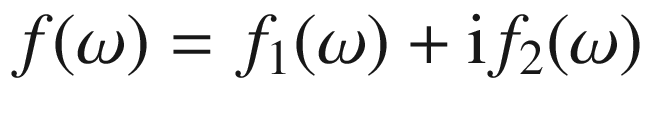
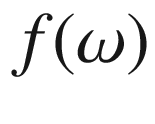
## Kramers–Kronig Relations

The Kramers–Kronig relations (KKR) are relations between the real and imaginary part of the dielectric function. They are of a general nature and are based on the properties of a complex, analytical response function



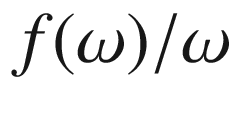
fulfilling the following conditions[1](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn1):

The poles of



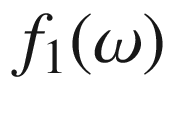
are below the real axis.

The integral of

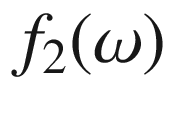


along a semicircle with infinite radius in the upper half of the complex plane vanishes.

The function

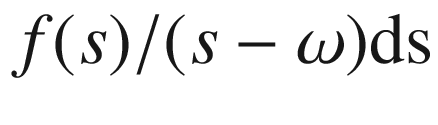


is even and the function

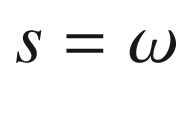


is odd for real values of the argument.

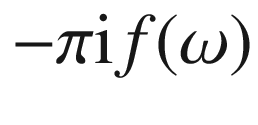
The integral of



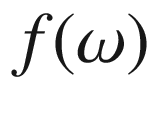
along the real axis and an infinite semicircle in the upper half of the complex plane is zero because the path is a closed line. The integral along a semicircle above the pole at



yields



, the integral over the infinite semicircle is zero. Therefore the value of

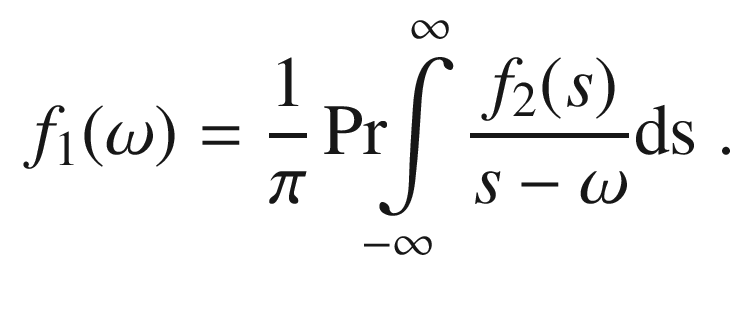


is given by[2](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn2)



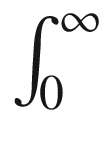
(C.1)

Equating the real and imaginary parts of ([C.1](#u116076_4_En_BookBackmatter_OnlinePDF-Equ23)) yields for the real part

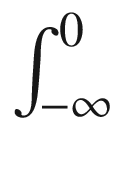


(C.2)

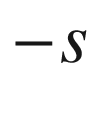
Splitting the integral into two parts



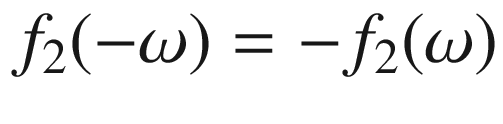
and



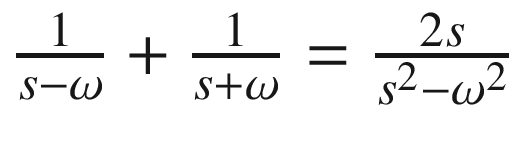
, going from *s* to



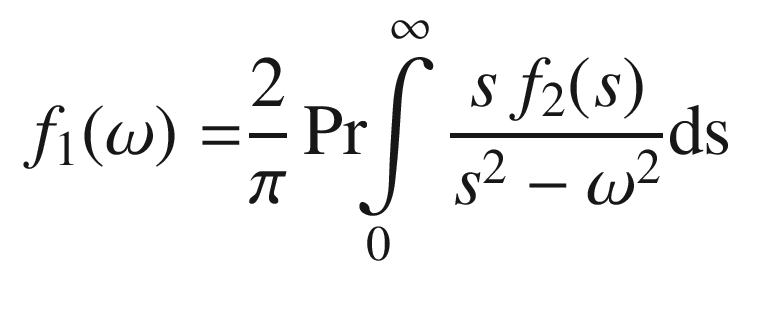
in the latter and using



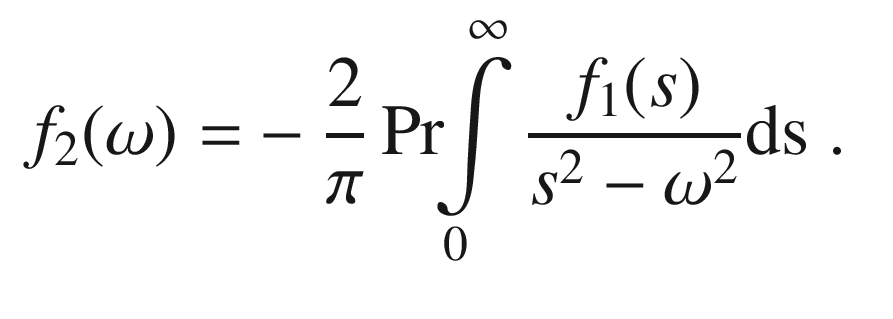
and



yields ([C.3a](#u116076_4_En_BookBackmatter_OnlinePDF-Equ25))



(C.3a)

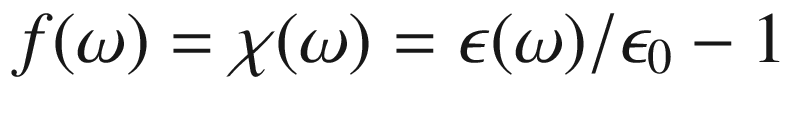


(C.3b)

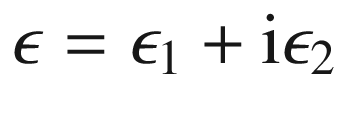
In a similar way, ([C.3b](#u116076_4_En_BookBackmatter_OnlinePDF-Equ26)) is obtained. These two relations are the Kramers–Kronig relations [[2152](#u116076_4_En_BookBackmatter_OnlinePDF-CR2152), [2153](#u116076_4_En_BookBackmatter_OnlinePDF-CR2153)]. They are most often applied to the dielectric function

$$\epsilon $$

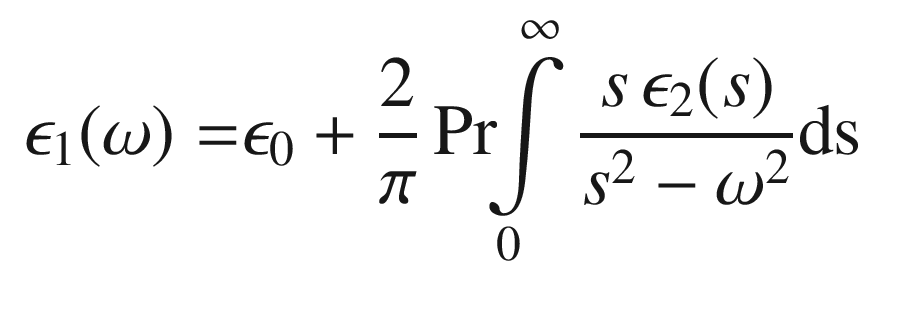
. In this case, they apply to the susceptibility , i.e.



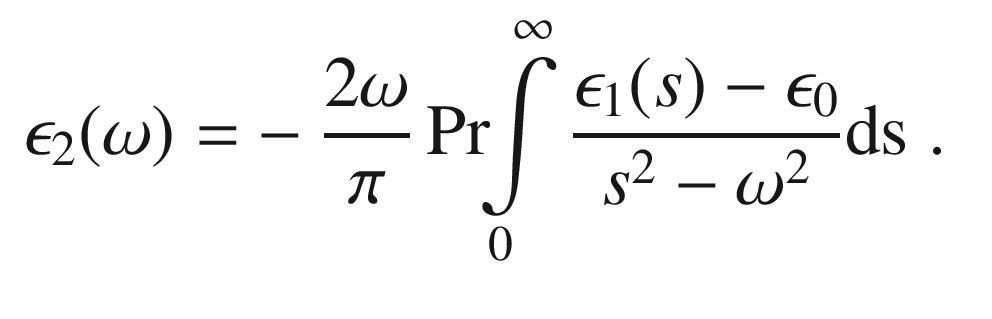
. The susceptibility can be interpreted as the Fourier transform of the time-dependent polarization  in the semiconductor after an infinitely short pulsed electric field, i.e. the impulse response of the polarization . For the dielectric function



, the following KKR relations hold:

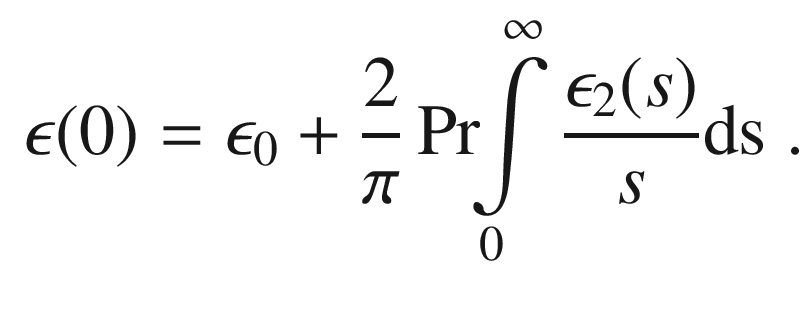


(C.4a)



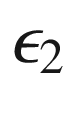
(C.4b)

The static dielectric constant is thus given by

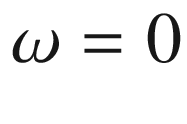


(C.5)

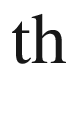
The integral does not diverge since



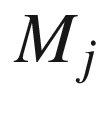
is an odd function and zero at



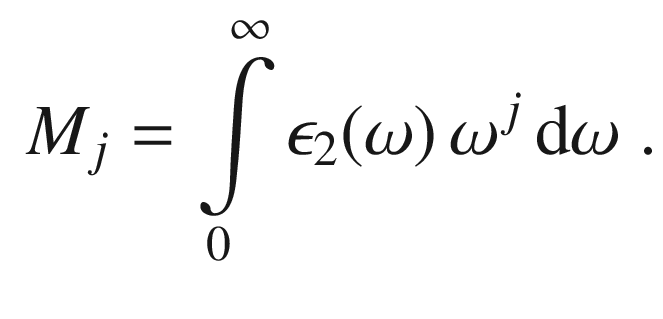
. Generally the *j*-



momentum

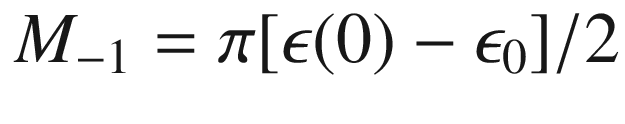


of the imaginary part of the dielectric function is



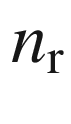
(C.6)

Thus,



.

Other KKRs are, e.g., the relation between the index of refraction



and the absorption coefficient

$$\alpha $$

:



(C.7)

If the imaginary (real) part of the dielectric function is known (for all frequencies), the real (imaginary) part can be calculated via the KKR. If the dependence is not known for the entire frequency range, assumptions about the dielectric function in the unknown spectral regions must be made that limits the reliability of the transformation.

Appendix D

## Oscillator Strength

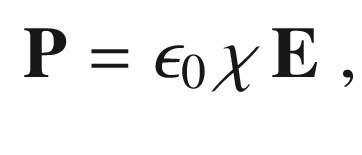
The response of an oscillator to an electric field



is formulated with the dielectric function. The resulting polarization

$$\mathbf{P}$$

is related to the electric field via



(D.1)

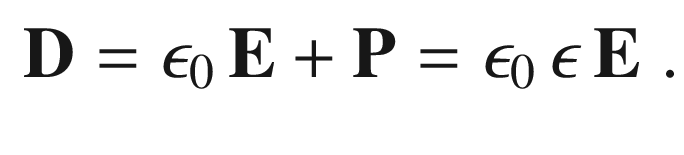
with

$$\chi $$

being the electric susceptibility, and the displacement field

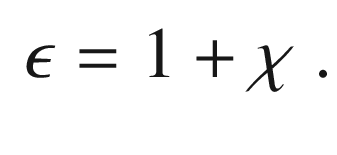


is given by



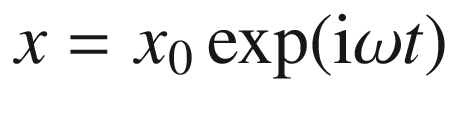
(D.2)

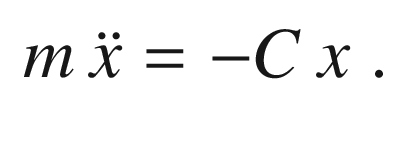
Thus the (relative) dielectric constant is



(D.3)

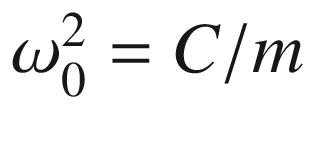
We assume a harmonic oscillator model for an electron, i.e. an equation of motion for the amplitude



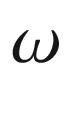


(D.4)

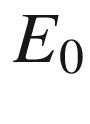
The resonance frequency is



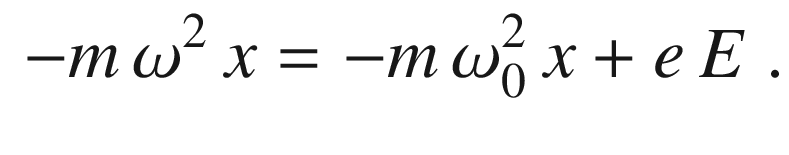
. The presence of a harmonic electric field *E* of frequency



and amplitude

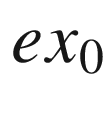


adds a force *eE*. Thus,

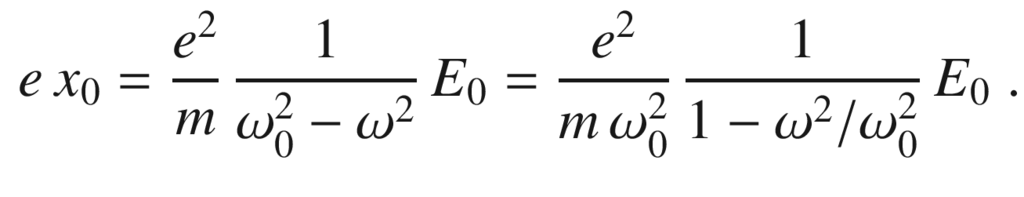


(D.5)

The polarization

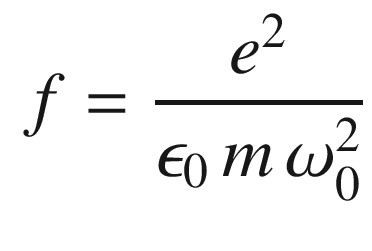


is given by



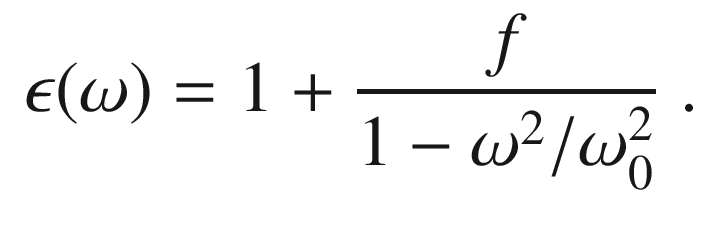
(D.6)

The pre-factor is called the (dimensionless) *oscillator strength* and will be denoted as



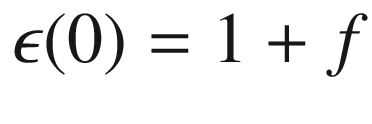
(D.7)

in the following. The frequency-dependent dielectric function of the resonance is thus

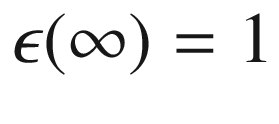


(D.8)

In the low-frequency limit, the dielectric function is



, in the high-frequency limit



. The oscillator strength is the difference of

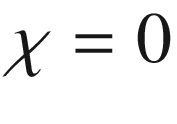
$$\epsilon $$

for frequencies below and above the resonance.

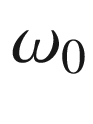
For all systems, the high-frequency limit of

$$\epsilon $$

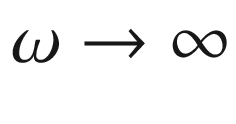
is 1. This means that



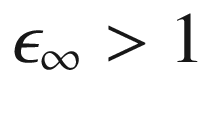
, i.e. there are no more oscillators to be polarized. The low-frequency limit includes all possible oscillators. If there are further oscillators between frequencies well above



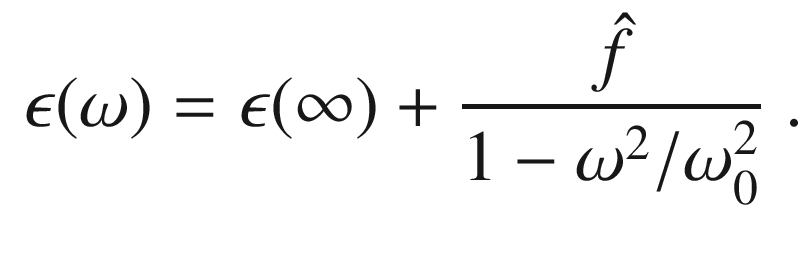
and



, these are summarized as the high-frequency dielectric constant

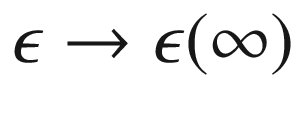


. Equation ([D.8](#u116076_4_En_BookBackmatter_OnlinePDF-Equ39)) then reads

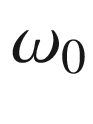


(D.9)

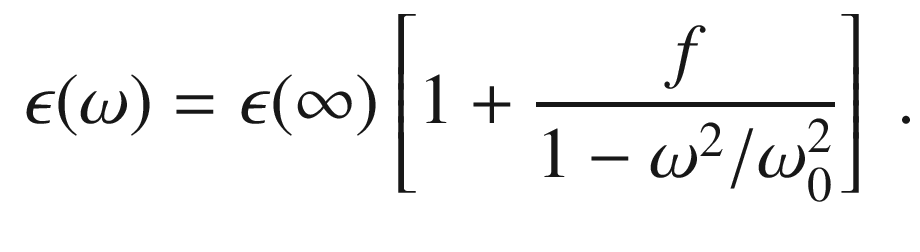
The limit



is only valid for frequencies above

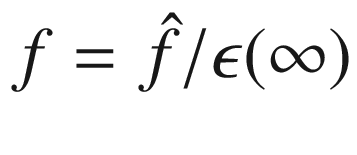


but smaller than the next resonance(s) at higher frequencies.[3](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn3) Another common form is to include the background dielectric constant via



(D.10)

Obviously,

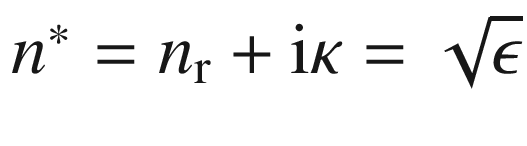


, making the two forms equivalent.

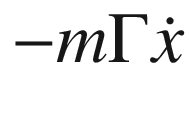
In order to discuss the lineshape, not only for

$$\epsilon $$

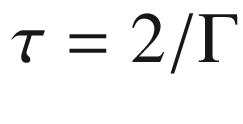
but also for the index of refraction



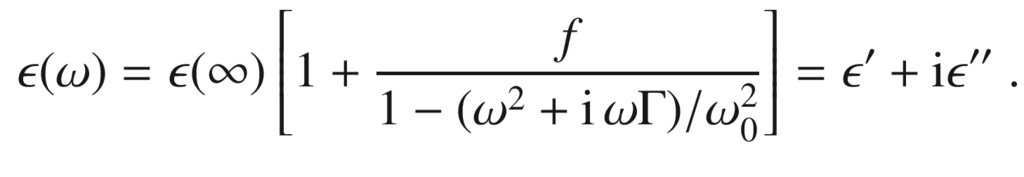
, we introduce damping to our calculation by adding a term



to the left side of ([D.5](#u116076_4_En_BookBackmatter_OnlinePDF-Equ36)). This term is something like a ‘friction’ and would cause the oscillation amplitude to decay exponentially with a time constant

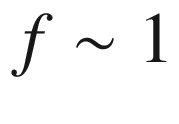


without external stimulus. The dielectric constant is

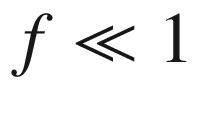


(D.11)

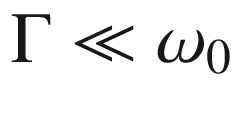
The real and imaginary part fulfill the Kramers–Kronig relations  ([C.3a](#u116076_4_En_BookBackmatter_OnlinePDF-Equ25)) and ([C.3b](#u116076_4_En_BookBackmatter_OnlinePDF-Equ26)). For the oscillator strength, the regimes of large oscillator strength (



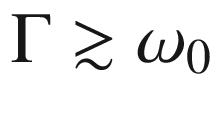
) and small oscillator strength (



) are distinguished. For the damping, two regimes should be distinguished: Small damping (



) and strong damping (



). Typical lineshapes are shown in Figs. [D.1](#u116076_4_En_BookBackmatter_OnlinePDF-Fig2) and [D.2](#u116076_4_En_BookBackmatter_OnlinePDF-Fig3).

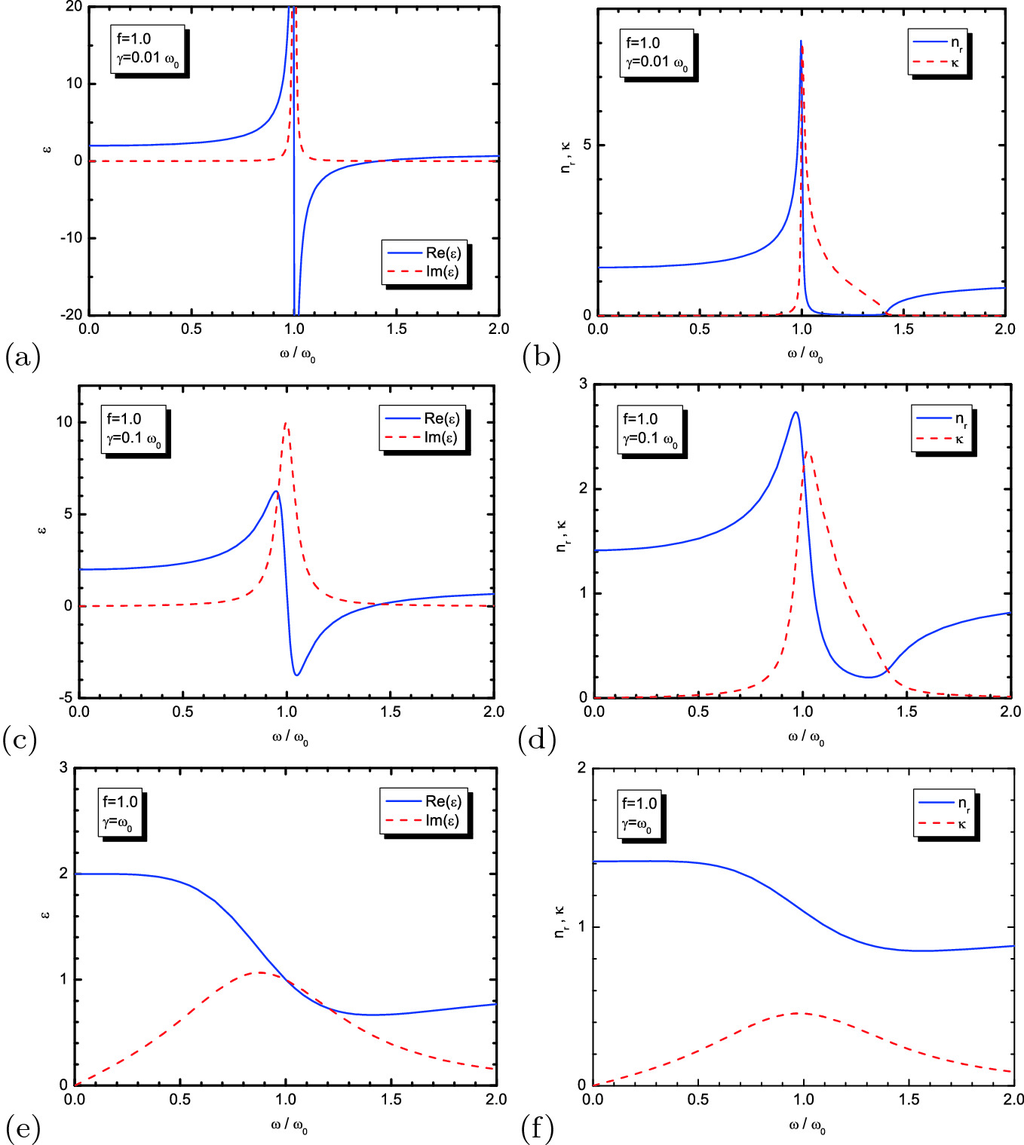
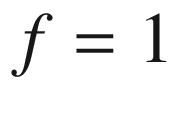
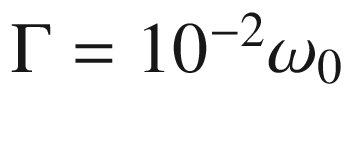


Fig. D.1

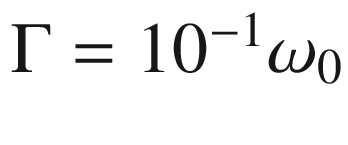
Real (*solid lines*) and imaginary (*dashed lines*) parts of the dielectric constant (**a**, **c**, **e**) and index of refraction (**b**, **d**, **f**) ([D.11](#u116076_4_En_BookBackmatter_OnlinePDF-Equ42)) for oscillator strength



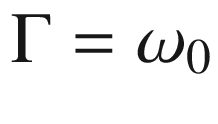
and various values of damping: (**a**, **b**)



, (**c**, **d**)



, and (**e**, **f**)



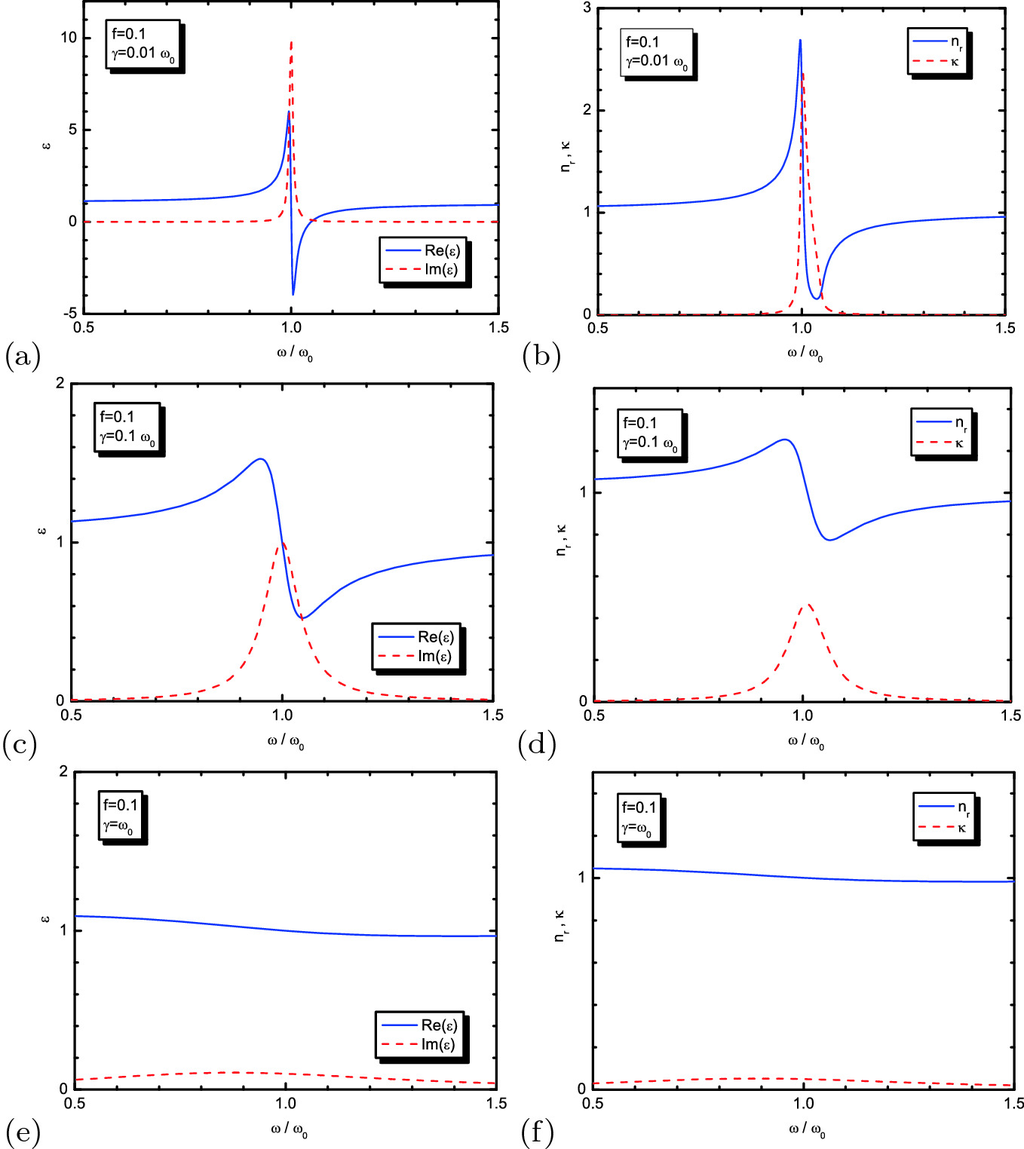
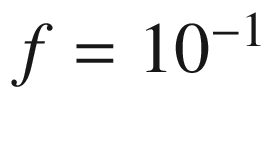
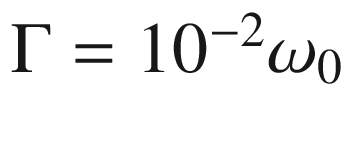


Fig. D.2

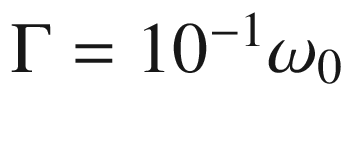
Real (*solid lines*) and imaginary (*dashed lines*) parts of the dielectric constant (**a**, **c**, **e**) and index of refraction (**b**, **d**, **f**) ([D.11](#u116076_4_En_BookBackmatter_OnlinePDF-Equ42)) for oscillator strength



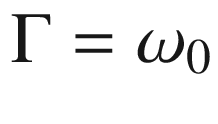
and various values of damping: (**a**, **b**)



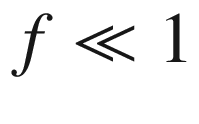
, (**c**, **d**)



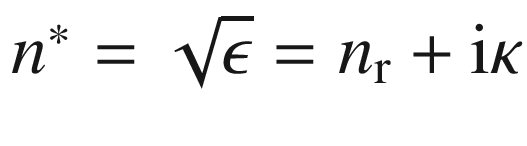
, and (**e**, **f**)



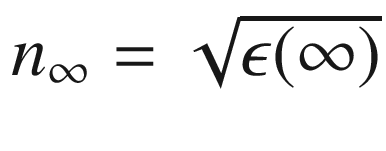
For small oscillator strength, i.e.



