystal, showing the Γ , X and L symmetry points. (b) Schematic band-structure of a direct band-gap semiconductor showing the Γ , X and L valleys.

Surfaces of constant energy in the Brillouin zone

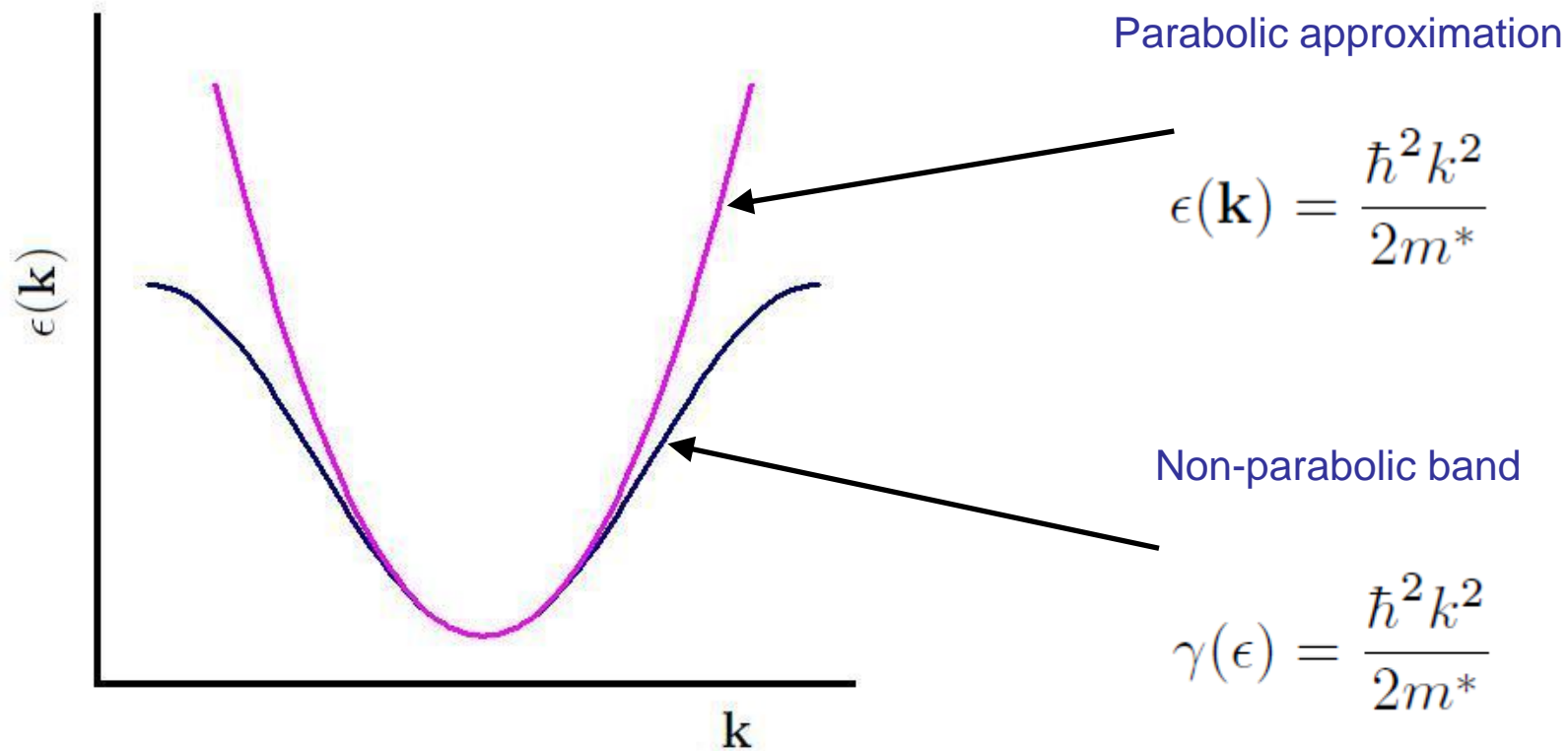


Spherical valley
(here centred on Γ point)



Spheroidal valley
(here lying along the Δ line)

Dispersion relations



The effective mass m^* is inversely proportional to the curvature of the band ($d^2\epsilon/dk^2$) at the band edge

The γ function describing the dispersion relations modifies:

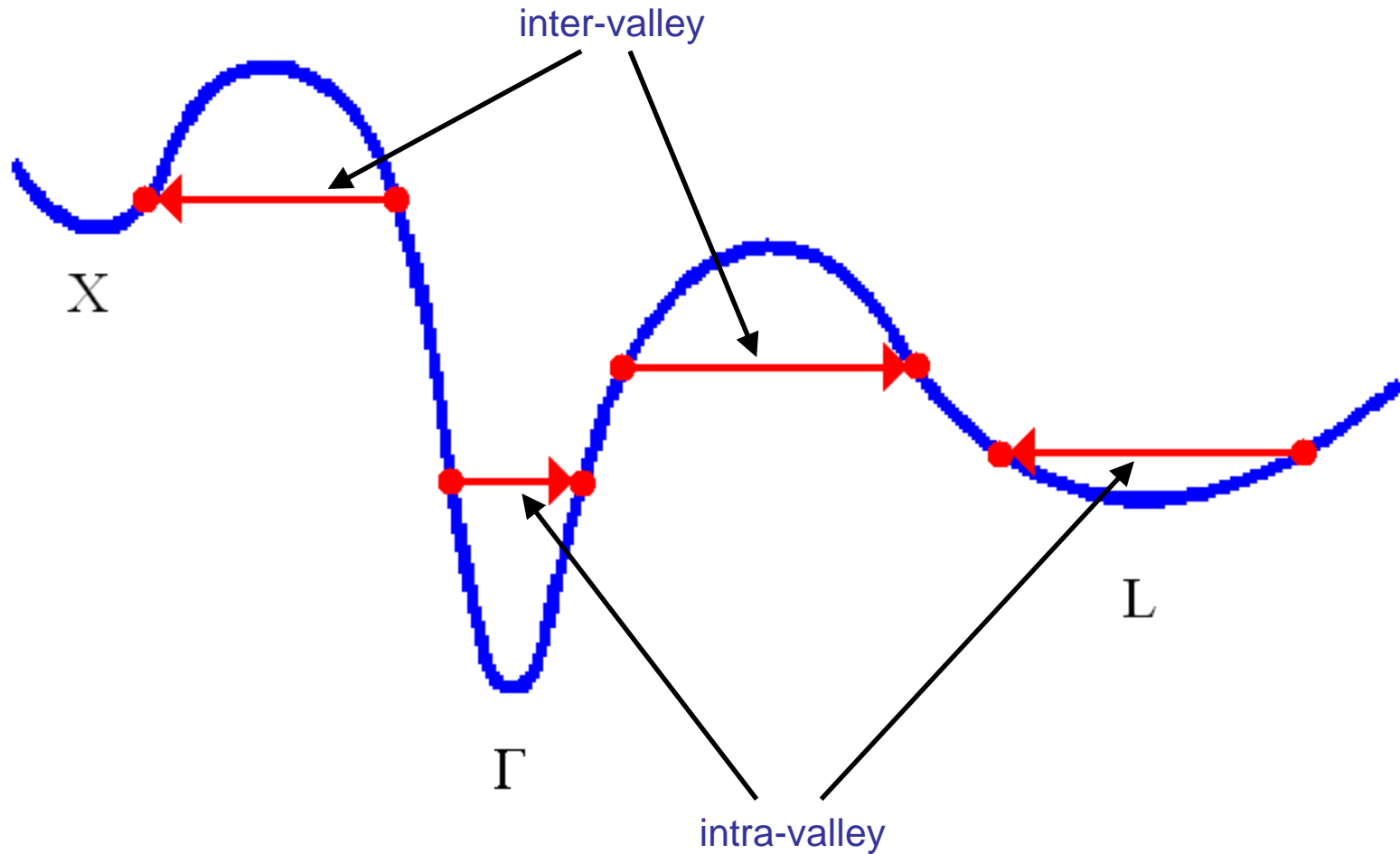
The electron group velocity

(here just the energy dependent magnitude is given)

$$v(\epsilon) = \left(\frac{2\gamma(\epsilon)}{m^*} \right)^{1/2} \left(\frac{d\gamma}{d\epsilon} \right)^{-1}$$

The density of states (DOS)

$$D(\epsilon) = V_C \frac{(2m^*)^{3/2}}{4\pi^2 \hbar^3} \gamma(\epsilon)^{1/2} \frac{d\gamma}{d\epsilon}$$



- The Fermi-Dirac distribution $f_0(\epsilon)$ gives the energetic electron distribution function in equilibrium
- We assume that under non-equilibrium conditions, there exists a distribution function $f(\mathbf{k})$, giving the probability a state in \mathbf{k} -space near to \mathbf{k} is occupied.
- This is the basis of the *semi-classical approach*
- **The principal task of semi-classical transport calculations is to find $f(\mathbf{k})$**

The **current density** is the integral of the group velocity times the probability of occupation, integrated over all states.

$$\mathbf{j} = -\frac{2e}{(2\pi)^3} \int \mathbf{v}(\mathbf{k}) f(\mathbf{k}) d^3\mathbf{k}$$

Note that phenomenologically:

$$\mathbf{j} = \sigma(\mathbf{E})\mathbf{E}$$

where σ is the conductivity tensor and \mathbf{E} must now be embedded in $f(\mathbf{k})$ somehow.

Note also that when the integral above is turned into an integral over energy, because $v(\epsilon)D(\epsilon) \sim m^*$, the conductivity must be (roughly) proportional to the effective mass.

The mobility is defined as

$$\mu(\mathbf{E}) = \frac{\sigma(\mathbf{E})}{en}$$

where the **free carrier density** is given by

$$n = \frac{2}{(2\pi)^3} \int_{CB} f(\mathbf{k}) d^3\mathbf{k}$$

The current density can then be written

$$\mathbf{j} = ne\mu(\mathbf{E})\mathbf{E} = ne\mathbf{v}_D(\mathbf{E})$$

where \mathbf{v}_D is the drift velocity (an average quantity)

Note that the mobility will also be proportional to the effective mass

Balance of energy:

$$\frac{d\epsilon}{dt} = -e\mathbf{E} \cdot \mathbf{v}_D - \left\langle \frac{d\epsilon}{dt} \right\rangle_s$$

Rates of change due to scattering, averaged over $f(\mathbf{k})$

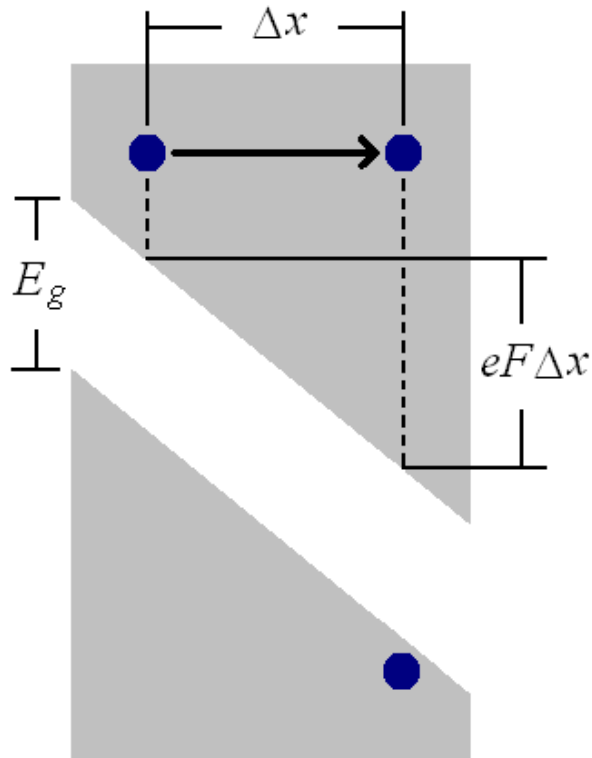
Balance of momentum:

$$\frac{d\hbar\mathbf{k}}{dt} = -e\mathbf{E} - \left\langle \frac{d\hbar\mathbf{k}}{dt} \right\rangle_s$$

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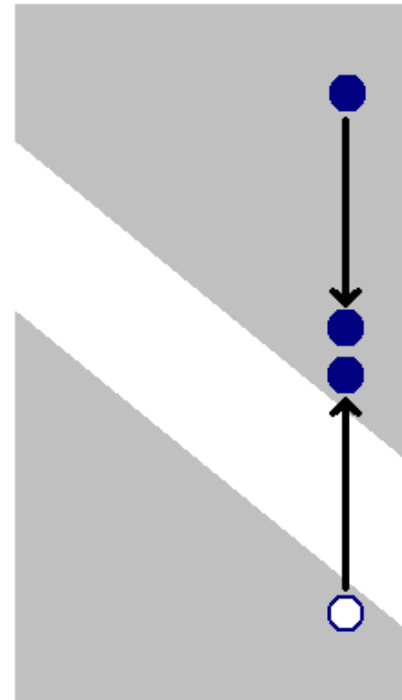
- **Avalanche multiplication**
- **Negative differential resistance**
- **Microwave oscillations**

Schematic of impact ionization for electrons



(a) An electron gains an energy $eF\Delta x$ ($> E_g$) from the field.