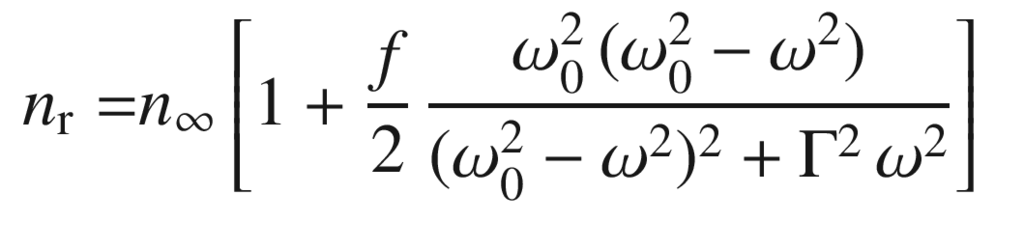
, the index of refraction



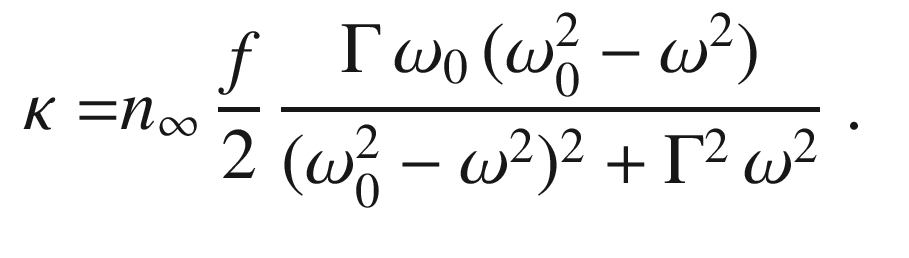
is given by (



)

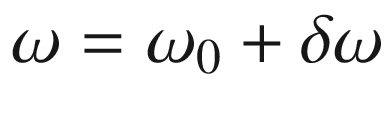


(D.12a)

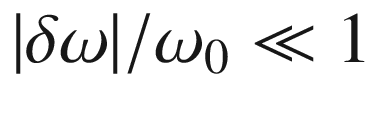


(D.12b)

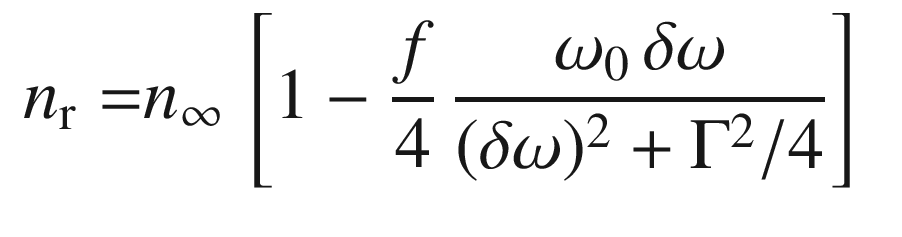
For small detuning from the resonance frequency, i.e.



with



, the index of refraction is given by

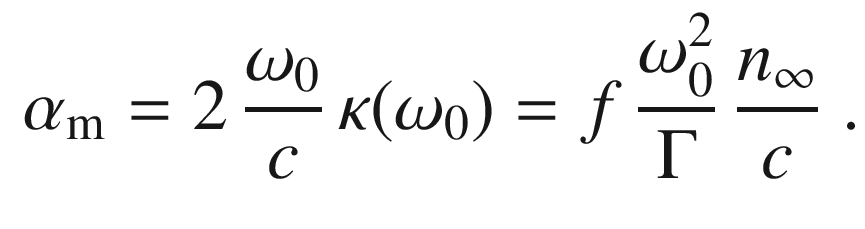


(D.13a)



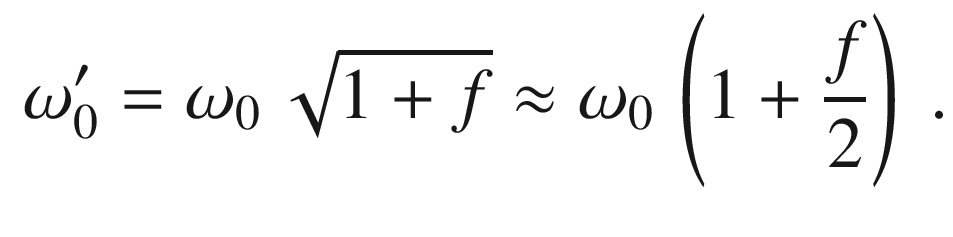
(D.13b)

The maximum absorption is given as



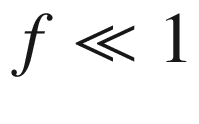
(D.14)

For zero damping, the dielectric function has a zero at

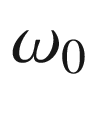


(D.15)

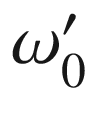
The latter approximation is valid for



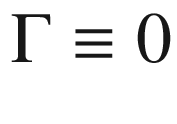
. In the region between



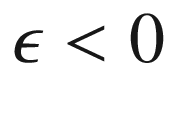
and



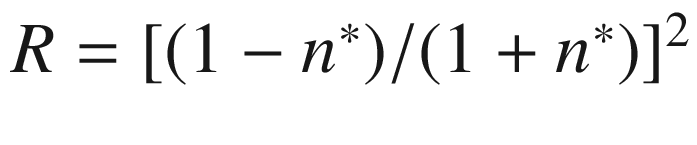
, the real part of the index of refraction is very small (for the physically unrealistic case of



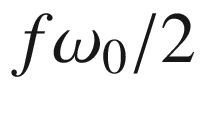
it is exactly zero since



). The reflectance (for vertical incidence

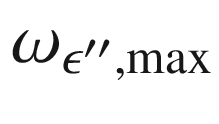


) in this region (width:

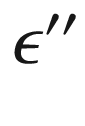


) is thus very high. For larger damping (and small oscillator strength), this effect is washed out.

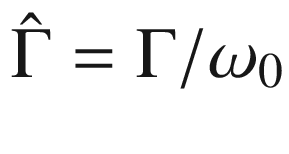
The frequency



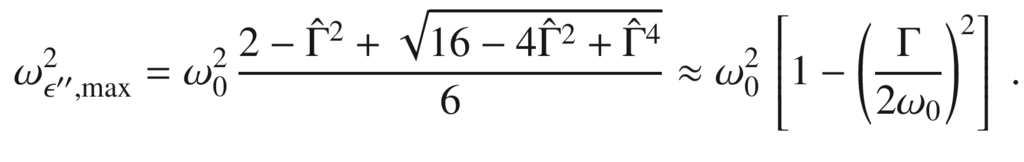
of the maximum of the imaginary part of



of the dielectric function (

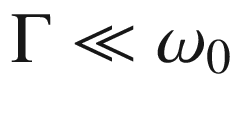


) is

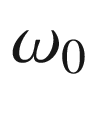


(D.16)

The approximation is valid for small damping



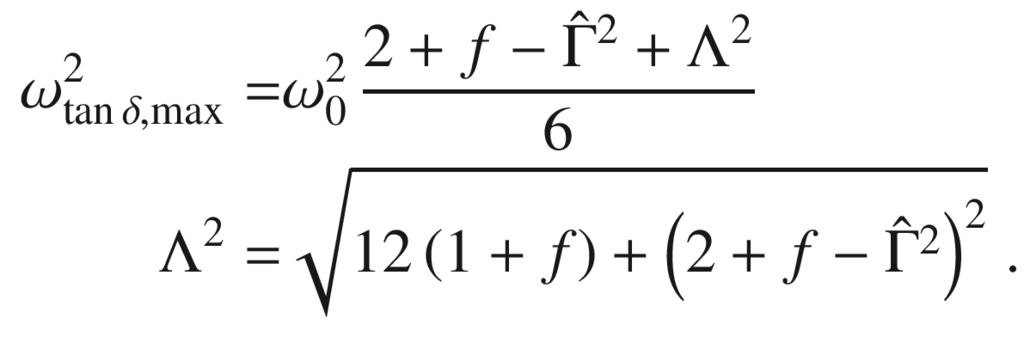
. In this case, the detuned frequency of the maximum is close to



(Fig. [D.3](#u116076_4_En_BookBackmatter_OnlinePDF-Fig4)). The frequency position of the maximum of

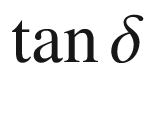


 is



(D.17)

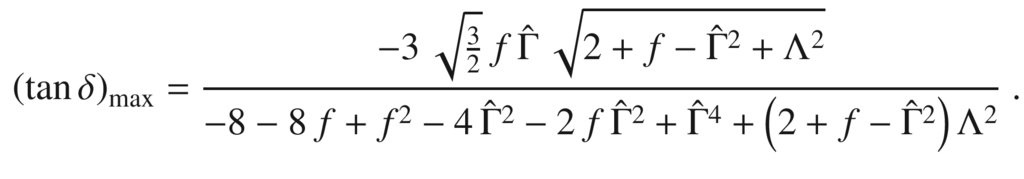
The value of



at its maximum is (



has the same meaning as in ([D.17](#u116076_4_En_BookBackmatter_OnlinePDF-Equ50)))



(D.18)

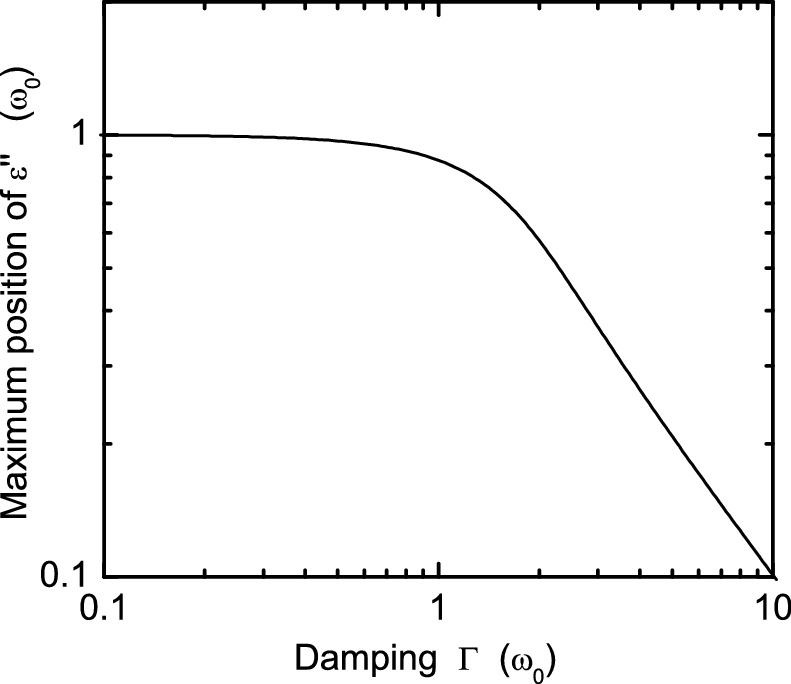


Fig. D.3

Frequency position of the maximum of

$$\epsilon $$

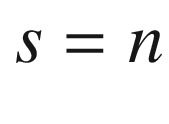
as a function of the damping

Appendix E

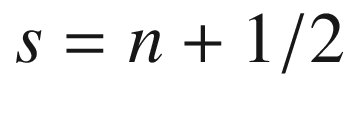
## Quantum Statistics

### E.1 Introduction

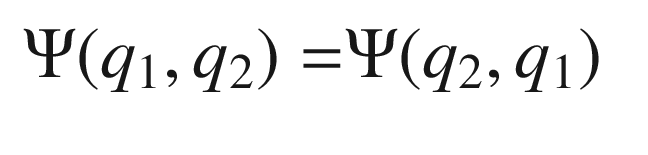
Bosons  are particles with integer spin



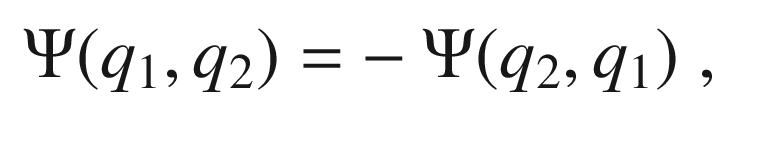
, fermions  are particles with spin



with *n* being an integer including zero. The fundamental quantum-mechanical property of the wavefunction of a system with *N* such particles is that under exchange of any two particles, the wavefunction is symmetric in the case of bosons and antisymmetric in the case of fermions. For two particles, these conditions read

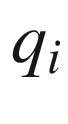


(E.1a)



(E.1b)

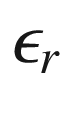
where ([E.1a](#u116076_4_En_BookBackmatter_OnlinePDF-Equ52)) holds for bosons and ([E.1b](#u116076_4_En_BookBackmatter_OnlinePDF-Equ53)) holds for fermions. The variables



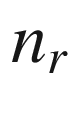
denote the coordinates and spin of the *i*-th particle. The Pauli principle allows bosons to populate the same single particle state with an arbitrary number of particles (at least more than one). For fermions, the exclusion principle  holds that each single particle state can only be populated once.

### E.2 Partition Sum

We consider a gas of *N* identical particles in a volume *V* in equilibrium at a temperature *T*. The possible quantum-mechanical states of a particle is denoted as *r*. The energy of a particle in the state *r* is

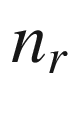


, the number of particles in the state *r* is

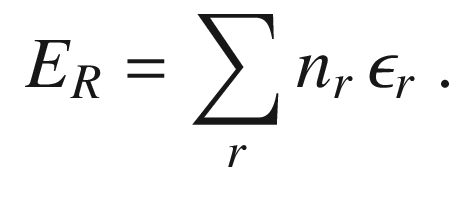


.

For vanishing interaction of the particles, the total energy of the gas in the state *R* (with

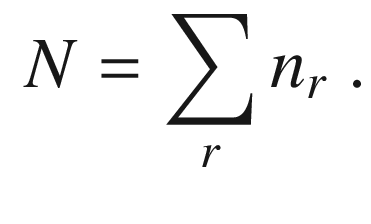


particles in the state *r*) is



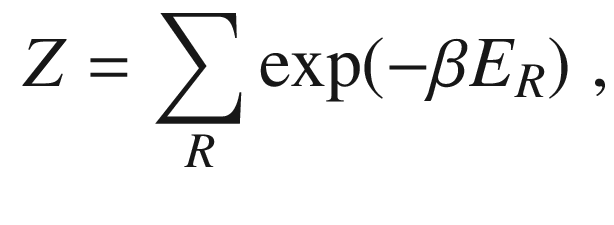
(E.2)

The sum runs over all possible states *r*. The total number of particles imposes the condition



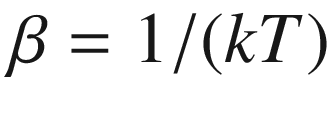
(E.3)

In order to calculate the thermodynamic potentials, the partition sum *Z* needs to be calculated

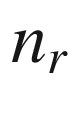


(E.4)

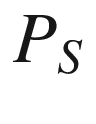
with



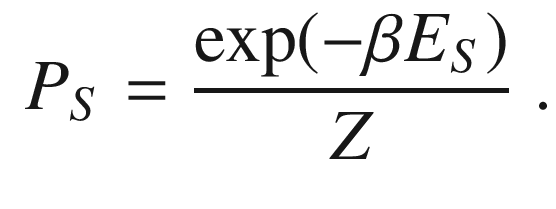
. The sum runs over all possible microscopic states *R* of the gas, i.e. all combinations of the



that fulfill ([E.3](#u116076_4_En_BookBackmatter_OnlinePDF-Equ55)). The probability

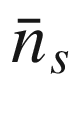


to find the system in a particular state *S* is given by (canonical ensemble)

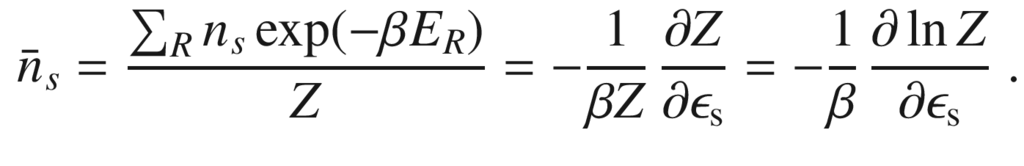


(E.5)

The average number

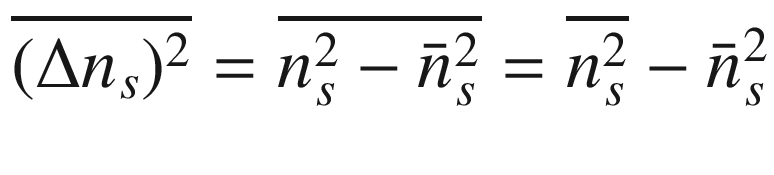


of particles in a state *s* is given by

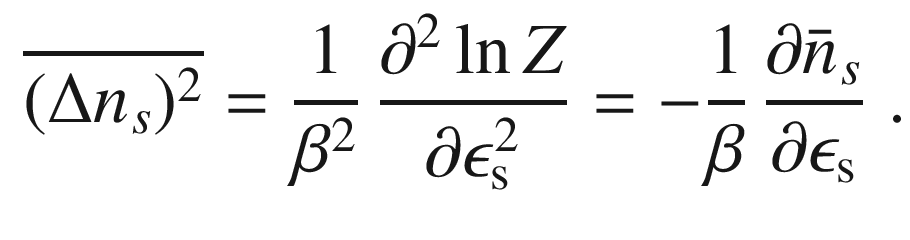


(E.6)

We note that the average deviation

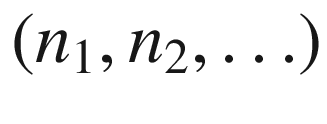


is given by

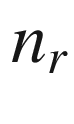


(E.7)

In the Bose–Einstein statistics (for bosons), the particles are fundamentally indistinguishable. Thus, a set of



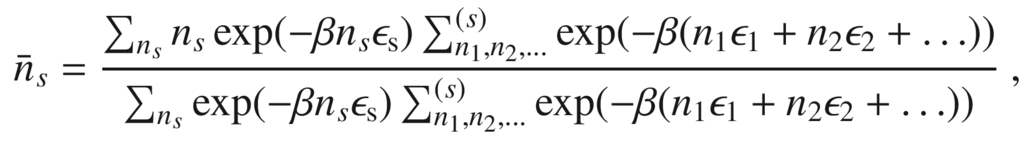
uniquely describes the system. In the case of fermions, for each state



is either 0 or 1. In both cases, ([E.3](#u116076_4_En_BookBackmatter_OnlinePDF-Equ55)) needs to be fulfilled.

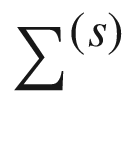
### E.3 Photon Statistics

This case is the Bose–Einstein statistics  (cf. ([E.24](#u116076_4_En_BookBackmatter_OnlinePDF-Equ76))) with undefined particle number. We rewrite ([E.6](#u116076_4_En_BookBackmatter_OnlinePDF-Equ58)) as

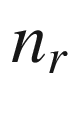


(E.8)

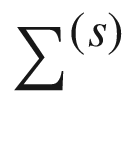
where



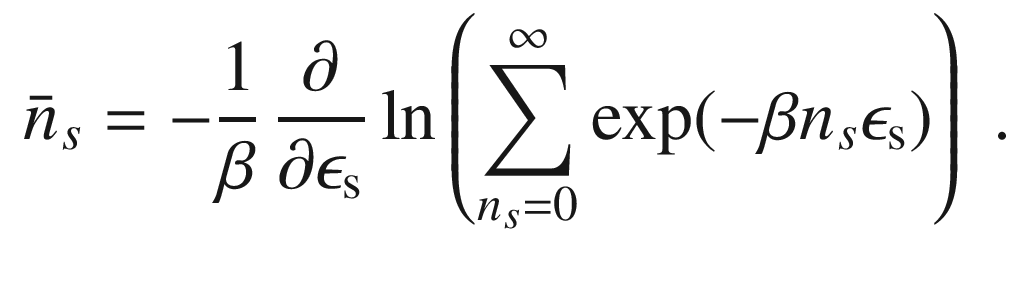
denotes a summation that does not include the index *s*. In the case of photons, the values



can take any value (integers including zero) without restriction and therefore the sums

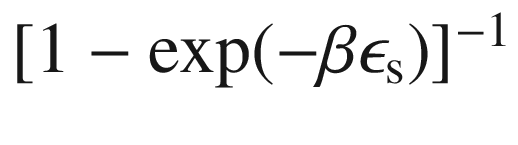


in the numerator and denominator of ([E.8](#u116076_4_En_BookBackmatter_OnlinePDF-Equ60)) are identical. After some calculation we find



(E.9)

The argument of the logarithm is a geometrical series with the limit



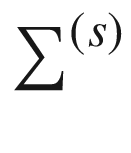
. This leads to the so-called Planck distribution



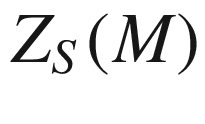
(E.10)

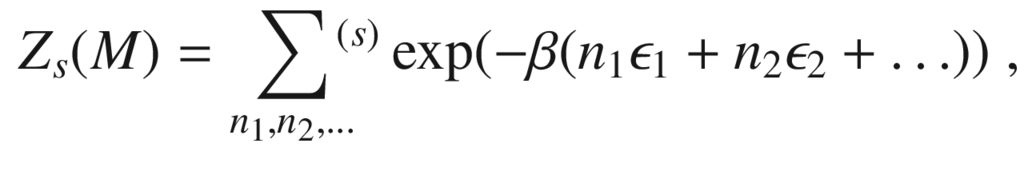
### E.4 Fermi–Dirac Statistics

Now, the particle number is fixed to *N*. For the sum



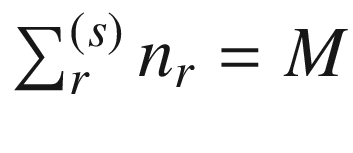
from ([E.6](#u116076_4_En_BookBackmatter_OnlinePDF-Equ58)), we introduce the term



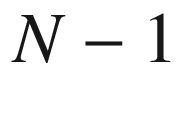


(E.11)

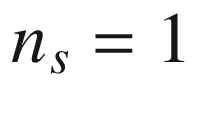
when *M* particles are to be distributed over all states except *s* (



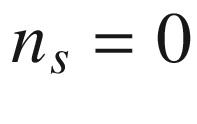
). *M* is either



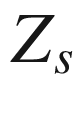
if



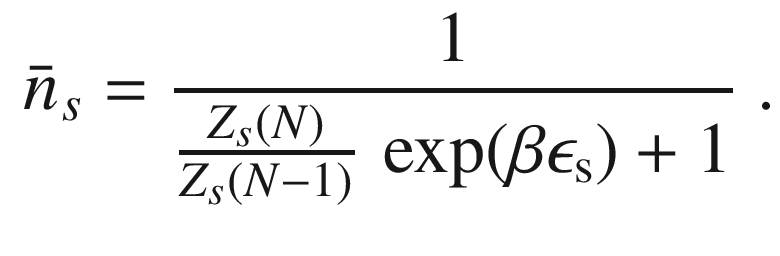
and *N* if



. Using

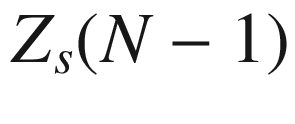


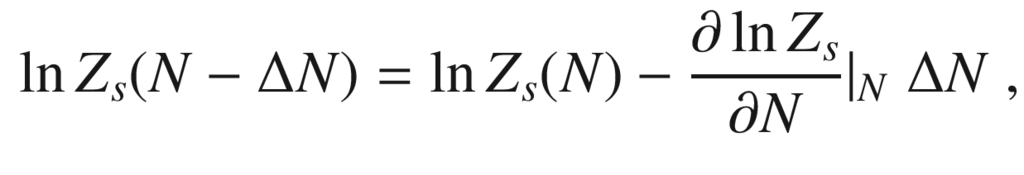
, we can write



(E.12)

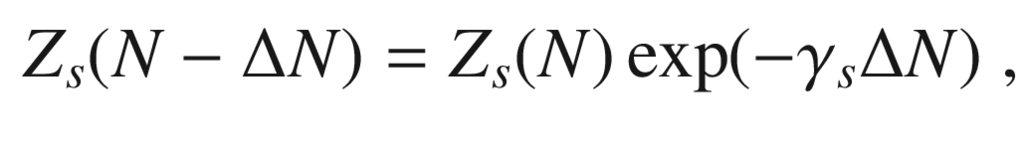
We evaluate





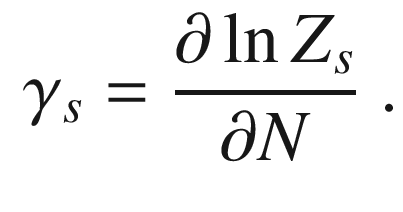
(E.13)

or



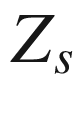
(E.14)

with

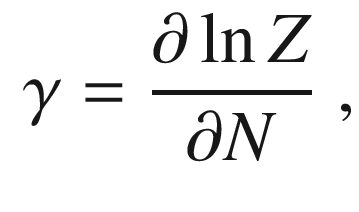


(E.15)

Since

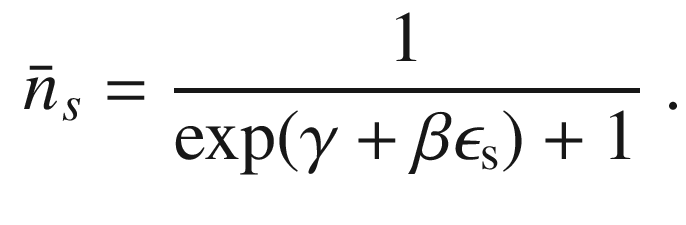


runs over many states, the derivative is approximately equal to



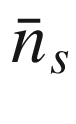
(E.16)

as will be shown below. Thus, we obtained so far

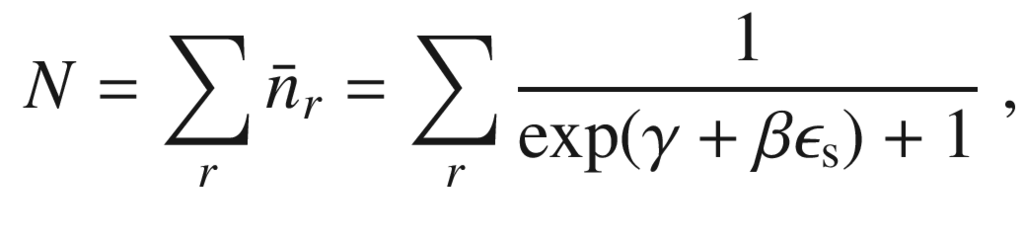


(E.17)

Equation ([E.3](#u116076_4_En_BookBackmatter_OnlinePDF-Equ55)) holds also for the average values



, i.e.

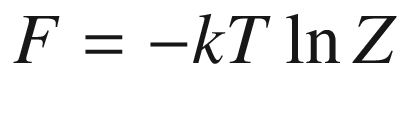


(E.18)

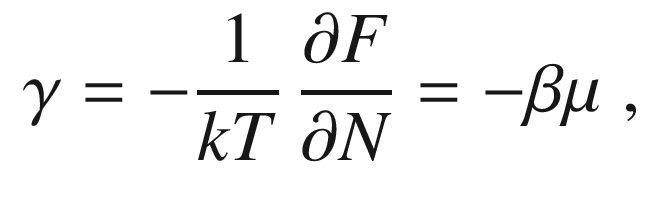
from which the value of

$$\gamma $$

can be calculated. Given that the free energy is given as



, we find that

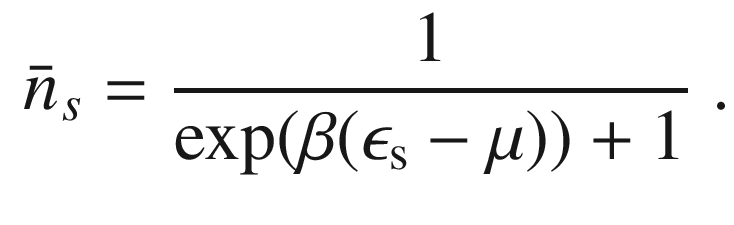


(E.19)

where

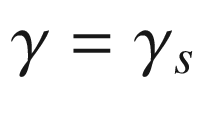
$$\mu $$

is the chemical potential by definition. Therefore, the distribution function for the Fermi–Dirac statistics (also called the Fermi function) is



(E.20)

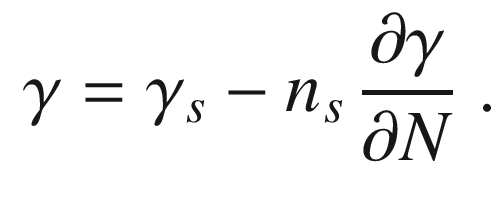
Now, we briefly revisit the approximation



. Exactly,

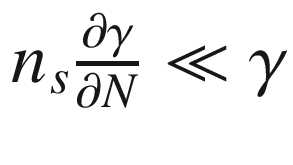
$$\gamma $$

fulfills

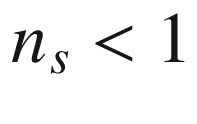


(E.21)

Thus, the approximation is valid if

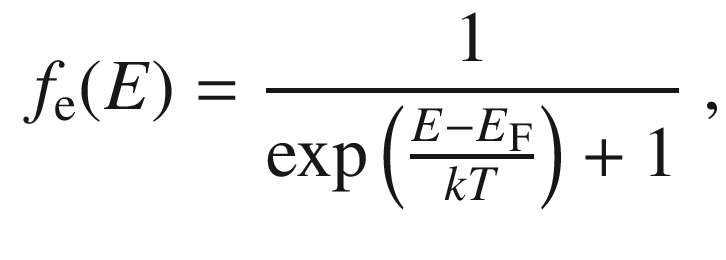


. Since



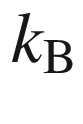
, this means that the chemical potential does not change significantly upon addition of another particle.

The Fermi–Dirac distribution function ([E.20](#u116076_4_En_BookBackmatter_OnlinePDF-Equ72)) for electrons is typically written as

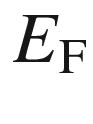


(E.22)

where *k* (or



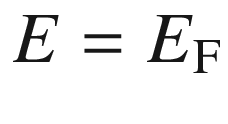
) denotes the Boltzmann constant, *T* is the temperature, and



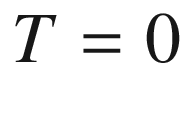
is the Fermi level, which is called the chemical potential

$$\mu $$

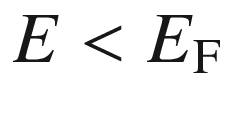
in thermodynamics. The Fermi distribution is shown in Fig. [E.1](#u116076_4_En_BookBackmatter_OnlinePDF-Fig5) for various parameters. The distribution function gives the probability that a state at energy *E* is populated in thermodynamic equilibrium. For



the population is 1/2 for all temperatures. At (the unrealistic case of)



, the function makes a step from 1 (for



) to 0.

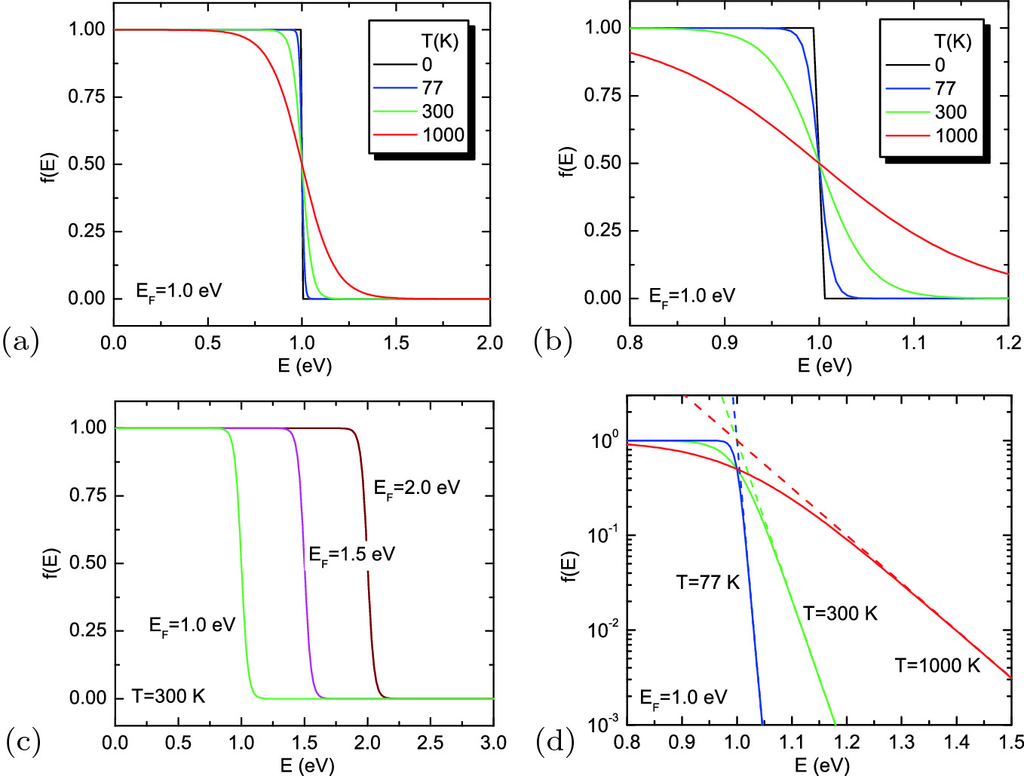
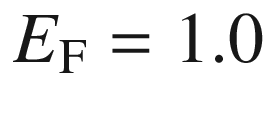
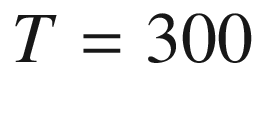


Fig. E.1

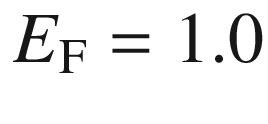
Fermi function for **a**, **b** different temperatures (for



 eV) and **c** for different chemical potentials (for

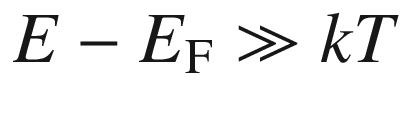


 K). **d** Fermi function (*solid lines*) compared with Boltzmann approximation (*dashed lines*) for various temperatures and

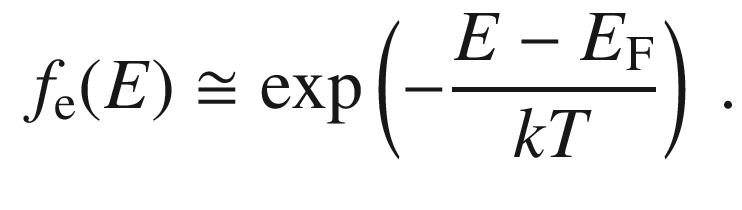


 eV on semilogarithmic plot

The high-energy tail of the Fermi distribution, i.e. for



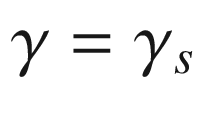
, can be approximated by the Boltzmann distribution:



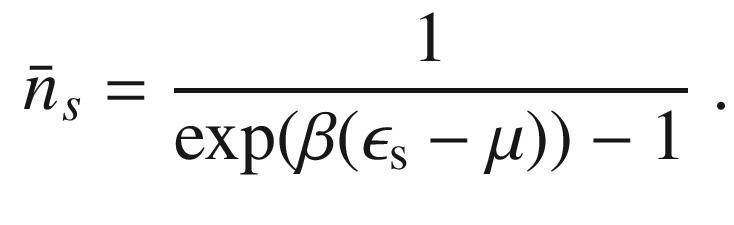
(E.23)

### E.5 Bose–Einstein Distribution

Executing ([E.8](#u116076_4_En_BookBackmatter_OnlinePDF-Equ60)) with the approximation



, the Bose–Einstein distribution is found to be



(E.24)

Appendix F

## Kronig-Penney Model

The Kronig-Penney model [[71](#u116076_4_En_BookBackmatter_OnlinePDF-CR71)] is a simple, one-dimensional analytically solvable model that visualizes the effect of the periodic potential on the dispersion relation of electrons, i.e. the formation of a band structure.