N.B. This is the inverse process to Auger recombination



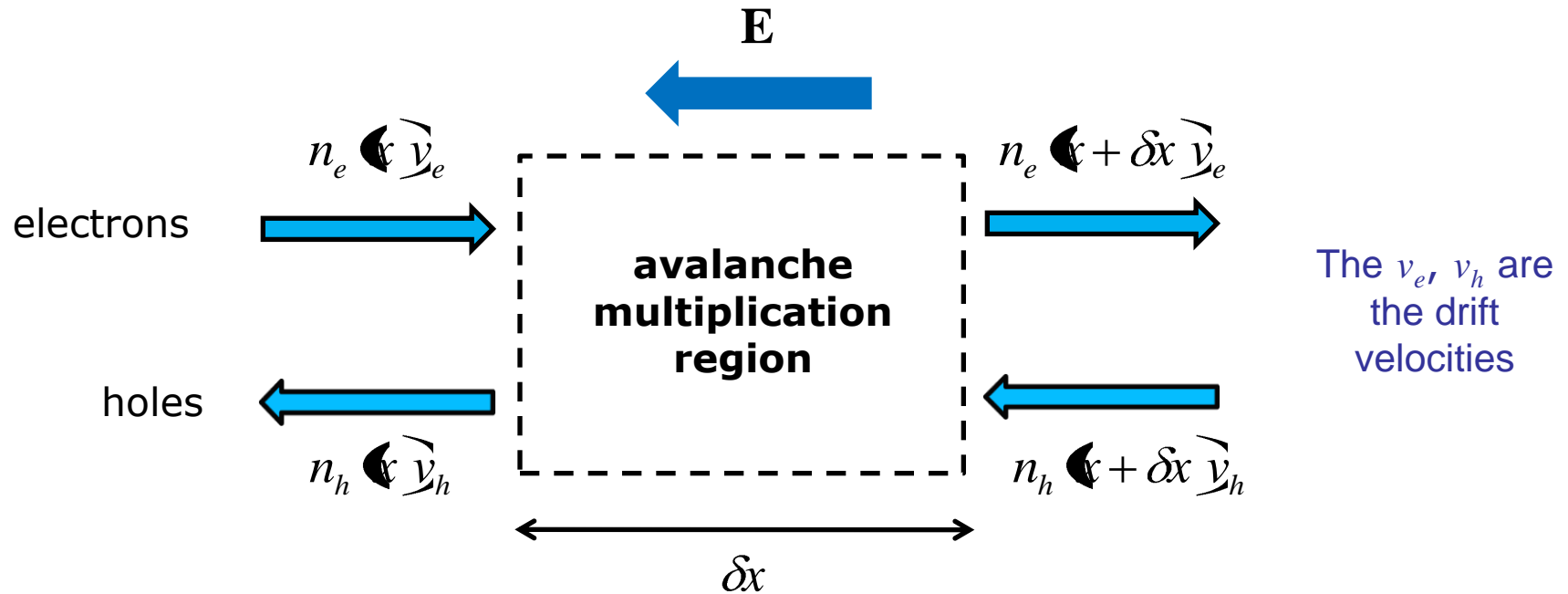
(b) After colliding with an ion, the electron gives up its energy to form an electron-hole pair.

We can define the probability that a given carrier will ionize an electron-hole pair in distance dx by $\alpha(E)dx$ (for electrons) or $\beta(E)dx$ (for holes), where

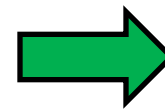
- $\alpha(E)$ is the **electron ionization coefficient** and
- $\beta(E)$ is the **hole ionization coefficient**

Here, $\alpha(E)$ and $\beta(E)$ are interpreted as *rates* (per unit distance). Alternatively, we can think in terms of the quantities

- $1/\alpha(E)$ the average distance an electron travels between ionizing collisions and
- $1/\beta(E)$ the average distance a hole travels between ionizing collisions.



$$\begin{aligned}
 n_e \ll + \delta x \ll_e &= n_e \ll \ll_e \\
 &+ \ll n_e \ll \ll_e + \beta n_h \ll + \delta x \ll_h \ll \delta x \\
 n_h \ll \ll_h &= n_h \ll + \delta x \ll_h \\
 &+ \ll n_e \ll \ll_e + \beta n_h \ll + \delta x \ll_h \ll \delta x
 \end{aligned}$$



$$\begin{aligned}
 \frac{dj_e}{dx} &= \alpha j_e \ll + \beta j_h \\
 \frac{dj_h}{dx} &= -\alpha j_e \ll - \beta j_h
 \end{aligned}$$

Solving the differential equations

$$\frac{dj_e}{dx} = \alpha j_e + \beta j_h$$

$$\frac{dj_h}{dx} = -\alpha j_e - \beta j_h$$

with boundary conditions

$$j_e(0) = J_0$$

$$j_e(\Delta x) = J$$

$$j_h(\Delta x) = 0$$

leads to

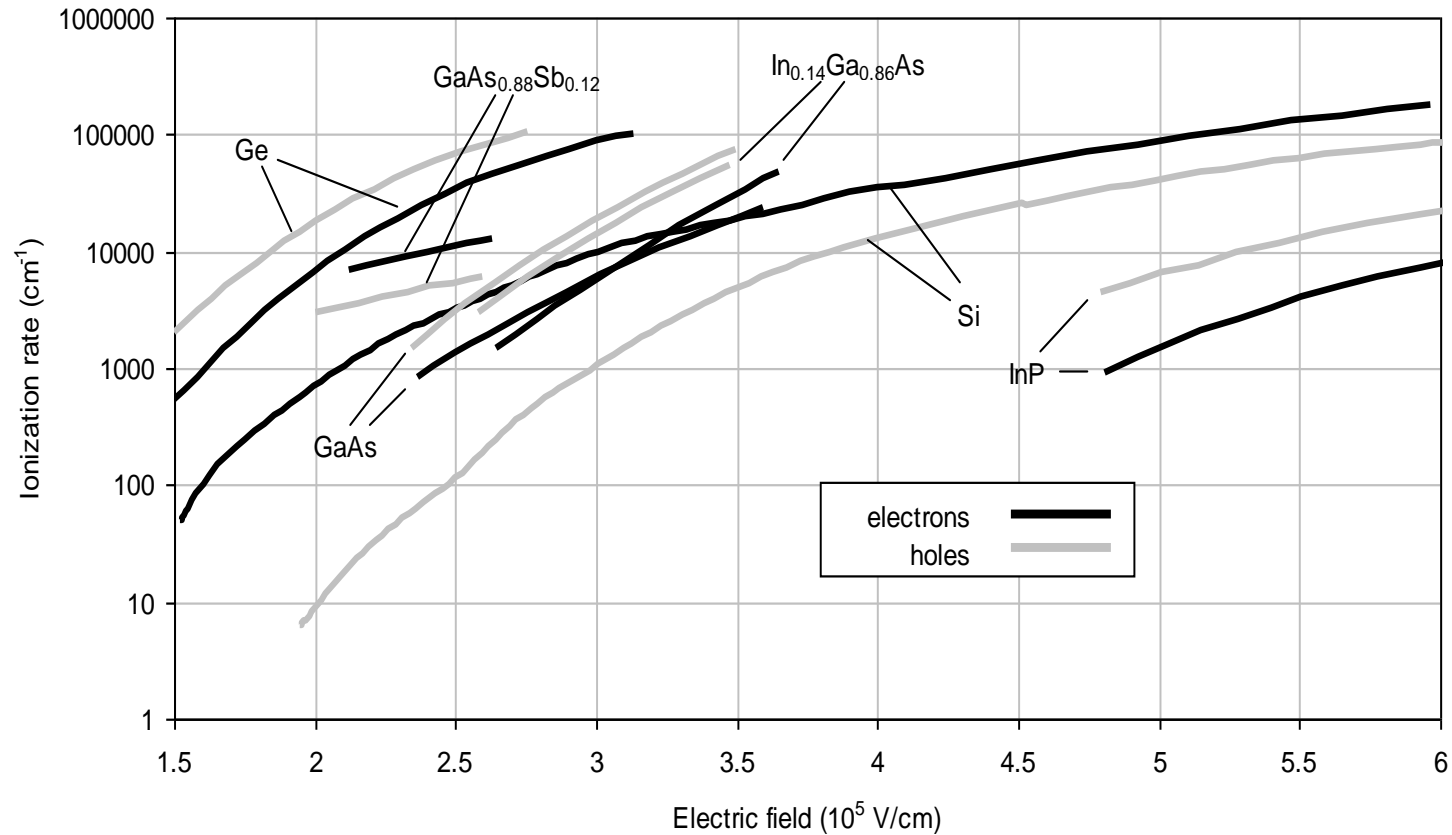
$$\frac{J}{J_0} = \frac{\alpha - \beta e^{(\alpha - \beta)\Delta x}}{\alpha - \beta e^{-(\alpha - \beta)\Delta x}}$$

This solution becomes infinite when

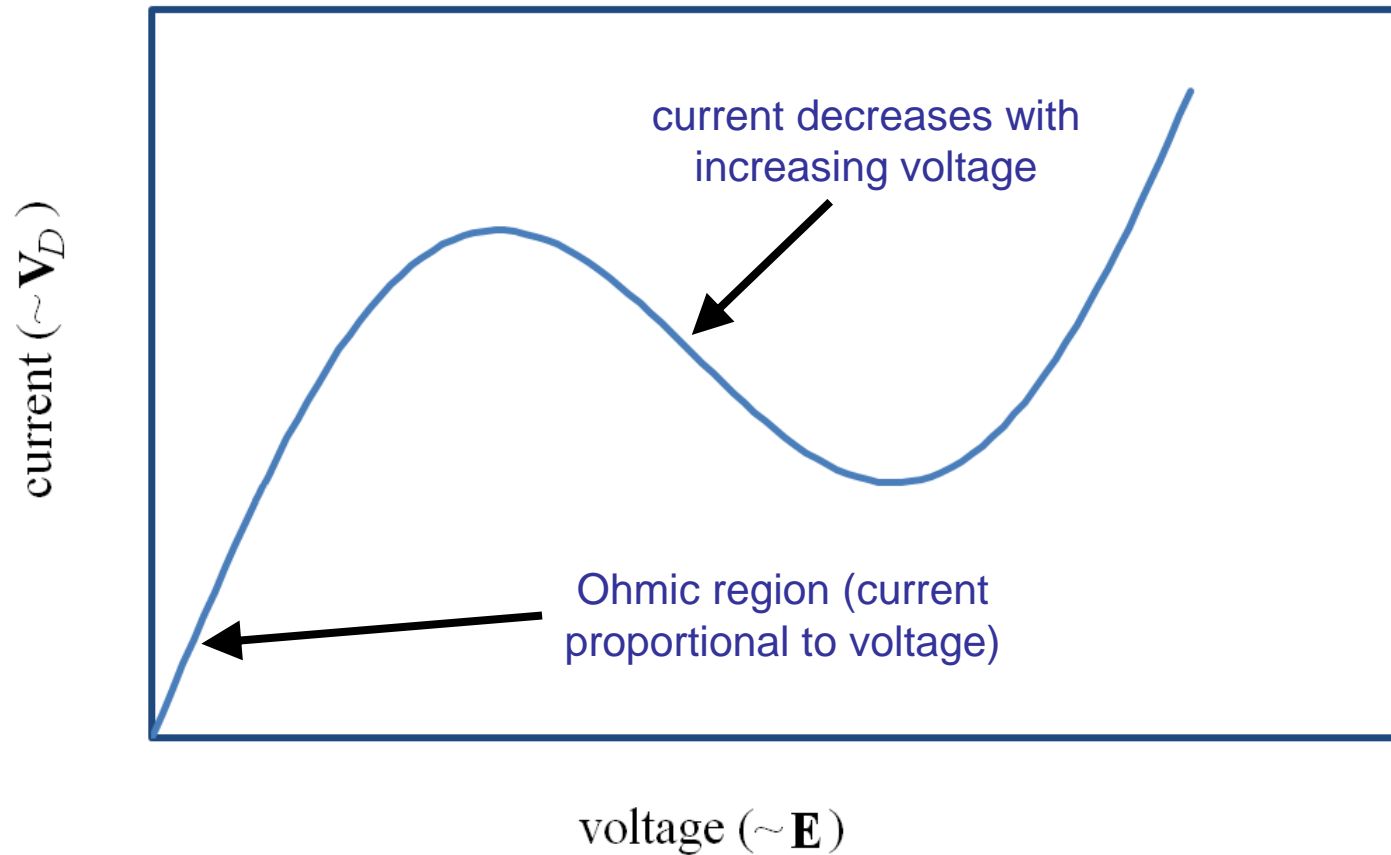
$$\alpha = \beta e^{-(\alpha - \beta)\Delta x}$$

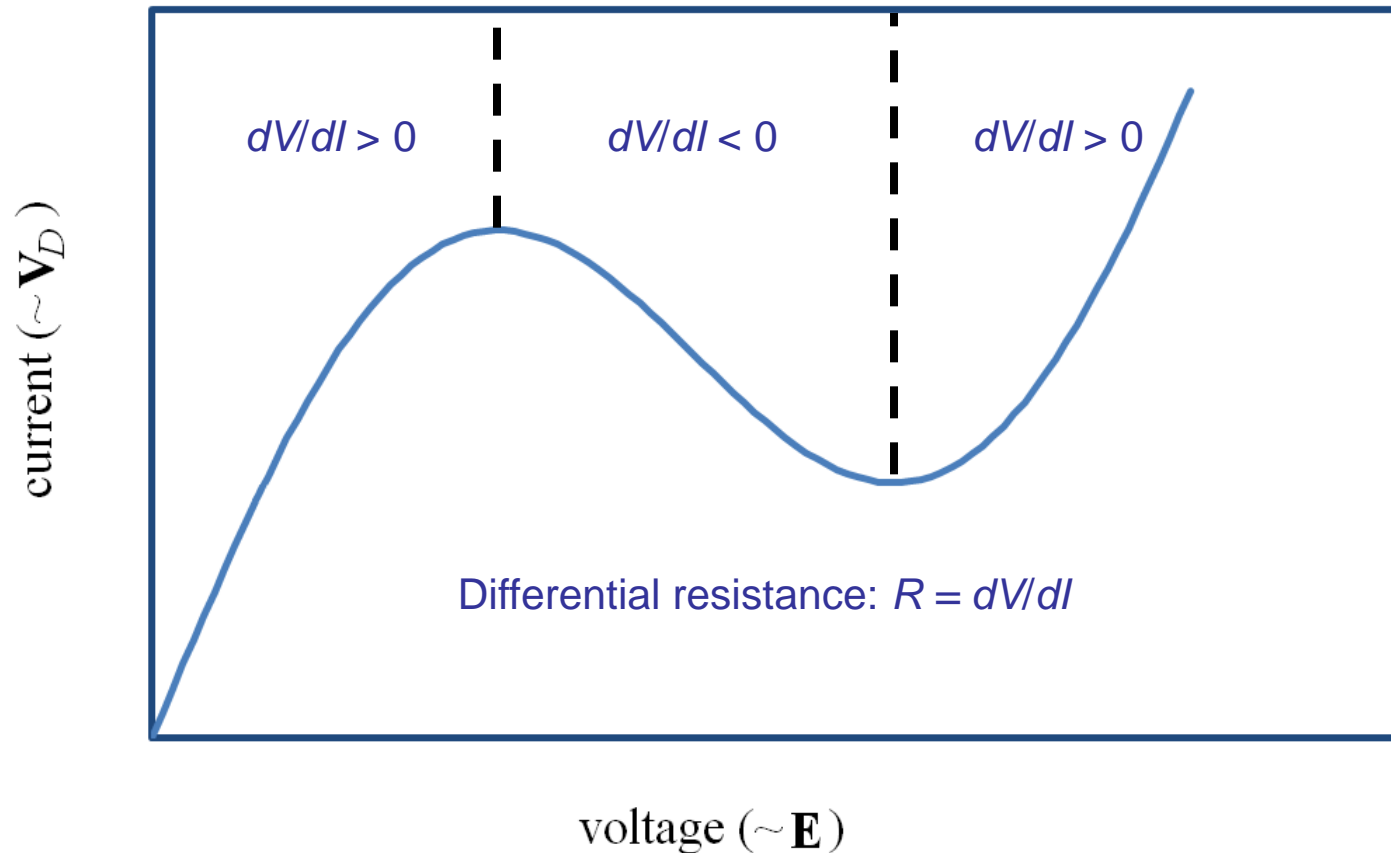
implying **avalanche breakdown**

Avalanche multiplication is exploited as a gain mechanism in **avalanche photodiodes (APDs)**

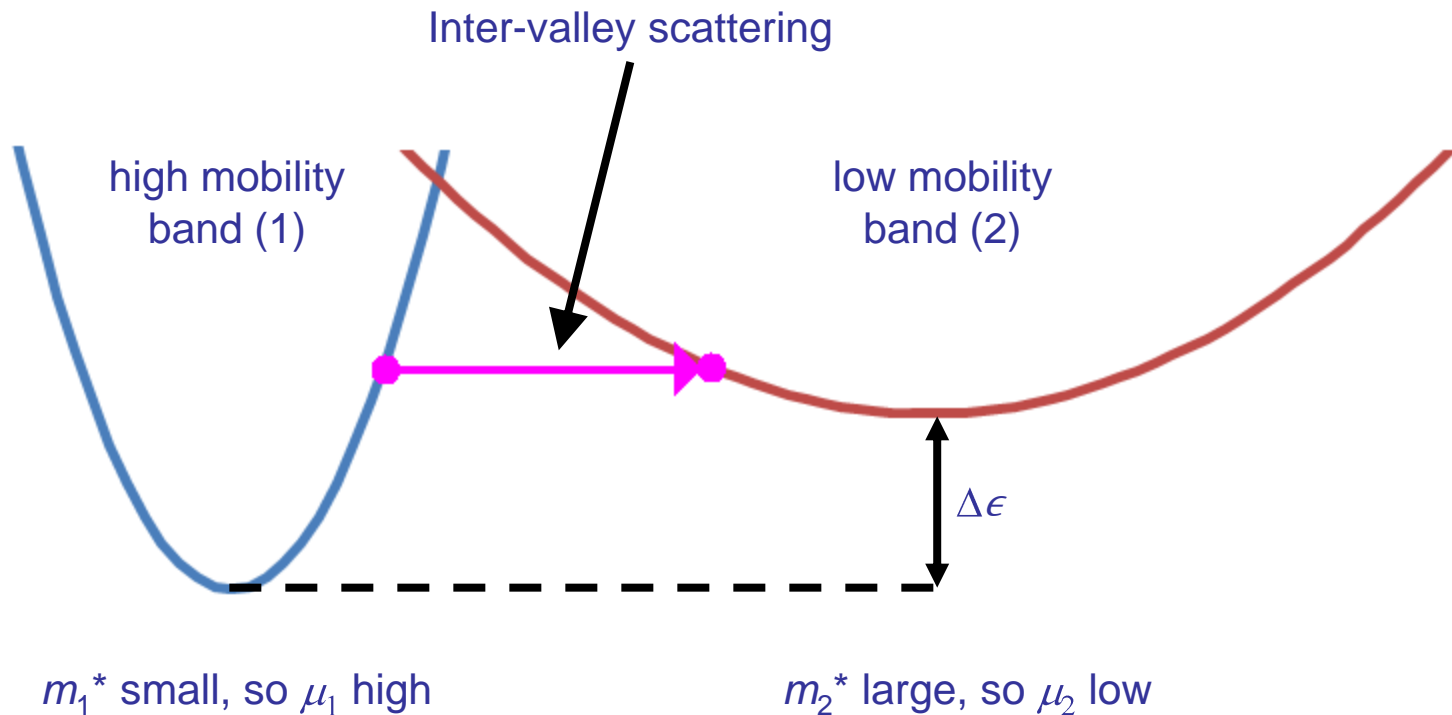


Taken from: T.P. Lee & T. Li in, Optical Fiber Telecommunications I, S.E. Miller & A.G. Chynoweth, Eds., Academic Press, San Diego, CA, 1979, Chap. 18.



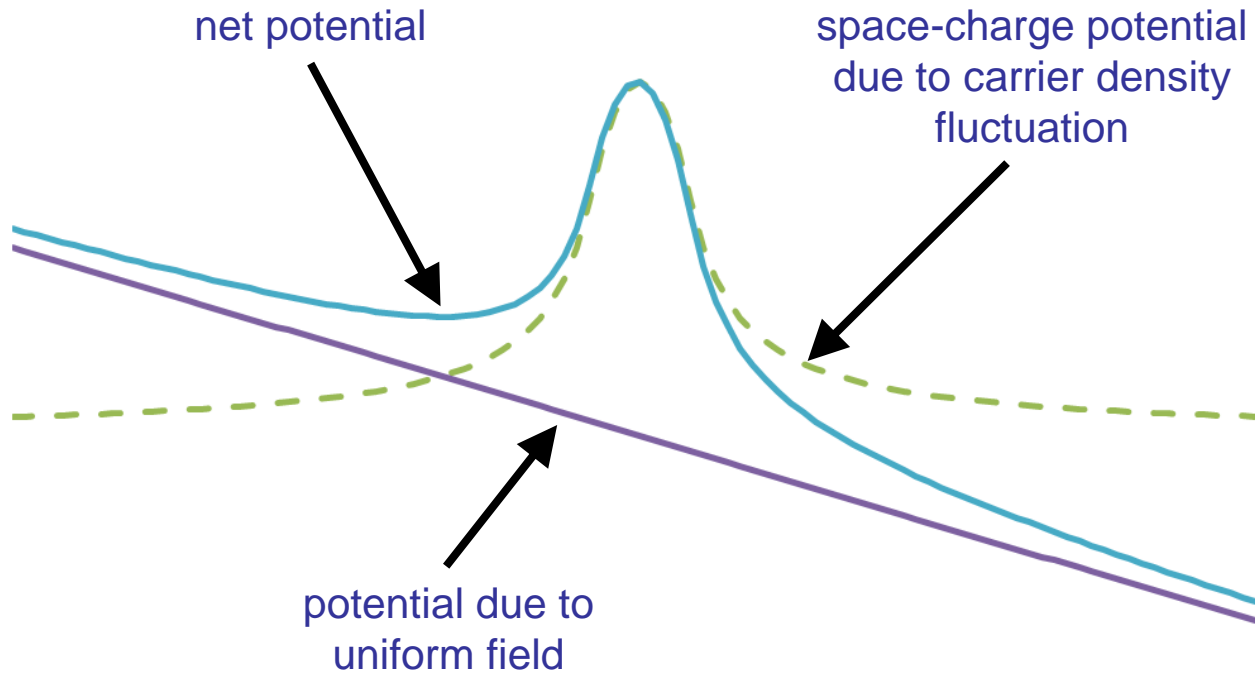


Such an NDR and the consequent microwave oscillations observed can be explained by the **Ridley-Watkins-Hilsum mechanism**