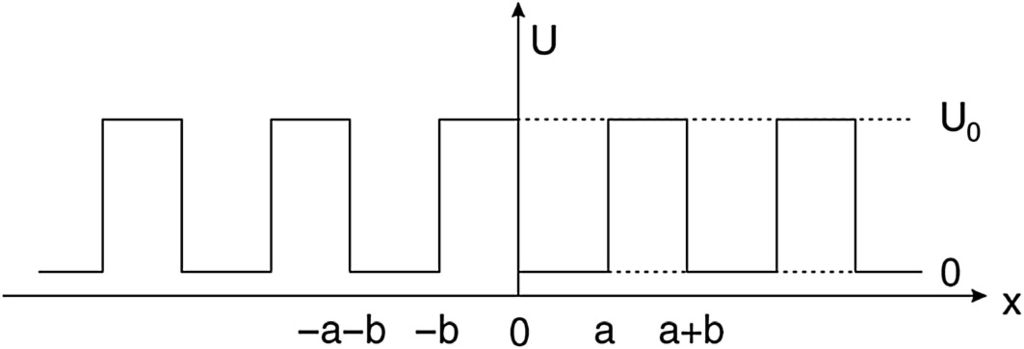
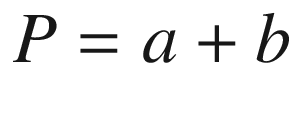


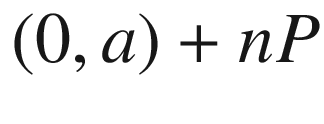
Fig. F.1

One-dimensional periodic hard-wall potential (Kronig-Penney model)

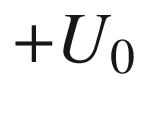
A one-dimensional periodic hard-wall potential of finite height is assumed (Fig. [F.1](#u116076_4_En_BookBackmatter_OnlinePDF-Fig6)). The well width is *a*, the barrier width *b* and thus the period



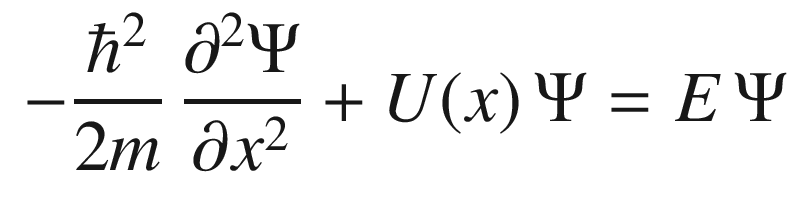
. The potential is zero in the well (regions



) and

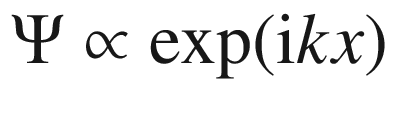


in the barrier. The Schrödinger equation

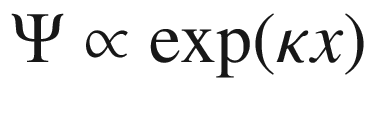


(F.1)

has to be solved. The solutions for a single hard-wall potential well are well known. In the well, they have oscillatory character, i.e.



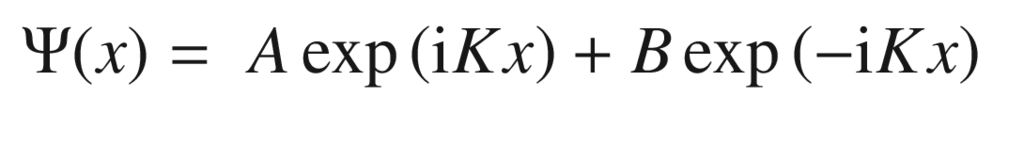
with real *k*. In the barrier, they have exponential character, i.e.



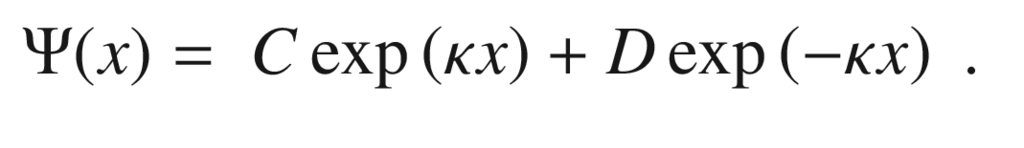
with real

$$\kappa $$

. Thus we chose

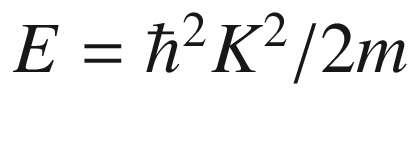


(F.2a)

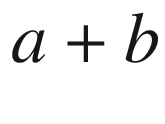


(F.2b)

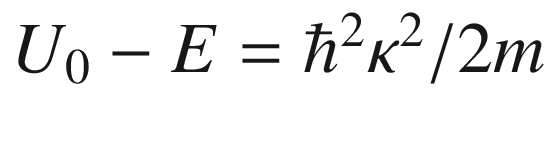
The wavefunction from ([F.2a](#u116076_4_En_BookBackmatter_OnlinePDF-Equ78)) is for the well between 0 and *a* with



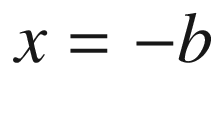
. The wavefunction from ([F.2b](#u116076_4_En_BookBackmatter_OnlinePDF-Equ79)) is for the barrier between *a* and



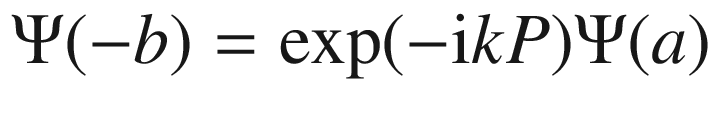
with



. From the periodicity and Bloch’s theorem ([6.​3](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter)) the wavefunction at



must have the form



, i.e. between the two wavefunctions is only a phase factor. The wavevector *k* of the Bloch function (plane-wave part of the solution) is a new quantity and must be carefully distinguished from *K* and

$$\kappa $$

, both coding the eigenenergy.

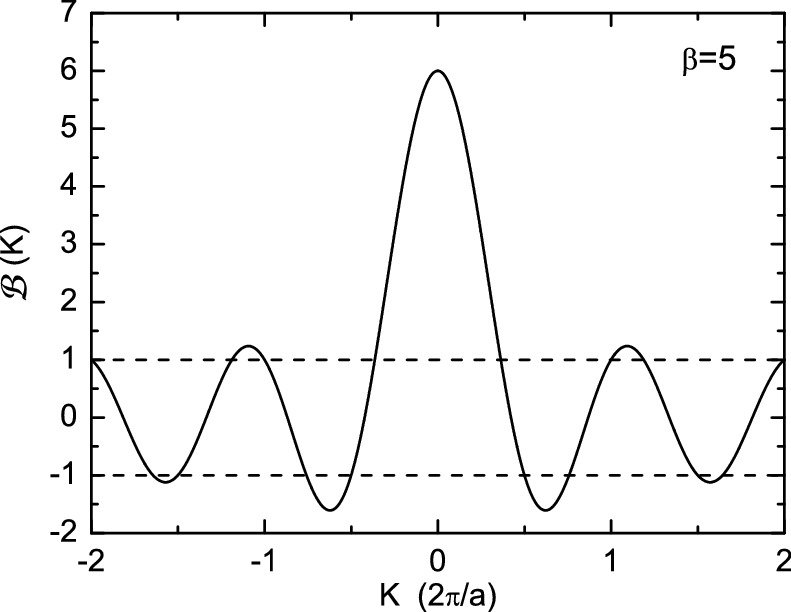
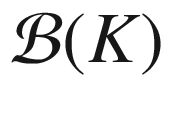
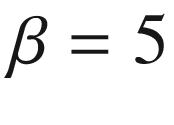


Fig. F.2

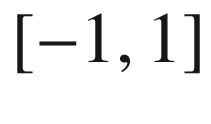
Transcendental function



from ([F.5](#u116076_4_En_BookBackmatter_OnlinePDF-Equ85)) for



. The *dashed lines* indicate the



interval for which solutions exist for ([F.5](#u116076_4_En_BookBackmatter_OnlinePDF-Equ85))

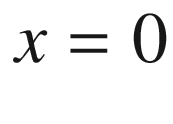
As boundary conditions, the continuity of



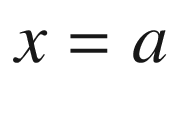
and



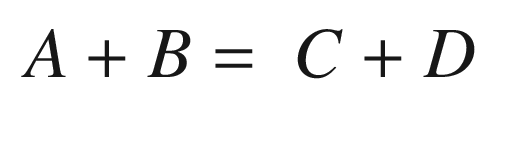
are used.[4](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn4) At



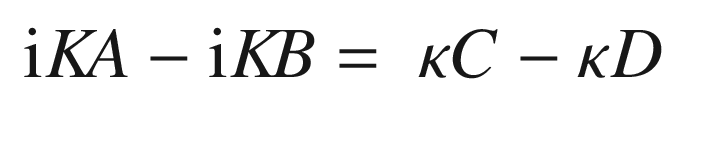
and



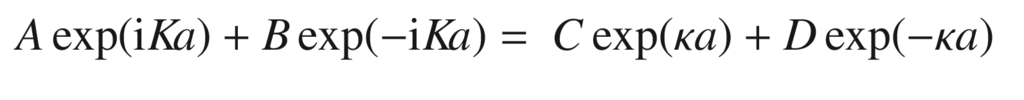
this yields



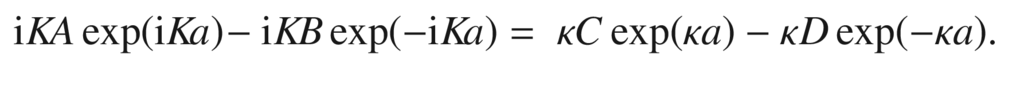
(F.3a)



(F.3b)



(F.3c)



(F.3d)

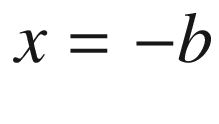
The continuity of



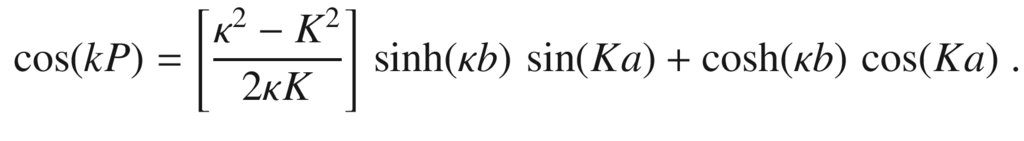
and



at

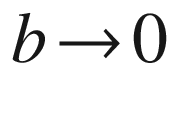


is used in the left sides of ([F.3c](#u116076_4_En_BookBackmatter_OnlinePDF-Equ82), [F.3d](#u116076_4_En_BookBackmatter_OnlinePDF-Equ83)). A nontrivial solution arises only if the determinant of the coefficient matrix is zero. This leads (after some tedious algebra) to

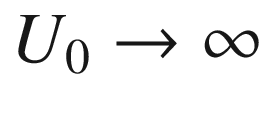


(F.4)

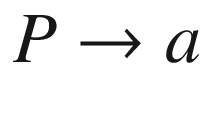
Further simplification are obtained by letting the barrier thickness



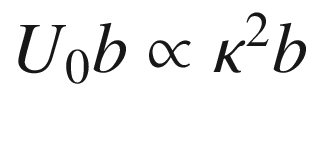
and



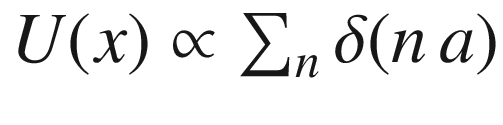
; then



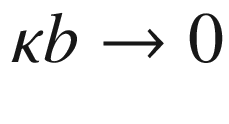
. The limit, however, is performed in such a way that the barrier ‘strength’



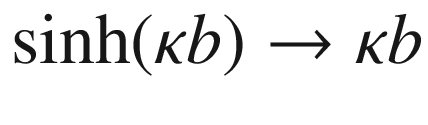
remains constant and finite, i.e.



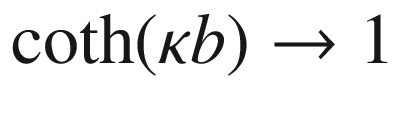
. Equation ([F.4](#u116076_4_En_BookBackmatter_OnlinePDF-Equ84)) then reads (for



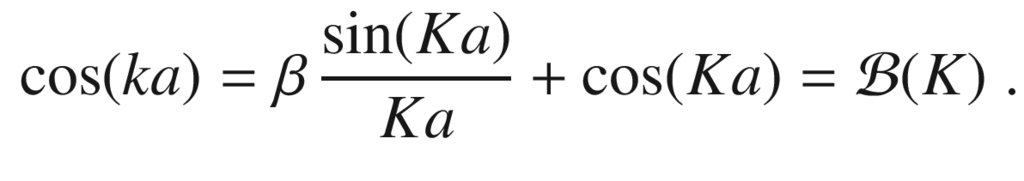
:



and

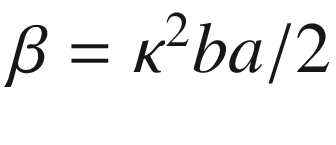


):

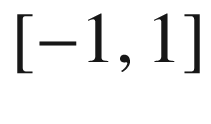


(F.5)

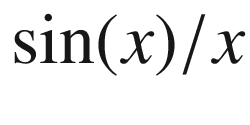
The dimensionless coupling parameter



represents the strength of the barrier. Equation ([F.5](#u116076_4_En_BookBackmatter_OnlinePDF-Equ85)) only has a solution if the right side is in the interval



(Fig. [F.2](#u116076_4_En_BookBackmatter_OnlinePDF-Fig7)). The function



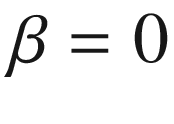
oscillates with decreasing amplitude such that for sufficiently high values of *Ka* a solution can always be found (



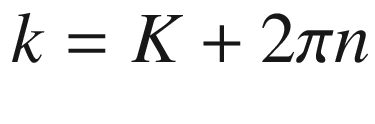
). The resulting dispersion is shown in Fig. [F.3](#u116076_4_En_BookBackmatter_OnlinePDF-Fig8)a, b for two different values of

$$\beta $$

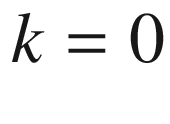
. The dispersion is different from the free-electron dispersion (for



, i.e.



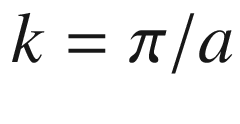
) and has several bands separated by gaps. The band gaps are related to the *K*-values for which ([F.5](#u116076_4_En_BookBackmatter_OnlinePDF-Equ85)) cannot be fulfilled. At the center (



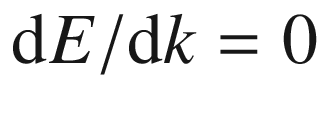
,

$$\Gamma $$

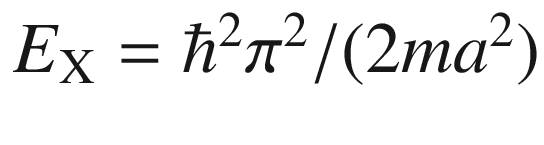
-point) and the zone boundary (X-point), (



) the bands are split and the tangent is horizontal (



). The form of the dispersion  is similar to the arccos function. The first band has the value



at the X-point for all values of

$$\beta $$

.

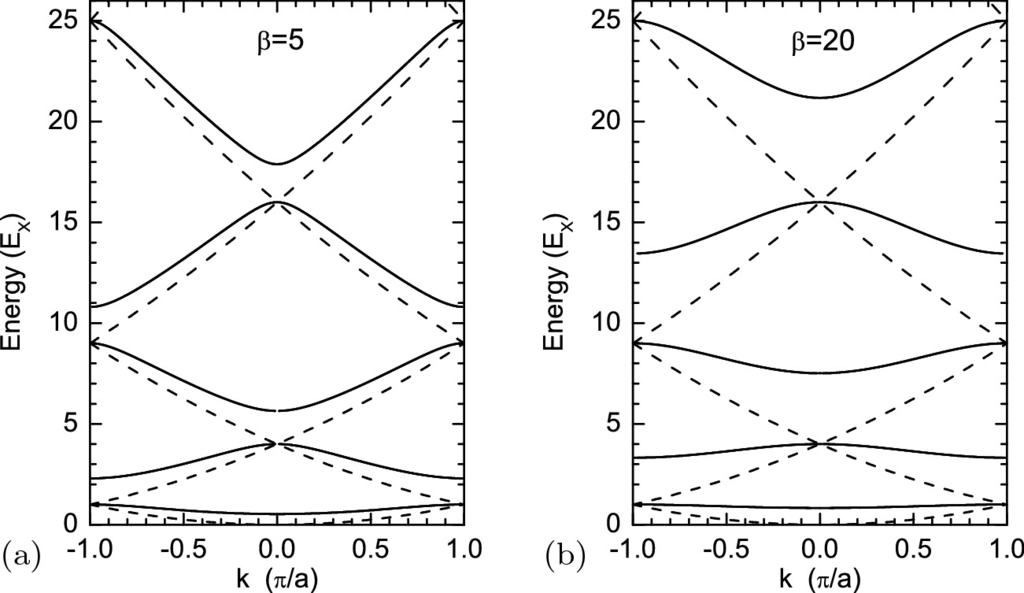
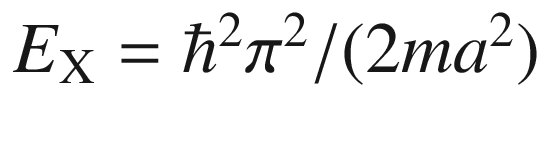
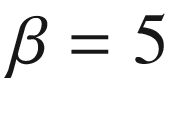


Fig. F.3

Energy dispersion of Kronig-Penney model (in units of



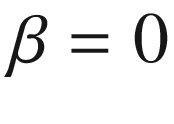
) as a function of the superlattice wavevector *k* for (**a**)



and (**b**)



in ([F.5](#u116076_4_En_BookBackmatter_OnlinePDF-Equ85)). The *dashed lines* are the free-electron dispersion (for



) (cf. Fig. [6.​2](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter-Fig2)a)

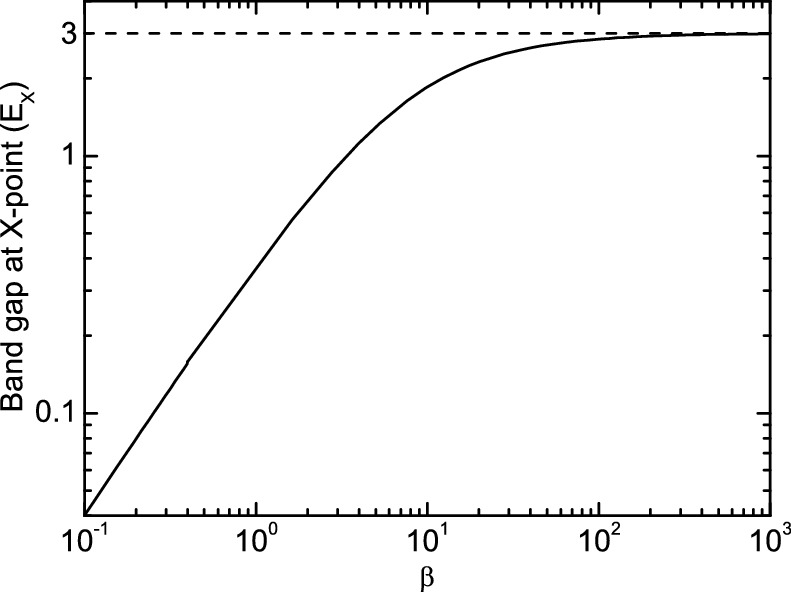
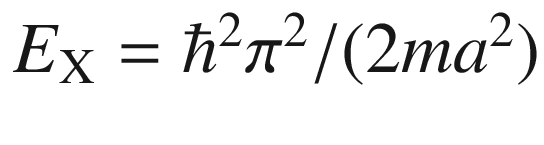


Fig. F.4

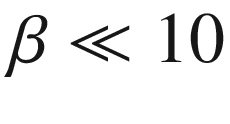
Band gap between first and second subband (at X-point, in units of



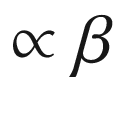
) as a function of

$$\beta $$

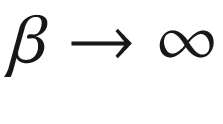
. For small



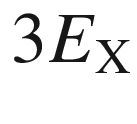
, the band gap is



. For thick barriers (



) the band gap saturates towards



as expected for uncoupled wells

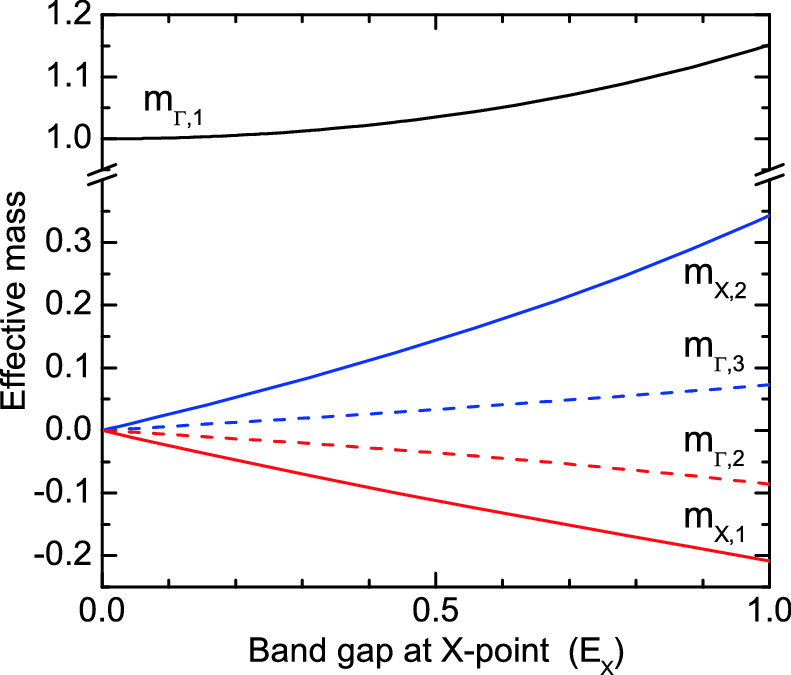
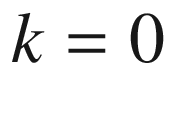


Fig. F.5

Effective mass (in units of *m*) of the first band extrema at the

$$\Gamma $$

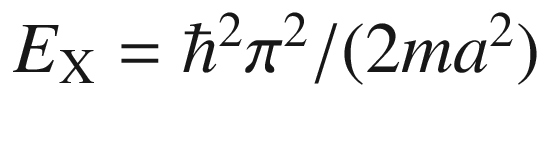
- and X-points (



and



, respectively) as a function of the band gap at the X-point (in units of

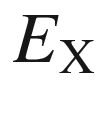


). The number in the index of the mass denotes the band

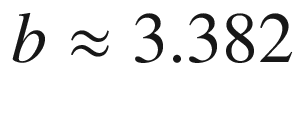


Fig. F.6

**a** Band dispersion and **b** density of states from the Kronig-Penney model for the first band gap being equal to

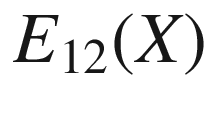


(



)

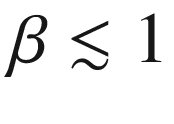
The band gap



between the first and the second subband (at the X-point) is shown in Fig. [F.4](#u116076_4_En_BookBackmatter_OnlinePDF-Fig9). For large coupling between the potential wells (small

$$\beta $$

,



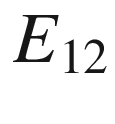
) it is



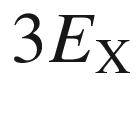
. In this case, the width of the subbands is wide. For small coupling (large

$$\beta $$

) the band gap



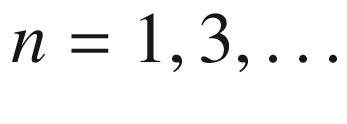
converges towards



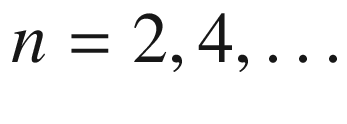
, as expected for decoupled potential wells with energy levels



. In this case, the width of the bands is small. Also, the character of the wavefunction is that of the solution for the individual quantum wells, i.e. even or s-type (for

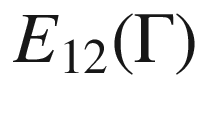


) or odd or p-type (for

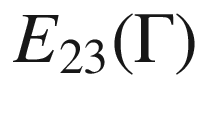


).

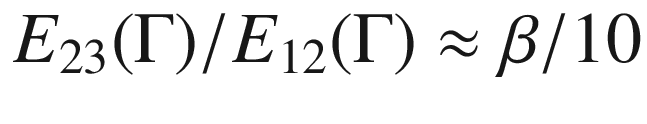
Other interesting quantities related to real bandstructures are the width of the valence band



and the fundamental bandgap



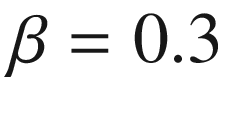
. Typical values of



(for



) of real semiconductors are in the range of 0.03–0.3, i.e. for



–3.

In Fig. [F.5](#u116076_4_En_BookBackmatter_OnlinePDF-Fig10) the effective masses are shown for the first five band extrema. The mass at the lowest minimum remains close to 1, i.e. keeps the carrier mass *m* from ([F.1](#u116076_4_En_BookBackmatter_OnlinePDF-Equ77)). Around the first gaps at the X- and the

$$\Gamma $$

-point, the effective masses are pairwise positive and negative, according to the character of the extremum as minimum or maximum, respectively. The absolute values are smaller than 1 for the given range of gaps. The mass increases initially linearly from zero with increasing gap.

The one-dimensional density of states (1D-DOS) has peaks (poles) at the band edges and is flat throughout most of the bands where the dispersion is linear (Fig. [F.6](#u116076_4_En_BookBackmatter_OnlinePDF-Fig11)).

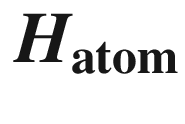
Appendix G

## Tight-Binding Model

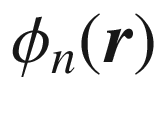
### G.1 Concept

The tight-binding model of electronic states rests on the concept of linear combination of atomic orbitals for finding a solution of the Hamiltonian of a periodic lattice. The ingredients of the model are the lattice structure and overlap matrix elements.[5](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn5)

Let us for now assume that there is one atom per lattice site. The atomic Hamiltonian



has the solutions

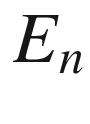


with

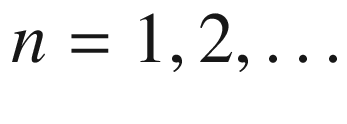


(G.1)

where

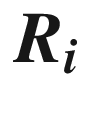


the energy of the *n*-th energy level (



) of the free atom.

The lattice shall be spanned by the lattice vectors



with the index *i* running over all *N* sites. For bulk-like solutions, a Bloch-type wave function, fulfilling ([6.​3](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter)), can be constructed from the atomic orbitals,



(G.2)

and will be taken as Ansatz for the solution of the crystal Hamiltonian

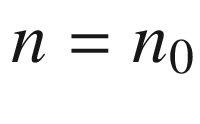


that is the sum of the atomic Hamiltonians plus a deviation

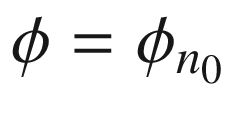


due to the crystal, which is small at the atomic site.

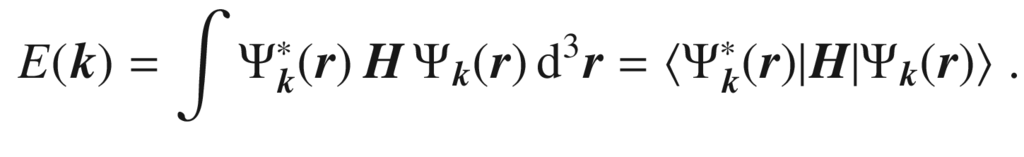
For now we consider only a single atomic state[6](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn6)



forming the band structure and write simple

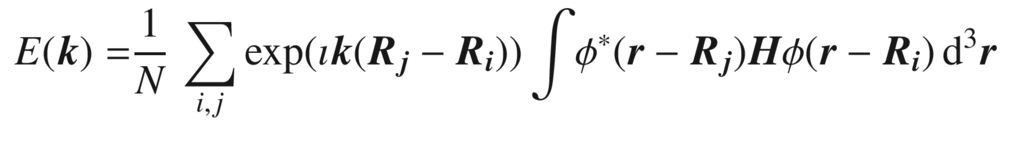


. The single particle energy in the crystal is then given by

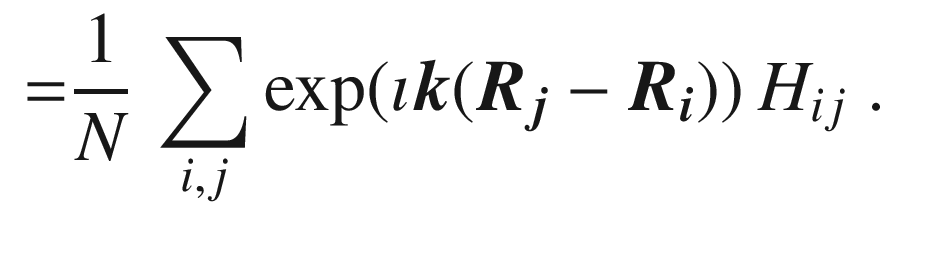


(G.3)

Equation ([G.3](#u116076_4_En_BookBackmatter_OnlinePDF-Equ88)) contains a double sum over the lattice sites *i* and *j*,

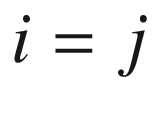


(G.4)

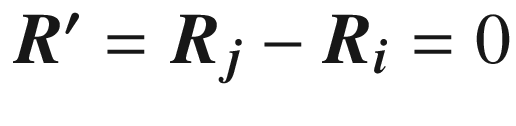


(G.5)

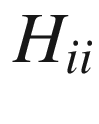
Now, for



, i.e.