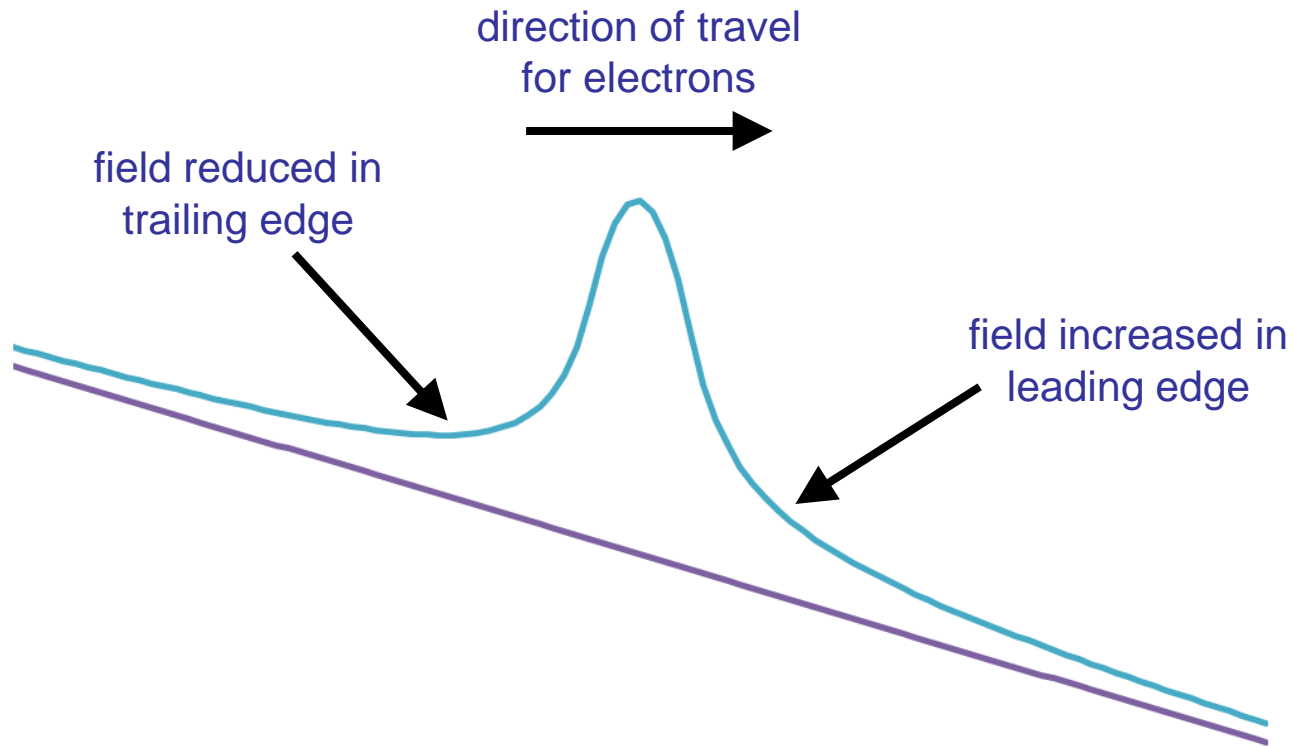


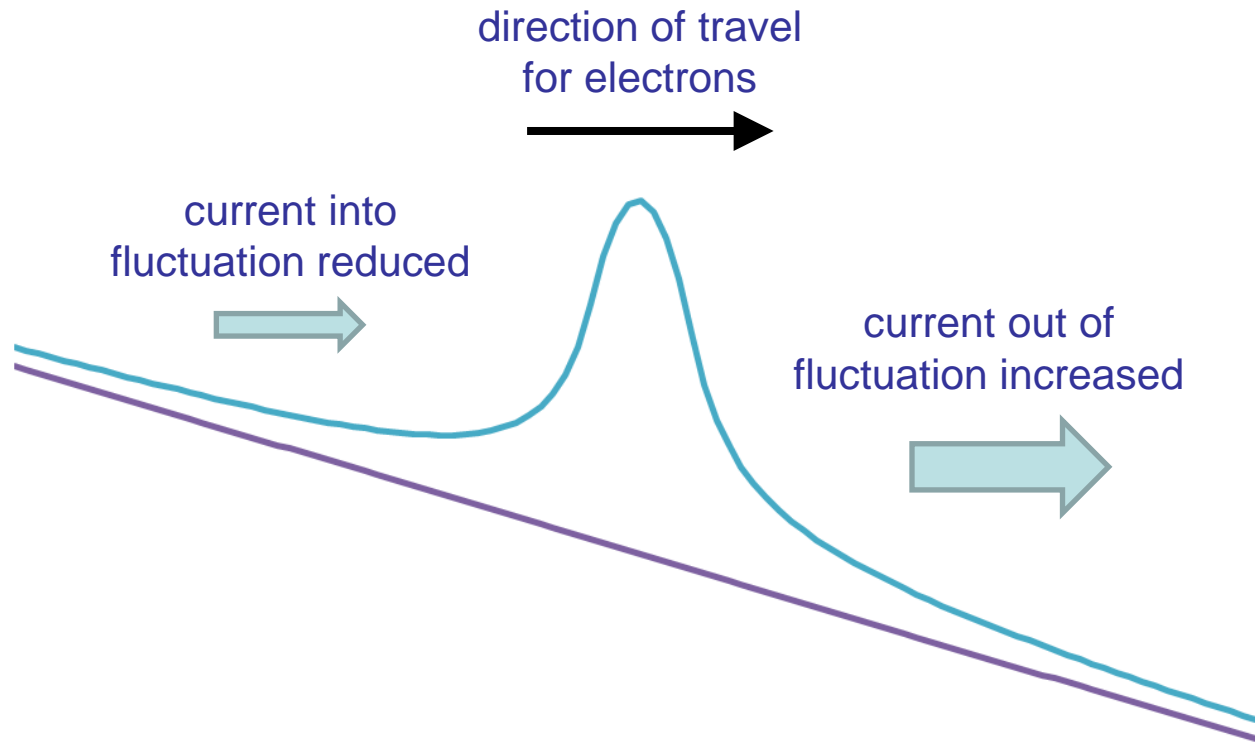
[1] B.K. Ridley and T.B. Watkins, *Proc. Phys. Soc.* **78**, 293 (1961)

[2] C. Hilsum, *Proc. IRE* **50**, 185 (1962)

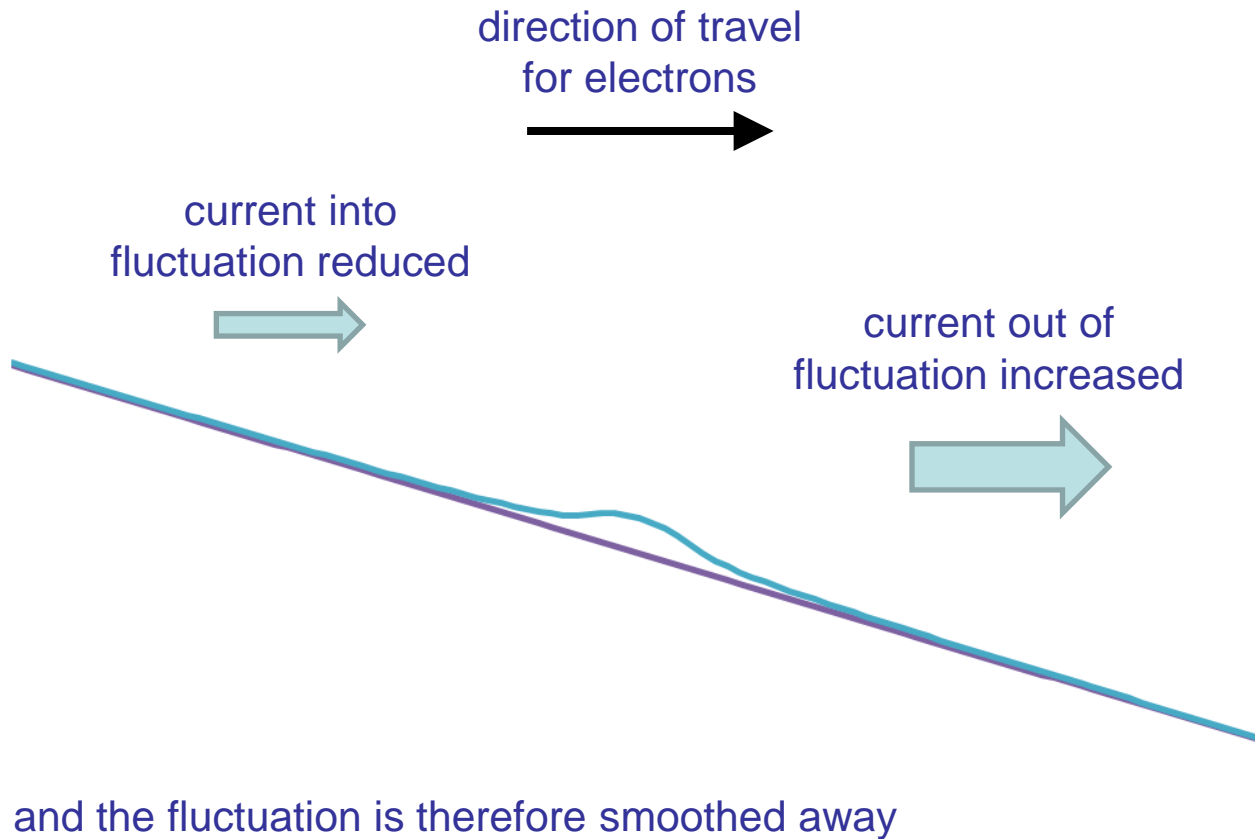


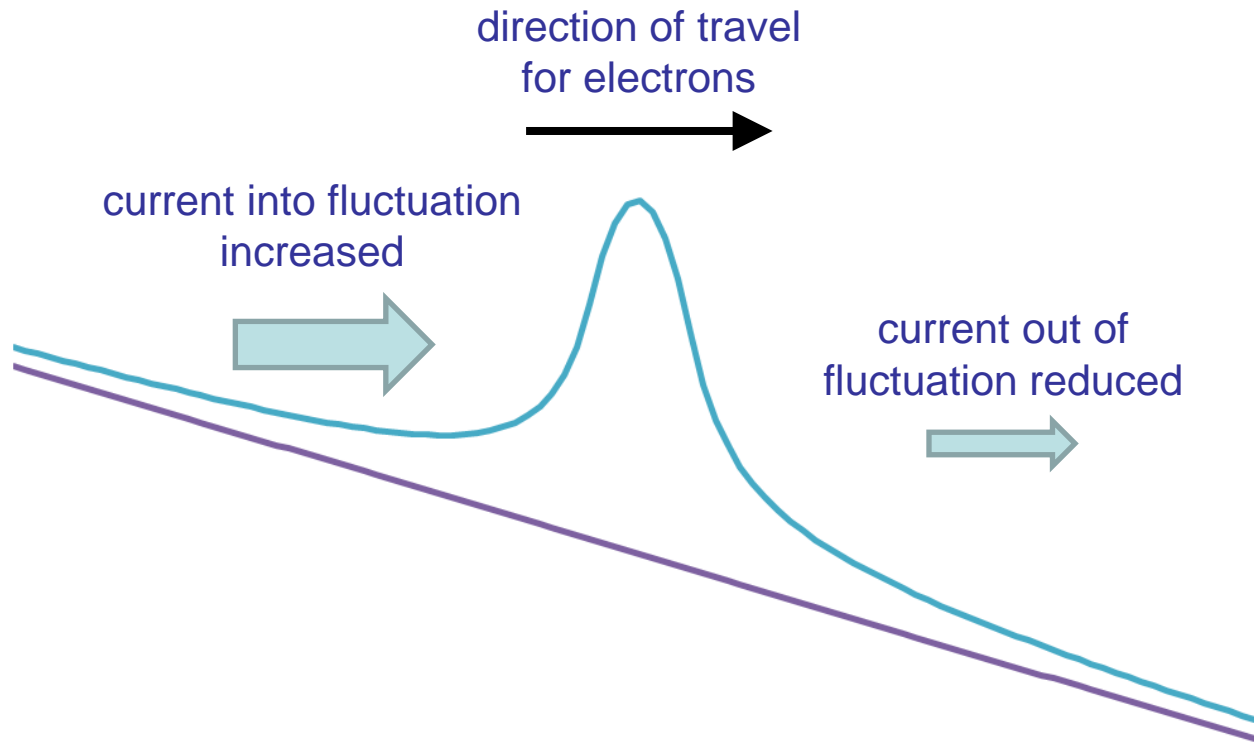
[1] B.K. Ridley and T.B. Watkins, *Proc. Phys. Soc.* **78**, 293 (1961)



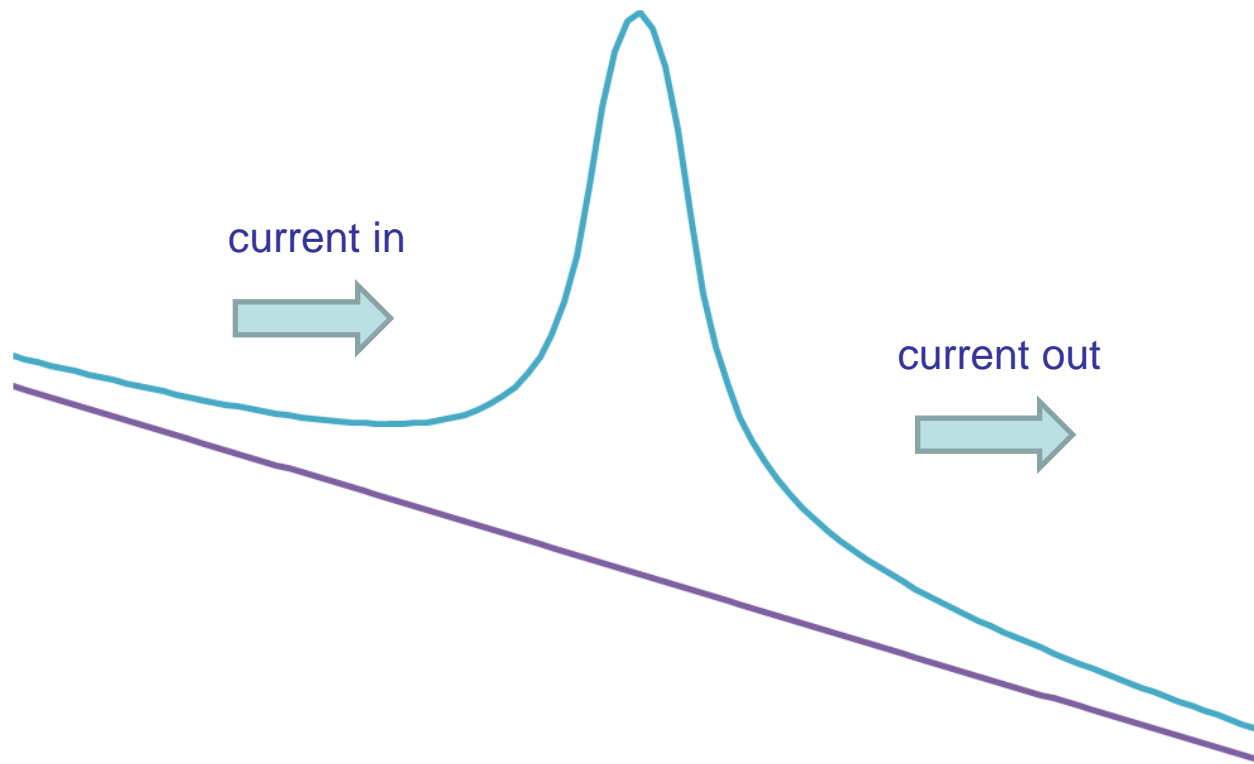


Under normal conditions of positive differential resistance, there is a net current out of the space-charge fluctuation