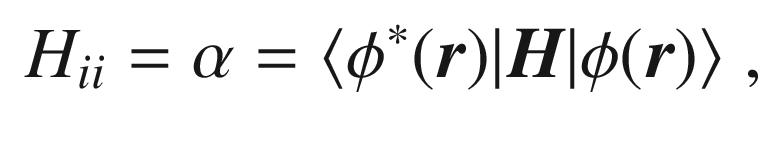
, the matrix element



gives a value

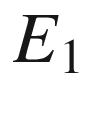
$$\alpha $$

,



(G.6)

which is nothing else but the atomic energy level



. Since the wave function

$$\phi $$

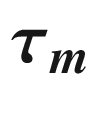
decays (rather quickly) with increasing distance



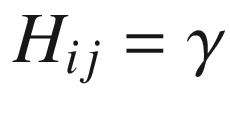
from the atom, the matrix elements will decrease as well. In the nearest-neighbor approximation, the sum of the



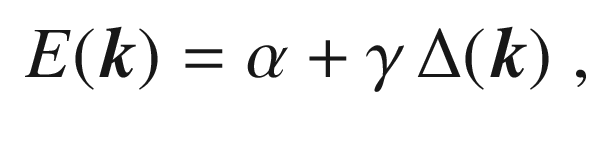
runs only over the *m* (equivalent) nearest neighbors



and we only consider one more matrix element

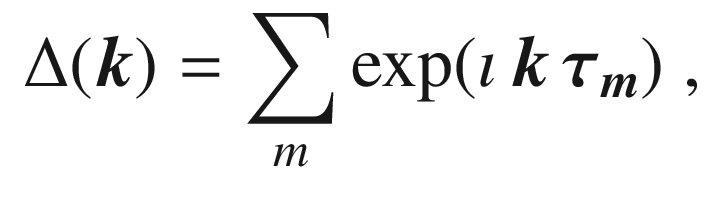


, when *i* and *j* are neighboring sites. This matrix element is not calculated explicitly but adjusted empirically to match experiments (empirical tight-binding model). Thus we find the energy dispersion



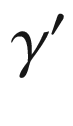
(G.7)

with the sum

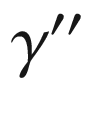


(G.8)

running over the nearest-neighbor sites. Extensions of the model consider second or even third next-neighbor sites with parameters



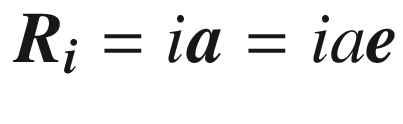
and



. Also, a larger number of atomic orbitals than a single one can be included, forming further bands.

### G.2 One-Dimensional Model

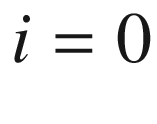
In a one-dimensional model,



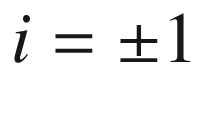
,

$$\varvec{e}$$

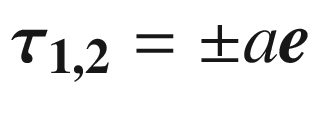
being the unit vector. The nearest neighbors to the atom at



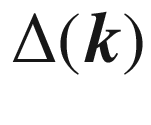
are at



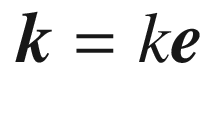
and



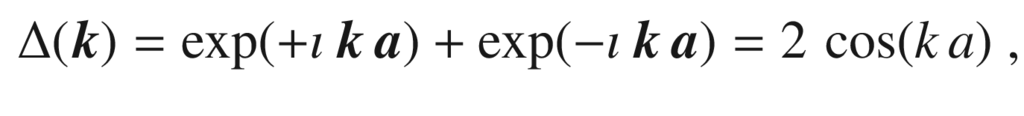
. Therefore,



([G.8](#u116076_4_En_BookBackmatter_OnlinePDF-Equ93)) is given by (

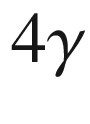


)

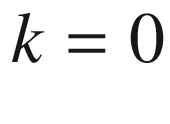


(G.9)

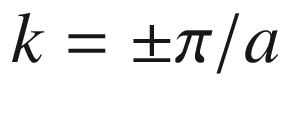
and the dispersion relation represents a band of width



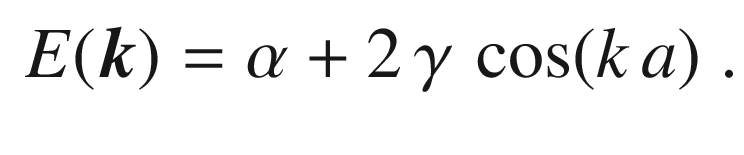
with extrema at



and



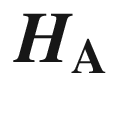
,



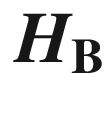
(G.10)

It is straightforward to extend this scheme to the case of a two-dimensional square lattice with four nearest neighbors (Appendix [G.3.1](#u116076_4_En_BookBackmatter_OnlinePDF-Sec19)) or to three-dimensional cubic lattices.

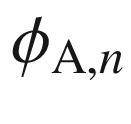
In the usual semiconductor cases, the basis has more than one atom; here we consider a two-atom basis with an A- and a B-site (like Fig. [5.​5](The_Physics_of_Semiconductors00002.docx#u116076_4_En_5_Chapter-Fig5)). Two different (the sites A and B having the same atom is a special case discussed below) atomic Hamiltonians



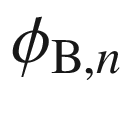
and



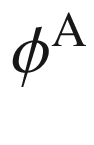
exist with sets of eigenfunctions



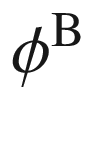
and



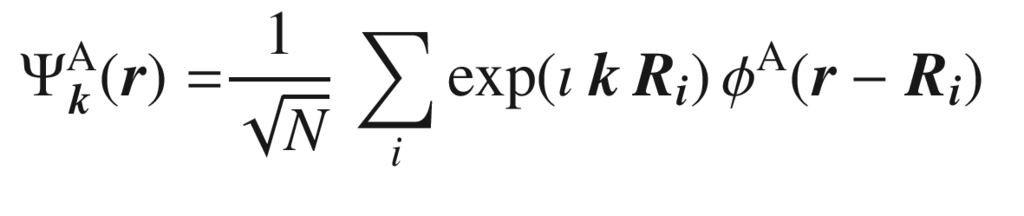
. We again consider only a single state at this point, i.e. we use



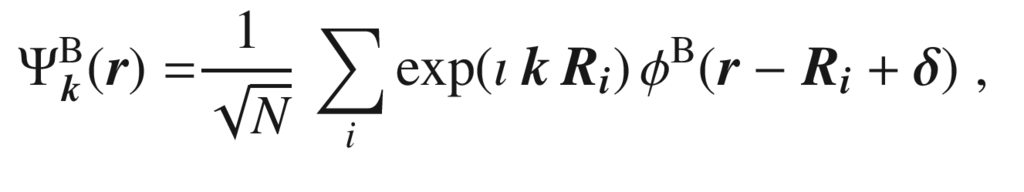
and



. Bloch-like functions ([6.​3](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter)) with these two orbitals are,



(G.11)

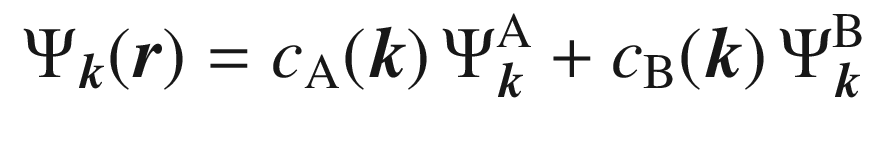


(G.12)

according to ([G.2](#u116076_4_En_BookBackmatter_OnlinePDF-Equ87)) with

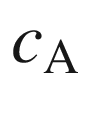
$$\varvec{\delta }$$

being the vector pointing from the A- to the B-site. The total wave function is given by

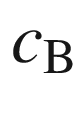


(G.13)

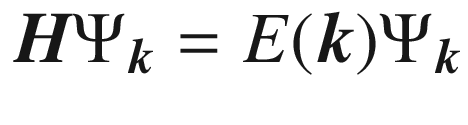
with complex coefficients



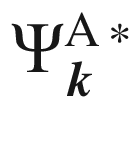
and



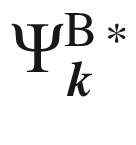
, denoting amplitudes and phases on the A- and B-site. This scheme can be generalized to larger number of atoms in the unit cell. Multiplying



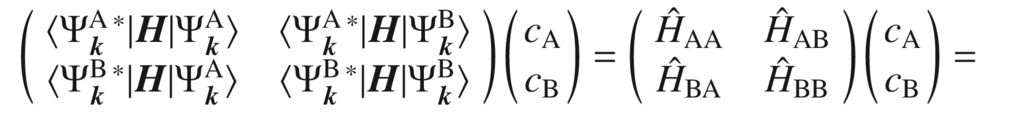
with



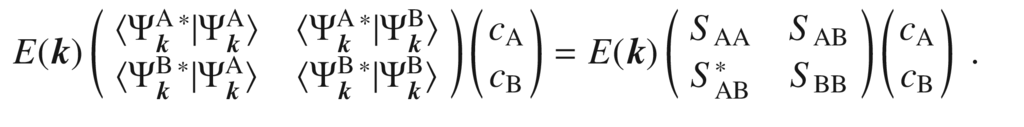
and



from the left side, respectively, and integration leads to the equation system,



(G.14)



(G.15)

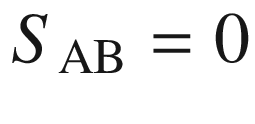
The overlap matrix

$$\varvec{S}$$

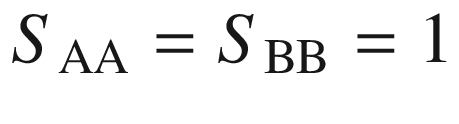
is approximately the unity matrix

$$\varvec{1}$$

, assuming the overlap integral of the atomic A and B wave functions



(of course, always



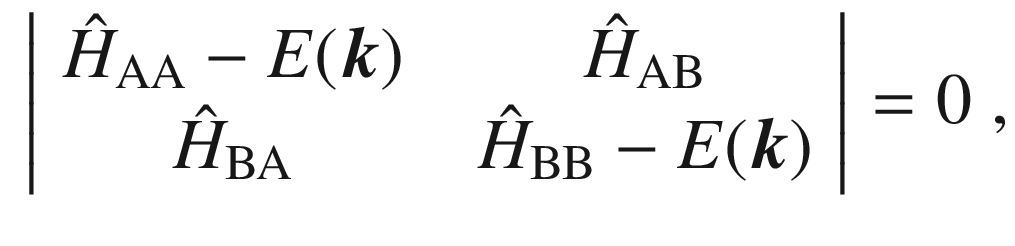
). The matrix



belongs to the Hamiltonian in the

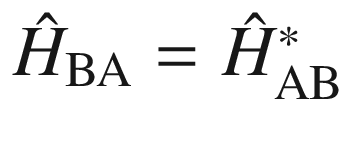
$$\varvec{k}$$

-representation. A non-trivial solution is only possible if the determinant fulfills,

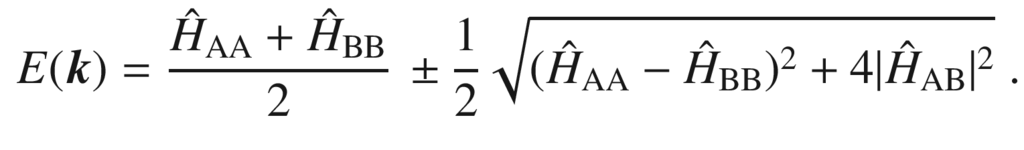


(G.16)

With



, the solutions are

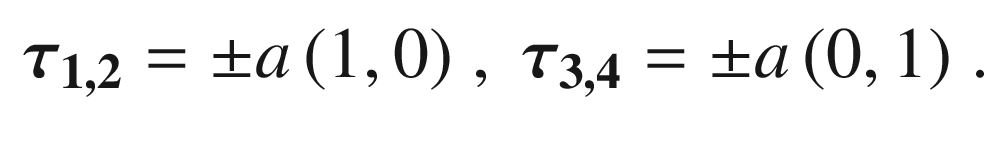


(G.17)

### G.3 Two-Dimensional Lattices

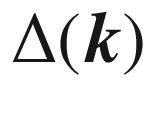
#### G.3.1 Square Lattice

The nearest neighbors in the square lattice (with simple base) with lattice constants *a* and *b*, are in orthogonal directions,

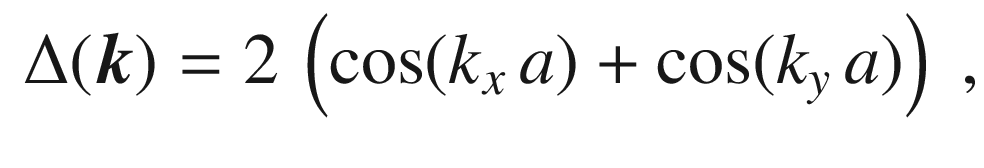


(G.18)

Thus

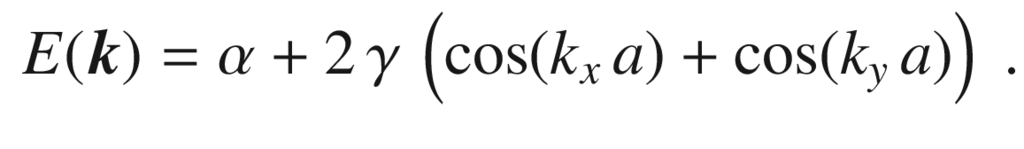


from ([G.8](#u116076_4_En_BookBackmatter_OnlinePDF-Equ93)) is given as



(G.19)

yielding the dispersion relation,



(G.20)

It should be mentioned that such model with an additional magnetic field perpendicular to the plane was treated by Hofstadter [[1471](#u116076_4_En_BookBackmatter_OnlinePDF-CR1471)] leading to a fractal behavior as function of the tight-binding energy

$$\gamma $$

and the magnetic field (‘Hofstadter butterfly’). Experiments on moiré graphene bilayers (cf. Sect. [13.​3](The_Physics_of_Semiconductors00006.docx#u116076_4_En_13_Chapter)) seemingly show such effects. Also the Hofstadter butterfly is the blueprint for assigning topological quantum numbers to the quantum Hall phases (cf. Sect. [15.​2.​8](The_Physics_of_Semiconductors00006.docx#u116076_4_En_15_Chapter)) [[1472](#u116076_4_En_BookBackmatter_OnlinePDF-CR1472)].

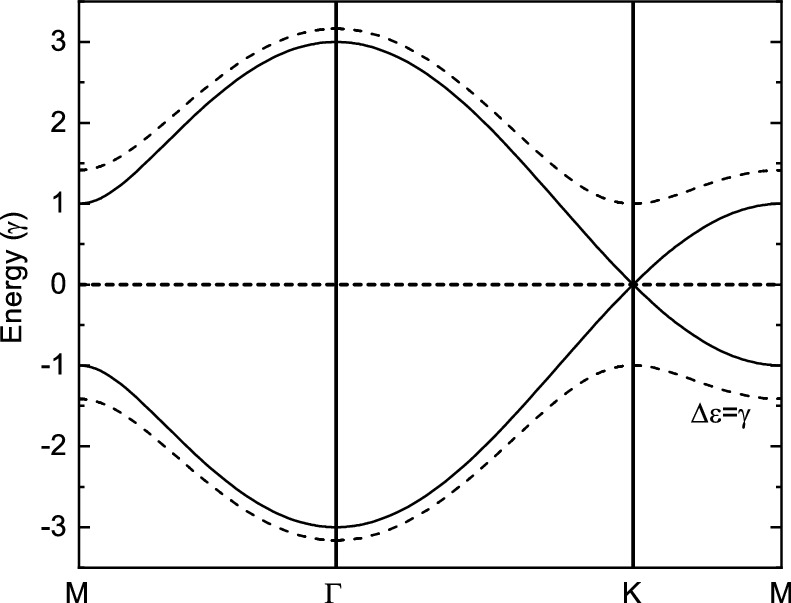


Fig. G.1

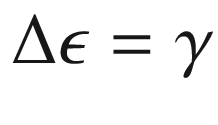
Tight-binding model band structure for honeycomb lattice with A

$$=$$

B according to ([G.24](#u116076_4_En_BookBackmatter_OnlinePDF-Equ109)) (solid line) and A

$$\ne $$

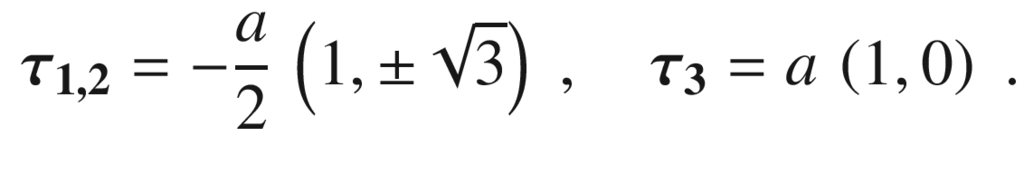
B according to ([G.25](#u116076_4_En_BookBackmatter_OnlinePDF-Equ110)) with



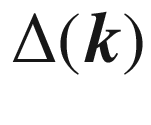
(*dashed line*)

#### G.3.2 Honeycomb Lattice

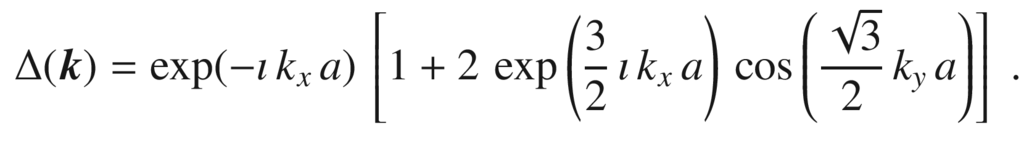
We now look at the honeycomb lattice which is a model for graphene or other two-dimensional semiconductors (cf. Fig. [13.​1](The_Physics_of_Semiconductors00006.docx#u116076_4_En_13_Chapter-Fig1)a). For an A-atom, the three vectors to the neighboring B-sites are



(G.21)

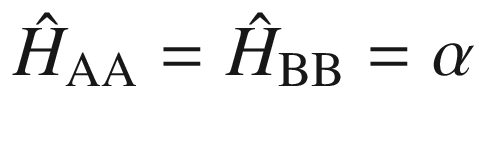


from ([G.8](#u116076_4_En_BookBackmatter_OnlinePDF-Equ93)) is given by

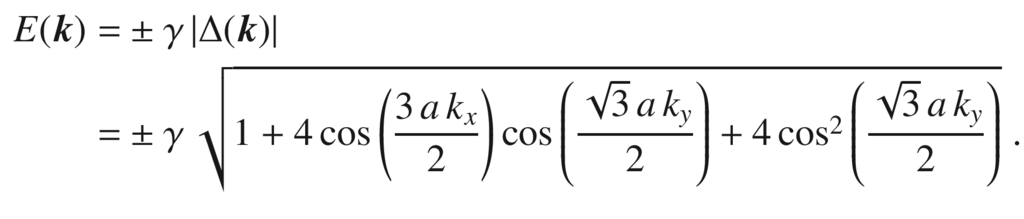


(G.22)

For the A- and B-atoms being the same (as for graphene),

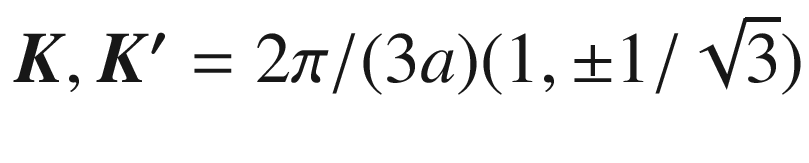


, giving a constant part to the energy that is ignored in the following. The square root in ([G.17](#u116076_4_En_BookBackmatter_OnlinePDF-Equ102)) yields a band structure (cf. Fig. [G.1](#u116076_4_En_BookBackmatter_OnlinePDF-Fig12))

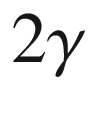


(G.23)

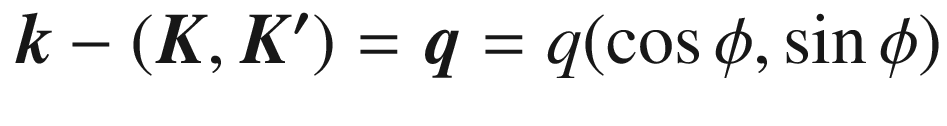
The energy is zero for at the K-points



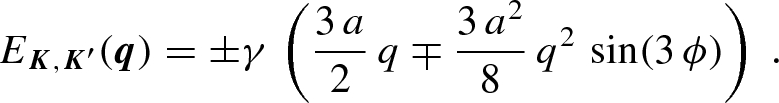
and their other equivalents (cmp. Fig. [13.​1](The_Physics_of_Semiconductors00006.docx#u116076_4_En_13_Chapter-Fig1)b). The band gap at the M-point is



. Around the K-points, the energy can be expanded with

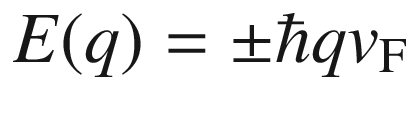


. We find

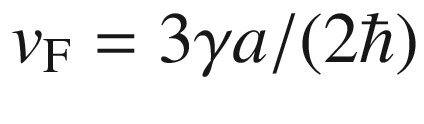


(G.24)

This shows that the dispersion is linear and isotropic around the K- and K’-points (Dirac points)  and (further away) has threefold symmetry (triangular warping, cmp. Sect. [6.​10.​2](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter)). The dispersion at the Dirac points is often written as



with

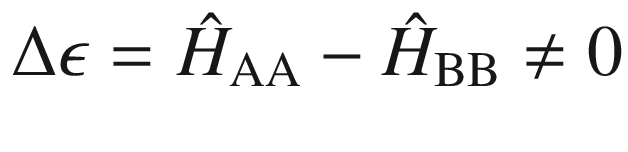


. Also, the K- and K’-points are non-equivalent, reflecting the two-atomic base. The winding sense in the

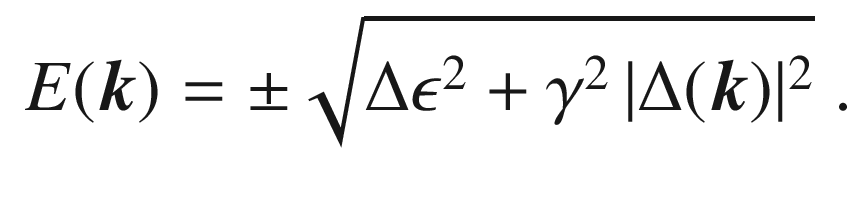
../images/116076_4_En_BookBackmatter_IEq516_HTML.gif

-term around K and K’ is opposite which leads to further ‘pseudo-spin’ physics.

For the case of the A- and B-sites being non-identical (e.g. for BN),

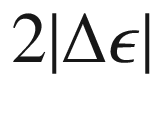


, the (non-constant part of the dispersion) is,

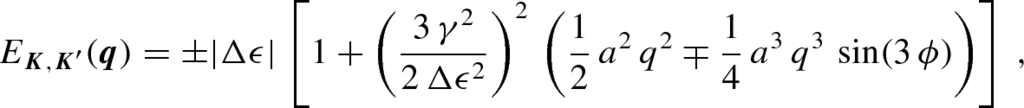


(G.25)

Thus a gap of



opens up at the K- and K’-points. Developing the solution around the K-points yields



(G.26)

and therefore (isotropic) parabolic extrema close to K and K’; the different winding sense of K and K’ appears in the

../images/116076_4_En_BookBackmatter_IEq519_HTML.gif

-term.

### G.4 Edge States and Topological Aspects

#### G.4.1 One-Dimensional Model

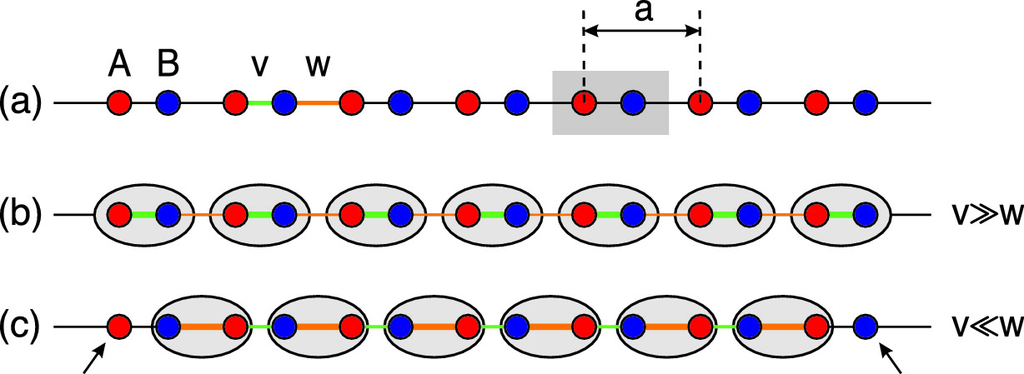
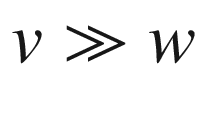
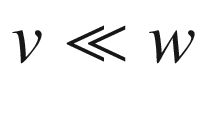


Fig. G.2

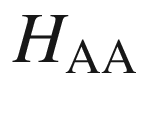
Schematic of the Su-Schrieffer-Heeger (SSH) model. (**a**) One-dimensional chain of unit cells (*grey area*) with A- and B-sites. The lattice constant is *a*. The hopping potentials *v* (intra-base, *green line*) and *w* (inter-base, *orange line*) are indicated. Dimers (*grey ellipses*) are shown for the cases (**b**)



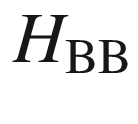
and (**c**)



The Su-Schrieffer-Heeger (SSH) model [[370](#u116076_4_En_BookBackmatter_OnlinePDF-CR370), [2154](#u116076_4_En_BookBackmatter_OnlinePDF-CR2154), [2155](#u116076_4_En_BookBackmatter_OnlinePDF-CR2155)] is a tight-binding model very much like the one in Appendix [G.2](#u116076_4_En_BookBackmatter_OnlinePDF-Sec17), describing a single spin-less electron on a one-dimensional lattice with a two-sites (A and B) unit cell (Fig. [G.2](#u116076_4_En_BookBackmatter_OnlinePDF-Fig13)a), suitable e.g. to describe an polyacetylene molecule. One electron per unit cell is assumed such that states are half filled. Also, the length of the chain will eventually be finite (*N* unit cells). The model has no on-site potential, which means that the constant energy parts



and

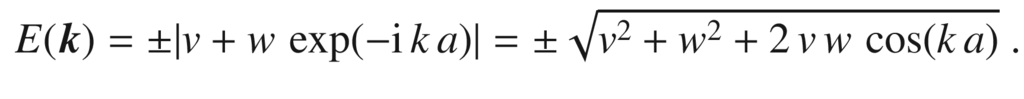


in ([G.16](#u116076_4_En_BookBackmatter_OnlinePDF-Equ101)) are now considered non-essential. The momentum-space Hamiltonian can be then written as



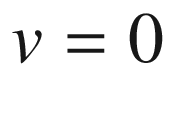
(G.27)

with the energy eigenvalues[7](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn7) given by

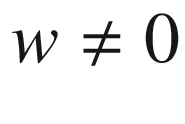


(G.28)

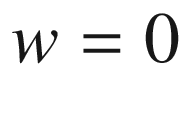
The parameters *v* and *w* are real positive numbers[8](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn8); *v* denotes the intra-base hopping amplitude between A and B, while *w* denotes the hopping between A and B belonging to different lattice points, i.e. from B to the right-neighbor A (Fig. [G.2](#u116076_4_En_BookBackmatter_OnlinePDF-Fig13)a). The band structure from ([G.28](#u116076_4_En_BookBackmatter_OnlinePDF-Equ113)) is shown in Fig. [G.3](#u116076_4_En_BookBackmatter_OnlinePDF-Fig14) for which we discuss five cases: in (a)



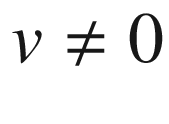
(



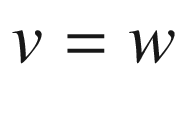
) and (e)



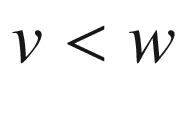
(



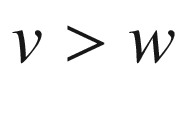
), the bands are flat with a gap (of size 2*v* or 2*w*). For (c)



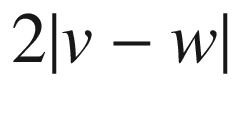
, the bands have no gap (similar to the graphene case). For the last two cases, (b)



and (d)



, the bands are curved with a gap (of size



).

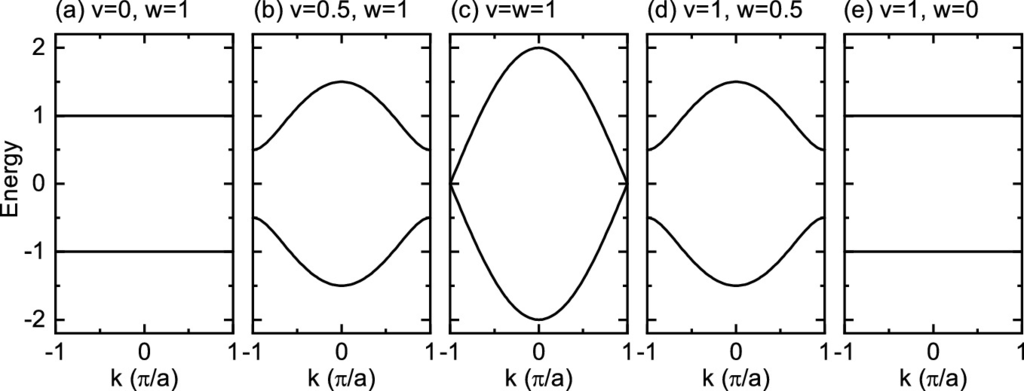
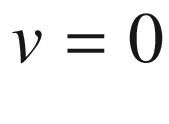
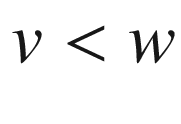


Fig. G.3

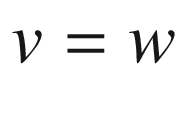
Band structure of the SSH model ([G.28](#u116076_4_En_BookBackmatter_OnlinePDF-Equ113)) for the cases



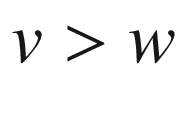
,



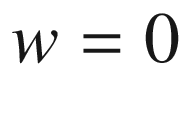
,



,



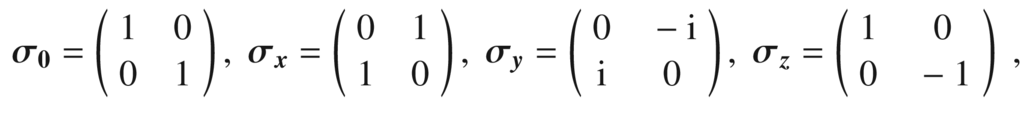
and



, as labeled

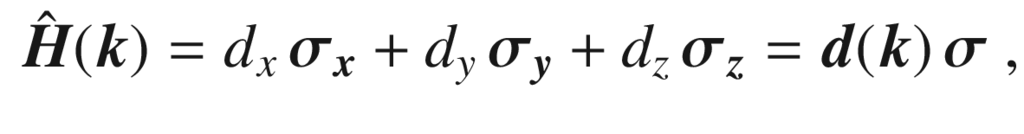
The point is now that the two seemingly similar cases Fig. [G.3](#u116076_4_En_BookBackmatter_OnlinePDF-Fig14)b and d result in the same band structure (i.e. the same eigenvalues), but they are different in other, maybe more subtle but actually very fundamental aspects, namely their eigenstates and eventually their topology .

The Hamiltonian for this two-band model ([G.27](#u116076_4_En_BookBackmatter_OnlinePDF-Equ112)) can be rewritten using the Pauli matrices,



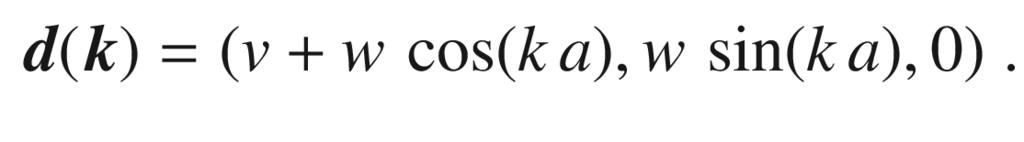
(G.29)

as



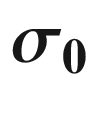
(G.30)

with the vector

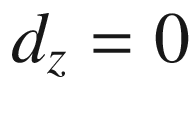


(G.31)

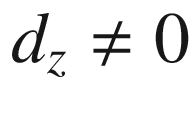
The coefficient of



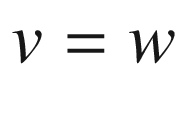
is zero in the SSH model (zero potential). Also



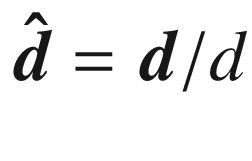
(due to ‘chiral’  symmetry,[9](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn9)



would open a gap[10](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn10) for



). Generally, the normalized vector



can be displayed on the Bloch sphere. In Fig. [G.4](#u116076_4_En_BookBackmatter_OnlinePDF-Fig15) the mapping of the Brillouin (torus, cf. Fig. [6.​6](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter-Fig6)) to the Bloch sphere to represent a unit vector.

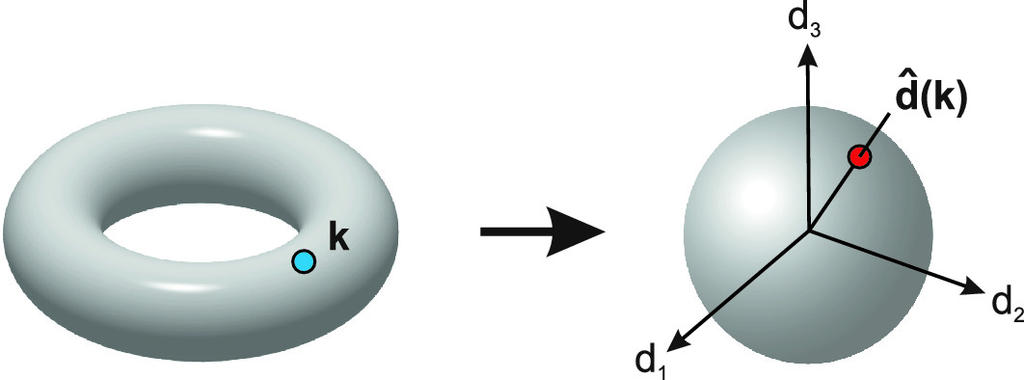


Fig. G.4

Mapping of the

$$\varvec{k}$$

-values from a 2D Brillouin zone (torus) to the vectors

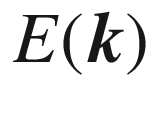
$$\varvec{\hat{d}}$$

(Bloch sphere). Designed after a graph in [[2157](#u116076_4_En_BookBackmatter_OnlinePDF-CR2157)]

Here, the vector

$$\varvec{d}$$

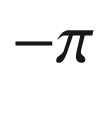
is two-dimensional and its length is equal to



(positive value). While

$$\varvec{k}$$

runs through the entire Brillouin zone, i.e. from



to

$$\pi $$

,

$$\varvec{d}$$

forms a circle of radius *w* around the point (*v*, 0); it is visualized in Fig. [G.5](#u116076_4_En_BookBackmatter_OnlinePDF-Fig16) for the cases (b) and (d).

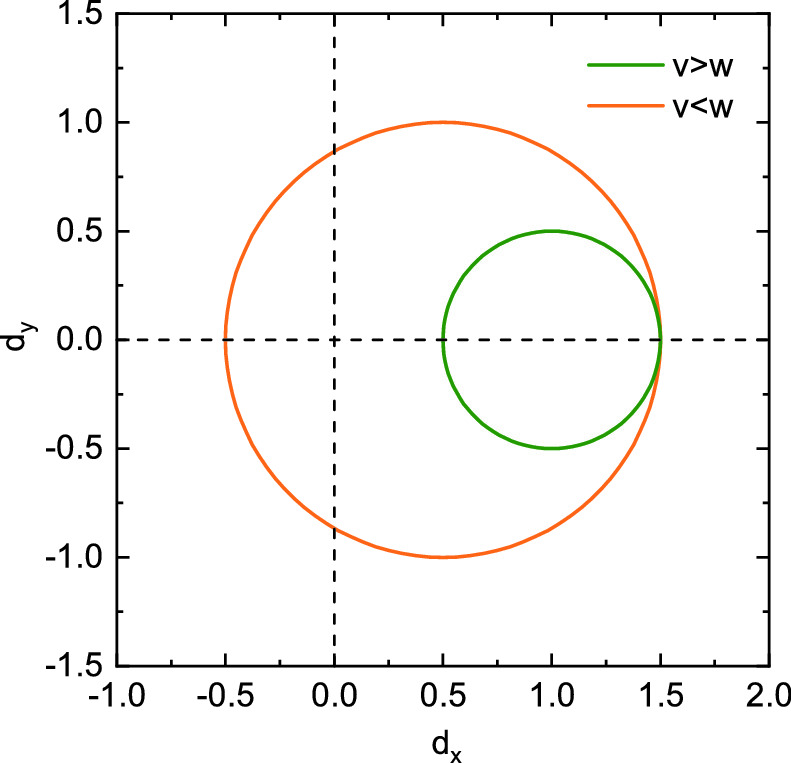
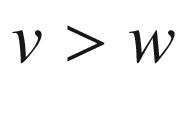


Fig. G.5

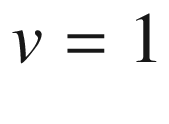
Vector

$$\varvec{d}$$

according to ([G.30](#u116076_4_En_BookBackmatter_OnlinePDF-Equ115)) for the cases



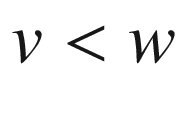
(*green*,



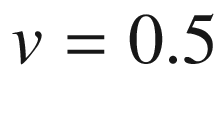
,



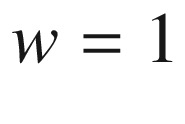
) and



(*orange*,

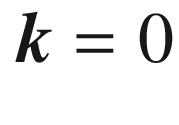


,

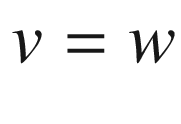


)

The main and *qualitative* difference of the two trajectories is that the origin (



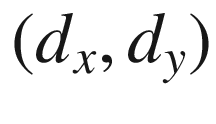
) is contained or not contained in the circle. Note, that for



, the circle touches the origin and the case (c) is undefined with that respect; such material, however, does not have a gap and is no insulator but a metal. Now, a number as topological invariant  can be defined as the number of rotations that

$$\varvec{d}$$

makes in the



-plane around the origin (while

$$\varvec{k}$$

runs through the entire Brillouin zone and avoids the origin for any wave vector since the material should have a gap); this quantity should be termed the ‘bulk winding number’

$$\nu $$

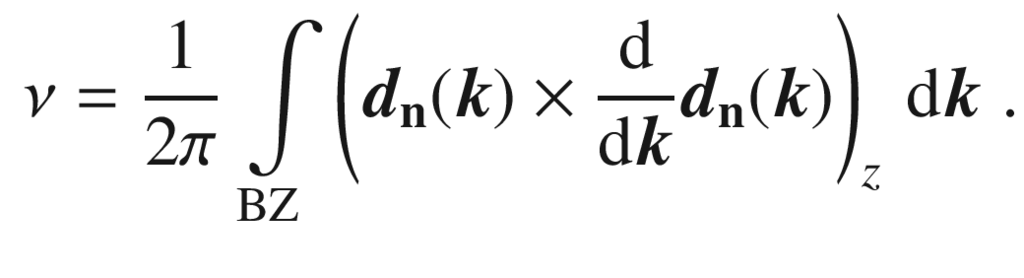
. We note that in general, the trajectory of

$$\varvec{d}$$

will be deformed from a circle, but it will be a closed loop due to the periodicity of the bulk

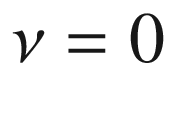
$$\varvec{k}$$

-space. Also, it might wind more than once around the origin. The calculation of the winding number can be generalized to an integral in reciprocal space,

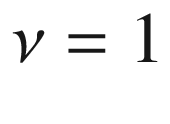


(G.32)

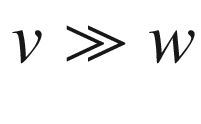
A look at the states of a finite chain model reveals another important distinction between the two cases



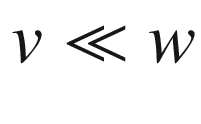
and



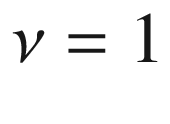
. Going to the extreme cases (a) and (e), the situation can be cartooned as shown in Fig. [G.2](#u116076_4_En_BookBackmatter_OnlinePDF-Fig13)b, c. For



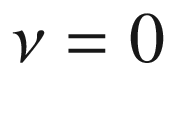
, the coupling within the base is strong and the chain disintegrates in *N* bases; this is called the ‘dimerized limit’. Then *N* identical uncoupled (or very weakly coupled) bases, split into their symmetric and anti-symmetric state, make up the flat bands. In the case



, the dimers group differently, giving the same flat bulk band structure. But, for a finite chain, at the edges two sites, indicated by arrows in Fig. [G.2](#u116076_4_En_BookBackmatter_OnlinePDF-Fig13)c remain unconnected to the bulk of the chain. Their energy is zero (since no on-site potentials are used in the SSH model). The discussed model is the simplest one to generate edge states. The edge states are only present for

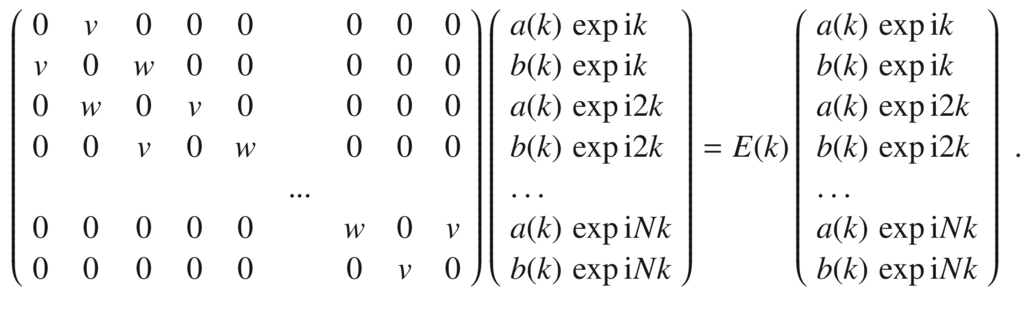


and not for the ‘topologically trivial’ case



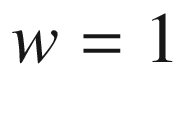
.

For finite *N*, the problem must be solved numerically. The Schrödinger equation ([G.27](#u116076_4_En_BookBackmatter_OnlinePDF-Equ112)) leads to the matrix eigenvalue problem,

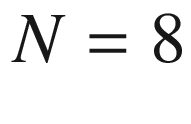


(G.33)

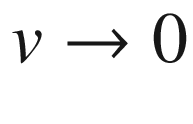
The eigenvalues for constant



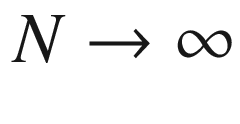
and *v* varying between 0 and 2 are shown in Fig. [G.6](#u116076_4_En_BookBackmatter_OnlinePDF-Fig17)a for a chain with



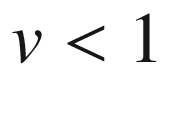
bases. For



, two edges states develop with zero energy in the gap. For



, the edge states develop for



. The wave function amplitudes of the edge states are shown together with those of the HOMO/LUMO in Fig. [G.6](#u116076_4_En_BookBackmatter_OnlinePDF-Fig17)b. The edge states have significant amplitude only on the A- or B-site and are strongly localized at the edges.

For a system with periodic boundary conditions, the upper right and the lower left element in the matrix of ([G.33](#u116076_4_En_BookBackmatter_OnlinePDF-Equ118)) are equal to *w* and no edge states are present.

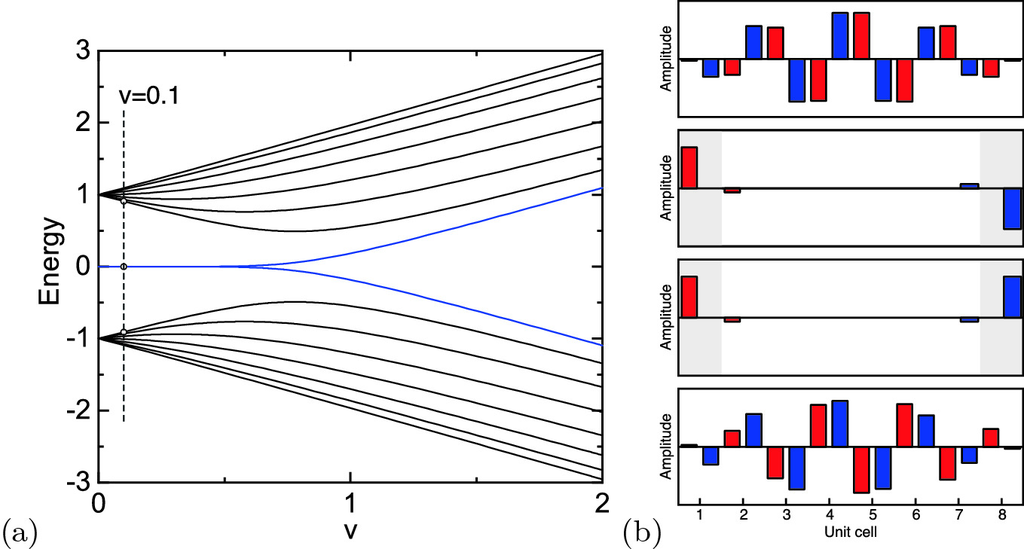
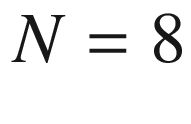
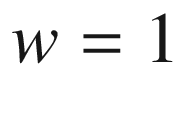


Fig. G.6

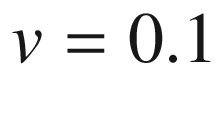
**a** Eigenvalues for SSH finite chain model ([G.33](#u116076_4_En_BookBackmatter_OnlinePDF-Equ118)) with



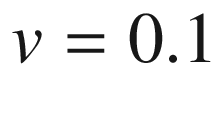
and



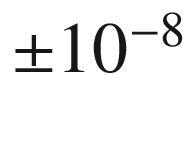
. For sufficiently small *v*, two zero energy edge states (*blue lines*) develop. The case



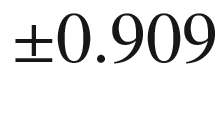
is highlighted with a *dashed line* and the HOMO, the LUMO and the two edge states are indicated by *circles*. **b** Mode patterns (for



) of the two edge states (center graphs) (energy:



) and the HOMO (bottom graph) and LUMO (top graph) (energy:



) as indicated in panel (**a**). The *red* (*blue*) bars denote the amplitude on the A (B) sites. The *greyed areas* denote the first and last unit cell of the chain

#### G.4.2 Two-Dimensional Models

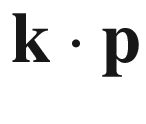
Topological edge states  in two-dimensional lattices with alternating hopping potentials  have been investigated for square and honeycomb lattices in [[2156](#u116076_4_En_BookBackmatter_OnlinePDF-CR2156), [2158](#u116076_4_En_BookBackmatter_OnlinePDF-CR2158)]. Topological aspects of graphene  are discussed in [[2159](#u116076_4_En_BookBackmatter_OnlinePDF-CR2159), [2160](#u116076_4_En_BookBackmatter_OnlinePDF-CR2160)]. The gap due to breaking parity symmetry (graphene



BN as discussed above) has been described in [[2161](#u116076_4_En_BookBackmatter_OnlinePDF-CR2161)]. It is topologically trivial while gaps in graphene due to next-nearest neighbor coupling [[1616](#u116076_4_En_BookBackmatter_OnlinePDF-CR1616)] or spin-orbit  interaction [[2162](#u116076_4_En_BookBackmatter_OnlinePDF-CR2162)] lead to non-trivial bulks. Two-dimensional topological insulators with arbitrary Chern number  can be constructed with the scheme given in [[2163](#u116076_4_En_BookBackmatter_OnlinePDF-CR2163)].

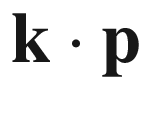
It was also found that zigzag graphene ribbons (cmp. Fig. [14.​16](The_Physics_of_Semiconductors00006.docx#u116076_4_En_14_Chapter-Fig16)) feature zero energy edge states, while armchair ribbons do not [[2164](#u116076_4_En_BookBackmatter_OnlinePDF-CR2164)].

Appendix H

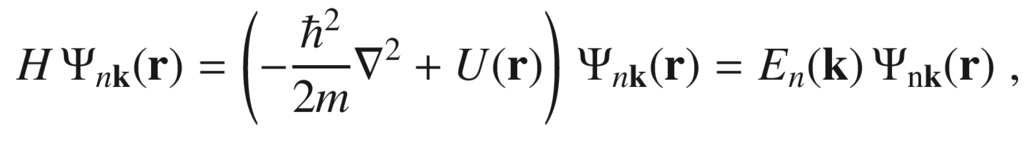


## Perturbation Theory

The

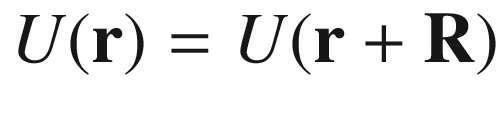


method is described in great detail in [[461](#u116076_4_En_BookBackmatter_OnlinePDF-CR461)] for various crystal symmetries. The solutions of the Schrödinger equation  (cf. Sect. [6.​2.​1](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter))



(H.1)

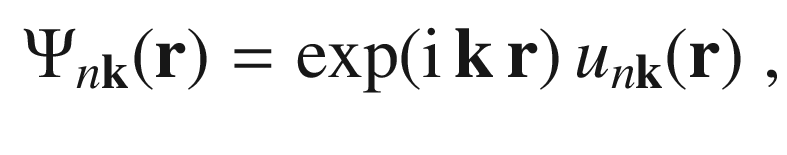
with a lattice periodic potential *U*, i.e.



for direct lattice vectors

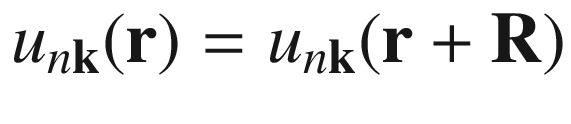


, are Bloch waves of the form



(H.2)

with the lattice periodic Bloch function



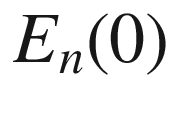
.

Inserting the Bloch wave into ([H.1](#u116076_4_En_BookBackmatter_OnlinePDF-Equ119)), the following equation is obtained for the periodic Bloch function:

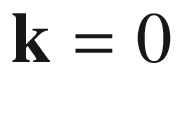


(H.3)

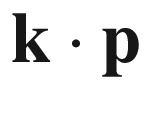
For simplicity, we assume a band edge



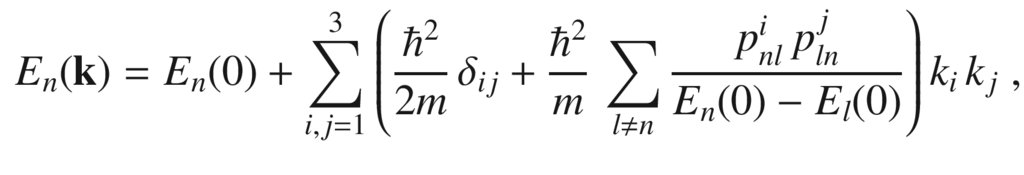
at



. In its vicinity, the



term can be treated as a perturbation. The dispersion for a nondegenerate band[11](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn11) is given up to second order in *k*

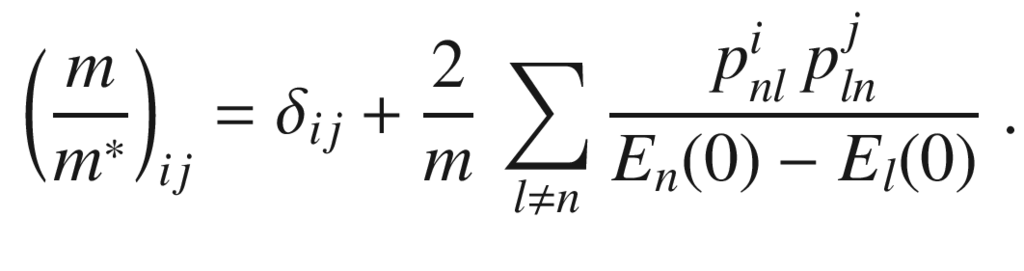


(H.4)

with *l* running over other, so-called *remote* bands. The momentum matrix element is given by

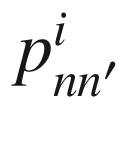


(cf. ([6.​39](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter))). The coefficients in front of the quadratic terms are the components of the dimensionless inverse effective-mass tensor (cf. ([6.​43](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter)))

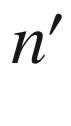


(H.5)

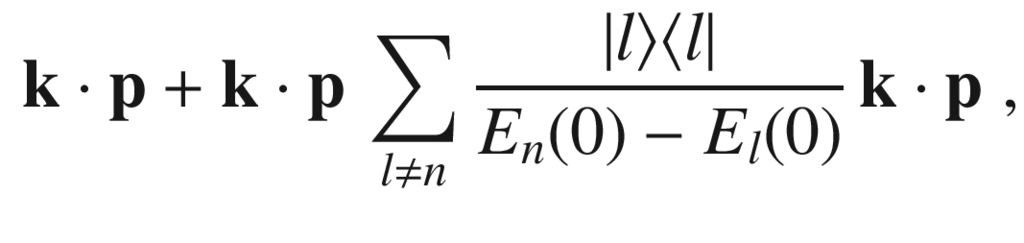
For degenerate bands, the



vanish when *n* and



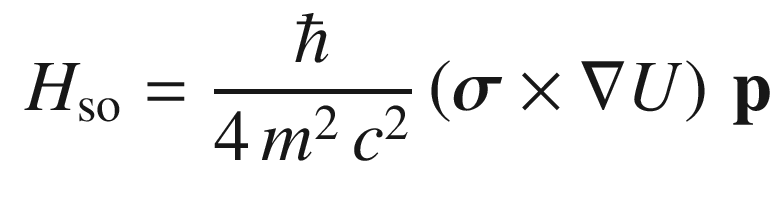
belong to the degenerate set and also the first-order correction is zero. In the  Löwdin perturbation theory [[2165](#u116076_4_En_BookBackmatter_OnlinePDF-CR2165)], the bands are separated into the close-by degenerate or nearly degenerate bands and the remote bands. The effect of the remote bands is taken into account by an effective perturbation



(H.6)

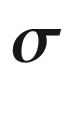
with the index *l* running over all bands not being in the degenerate set. The dispersion relation is obtained by diagonalization of the Hamiltonian ([H.3](#u116076_4_En_BookBackmatter_OnlinePDF-Equ121)) in the degenerate basis but with the perturbation given by ([H.6](#u116076_4_En_BookBackmatter_OnlinePDF-Equ124)).

The spin-orbit interaction [[1547](#u116076_4_En_BookBackmatter_OnlinePDF-CR1547)] adds an additional term

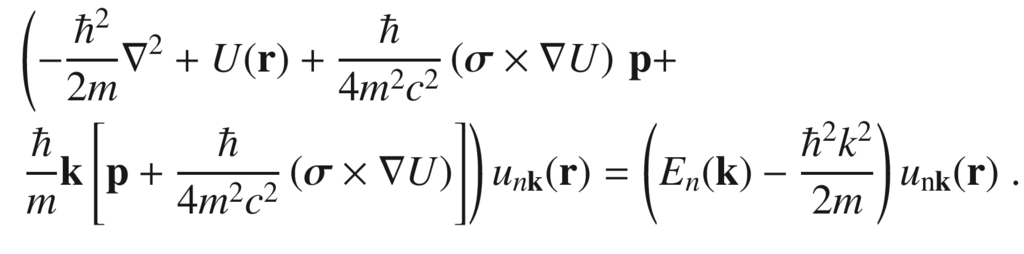


(H.7)

to the Hamiltonian, where



are the Pauli spin matrices and *c* the vacuum speed of light. In the Schrödinger equation for the Bloch functions two new terms arise:

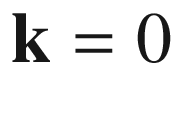


(H.8)

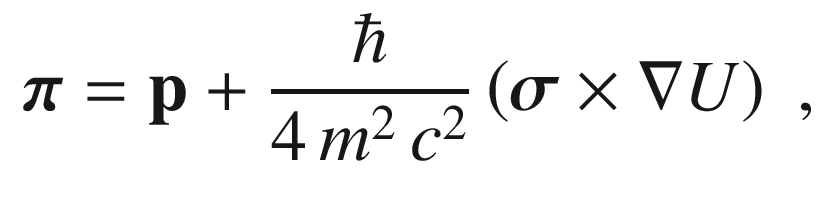
The linear term in

$$\mathbf{k}$$

is again treated as a perturbation. The first spin-orbit term in ([H.8](#u116076_4_En_BookBackmatter_OnlinePDF-Equ126)) is lattice periodic, thus the solutions at



are still periodic Bloch functions, however, different ones from previously. If the band edge is not degenerate, the momentum operator in ([H.3](#u116076_4_En_BookBackmatter_OnlinePDF-Equ121)) is simply replaced by



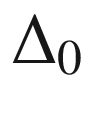
(H.9)

and the band edge is still parabolic. For a degenerate band edge, the effect can be more profound, in particular it can lead to the lifting of a degeneracy.Table H.1

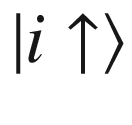
Basis set that diagonalizes the spin-orbit interaction

| $$| J, m_j \rangle $$ | Wavefunction | Symmetry |
| --- | --- | --- |
| $$| \frac{1}{2}, \frac{1}{2} \rangle $$ | $${\mathrm {i}}| s \uparrow \rangle $$ | $$\Gamma _6$$ |
| $$| \frac{1}{2}, -\frac{1}{2} \rangle $$ | $${\mathrm {i}}| s \downarrow \rangle $$ | $$\Gamma _6$$ |
| $$| \frac{3}{2}, \frac{3}{2} \rangle $$ | $$ \frac{1}{\sqrt{2}} | (x+{\mathrm {i}}y) \uparrow \rangle $$ | $$\Gamma _8$$ |
| $$| \frac{3}{2}, \frac{1}{2} \rangle $$ | $$ \frac{1}{\sqrt{6}} | (x+{\mathrm {i}}y) \downarrow \rangle - \sqrt{\frac{2}{3}} | z \uparrow \rangle $$ | $$\Gamma _8$$ |
| $$| \frac{3}{2}, -\frac{1}{2} \rangle $$ | $$ -\frac{1}{\sqrt{6}} | (x-{\mathrm {i}}y) \uparrow \rangle - \sqrt{\frac{2}{3}} | z \downarrow \rangle $$ | $$\Gamma _8$$ |
| $$| \frac{3}{2}, -\frac{3}{2} \rangle $$ | $$ \frac{1}{\sqrt{2}} | (x-{\mathrm {i}}y) \uparrow \rangle $$ | $$\Gamma _8$$ |
| $$| \frac{1}{2}, \frac{1}{2} \rangle $$ | $$ \frac{1}{\sqrt{3}} | (x+{\mathrm {i}}y) \downarrow \rangle + \sqrt{\frac{1}{3}} | z \uparrow \rangle $$ | $$\Gamma _7$$ |
| $$| \frac{1}{2}, -\frac{1}{2} \rangle $$ | $$ -\frac{1}{\sqrt{3}} | (x-{\mathrm {i}}y) \uparrow \rangle + \sqrt{\frac{1}{3}} | z \downarrow \rangle $$ | $$\Gamma _7$$ |

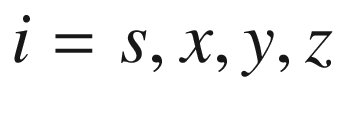
In the 8-band Kane model [[510](#u116076_4_En_BookBackmatter_OnlinePDF-CR510)], four bands (lowest conduction band, heavy, light and split-off hole band) are treated explicitly and the others through Löwdin perturbation theory. The basis is chosen to be diagonal in the spin-orbit interaction  leaving the spin-orbit interaction



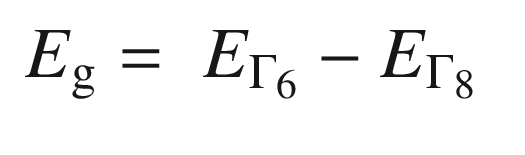
as parameter. The band- edge Bloch functions are denoted as



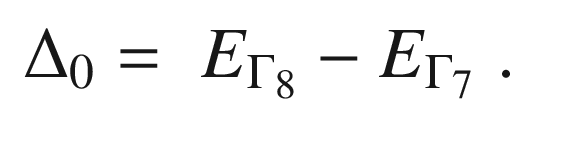
, where the index



labels the symmetry of the different bands. The linear combinations that diagonalize the spin-orbit interaction are given in Table [H.1](#u116076_4_En_BookBackmatter_OnlinePDF-Tab4). The band gap and the spin-orbit interaction are given by

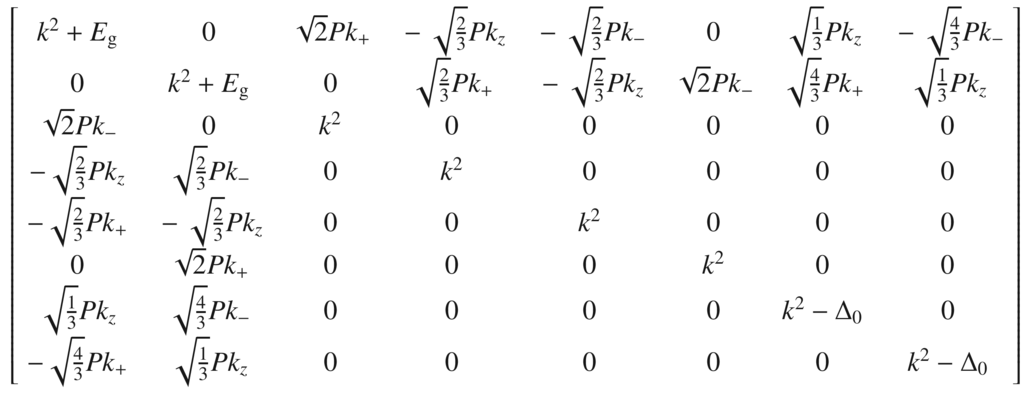


(H.10a)



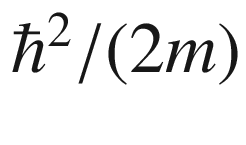
(H.10b)

The Hamiltonian in the basis states of Table [H.1](#u116076_4_En_BookBackmatter_OnlinePDF-Tab4) is given by



(H.11)

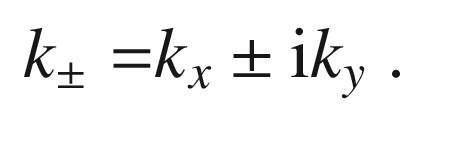
with the energy measured from the valence-band edge in units of



and

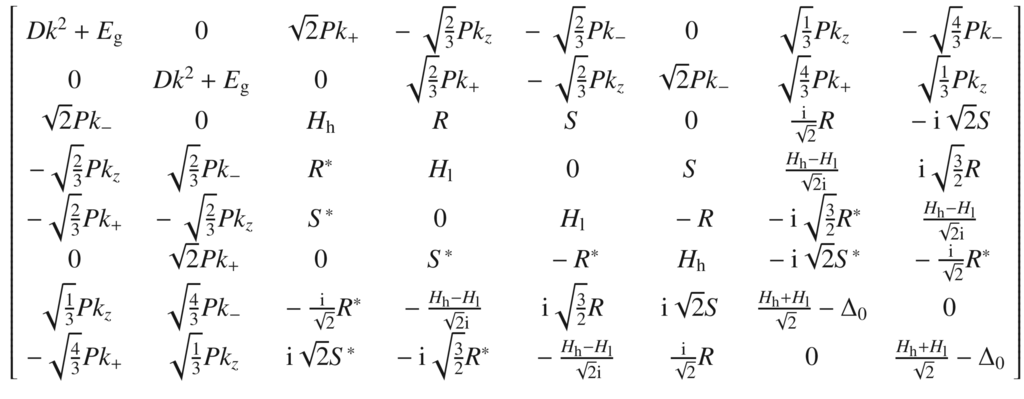


(H.12a)