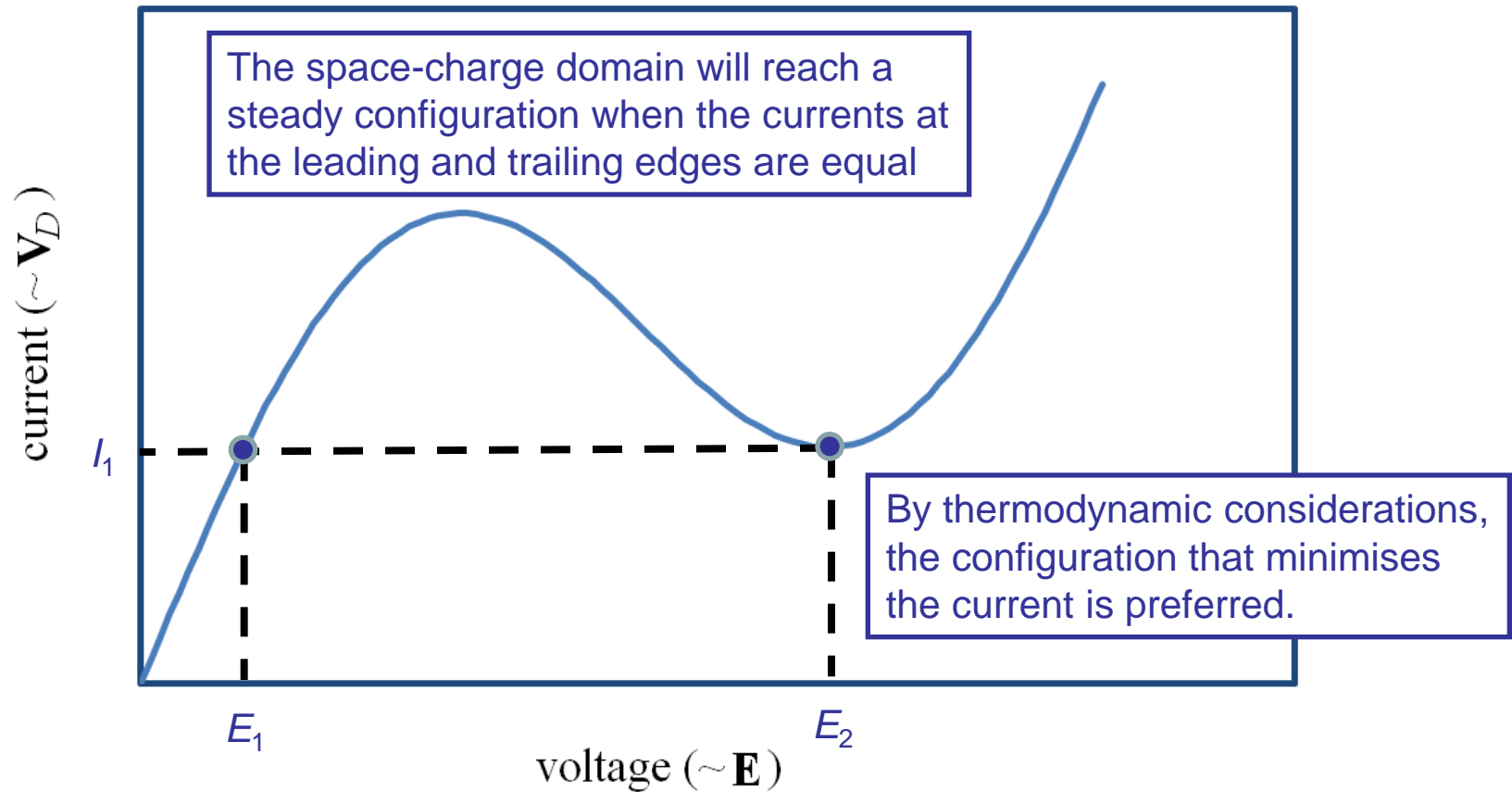




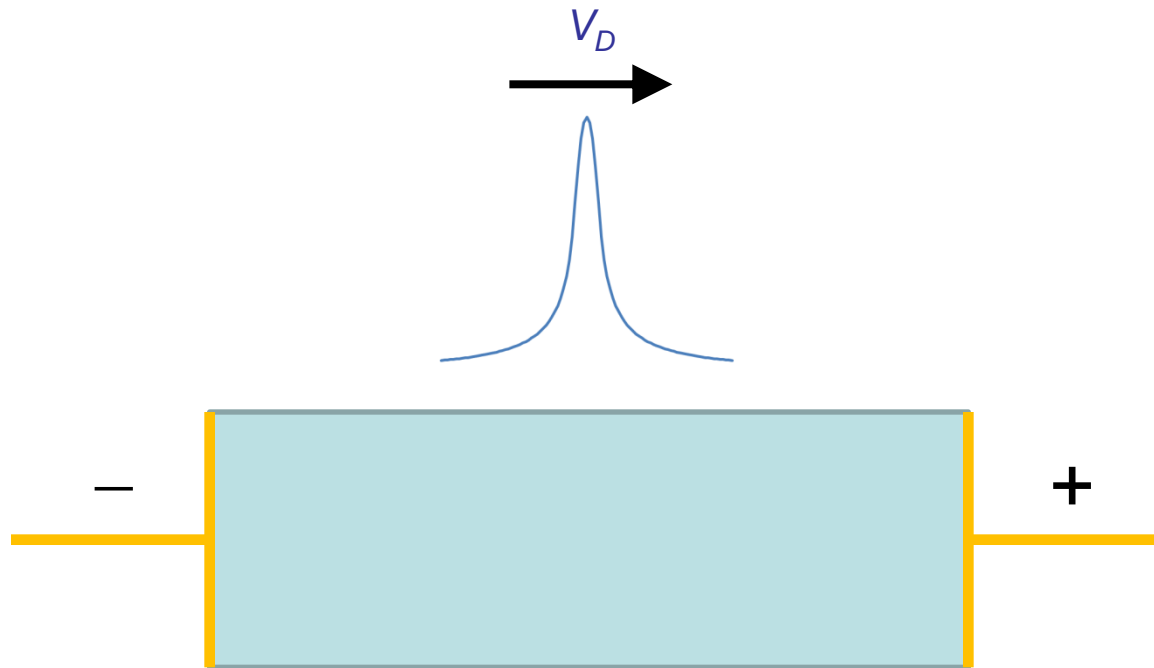
In the case of negative differential resistance, the reverse situation pertains and we have a net flow of charge into the fluctuation



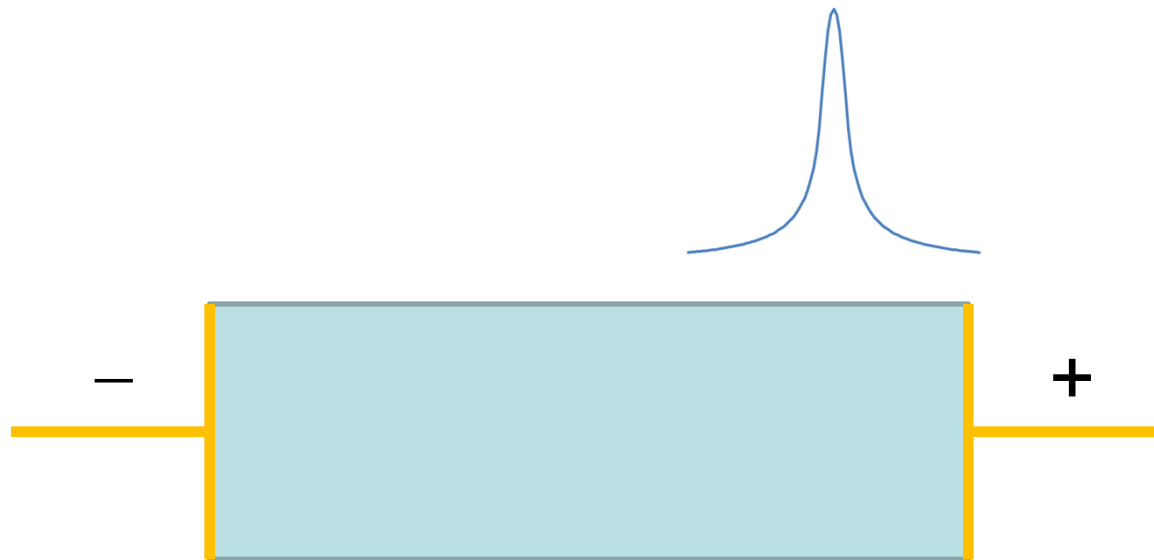
Hence the space charge increases until the currents in and out of the fluctuation equalise



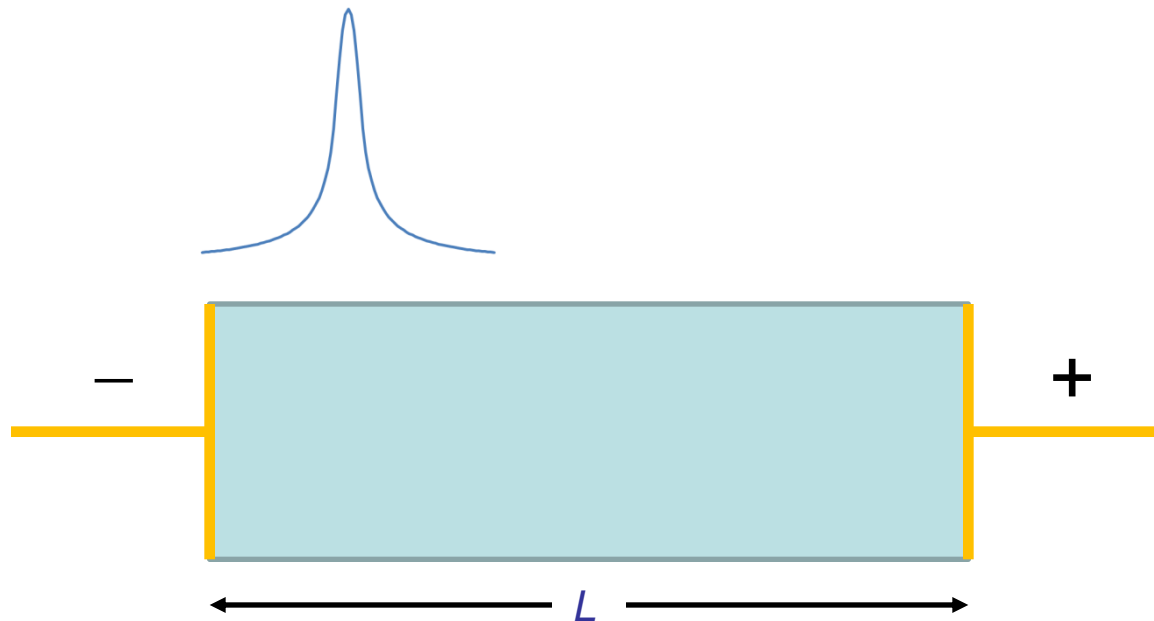
[1] B.K. Ridley , *Proc. Phys. Soc.* **82**, 954 (1963)



The high-field domain travels along the field with the drift velocity V_D associated with I_1 . For short devices, there is likely to be only one domain in the device at a time.



As the domain leaves the device at the positive terminal,



another is nucleated at the negative terminal.

Hence we obtain current oscillations with a frequency of approximately V_D/L . This is the mechanism of the **Gunn diode**.