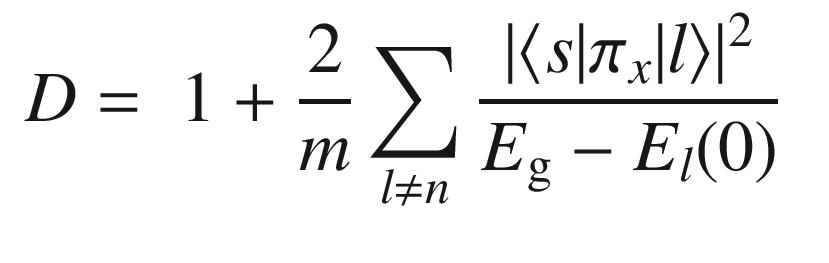
(H.12b)

The inclusion of remote bands renormalizes the above Hamiltonian to

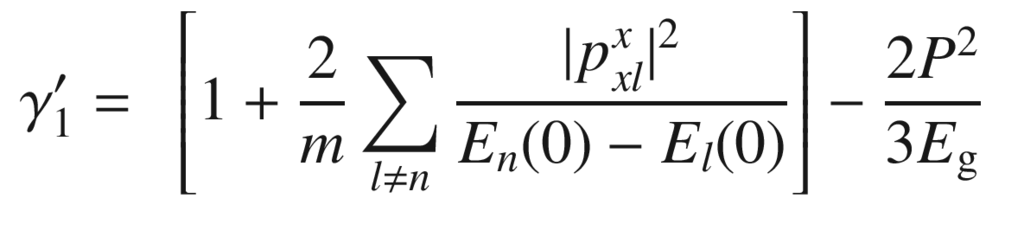


(H.13)

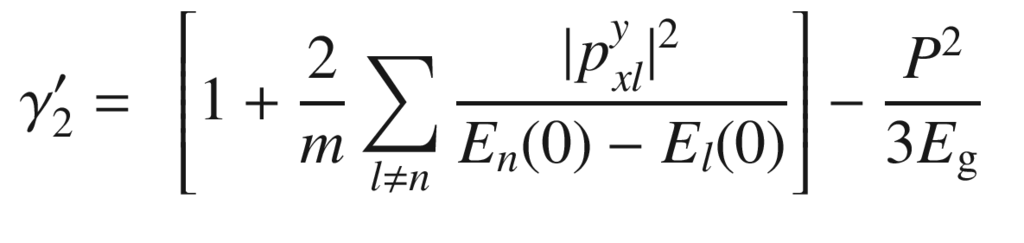
with



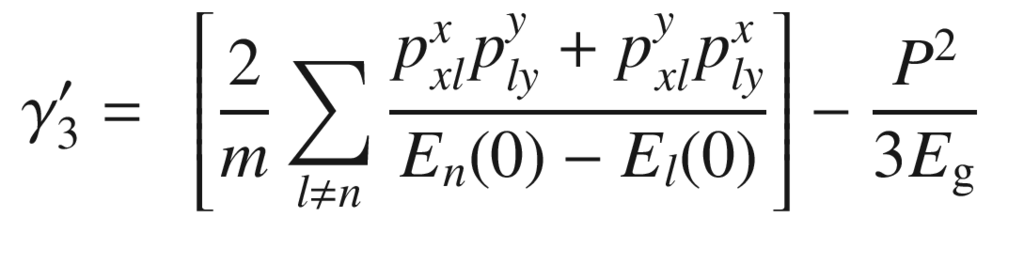
(H.14a)



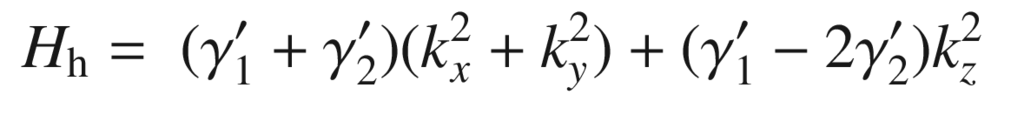
(H.14b)



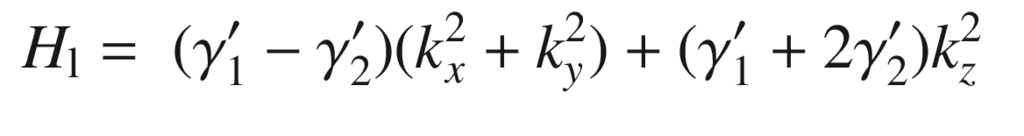
(H.14c)



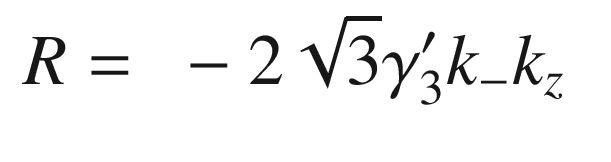
(H.14d)



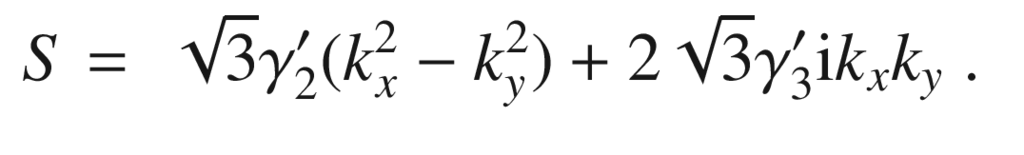
(H.14e)



(H.14f)

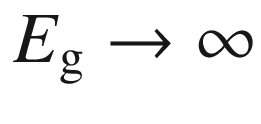


(H.14g)

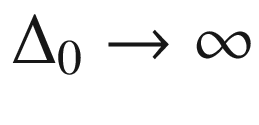


(H.14h)

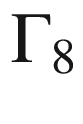
The Hamiltonian in the presence of inhomogeneous strain is given in [[536](#u116076_4_En_BookBackmatter_OnlinePDF-CR536)]. The hole bands decouple from the conduction band for



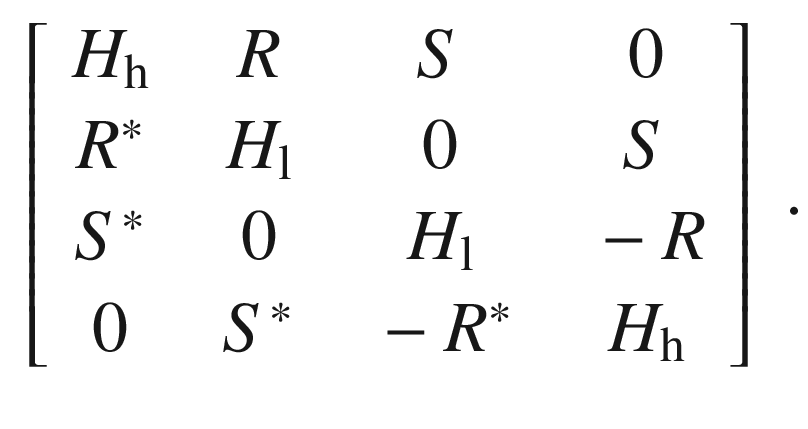
(six-band model [[1423](#u116076_4_En_BookBackmatter_OnlinePDF-CR1423)]). The heavy and light holes can be treated separately for



(Luttinger Hamiltonian). For the



states, the Hamiltonian is then given by



(H.15)

Appendix I

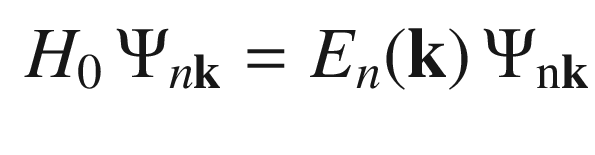
## Effective-Mass Theory

The effective-mass theory or approximation (EMA), also termed the envelope function approximation, is widely used for calculating the electronic properties of carriers in potentials in an otherwise periodic crystal. The strength of the method is that the complexities of the periodic potential are hidden in the effective-mass tensor



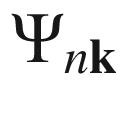
. The effective-mass theory is a useful approximation for the treatment of shallow impurities (Sect. [7.​5](The_Physics_of_Semiconductors00003.docx#u116076_4_En_7_Chapter)) or quantum wells (Sect. [12.​3.​2](The_Physics_of_Semiconductors00005.docx#u116076_4_En_12_Chapter)) with a potential that is slowly varying with respect to the scale of the lattice constant.

For the lattice-periodic potential, the Schrödinger equation

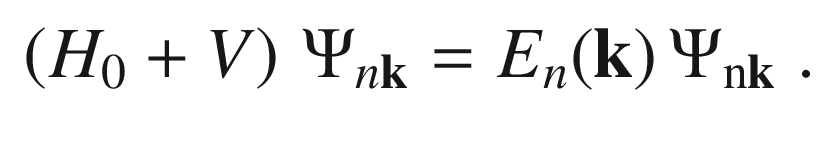


(I.1)

is solved by the Bloch wave

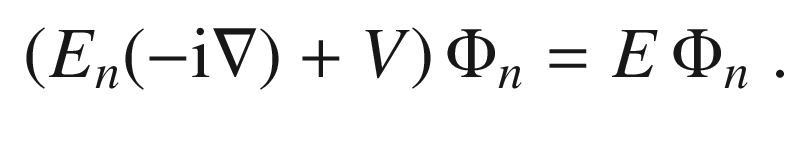


. With a perturbing potential *V*, the Schrödinger equation reads



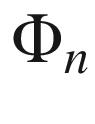
(I.2)

According to  Wannier’s theorem [[2166](#u116076_4_En_BookBackmatter_OnlinePDF-CR2166)], the solution is approximated by the solution of the equation

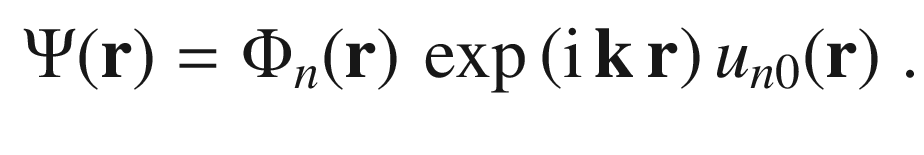


(I.3)

The dispersion relation is expanded to second order as described in Appendix [H](#u116076_4_En_BookBackmatter_OnlinePDF-Sec24). The function



is termed the *envelope function* since it varies slowly compared to the lattice constant and the exact wavefunction is approximated (in lowest order) by



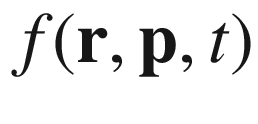
(I.4)

Appendix J

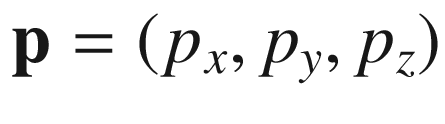
## Boltzmann Transport Theory

### J.1 Boltzmann Transport Equation

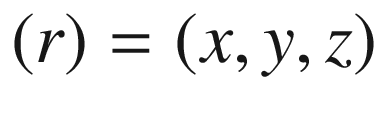
The Boltzmann treatment of transport  in semiconductors goes beyond the relaxation time approximation (cmp. Sect. [8.​2](The_Physics_of_Semiconductors00004.docx#u116076_4_En_8_Chapter)) and contains this approach as its simplest approximation. The distribution function of carriers



is considered with regard to their momentum

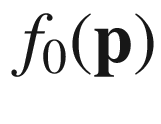


, their position



and time *t*. Via the dispersion relation(s) the momentum distribution also determines the energy distribution.

In thermodynamical equilibrium, the distribution function shall be termed



. In a homogeneous semiconductor it should be independent of

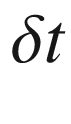
$$\mathbf{r}$$

, not depend explicitly on time and the momentum distribution be such that the resulting energy distribution should match the Fermi-Dirac distribution.

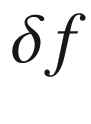
In non-equilibrium, the flow of electrons and heat is determined by the external forces

$$\mathbf{F}$$

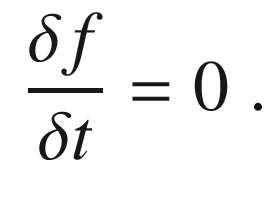
(electrical and magnetic fields) and the scattering  of charge carriers via various processes (termed here collisions). In a (non-equilibrium) steady-state situation with constant forces, the distribution function *f* is constant in time; thus in a given time interval



the change



is zero,

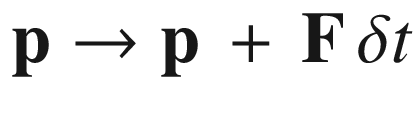


(J.1)

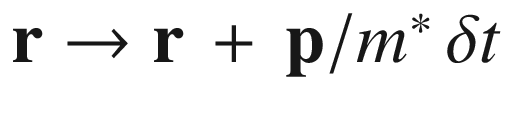
Within the time interval



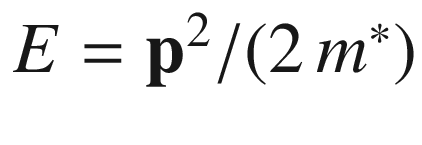
the momenta change as



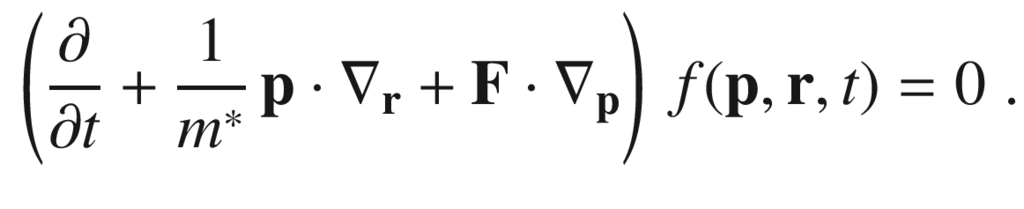
and the coordinates as



. We assume here for simplicity an isotropic mass and also the particle energy given by

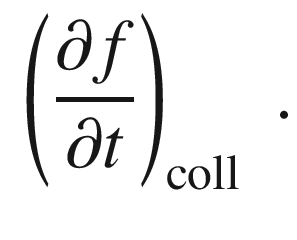


. The condition ([J.1](#u116076_4_En_BookBackmatter_OnlinePDF-Equ147)) written in partial derivatives reads



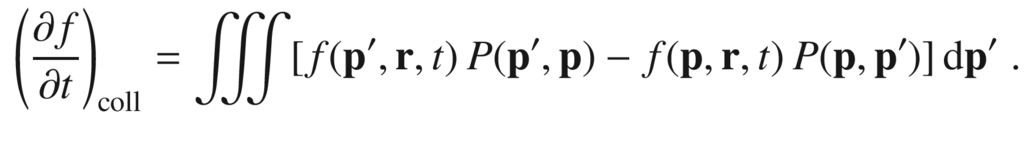
(J.2)

The force may be taken as the Lorentz force. So far no collisions  have been considered. Without giving an explicit form for the microscopic details of the collisions, the change of the distribution function due to collisions is written as



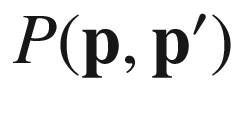
(J.3)

Assuming that only two-particle collisions play a role, sample boundaries play no role and that position and velocity of particles are uncorrelated, the collision term can be written as



(J.4)

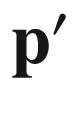
with



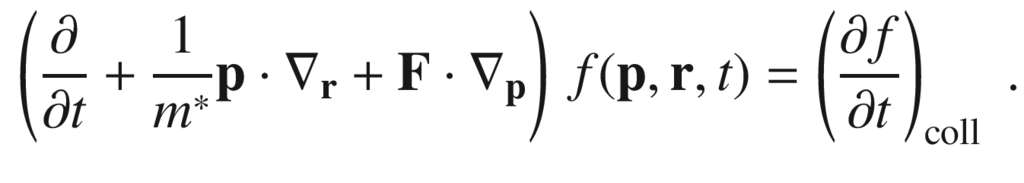
being the transition probability per time that a momentum

$$\mathbf{p}$$

is changed into

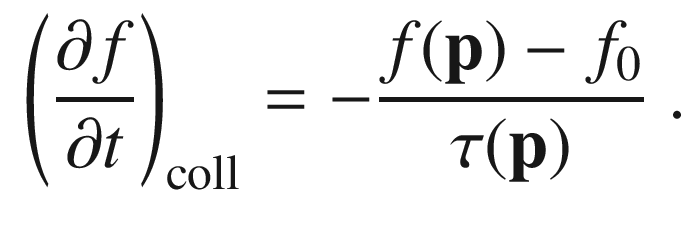


by collisions. The collision integral must be calculated explicitly using microscopic and eventually quantum mechanical models. This leads now to the Boltzmann transport equation



(J.5)

Under certain circumstances, the collision term can be effectively written as (for a homogeneous semiconductor and homogeneous fields, neglecting the spatial dependence of *f*)

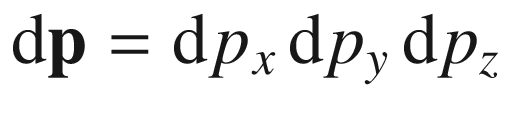


(J.6)

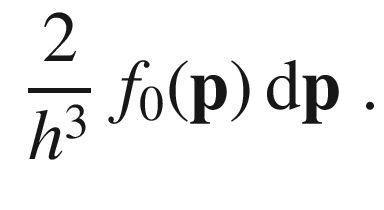
Compared to the relaxation time approximation, the major difference on the level of ([J.6](#u116076_4_En_BookBackmatter_OnlinePDF-Equ152)) here is the consideration of the momentum (and energy) dependence of the distribution function and the relaxation time.

### J.2 Conductivity

In thermodynamical equilibrium the number of electronic states per unit volume associated with an element



, including spin degeneracy of 2 is

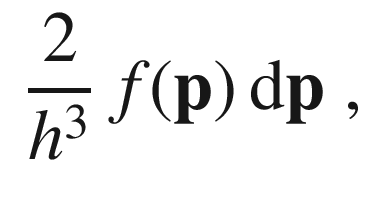


(J.7)

In the presence of an electric field

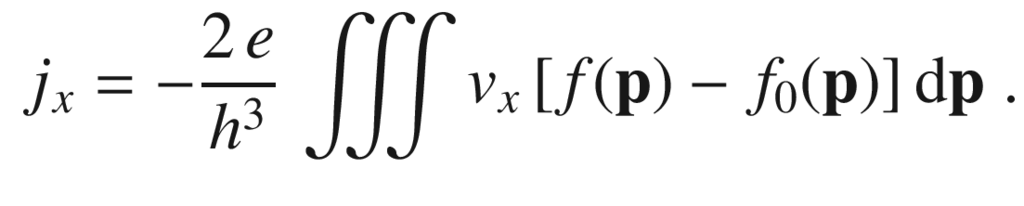


, which we assume here in *x*-direction, a steady-state current will arise and the number of electronic states changes to



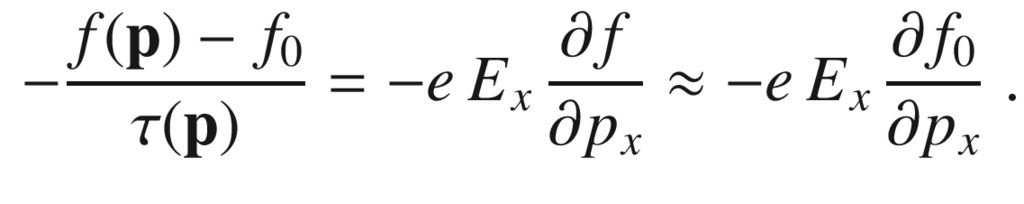
(J.8)

making the (electron) current density (along *x*-direction)



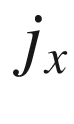
(J.9)

This is a generalization of ([8.​4](The_Physics_of_Semiconductors00004.docx#u116076_4_En_8_Chapter)). The Boltzmann transport equation ([J.5](#u116076_4_En_BookBackmatter_OnlinePDF-Equ151)) with ([J.6](#u116076_4_En_BookBackmatter_OnlinePDF-Equ152)) simplifies to

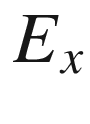


(J.10)

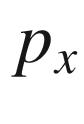
The last approximation is valid for small fields and makes



proportional to



(ohmic regime). The derivative with respect to

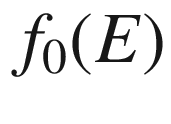


is converted to a derivative with respect to energy, yielding

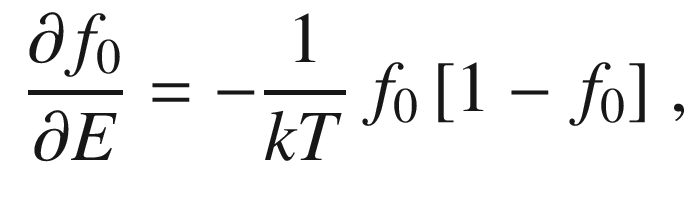


(J.11)

We note that for the Fermi-Dirac distribution ([E.22](#u116076_4_En_BookBackmatter_OnlinePDF-Equ74))

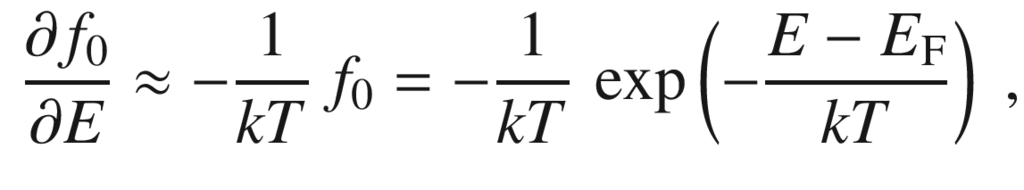


:



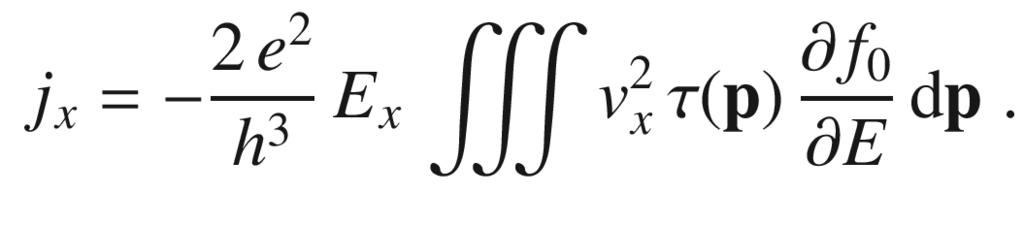
(J.12)

and in the case of a non-degenerate semiconductor (Boltzmann approximation), the right-hand side simplyfies to



(J.13)

Now the current density is given as

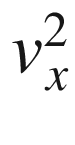


(J.14)

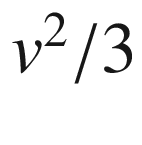
If we assume that

$$\tau $$

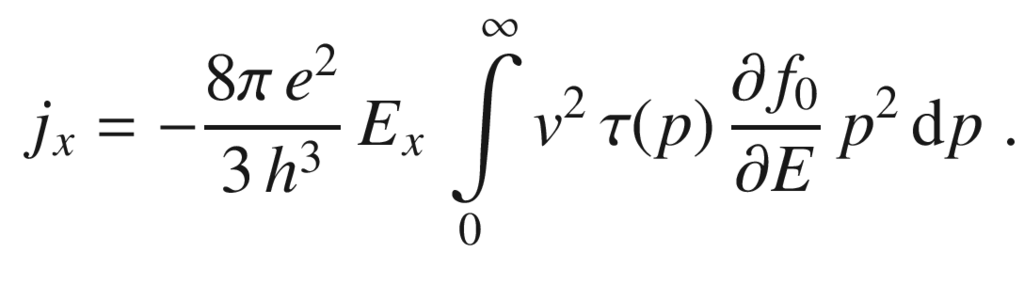
depends only on the momentum and not its direction[12](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn12), and replace



by

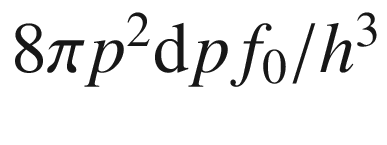


assuming isotropy, the integral reads[13](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn13)

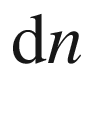


(J.15)

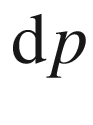
The quantity



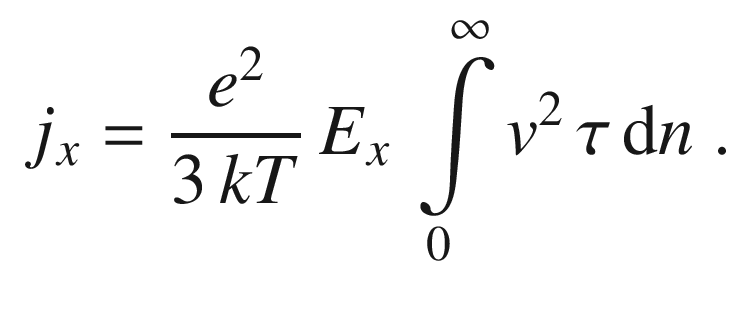
(cmp. [J.7](#u116076_4_En_BookBackmatter_OnlinePDF-Equ153)) denotes the number



of electrons with momentum in the range

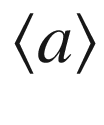


. Thus the integral can also be written as (in Boltzmann approximation)

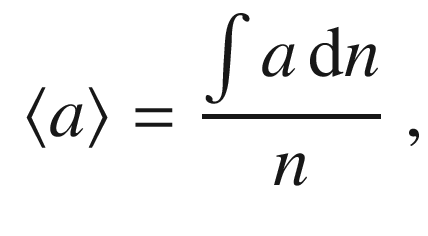


(J.16)

Denoting the average of a quantity *a* over the electron distribution with

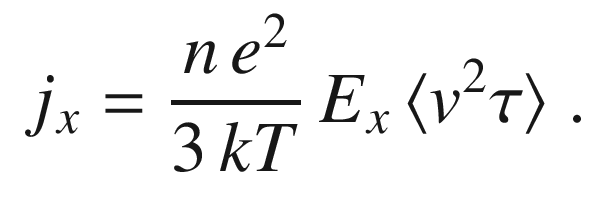


according to



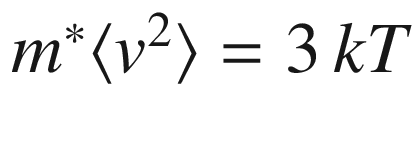
(J.17)

the equation ([J.16](#u116076_4_En_BookBackmatter_OnlinePDF-Equ162)) can be written as

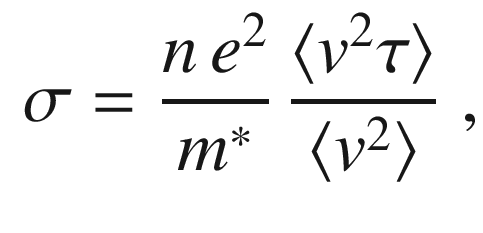


(J.18)

Using

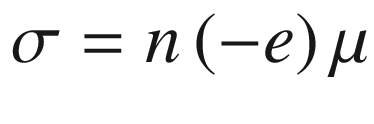


, we thus have obtained

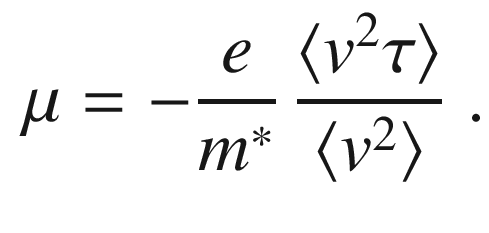


(J.19)

and with

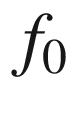


(for electrons), the mobility

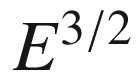


(J.20)

For degenerate semiconductors, similar as for metals, the derivative of



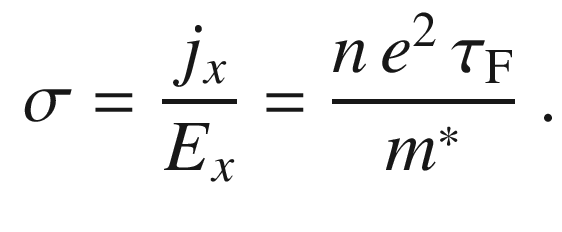
in ([J.15](#u116076_4_En_BookBackmatter_OnlinePDF-Equ161)) has a significant value only in the few-*kT* vicinity of the Fermi level. In an approximation we can evaluate the integral by replacing



and

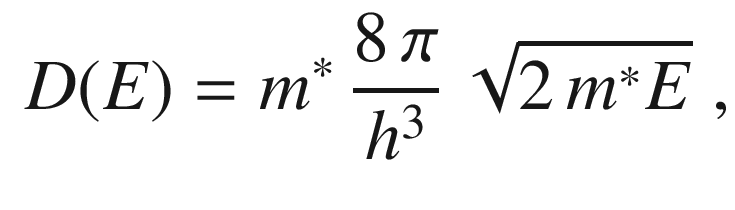
$$\tau $$

by their values at the Fermi level and find[14](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn14) (using ([6.​70](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter)))



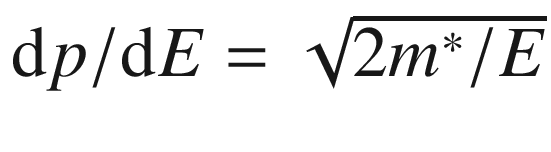
(J.21)

Starting again with ([J.15](#u116076_4_En_BookBackmatter_OnlinePDF-Equ161)), using the density of states ([6.​71](The_Physics_of_Semiconductors00003.docx#u116076_4_En_6_Chapter)) in the form (per volume)

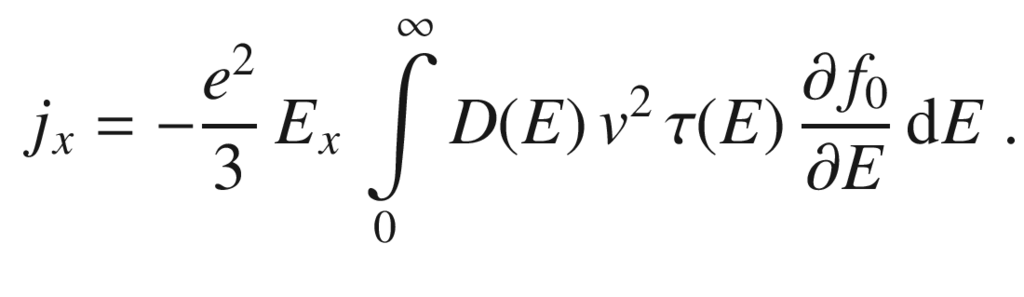


(J.22)

and

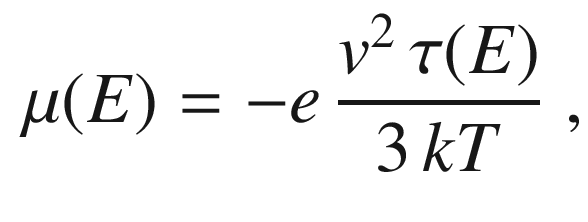


we write



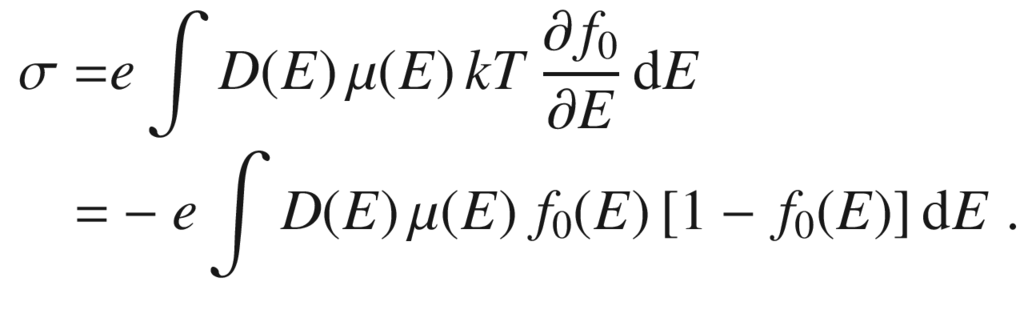
(J.23)

Using an energy-dependent mobility, in the spirit of ([J.20](#u116076_4_En_BookBackmatter_OnlinePDF-Equ166)) defined as



(J.24)

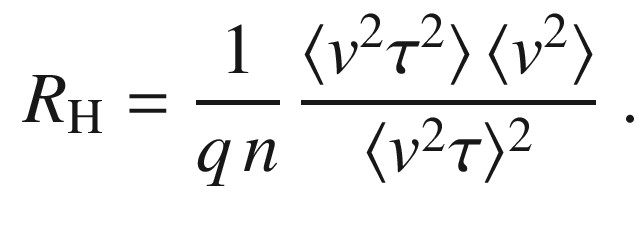
the conductivity can be written in a generalized form integrating over single electron states [[2167](#u116076_4_En_BookBackmatter_OnlinePDF-CR2167)] (neglecting correlation effects):



(J.25)

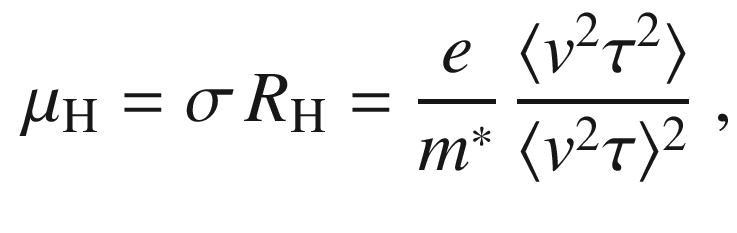
### J.3 Hall Effect

Treating the Hall effect with the Boltzmann transport equation and making the assumptions of isotropy, one obtains (cmp. ([15.​12](The_Physics_of_Semiconductors00006.docx#u116076_4_En_15_Chapter)) and ([15.​22](The_Physics_of_Semiconductors00006.docx#u116076_4_En_15_Chapter)))



(J.26)

The Hall mobility determined from the Hall coefficient is

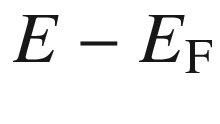


(J.27)

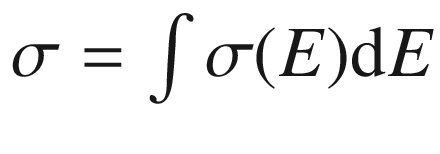
and thus different from the field mobility ([J.20](#u116076_4_En_BookBackmatter_OnlinePDF-Equ166)).