[1] J.B. Gunn, *IBM J. Res. & Dev.* **8**, 141 (1964)

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- The intrinsic scattering rate
- Phonons
- The Coulomb interaction
- Other scattering mechanisms

Scattering rate per
k-state from **k'** to **k**

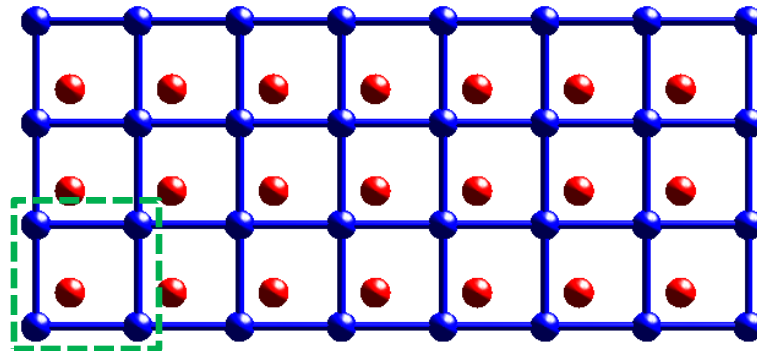
V_C is the volume of the
crystal; $2\pi^3/V_C$ is the
volume in reciprocal space
occupied by a **k**-state

$$s(\mathbf{k}', \mathbf{k}) = \frac{2\pi}{\hbar} |\langle \mathbf{k} | V | \mathbf{k}' \rangle|^2 \frac{V_C}{(2\pi)^3} \delta(\epsilon' - \epsilon)$$

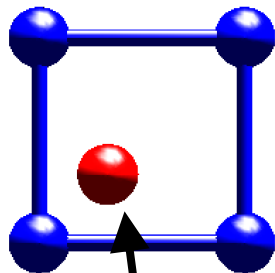
Matrix element for the
transition probability per unit
time from state **k'** to **k**

Here, the Dirac delta gives the
condition for conservation of energy
(in this case, for elastic scattering)

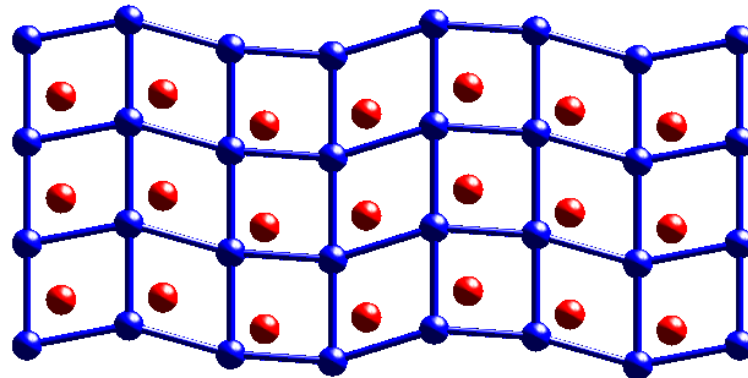
Schematic of
crystal lattice



unit cell



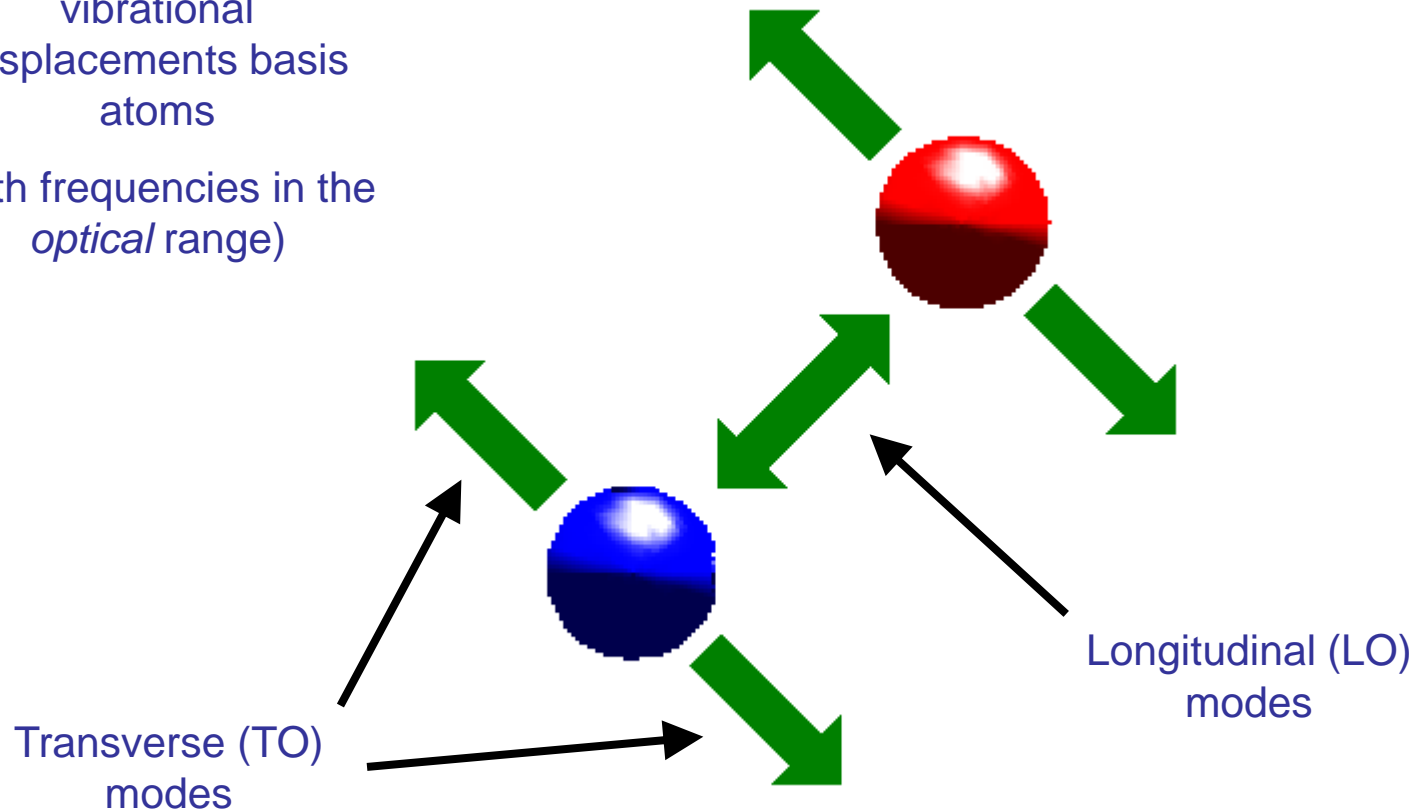
basis
atoms



Acoustic phonons are
vibrational
displacements of the
unit cells
(with frequencies in the
acoustic range)

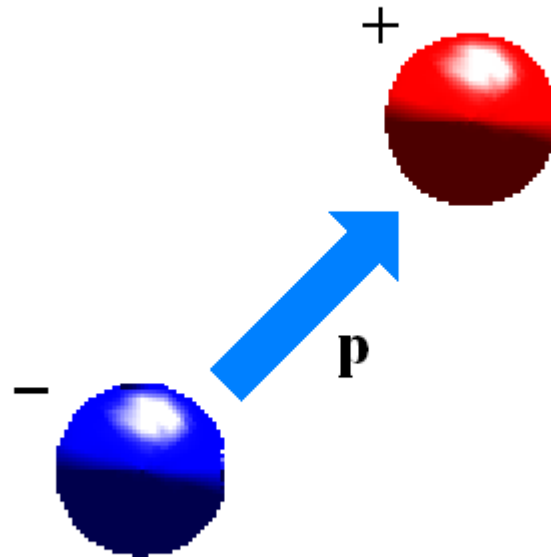
Optical phonons are
vibrational
displacements basis
atoms

(with frequencies in the
optical range)



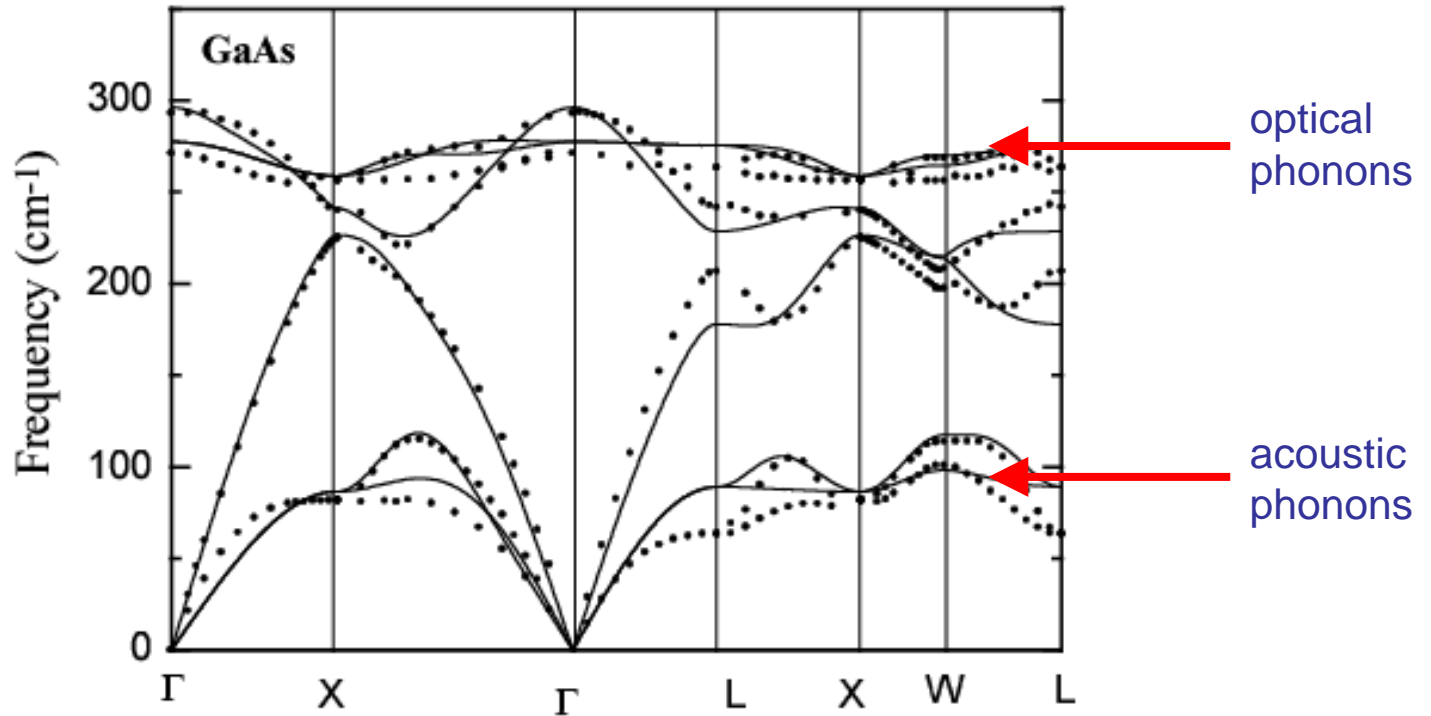
If the basis atoms are of a different type, there may be a redistribution of charge between them...

... giving rise to an electric dipole \mathbf{p} between them



Longitudinal polar optical phonons couple very strongly with electrons

M.Sternik, P.T.Jochym and Parlinski, *Comput. Materials Science* **13** 232 (1999).



Note that the frequency of the optical phonons is roughly constant, whilst, near the Γ -point, the frequency of acoustic phonons is proportional to wavevector

For phonons, the scattering is inelastic. The rate must also be decomposed into terms for emission and absorption of a phonon with energy $\hbar\omega$

$$s(\mathbf{k}', \mathbf{k}) = s_A(\mathbf{k}', \mathbf{k})\delta(\epsilon' - \epsilon + \hbar\omega) + s_E(\mathbf{k}', \mathbf{k})\delta(\epsilon' - \epsilon - \hbar\omega)$$

where

$$s_A(\mathbf{k}', \mathbf{k}) = \frac{2\pi}{\hbar} \left| M_{\mathbf{k}'\mathbf{k}}^{n'n'-1} \right|^2 \frac{V_C}{(2\pi)^3}$$

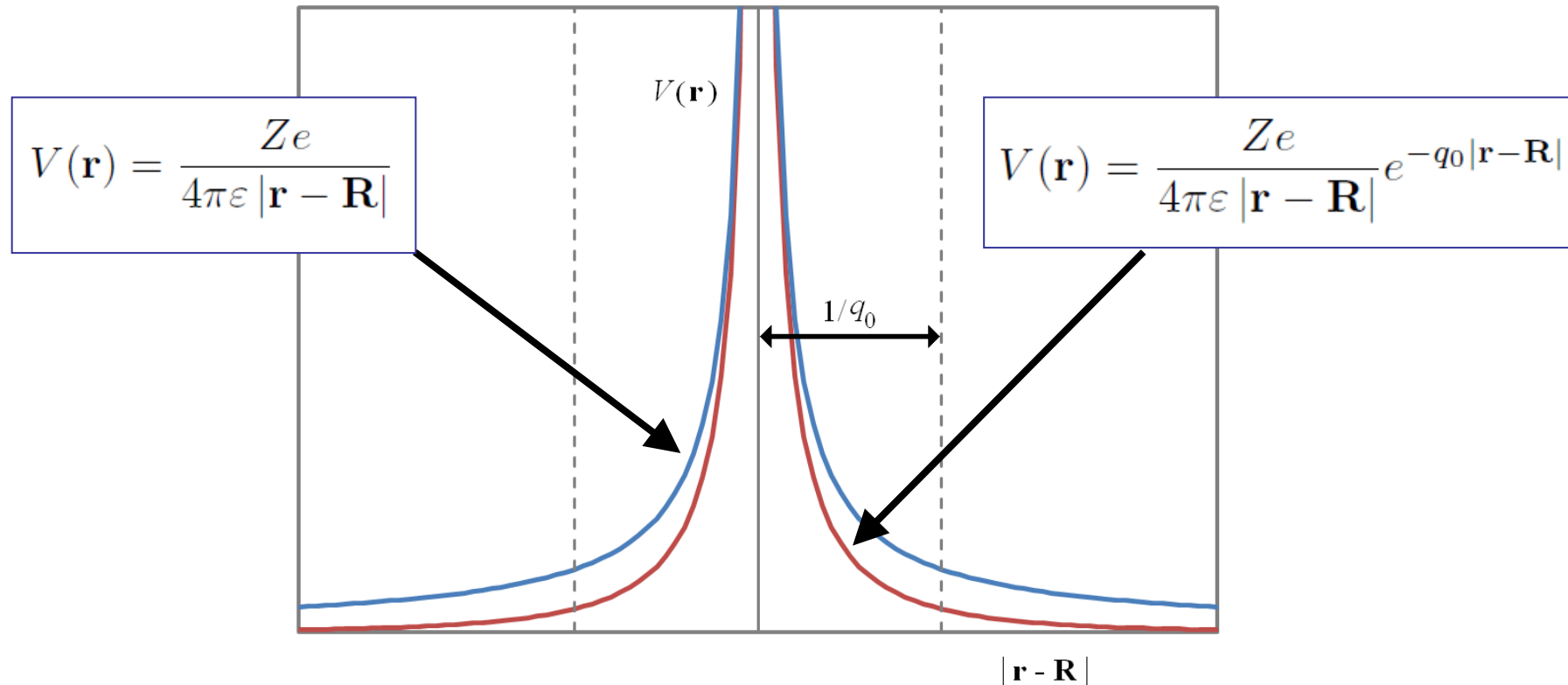
is for *absorption* of a phonon and

$$s_E(\mathbf{k}', \mathbf{k}) = \frac{2\pi}{\hbar} \left| M_{\mathbf{k}'\mathbf{k}}^{n'n'+1} \right|^2 \frac{V_C}{(2\pi)^3}$$

is for *emission*.

n is the phonon occupation number (given by the Bose-Einstein factor).

It is known that a bare Coulomb potential leads to electron scattering at all distances.



However, the redistribution of free charge around a charged particle usually gives rise to some kind of screening (here q_0 is the reciprocal screening length)

- Charged impurity scattering
 - Ionized donors and acceptors
 - Significant at low T_0
- Electron-hole scattering
 - Significant for narrow gap semiconductors at room temperature
- Electron-electron scattering
 - Does not relax net momentum but may randomize momentum, with consequences for the high-field distribution function
- Impact-ionization
 - Significant at high fields once free electrons attain sufficient energy to ionize a valence-band electron

- Neutral impurity scattering
 - For non-ionized donors and acceptors, only significant at very low T_0
 - More generally, may contribute to resistivity over all temperature ranges
 - Resonant states (such as N in GaAs) may give very strong scattering
- Alloy scattering
 - Arises from random deviations from the averaged potential due to substitutional atomic species in alloys
 - Can provide a mechanism of inter-valley scattering

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- High field devices

- General form of the BTE
- The linearized distribution function
- Low-field solution and the ladder method
- High-field solution for a single valley
- Inter-valley transfer

Temporal rate
of change

Force term



Ludwig Boltzmann (1844 – 1906)

$$\frac{df(\mathbf{k})}{dt} = \left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_s - \frac{d\mathbf{k}}{dt} \cdot \nabla_{\mathbf{k}} f(\mathbf{k}) - \mathbf{v}(\mathbf{k}) \cdot \nabla f(\mathbf{k})$$

Scattering
term

Density / temperature
gradient term

intrinsic scattering
from \mathbf{k}' to \mathbf{k}

probability \mathbf{k} not
occupied

probability \mathbf{k}
occupied

$$\left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_s = \int s(\mathbf{k}', \mathbf{k}) f(\mathbf{k}') [1 - f(\mathbf{k})] - s(\mathbf{k}, \mathbf{k}') f(\mathbf{k}) [1 - f(\mathbf{k}')] d^3 \mathbf{k}'$$

probability \mathbf{k}'
occupied

intrinsic scattering
from \mathbf{k} to \mathbf{k}'

probability \mathbf{k}' not
occupied

- Put $d\mathbf{k}/dt = \mathbf{F}/\hbar$, where \mathbf{F} is the applied force
- Assume no concentration / temperature gradient
- Assume steady state, so $df(\mathbf{k})/dt = 0$

Then we are left with

$$\frac{\mathbf{F}}{\hbar} \cdot \nabla_{\mathbf{k}} f(k) = \left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_s$$

We shall take $\mathbf{F} = -e\mathbf{E}$, where \mathbf{E} is the electric field

(1) Expand $f(\mathbf{k})$ to first order

$$f(\mathbf{k}) = f_0(\mathbf{k} - \delta\mathbf{k}) = f_0(\epsilon) - \nabla_{\mathbf{k}} f_0(\epsilon) \cdot \delta\mathbf{k}$$

(2) Use change rule and $\mathbf{v} = \nabla_{\mathbf{k}}\omega = \nabla_{\mathbf{k}}\epsilon/\hbar$ for group velocity

$$f(\mathbf{k}) = f_0(\epsilon) - \hbar \frac{df_0(\epsilon)}{d\epsilon} \mathbf{v}(\mathbf{k}) \cdot \delta\mathbf{k}$$

(3) Put $\hbar\delta\mathbf{k}$ as momentum gained from \mathbf{E} before scattering

$$\delta\mathbf{k} = -\frac{e\mathbf{E}\tau(\epsilon)}{\hbar}$$

(4) Substitute in $\delta\mathbf{k}$

$$f(\mathbf{k}) = f_0(\epsilon) + e\tau(\epsilon) \frac{df_0(\epsilon)}{d\epsilon} \mathbf{v}(\mathbf{k}) \cdot \mathbf{E}$$

(5) Define f_1 as asymmetric part of $f(\mathbf{k})$

$$f_1(\epsilon) = e\tau(\epsilon) \frac{df_0(\epsilon)}{d\epsilon} E v(\epsilon) x$$

(x is cosine of angle between \mathbf{v} and \mathbf{E})

Our task now is to determine $\tau(\epsilon)$

Inserting

$$f(\mathbf{k}) = f_0(\epsilon) + e\tau(\epsilon) \frac{df_0(\epsilon)}{d\epsilon} \mathbf{v}(\mathbf{k}) \cdot \mathbf{E}$$

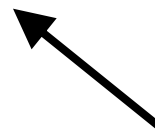
into

$$\mathbf{j} = -\frac{2e}{(2\pi)^3} \int \mathbf{v}(\mathbf{k}) f(\mathbf{k}) d^3\mathbf{k}$$

Recalling that

$$\mathbf{j} = \sigma(\mathbf{E}) \mathbf{E}$$

symmetric part of $f(\mathbf{k})$ disappears due to odd parity of $\mathbf{v}(\mathbf{k})$



leads to

$$\sigma = -\frac{2e^2}{3(2\pi)^3} \int v^2(\epsilon_{\mathbf{k}}) \tau(\epsilon_{\mathbf{k}}) \frac{df_0(\epsilon_{\mathbf{k}})}{d\epsilon} d^3\mathbf{k}$$

for the low-field conductivity

Using Boltzmann's equation in the steady state

$$\frac{\mathbf{F}}{\hbar} \cdot \nabla_{\mathbf{k}} f(\mathbf{k}) = \left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_s$$

neglecting terms in E^2 the left-hand-side becomes

$$-\frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f(\mathbf{k}) = -e \mathbf{E} \cdot \mathbf{v}(\mathbf{k}) \frac{df_0(\epsilon)}{d\epsilon} = -e E v(\epsilon) x \frac{df_0(\epsilon)}{d\epsilon}$$

and the right-hand-side is decomposed into zero and first-order scattering terms

$$\left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_s = \left(\frac{\partial f_0(\epsilon)}{\partial t} \right)_s + \left(\frac{\partial f_1(\epsilon)}{\partial t} \right)_s$$

For low-field $f_0(\epsilon)$ is the Fermi-Dirac factor (i.e. equilibrium distribution), hence

$$\left(\frac{\partial f_0(\epsilon)}{\partial t} \right)_s = \int s(\mathbf{k}', \mathbf{k}) f_0(\epsilon') [1 - f_0(\epsilon)] - s(\mathbf{k}, \mathbf{k}') f_0(\epsilon) [1 - f_0(\epsilon')] d^3 \mathbf{k}'$$

disappears, being an expression of the principle of detailed balance

which just leaves

$$\begin{aligned} \left(\frac{\partial f_1(\epsilon)}{\partial t} \right)_s = & \int s(\mathbf{k}', \mathbf{k}) \{ f_1(\epsilon') [1 - f_0(\epsilon)] - f_1(\epsilon) f_0(\epsilon') \} \\ & - s(\mathbf{k}, \mathbf{k}') \{ f_1(\epsilon) [1 - f_0(\epsilon')] - f_1(\epsilon') f_0(\epsilon) \} d^3 \mathbf{k}' \end{aligned}$$

on the right-hand-side.

Substituting for $f_1(\epsilon)$, the scattering integral becomes

$$\left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_s = -e \frac{df_0(\epsilon)}{d\epsilon} E v(\epsilon) x \times \int s(\mathbf{k}', \mathbf{k}) \frac{f_0(\epsilon')}{f_0(\epsilon)} \left\{ \tau(\epsilon) - \tau(\epsilon') \frac{v(\epsilon') x'}{v(\epsilon) x} \right\} d^3 \mathbf{k}'$$

The factor of x'/x can be dealt with by noting that

$$\hat{\mathbf{E}} \cdot \hat{\mathbf{k}}' = \cos \theta' = \cos \theta \cos \alpha' + \sin \theta \sin \alpha' \cos \phi$$

where α' is the angle between \mathbf{k} and \mathbf{k}' . Since the second term disappears on integration, x'/x is effectively equal to $\cos \alpha'$

On comparison of the left and right-hand-sides of the Boltzmann equation, we find

$$\int s(\mathbf{k}', \mathbf{k}) \frac{f_0(\epsilon')}{f_0(\epsilon)} \left\{ \tau(\epsilon) - \tau(\epsilon') \frac{v(\epsilon')}{v(\epsilon)} \cos \alpha' \right\} d^3 \mathbf{k}' = 1$$

Note that we also have

$$\left(\frac{\partial f_1(\epsilon)}{\partial t} \right)_s = -e \frac{df_0(\epsilon)}{d\epsilon} E v(\epsilon) x = -\frac{f_1(\epsilon)}{\tau(\epsilon)}$$

where the $\tau(\epsilon)$ are to be calculated using the top expression.

Putting

$$s(\mathbf{k}', \mathbf{k}) = s_e(\mathbf{k}', \mathbf{k}) \delta(\epsilon' - \epsilon)$$

for a general elastic process, the $\tau(\epsilon)$ become equal and may be taken outside the integral, whilst the $f_0(\epsilon)$ and $v(\epsilon)$ cancel out, leaving

$$\int s_e(\mathbf{k}', \mathbf{k}) \{1 - \cos \alpha\} \delta(\epsilon' - \epsilon) d^3 \mathbf{k}' = w_e(\epsilon) = \frac{1}{\tau_m(\epsilon)}$$

which is the definition of a **momentum relaxation time** $\tau_m(\epsilon)$.

Using the general expression for the intrinsic scattering rate, we have

$$\begin{aligned} w_e(\epsilon) &= \frac{2\pi}{\hbar} |\langle \mathbf{k} | V | \mathbf{k}' \rangle|^2 V_C \int \delta(\epsilon' - \epsilon) \frac{d^3 \mathbf{k}'}{(2\pi)^3} \\ &= \frac{2\pi}{\hbar} |\langle \mathbf{k} | V | \mathbf{k}' \rangle|^2 D(\epsilon) \end{aligned}$$

i.e. **Fermi's Golden Rule**.

In the case of phonon scattering we can put

$$s(\mathbf{k}', \mathbf{k}) = s_A(\mathbf{k}', \mathbf{k})\delta(\epsilon' - \epsilon + \hbar\omega) + s_E(\mathbf{k}', \mathbf{k})\delta(\epsilon' - \epsilon - \hbar\omega)$$

When this is inserted into the scattering integral, the effect of the Dirac delta is to bring out the $\tau(\epsilon)$ at different energies:

$$A(\epsilon)\tau(\epsilon - \hbar\omega) + B(\epsilon)\tau(\epsilon) + C(\epsilon)\tau(\epsilon + \hbar\omega) = 1$$

where the $A(\epsilon)$, $B(\epsilon)$ and $C(\epsilon)$ are the new scattering integrals.

For acoustic (deformation potential) and non-polar optical phonon scattering, the $A(\epsilon)$ and $C(\epsilon)$ disappear, giving the normal relaxation time.

However, this is **not** the case for polar optical phonon scattering!