### J.4 Thermopower

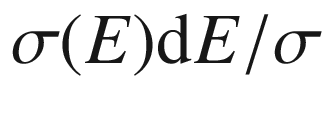
The electronic energy transported per electron is



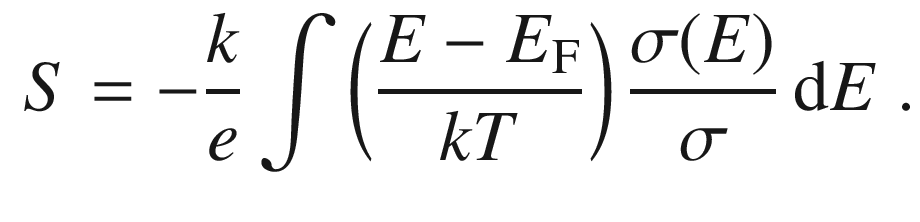
. Writing ([J.25](#u116076_4_En_BookBackmatter_OnlinePDF-Equ171)) as



, the weighing factor for electrons at energy *E* contributing to conduction is

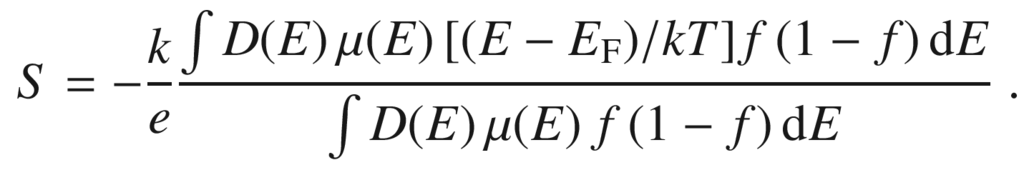


. Therefore the Seebeck coefficient (thermopower)  can be written [[823](#u116076_4_En_BookBackmatter_OnlinePDF-CR823)]



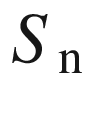
(J.28)

or

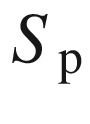


(J.29)

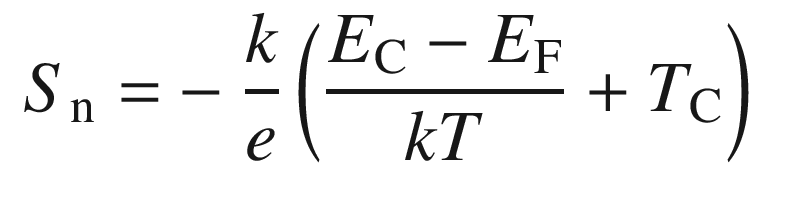
For band conduction the thermopower is obtained by integrating ([J.29](#u116076_4_En_BookBackmatter_OnlinePDF-Equ175)) for electrons (



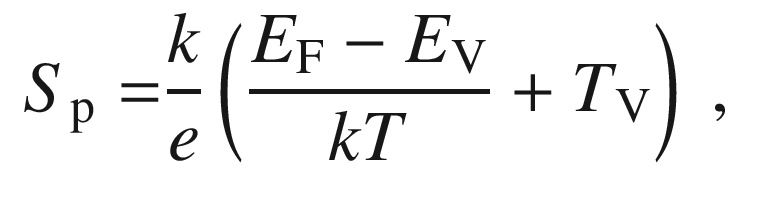
) and holes (



) (using the Boltzmann approximation) as [[823](#u116076_4_En_BookBackmatter_OnlinePDF-CR823)]

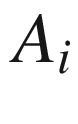


(J.30a)

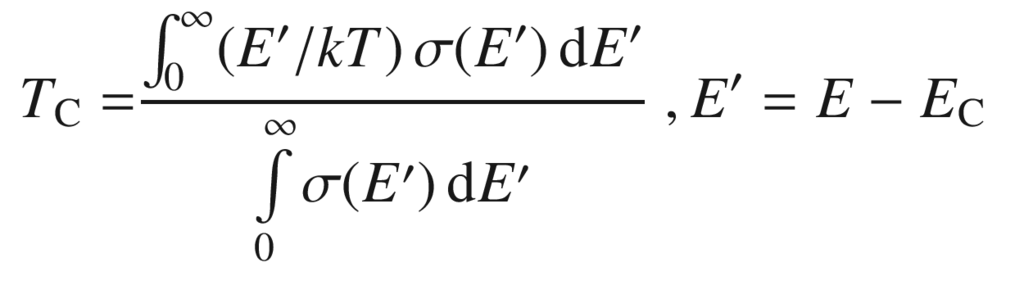


(J.30b)

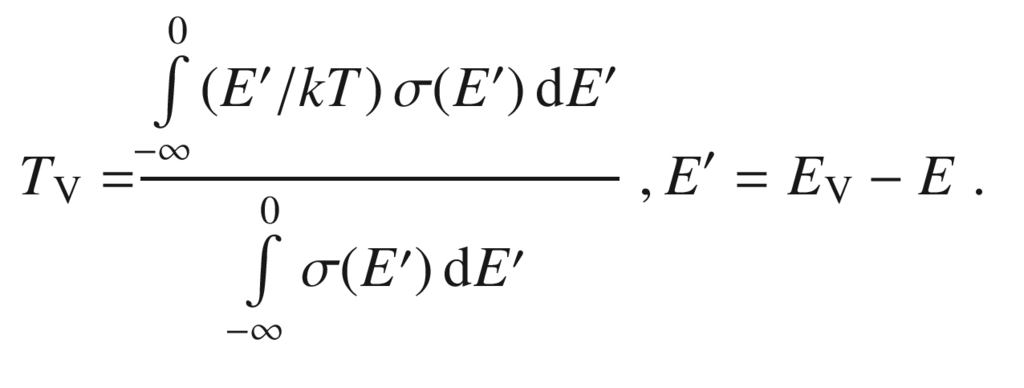
where



are constants depending on the energy dependence of the density of states and the mobility,

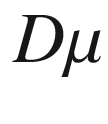


(J.31a)



(J.31b)

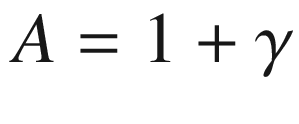
If the product of the density of states and the mobility



depends on the energy like



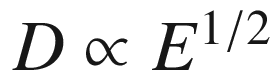
, the constant is



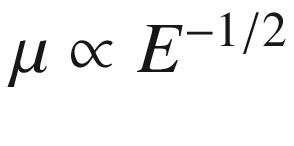
(for



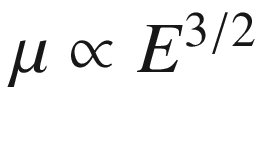
). For a parabolic band (



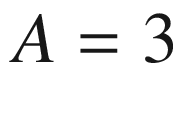
) and acoustic deformation potential scattering



(Sect. [8.​3.​4](The_Physics_of_Semiconductors00004.docx#u116076_4_En_8_Chapter)), A=1; for moderate ionized impurity scattering

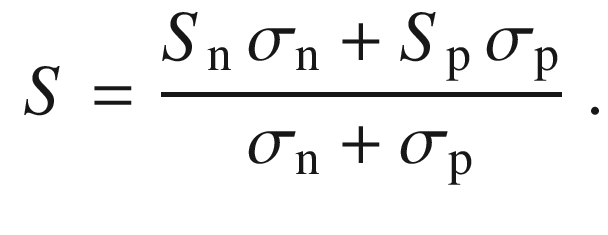


(Sect. [8.​3.​3](The_Physics_of_Semiconductors00004.docx#u116076_4_En_8_Chapter)) and



.

For two-band conduction, when electrons *and* holes contribute to transport,



(J.32)

At low temperatures the interaction of the phonon flow with the current via electron-phonon scattering (phonon-drag effect) leads to an increase of thermopower [[825](#u116076_4_En_BookBackmatter_OnlinePDF-CR825), [2168](#u116076_4_En_BookBackmatter_OnlinePDF-CR2168)–[2170](#u116076_4_En_BookBackmatter_OnlinePDF-CR2170)].

Appendix K

## Noise

Noise is a general phenomenon effecting every measurement process and the performance of semiconductor devices [[2171](#u116076_4_En_BookBackmatter_OnlinePDF-CR2171)–[2178](#u116076_4_En_BookBackmatter_OnlinePDF-CR2178)]. Eventually, always a signal-to-noise ratio  is measured instead of a ‘signal’. Electrical noise fundamentally limits the sensitivity and resolution of communication, navigation, measurement, and other electronic systems [[2176](#u116076_4_En_BookBackmatter_OnlinePDF-CR2176)].

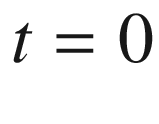
Behind the fluctuating signal stand microscopic classical and quantum mechanical processes that inherently contain randomness. From the physical standpoint, seemingly constant physical quantities even in thermodynamical equilibrium such as the free carrier density or the density of carriers on a trap are subject to fluctuations, e.g. leading to generation-recombination noise. Also the random motion of carriers, in equilibrium without net charge transport, leads to fluctuations , e.g. thermal noise on a resistor.

In this appendix necessary definitions, some mathematical basics and simple physical examples regarding noise are given.

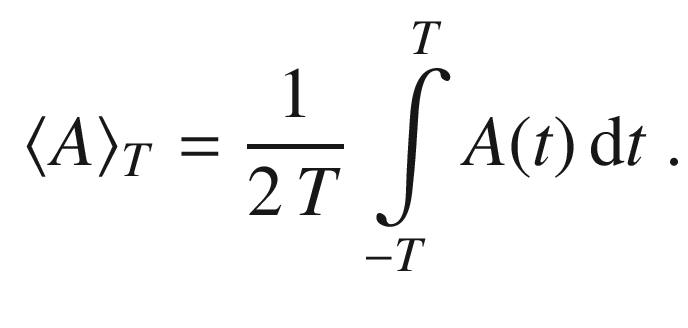
### K.1 Fluctuating signals

The noisy signal under consideration can be ‘analog’, for example in the case of a fluctuating current, voltage or power or it can be ‘digital’ for example a photon count rate.

Let *A*(*t*) be an analog signal that fluctuates in time. Even under constant experimental conditions, it will fluctuate due to possibly many reasons, at least due to thermal fluctuations. We note that another, identically set-up experiment will have another signal *B*(*t*). The time average  (of first moment) of the signal within a time interval 2*T* (symmetric around

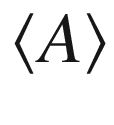


) is defined as



(K.1)

The time average of the signal

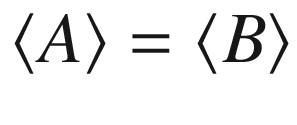


in general is the limit for large times,

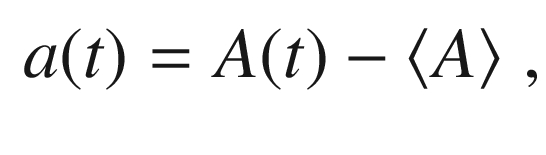


(K.2)

Two identical experiments will (should) share the same limits, i.e.

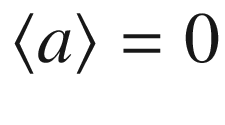


. The fluctuation or noise of *A* is defined as *a*(*t*) via

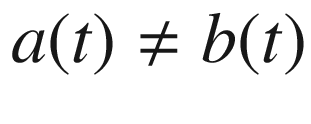


(K.3)

thus evidently

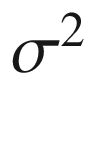


. For an identical but different experiment,

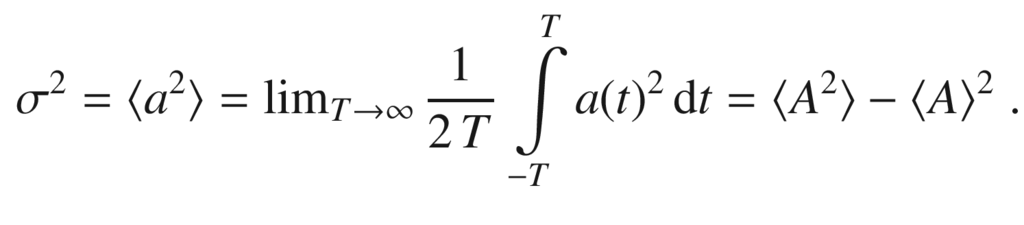


as stated before.

The *variance*

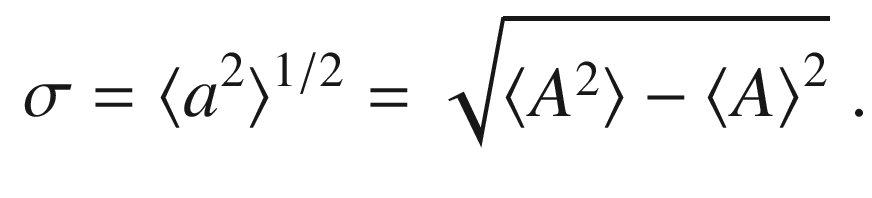


(or second moment) of the signal is the average of the squared fluctuation,



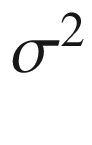
(K.4)

The *effective value* of the noise quantity *a* is the square root of the variance, also termed the ‘root mean square’ (or rms-value),

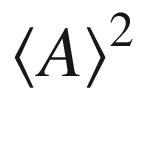


(K.5)

The quantity

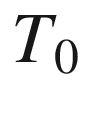


is a measure of the noise power, where

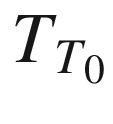


is a measure of the dc power.[15](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn15)

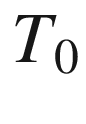
In a measurement procedure, the noise of a signal can be reduced by integrating or averaging over time; however, the time for a specific measurement is always finite and maybe constricted by many conditions. Given a fixed (finite) averaging time of



, the measured signals

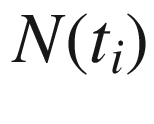


in a series of such subsequent identical measurements will still exhibit a fluctuation. How large this remaining fluctuation is depends on the choice of



and the noise spectrum discussed below.

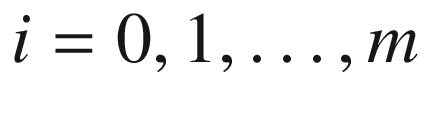
In the case of a digital signal, e.g. the count rate of a photomultiplier or from a scintillator, the signal consists of (integer) numbers



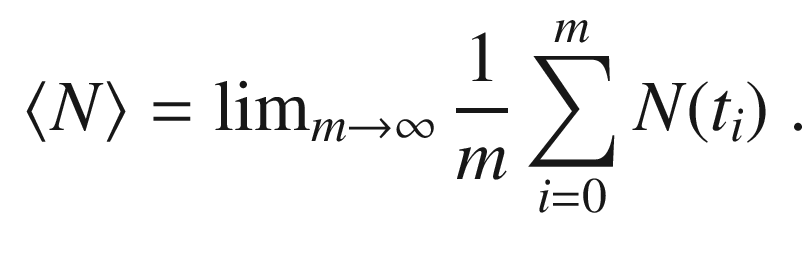
aggregated at times

$$t_i$$

,

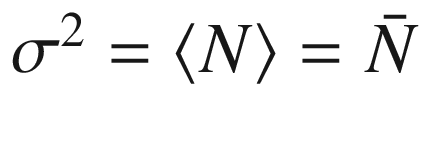


. The average is then defined as



(K.6)

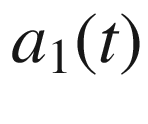
The definition of the variance and rms are analog to this definition. A well known result for photon counting, based on the Poisson statistics  of classical light is



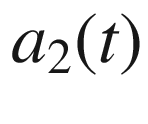
.

### K.2 Correlations

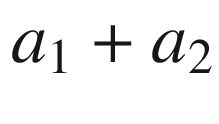
If a measurable quantity is subject to two fluctuating quantities



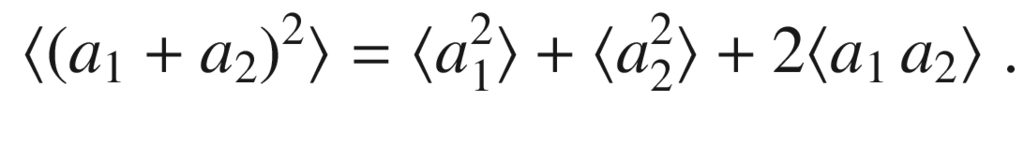
and



, the time average of

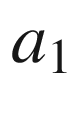


 is

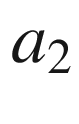


(K.7)

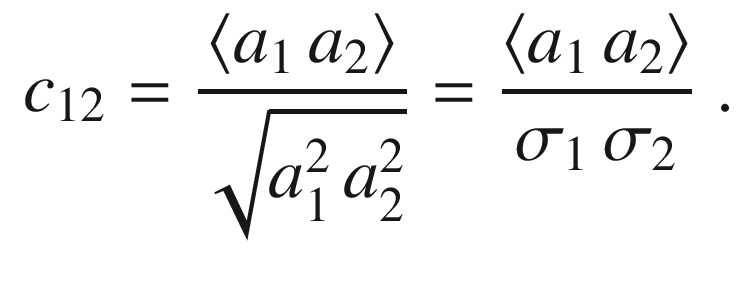
The third term is the decisive one; the correlation coefficient of noise quantities



and

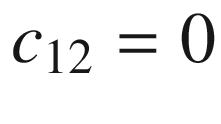


is defined as

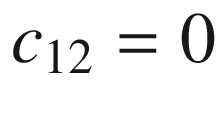


(K.8)

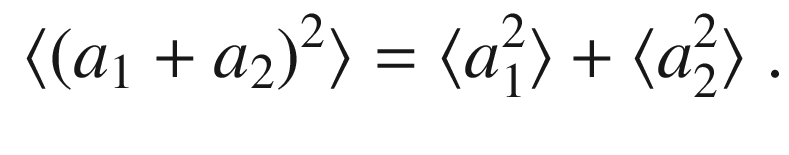
If the two noise quantities are independent of each other they are termed *uncorrelated* and



. In the following it will become clear that this is a necessary but not sufficient condition for two noise sources to be uncorrelated. In the case



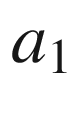
, the noise powers of the two processes are simply added,



(K.9)

This concept can be generalized to several noise sources.

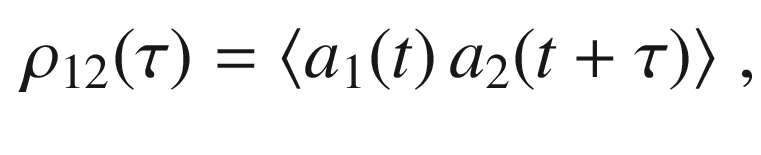
A more general concept to determine correlation of two functions



and

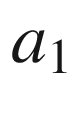


is the *cross correlation* function, defined by

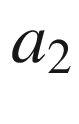


(K.10)

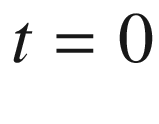
which is the average of function



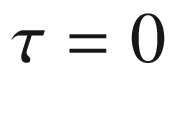
and time-shifted function



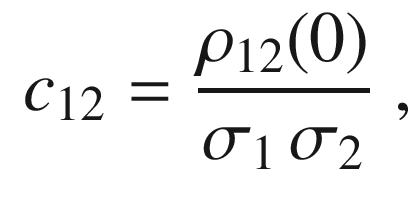
. Often



is used when the nature of the fluctuations does not change with time. An important time-shift is

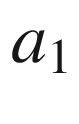


, and it follows that

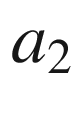


(K.11)

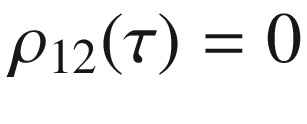
Two noise quantities



and



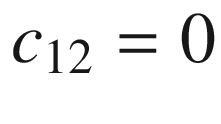
are uncorrelated if



holds for all times

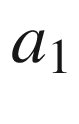
$$\tau $$

; thus

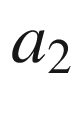


is a special but important case.[16](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn16)

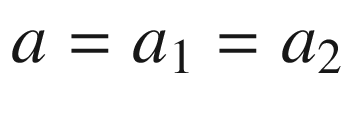
If



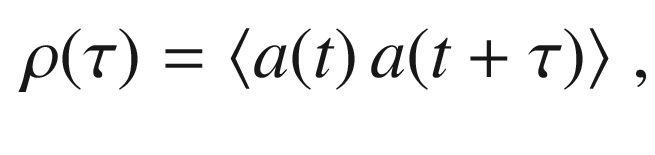
and



are the same function, i.e.



, ([K.10](#u116076_4_En_BookBackmatter_OnlinePDF-Equ190)) becomes the *auto correlation* function,

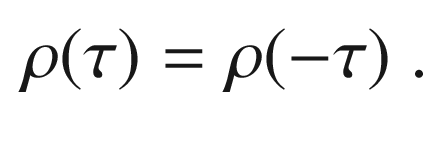


(K.12)

In stationary processes the auto correlation function must be symmetric with regard to

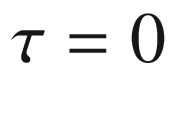
$$\tau $$

,

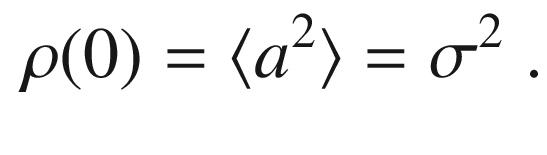


(K.13)

The value at



 is



(K.14)

Typically,



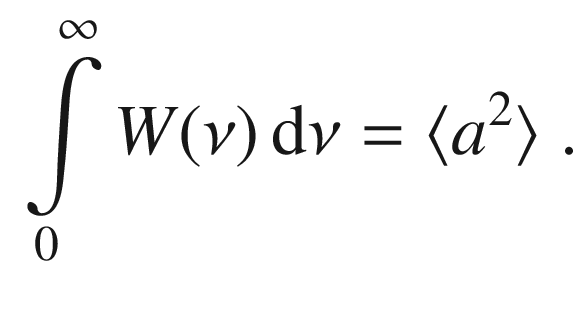
in a statistic (non-repetitive) process. For uncorrelated processes, the auto correlation function of the sum, is the sum of the individual auto correlation functions.

### K.3 Noise spectrum

Since the function *a*(*t*) is not known, the noise spectrum cannot be calculated from its Fourier transform. However, this is also unnecessary since we are not interested in the Fourier transform of *a* itself but rather the spectral power density for a given frequency

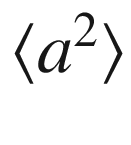


, with

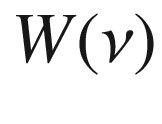


(K.15)

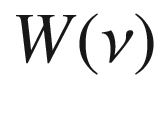
Since the quantity



is finite and the spectral power density



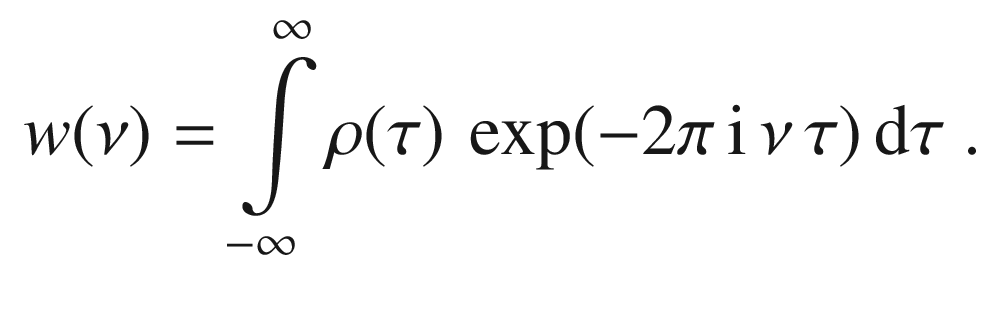
is positive, for high frequencies,



must decrease to zero. Starting from the auto correlation function

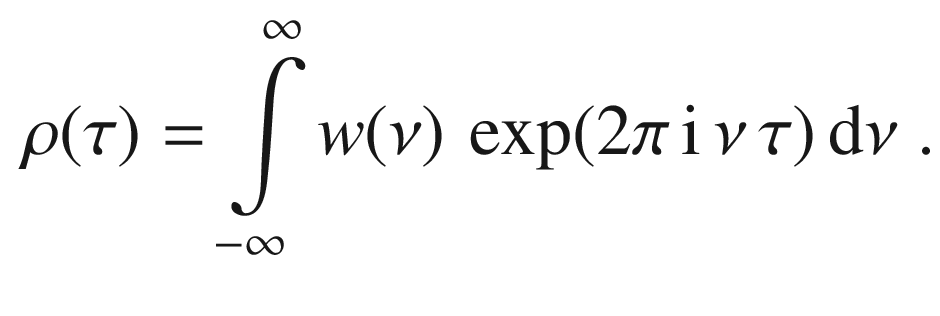
$$\rho $$

, its Fourier transform shall be denoted *w*,



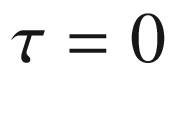
(K.16)

Also,

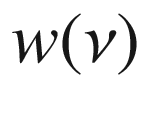


(K.17)

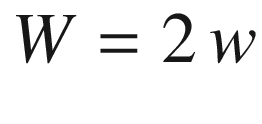
Using



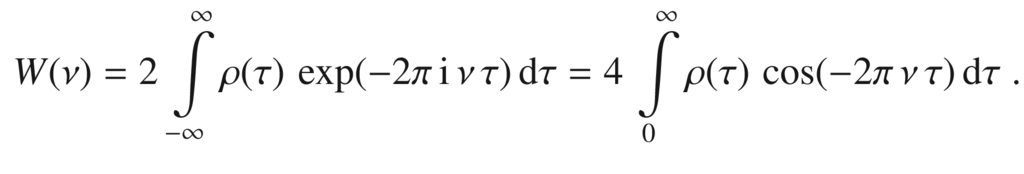
in this equation, we have obtained an equation similar to ([K.15](#u116076_4_En_BookBackmatter_OnlinePDF-Equ195)). With ([K.12](#u116076_4_En_BookBackmatter_OnlinePDF-Equ192))



can be identified as a spectral power density. Due to ([K.13](#u116076_4_En_BookBackmatter_OnlinePDF-Equ193)), *w* is a real and even function and we find for the noise power spectrum *W* in ([K.15](#u116076_4_En_BookBackmatter_OnlinePDF-Equ195))

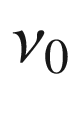


(Wiener–Khintchine theorem),

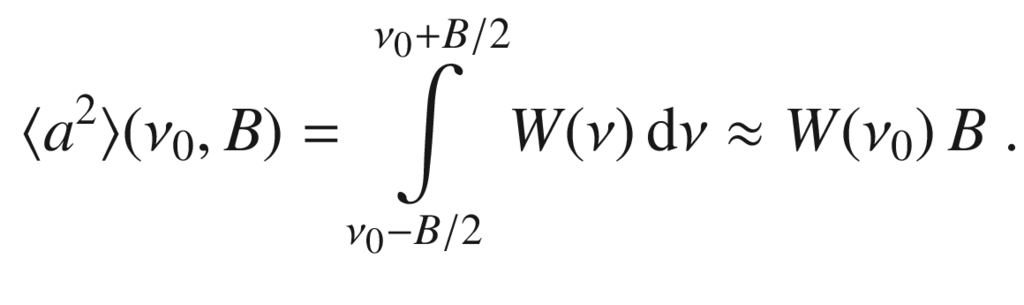


(K.18)

The noise power is practically measured in a finite frequency range, often in a narrow band of width  *B* (with varying central frequency). If the frequency dependence of *W* can be neglected within *B* around the frequency



, the variance is given by



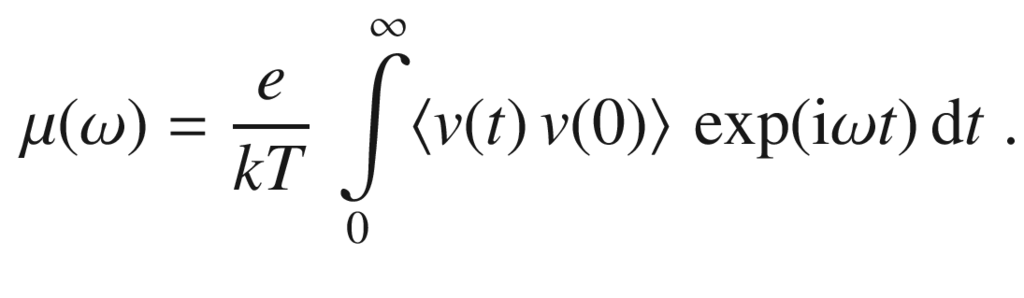
(K.19)

Typical noise mechanisms and spectra are discussed in the following sections.

#### K.3.1 Thermal Noise

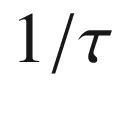
Finite temperature induces random motion of particles, e.g. as known from the theory of ideal gases and diffusion. In the case of charge carriers such motions lead to fluctuations of current or at a resistor to fluctuation of voltage. This happens also in the case of zero bias (no external fields). Such ‘thermal noise’ at a resistor was experimentally found by Johnson [[1820](#u116076_4_En_BookBackmatter_OnlinePDF-CR1820), [1821](#u116076_4_En_BookBackmatter_OnlinePDF-CR1821)] and theoretically derived by Nyquist [[1822](#u116076_4_En_BookBackmatter_OnlinePDF-CR1822)].