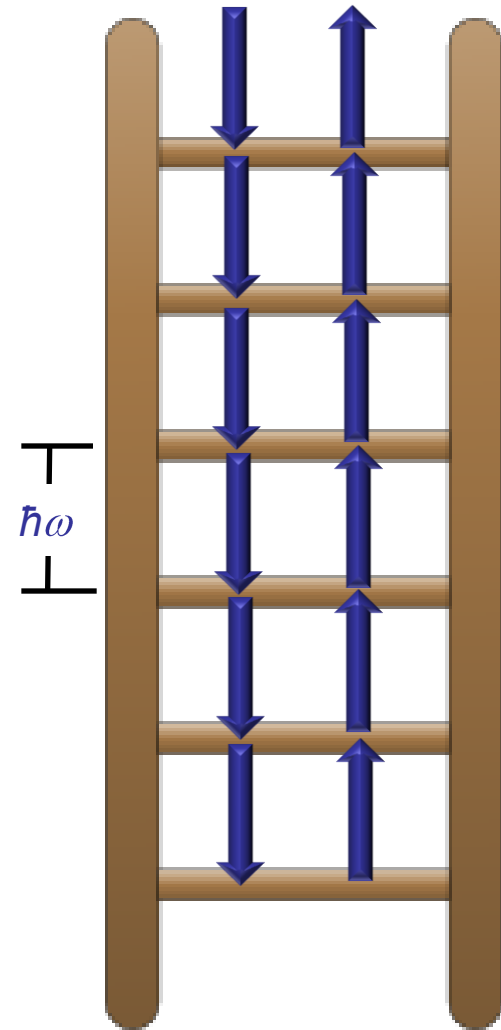
For polar optical phonon scattering we have

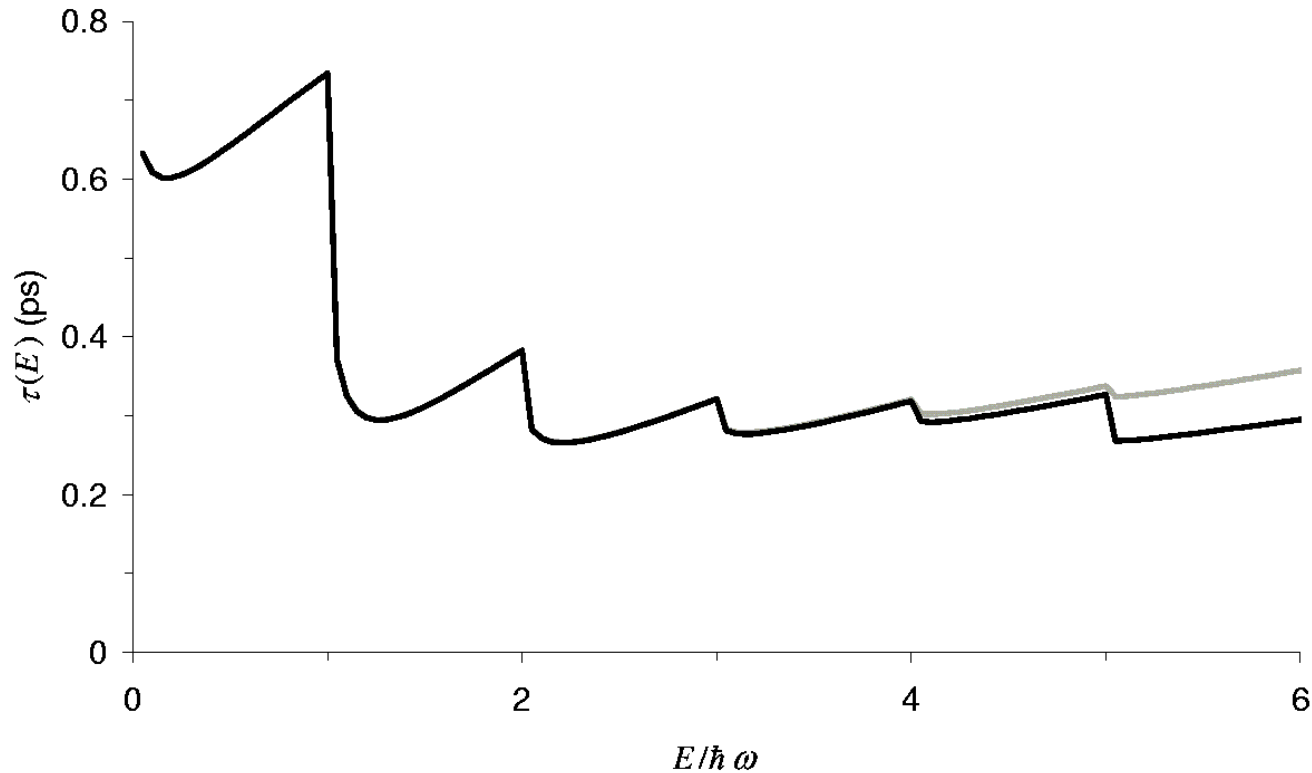
$$A(\epsilon)\tau(\epsilon - \hbar\omega) + B(\epsilon)\tau(\epsilon) + C(\epsilon)\tau(\epsilon + \hbar\omega) = 1$$

where the $A(\epsilon)$, $B(\epsilon)$ and $C(\epsilon)$ do not disappear.

Hence, $\tau(\epsilon)$ at any particular energy becomes coupled to $\tau(\epsilon + \hbar\omega)$ and $\tau(\epsilon - \hbar\omega)$.

This suggests the picture of a phonon ladder, with rungs $\hbar\omega$ apart, where the scattering at any rung is coupled to the rungs above and below it.



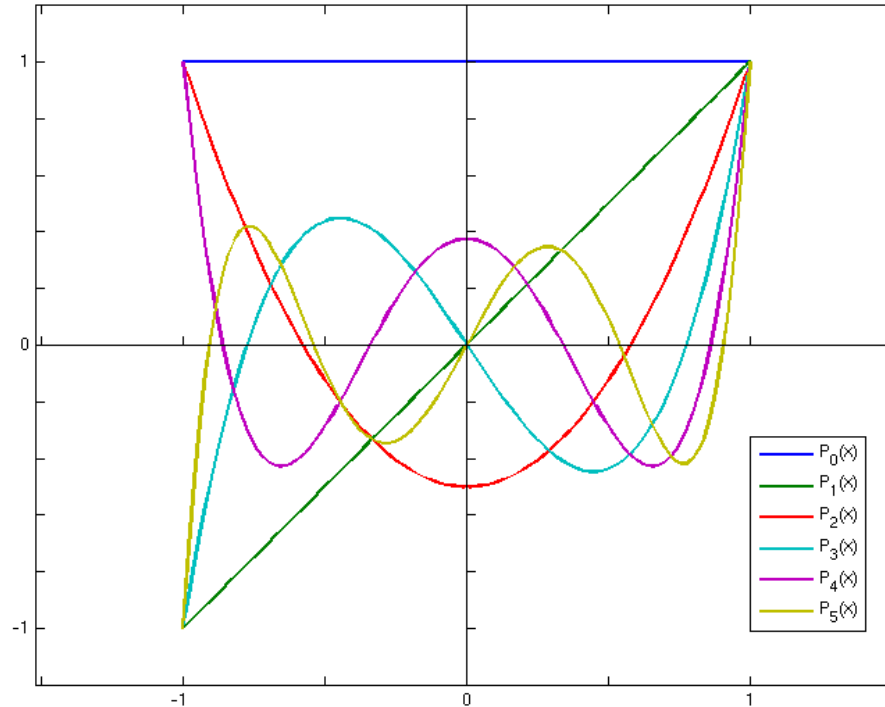


Example of the polar optical phonon scattering relaxation time (for GaAs). The black line is the calculation with the number of rungs truncated to 6.

The distribution function may be expanded as a series in the Legendre polynomials $P_j(x)$

$$f(\mathbf{k}) = \sum_j h_j(\epsilon) P_j(x)$$

Plot of the first six Legendre polynomials



Note that the even orders are symmetric in x ($\cos \theta$) whilst the odd orders are antisymmetric.

Inserting this into the left-hand-side of Boltzmann's equation gives for the force term

$$-\frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f(k) = -eE \sum_j \left\{ \frac{j+1}{2j+1} \left[v(\epsilon) \frac{dh_j}{d\epsilon} - j \frac{h_j(\epsilon)}{\hbar k} \right] P_{j+1}(x) \right. \\ \left. + \frac{j}{2j+1} \left[v(\epsilon) \frac{dh_j}{d\epsilon} + (j+1) \frac{h_j(\epsilon)}{\hbar k} \right] P_{j-1}(x) \right\}$$

Limiting this to terms up to $j=2$, this is

$$-\frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f(k) = -eE \left\{ \frac{1}{3} \left[v(\epsilon) \frac{dh_1}{d\epsilon} + 2 \frac{h_1(\epsilon)}{\hbar k} \right] P_0(x) + v(\epsilon) \frac{dh_0}{d\epsilon} P_1(x) + \frac{2}{3} \left[v(\epsilon) \frac{dh_1}{d\epsilon} - \frac{h_1(\epsilon)}{\hbar k} \right] P_2(x) \right\}$$

Decomposing the scattering integral into zero and first order integrals, we have

$$\left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_s = \left(\frac{\partial h_0(\epsilon)}{\partial t} \right)_s + \left(\frac{\partial h_1(\epsilon)x}{\partial t} \right)_s$$

where the zero-order integral is

$$P_0(x)I_0 = \int s(\mathbf{k}', \mathbf{k}) h_0(\epsilon') [1 - h_0(\epsilon)] - s(\mathbf{k}, \mathbf{k}') h_0(\epsilon) [1 - h_0(\epsilon')] d^3\mathbf{k}'$$

and the first-order integral is

$$\begin{aligned} P_1(x)I_1 = x \int s(\mathbf{k}', \mathbf{k}) \{ h_1(\epsilon') \cos \alpha [1 - h_0(\epsilon)] - h_1(\epsilon) h_0(\epsilon') \} \\ - s(\mathbf{k}, \mathbf{k}') \{ h_1(\epsilon) [1 - h_0(\epsilon')] - h_1(\epsilon') \cos \alpha' h_0(\epsilon) \} d^3\mathbf{k}' \end{aligned}$$

Equating the coefficients of the Legendre polynomials

$$-\frac{eE}{3} \left[v(\epsilon) \frac{dh_1}{d\epsilon} + 2 \frac{h_1(\epsilon)}{\hbar k} \right] = I_0$$

$$-eE v(\epsilon) \frac{dh_0}{d\epsilon} = I_1$$

or, in terms of the $\gamma(\epsilon)$ function and its derivative

$$-\frac{eE}{3} \left(\frac{2}{m^* \gamma(\epsilon)} \right)^{1/2} \left(\frac{d\gamma}{d\epsilon} \right)^{-1} \frac{d}{d\epsilon} [\gamma(\epsilon) h_1(\epsilon)] = I_0$$

$$-eE \left(\frac{2\gamma(\epsilon)}{m^*} \right)^{1/2} \left(\frac{d\gamma}{d\epsilon} \right)^{-1} \frac{dh_0}{d\epsilon} = I_1$$

Using the low-field result for the derivative of the first-order term in $f(\mathbf{k})$ due to scattering

$$\frac{1}{x} \left(\frac{dh_1(\epsilon)x}{dt} \right)_s = -\frac{h_1(\epsilon)}{\tau(\epsilon)}$$

we obtain the differential equation

$$-\frac{2e^2 E^2}{3m^*} \left(\frac{1}{\gamma(\epsilon)} \right)^{1/2} \left(\frac{d\gamma(\epsilon)}{d\epsilon} \right)^{-1} \frac{d}{d\epsilon} \left[\frac{\gamma^{3/2}(\epsilon)\tau(\epsilon)}{d\gamma/d\epsilon} \frac{dh_0}{d\epsilon} \right] = I_0$$

Note that the $\tau(\epsilon)$ are obtained from I_1 . The solution of the above equation is the electric field dependent part of $f(\mathbf{k})$, $h_0(\epsilon)$.

General overview:

To deal with inter-valley transfer, it is useful to decompose the distribution function into the distributions in each valley.

Each valley will have associated with it a differential equation like that just derived for the distribution function.

However, we must also bring in a scattering integral due to inter-valley transfer.

These additional terms will couple the differential equations together, which must then be solved simultaneously.

- The drifted Maxwellian approach

- The distribution function is assumed to be a Maxwellian shifted by an average drift k-vector
- Validity based on assumption that momentum has been randomised by electron-electron scattering
- Introduces the electron temperature T_e into the formulation explicitly

- Monte-Carlo simulation

- Monte Carlo techniques used to find the distribution function directly
- Employs a method of mapping a uniform random distribution into scattering probabilities
- If implemented correctly, can give very realistic results by reducing modelling assumptions

- Introduction
- Basic transport concepts
- High field phenomena
- Scattering mechanisms
- The Boltzmann transport equation

The Ridley-Watkins-Hilsum mechanism

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C. Hilsum, *Proc. IRE* **50**, 185 (1962)

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K. Fletcher and P.N. Butcher, *J. Phys. C: Solid State Phys.* **5**, 212 (1972)

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High-field solution of the Boltzmann equation

E.M. Conwell and M.O. Vassell, *Phys. Rev.* **166**, 797 (1967)

B.K. Ridley, 'Quantum processes in semiconductors' Oxford University Press (1999)

Recommended text book

B.K. Ridley, 'Quantum processes in semiconductors' Oxford University Press (1999)