Using the general result from Langevin theory of motion under a fluctuating force, the mobility[17](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn17) is given as

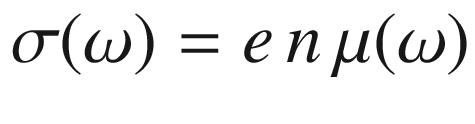


(K.20)

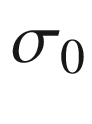
Now we restrict ourselves to times much longer than the relaxation time constant, and subsequently to frequencies much smaller than



. In this case the conductivity



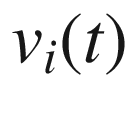
does not depend on frequency and can be taken as its low frequency limit



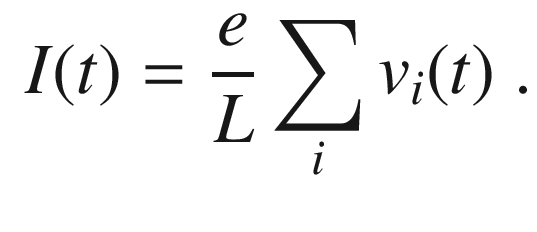
(cmp. Sect. [8.​5](The_Physics_of_Semiconductors00004.docx#u116076_4_En_8_Chapter)). In a conductor (resistor) of length *L* and cross section *A* shall be *N* electrons (



). With the electron velocities

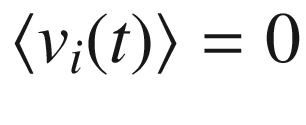


, the current is

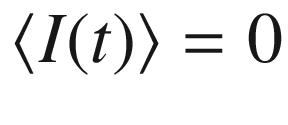


(K.21)

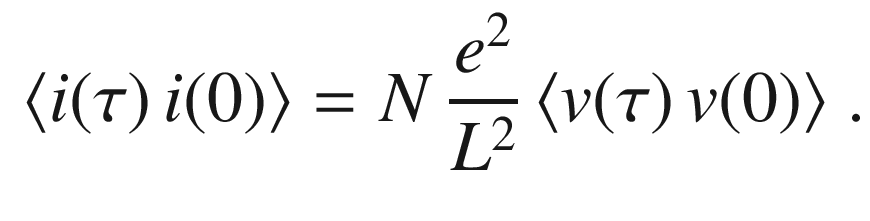
Without external field,



and

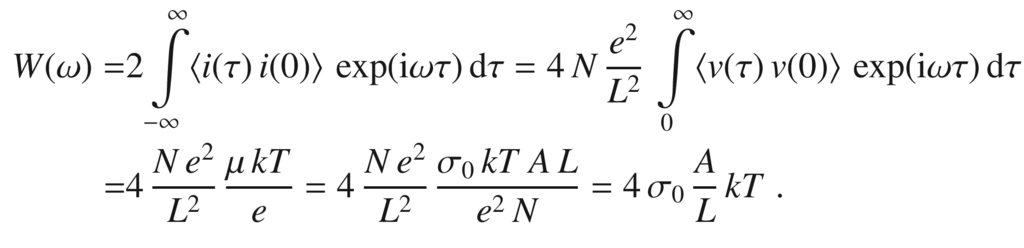


and we name this fluctuating current *i*(*t*). If all electrons move independently of each other,



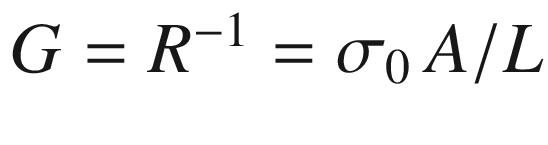
(K.22)

The power spectrum of *i*(*t*) is according to ([K.18](#u116076_4_En_BookBackmatter_OnlinePDF-Equ198)),

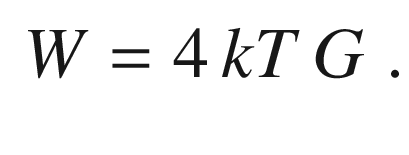


(K.23)

Then, using the conductance

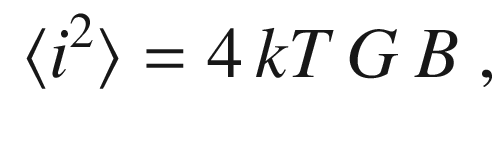


, we find the frequency independent spectral power



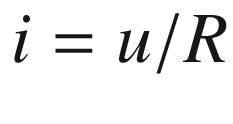
(K.24)

Therefore the fluctuation of the current induced by the thermal motion is

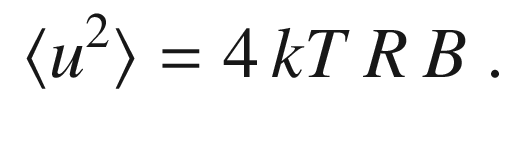


(K.25)

and the variance of the fluctuating voltage at a resistor with resistance *R* in a frequency range *B* is (

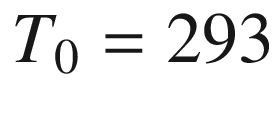


)

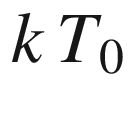


(K.26)

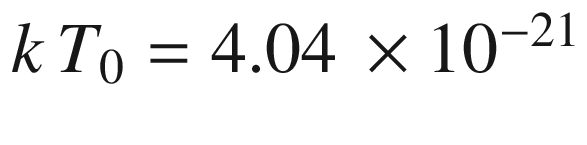
At room temperature (



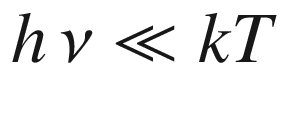
 K), the quantity



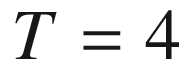
is about 26 meV; in the context here, the unit W s=W/Hz is the appropriate one, and



 W/Hz. This represents a fundamental limit to noise in devices. Since the power density is independent of frequency, this noise is ‘white’ noise. The formulas ([K.26](#u116076_4_En_BookBackmatter_OnlinePDF-Equ206)) and ([K.25](#u116076_4_En_BookBackmatter_OnlinePDF-Equ205)) are valid for frequencies

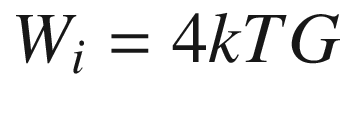


; for larger frequencies the quantum nature of electromagnetic radiation and photon statistics play a role. For practical purposes even cooled devices at

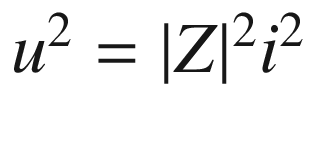


 K fulfill the limit condition for frequencies up in the 100 GHz regime. In the cases of heated electron (or hole) gases (cmp. Fig.[10.​3](The_Physics_of_Semiconductors00005.docx#u116076_4_En_10_Chapter-Fig3)), the lattice temperature must be replaced by the temperature of the carrier gas.

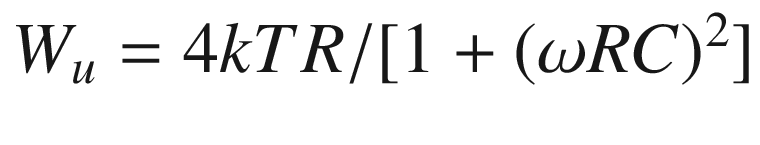
For a RC low pass, the power spectrum



at the resistor is converted using



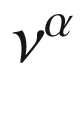
to



.

#### K.3.2 1/f Noise

For many processes a frequency dependent noise spectral power following a



-law is found with

$$\alpha $$

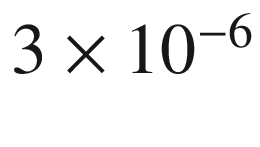
close to



. Such noise is termed ‘pink noise’, 1/*f*-noise or Flicker noise. The microscopic reasons for such behavior can be manifold and various models have been proposed [[2179](#u116076_4_En_BookBackmatter_OnlinePDF-CR2179), [2180](#u116076_4_En_BookBackmatter_OnlinePDF-CR2180)]. As an example, the noise spectrum of a RuO

$$_2$$

thick film resistor is depicted in Fig. [K.1](#u116076_4_En_BookBackmatter_OnlinePDF-Fig18)a; for this system, the fluctuation of tunneling current in metal-insulator-metal units was used to explain the observed frequency (and temperature) dependence of the 1/*f*-noise. At high frequencies, the 1/*f* spectral power vanishes and other noise sources such as thermal noise dominate, as depicted in Fig. [K.1](#u116076_4_En_BookBackmatter_OnlinePDF-Fig18)b for an a-Si thin film transistor. The 1/*f*-dependence of the noise spectral power (of a carbon sheet resistor) has been detected for frequencies down to



 Hz [[2181](#u116076_4_En_BookBackmatter_OnlinePDF-CR2181)].

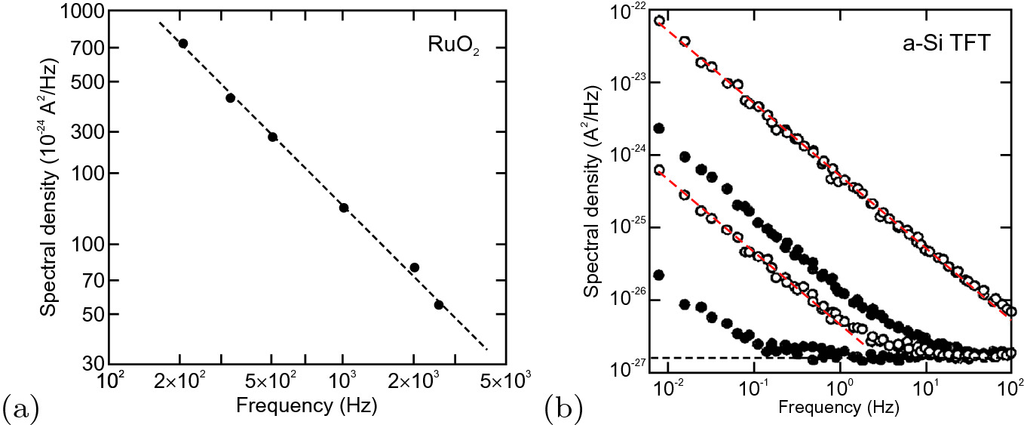
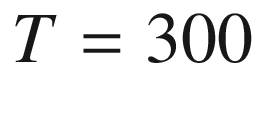
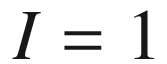


Fig. K.1

**a** Noise current density spectrum of a ruthenium oxide resistor (at



 K and current of

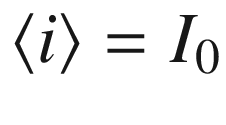


 mA), experimental data (*symbols*) and 1/*f*-dependency (*dashed line*). Adapted from [[2182](#u116076_4_En_BookBackmatter_OnlinePDF-CR2182)]. **b** Noise current density spectrum of an amorphous silicon thin film transistor, experimental data (*symbols*) for various source-drain voltages, thermal noise (*horizontal blue dashed line*) and 1/*f*-dependency (*red dashed lines*).

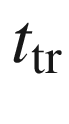
Adapted from [[2183](#u116076_4_En_BookBackmatter_OnlinePDF-CR2183)]

#### K.3.3 Shot Noise

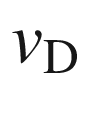
A dc current



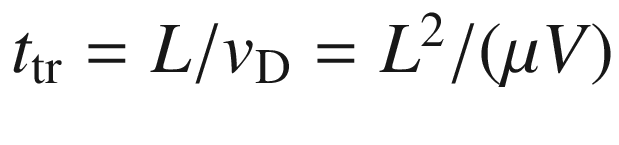
through a resistor is a sequence of electron transfers from one contact to the other. The transit time



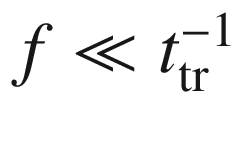
is given by the length *L* and the drift velocity



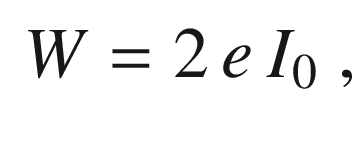
as



. The event times of these transits are random and thus lead to a noise (ac) component on top of the dc current. This is termed ‘shot’ noise, after the crackling arrival of shot pellets on a target. For low frequencies (

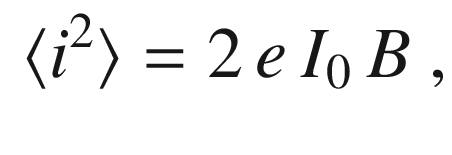


), the noise power is



(K.27)

and the current noise thus is given by



(K.28)

This noise term has been first found for vacuum diodes in the saturation regime which also serve as noise normals according to ([K.28](#u116076_4_En_BookBackmatter_OnlinePDF-Equ208)). It is important for the validity of ([K.28](#u116076_4_En_BookBackmatter_OnlinePDF-Equ208)) that in each event a full charge *e* is transferred. The situation in a semiconductor diode is more complicated since various currents contribute; if scattering events occur during transit, also fractional transferred charges can occur. The reverse current of an asymmetric diode if originating from the lowly doped region is due to carriers crossing the depletion layer. If generation in the depletion layer plays no role, the noise is also determined by the shot noise ([K.28](#u116076_4_En_BookBackmatter_OnlinePDF-Equ208)).

The maximal noise level ([K.28](#u116076_4_En_BookBackmatter_OnlinePDF-Equ208)) is present in absence of all correlations (Poisson process), both in the injection process as well as in the subsequent transport. Such value has been found, e.g., for intrinsic germanium in [[2184](#u116076_4_En_BookBackmatter_OnlinePDF-CR2184)] and in the limit of large currents for CdTe detectors [[2185](#u116076_4_En_BookBackmatter_OnlinePDF-CR2185)] (Fig. [K.2](#u116076_4_En_BookBackmatter_OnlinePDF-Fig19)). In a metallic conductor (or degenerate semiconductor) the noise is reduced to a third of that value due to correlations induced by the Pauli exclusion principle [[2186](#u116076_4_En_BookBackmatter_OnlinePDF-CR2186)]. The modification in non-degenerate semiconductors on length scales intermediate between the elastic and inelastic mean free paths is discussed in [[2187](#u116076_4_En_BookBackmatter_OnlinePDF-CR2187)]. The case of shot noise in semiconductors in the presence of transport of electrons and holes has been treated in [[2184](#u116076_4_En_BookBackmatter_OnlinePDF-CR2184), [2188](#u116076_4_En_BookBackmatter_OnlinePDF-CR2188)].

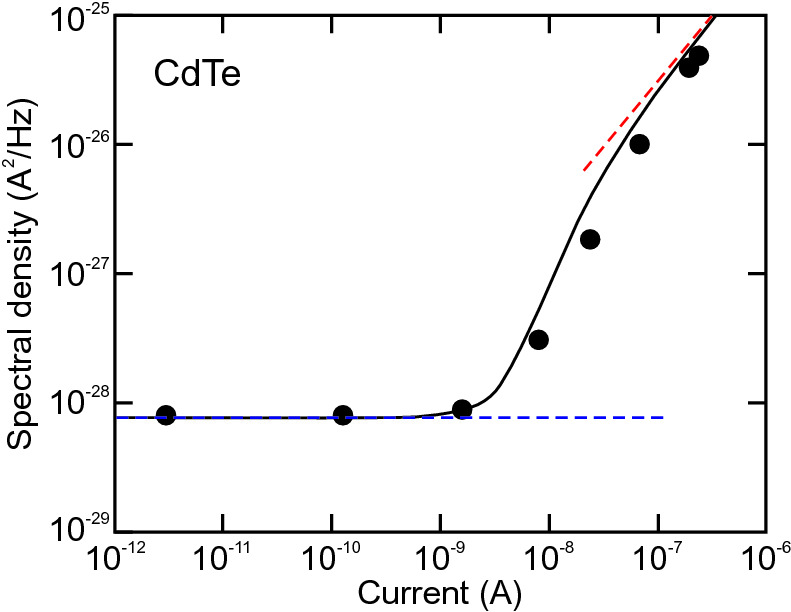
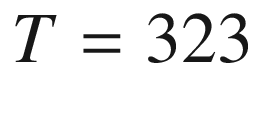


Fig. K.2

Noise of semi-insulating (dark) CdTe detector at



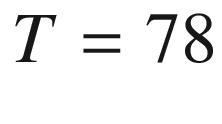
 K (at a frequency of about 1–2 kHz when 1/*f*-noise plays no role). Experimental data (*symbols*) and detailed theory (*black line*). The *dashed blue line* represents the thermal noise ([K.25](#u116076_4_En_BookBackmatter_OnlinePDF-Equ205)), the *dashed red line* the shot noise ([K.28](#u116076_4_En_BookBackmatter_OnlinePDF-Equ208)).

Adapted from [[2185](#u116076_4_En_BookBackmatter_OnlinePDF-CR2185)]

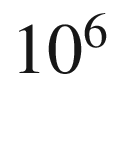
#### K.3.4 Generation-Recombination Noise

It is a semiconductor specific property that the carrier density is subject to fluctuations due to generation and recombination.[18](The_Physics_of_Semiconductors00011.docx#u116076_4_En_BookBackmatter_OnlinePDF-Fn18) A fluctuation in majority carrier density leads to a change of conductivity which will lead to a change in current if a constant voltage is applied. Typical examples of transitions leading to a fluctuation of the carrier density are between bands and localized levels and in between the conduction and valence bands. Usually, the sample remains neutral. Detailed treatments are given in [[2189](#u116076_4_En_BookBackmatter_OnlinePDF-CR2189), [2190](#u116076_4_En_BookBackmatter_OnlinePDF-CR2190)].

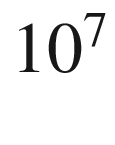
A simple example is the effect of carrier number fluctuation due to transitions between a conduction band and donor levels. This is manifested in the noise spectrum of a n-Si sample at



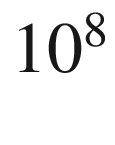
 K (Fig. [K.3](#u116076_4_En_BookBackmatter_OnlinePDF-Fig20)a) with the plateau at



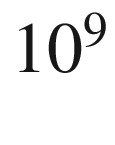
–



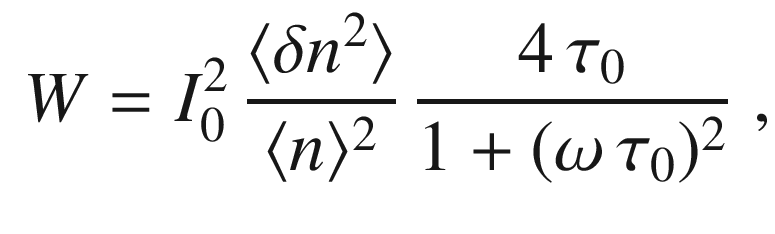
 Hz on top of the 1/*f* noise [[2191](#u116076_4_En_BookBackmatter_OnlinePDF-CR2191)] (The plateau at



–

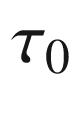


 Hz is due to velocity fluctuations). The spectral power of the generation-recombination noise contribution is given by

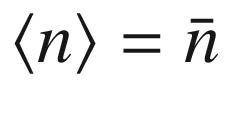


(K.29)

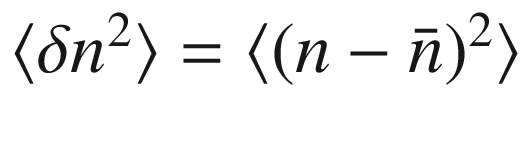
where



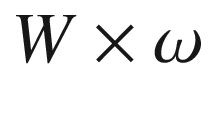
is the characteristic relaxation time,



is the average carrier density (average carrier number per given volume) and



is the fluctuation of the carrier density. In order to better visualize the generation-recombination noise with respect to the 1/*f* noise, the quantity



can be plotted (Fig. [K.3](#u116076_4_En_BookBackmatter_OnlinePDF-Fig20)b) which takes the shape of a peak (for logarithmic frequency axis) [[2192](#u116076_4_En_BookBackmatter_OnlinePDF-CR2192)].

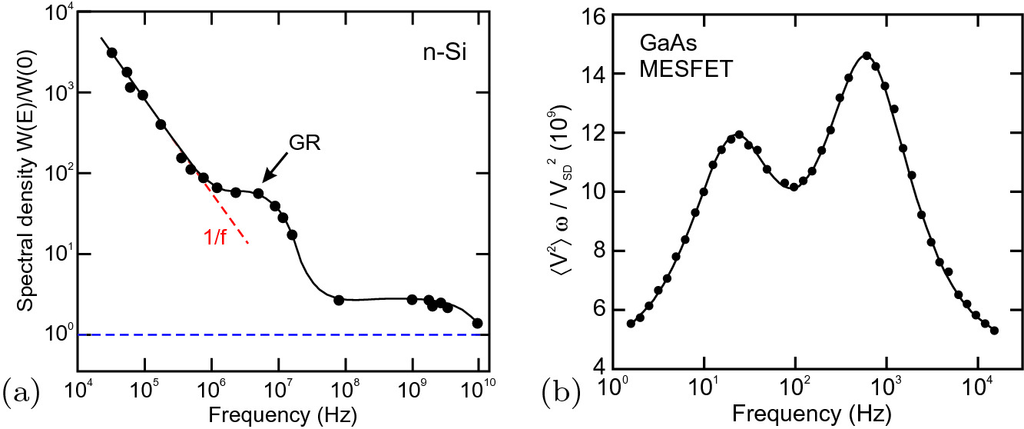
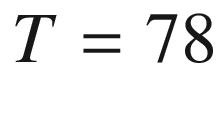
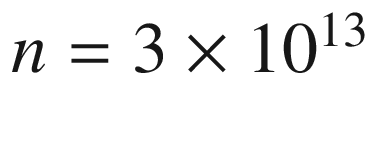


Fig. K.3

**a** Current noise spectrum of n-type Si (



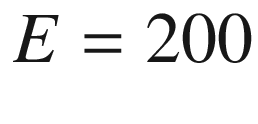
 K,



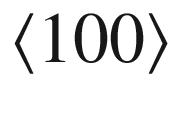
 cm



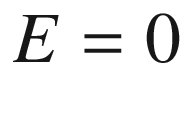
) for an electric field of



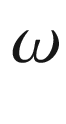
 V/cm along the



direction, in relative units to the noise spectrum for

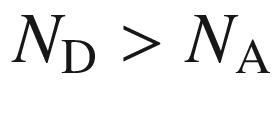


. The *dashed blue line* indicates the level of thermal noise, The *arrow* labeled ‘GR’ denotes the contribution of generation-recombination noise. Adapted from [[2191](#u116076_4_En_BookBackmatter_OnlinePDF-CR2191)]. **b** Voltage noise power times frequency of a GaAs MESFET. Experimental data (*symbols*) and fit (*solid line*) including two generation-recombination noise terms of the type ([K.29](#u116076_4_En_BookBackmatter_OnlinePDF-Equ209)) (times

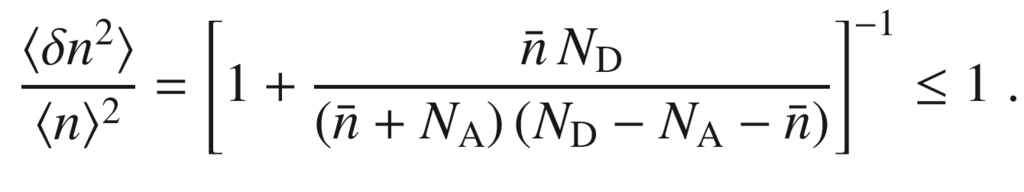


) for two different traps. Adapted from [[2192](#u116076_4_En_BookBackmatter_OnlinePDF-CR2192)]

For a partially compensated semiconductor with



it is found (if holes can be neglected) [[2190](#u116076_4_En_BookBackmatter_OnlinePDF-CR2190)]

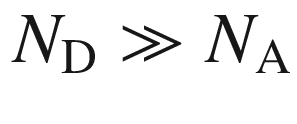


(K.30)

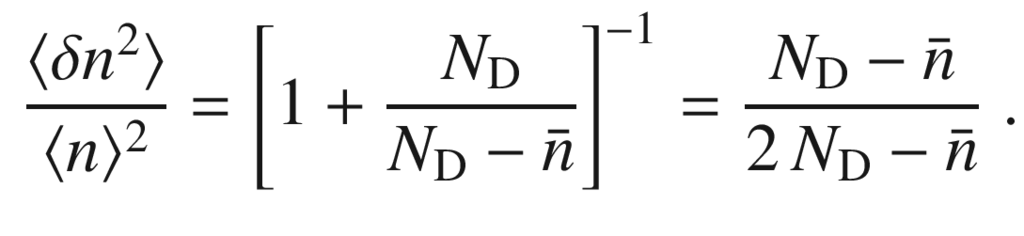
The fluctuation



is typically smaller than the Poisson value of 1; such sub-Poissonian statistics is typical of a repulsive correlation. For the case

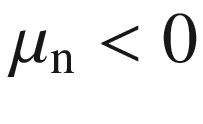


[[2190](#u116076_4_En_BookBackmatter_OnlinePDF-CR2190)], ([K.30](#u116076_4_En_BookBackmatter_OnlinePDF-Equ210)) simplifies to

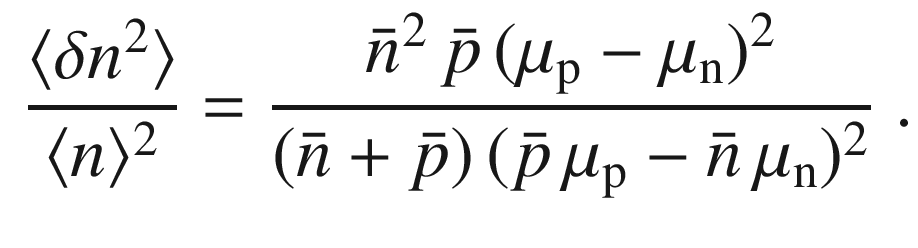


(K.31)

In the ambipolar regime, typically close to intrinsic conditions, when only free electrons and holes are important, it is found [[2190](#u116076_4_En_BookBackmatter_OnlinePDF-CR2190)] (

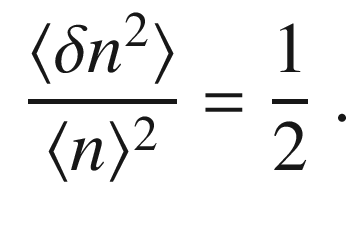


)



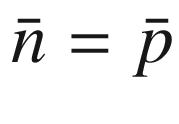
(K.32)

which simplifies to



(K.33)

in the intrinsic case (



).

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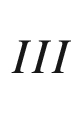
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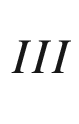


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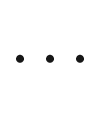
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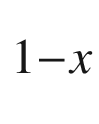
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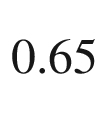
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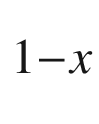
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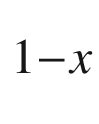
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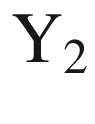
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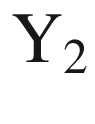


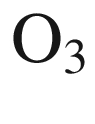
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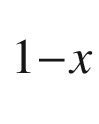
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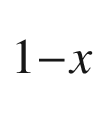
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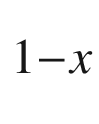
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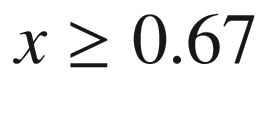
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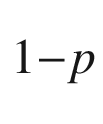
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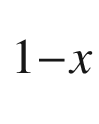
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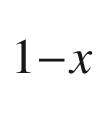
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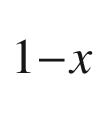


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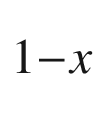
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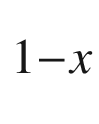
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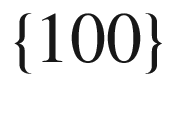
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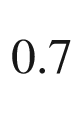
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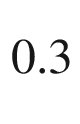
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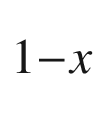
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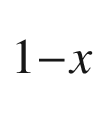
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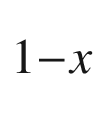
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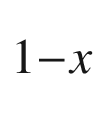


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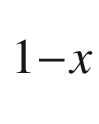
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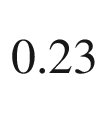
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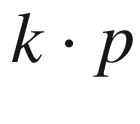
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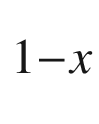
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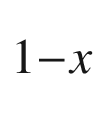
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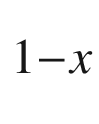
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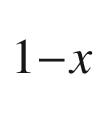


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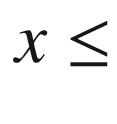
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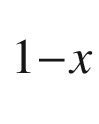


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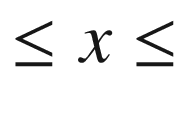
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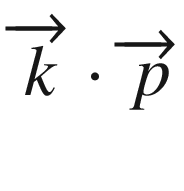
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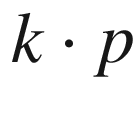
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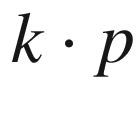
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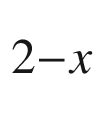
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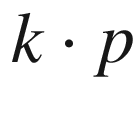
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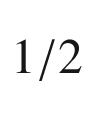
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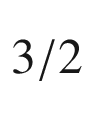


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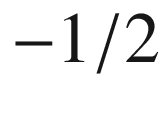
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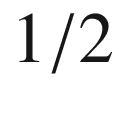
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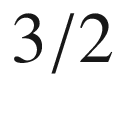
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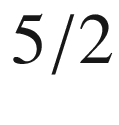
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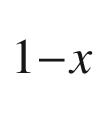
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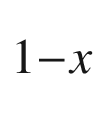
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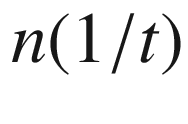
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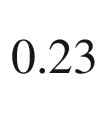
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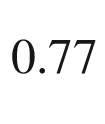
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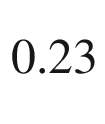
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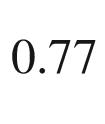
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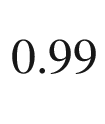
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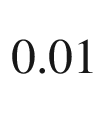
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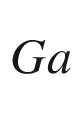
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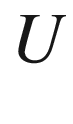
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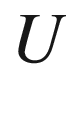
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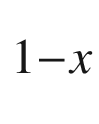
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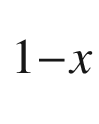
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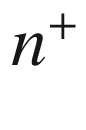
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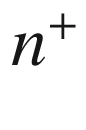
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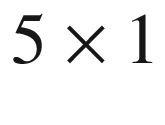
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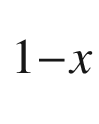
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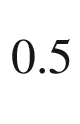
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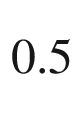
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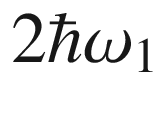
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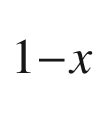
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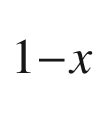
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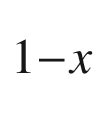
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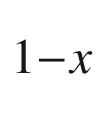


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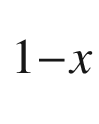
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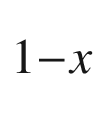
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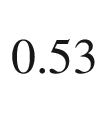
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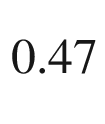


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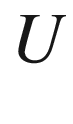
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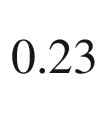
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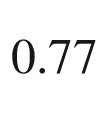
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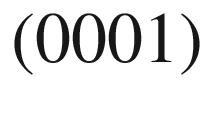
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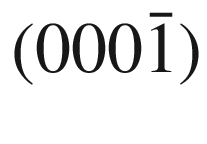
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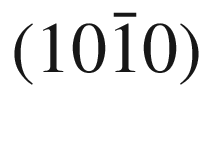
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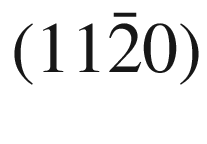
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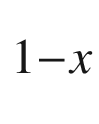
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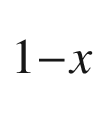
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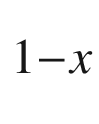
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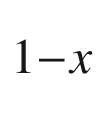
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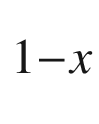
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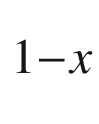
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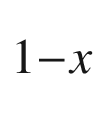
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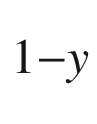
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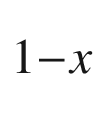
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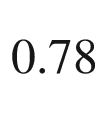
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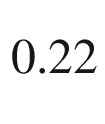
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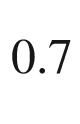


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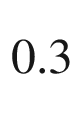


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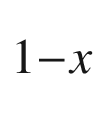


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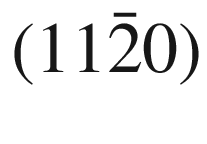
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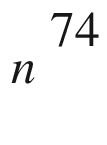


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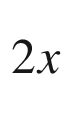
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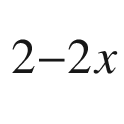
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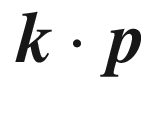
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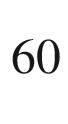
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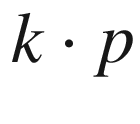
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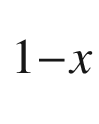
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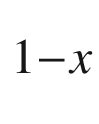
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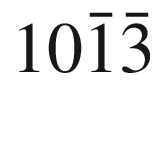
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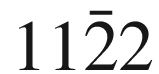
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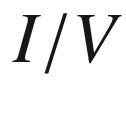
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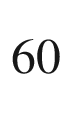
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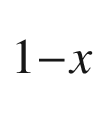
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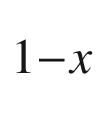
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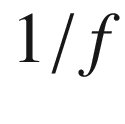
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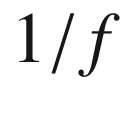
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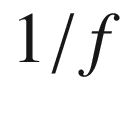
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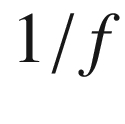
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