Appendix A
Tensors

A.1 Introduction

A physical quantity $T_{ij\ldots m}$ with a total of k indices that is independent of translations of the coordinate system and transforms with respect to all indices like a vector is called a tensor of rank k.

Often, Einstein's sum convention is used; a sum is built over indices with the same symbol. For example, $x_i' = D_{ij}\, x_j$ shall be read as $x_i' = \sum_{j=1}^{3} D_{ij}\, x_j$.

A.2 Rotation of Coordinate System

A rotation of the coordinate system is a transformation $\mathbf{x} \rightarrow \mathbf{x}'$ that is written in components as

$$x_i' = D_{ij}\, x_j. \tag{A.1}$$

$\mathbf{D}$ is called the rotation matrix. The inverse of the rotation matrix is $\mathbf{D}^{-1}$ with

$$D_{kl}^{-1} = D_{lk}, \tag{A.2}$$

i.e. it is the transposed matrix $\mathbf{D}$. The inverse transformation is $x_j = D_{ij}\, x_i'$. Thus,

$$D_{ij}\, D_{kj} = \delta_{ij}. \tag{A.3}$$

A simple example is the azimuthal rotation around the z-axis by an angle ϕ (in the mathematically positive direction)

$$\mathbf{D} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{A.4}$$

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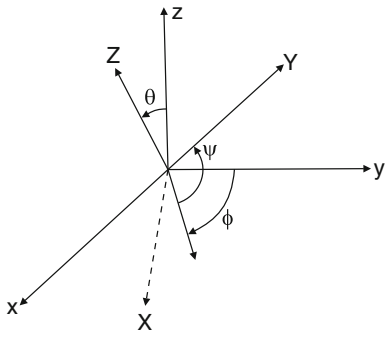

Fig. A.1 Rotation of a coordinate system (x, y, z) by the Euler angles (ϕ, θ, ψ) into the system (X, Y, Z)

For the description of an arbitrary rotation $(x, y, z) \rightarrow (X, Y, Z)$, generally three angles are necessary. Typically, the Euler angles (ϕ, θ, ψ) are used (Fig. A.1). First, the system is rotated by ϕ around the z-axis. The y-axis becomes the u-axis. Then, the system is tilted by θ around the u-axis and the z-axis becomes the Z-axis. Finally, the system is rotated by ψ around the Z-axis.

The matrix for the general rotation by the Euler angles is

$$\begin{pmatrix} \cos\psi\cos\theta\cos\phi - \sin\psi\sin\phi & -\sin\phi\cos\theta\cos\psi - \cos\phi\sin\psi & \sin\theta\cos\psi \\ \cos\phi\cos\theta\sin\psi + \sin\phi\cos\psi & -\sin\psi\cos\theta\sin\phi + \cos\psi\cos\phi & \sin\theta\sin\psi \\ -\cos\phi\sin\theta & \sin\phi\sin\theta & \cos\theta \end{pmatrix}. \quad \text{(A.5)}$$

A.3 Rank-*n* Tensors

Rank-0 Tensors

A tensor of rank 0 is also called a scalar. For example, the length $v_1^2 + v_2^2 + v_3^2$ of the vector $\mathbf{v} = (v_1, v_2, v_3)$ is a scalar since it is invariant under rotation of the coordinate system. However, 'scalar' is not equivalent to 'number' since, e.g. the number $v_1^2 + v_2^2$ is not rotationally invariant.

Rank-1 Tensors

A tensor of rank 1 is a vector. It transforms under coordinate rotation $\mathbf{D}$ as

$$v_i' = D_{ij}\, v_j. \quad \text{(A.6)}$$

Rank-2 Tensors

A tensor of rank 2 is also called a dyade and is a 3×3 matrix $\mathbf{T}$ that transforms under coordinate rotation as

$$T_{ij}' = D_{ik}\, D_{jl}\, T_{kl}. \quad \text{(A.7)}$$

The physical meaning is the following: Two vectors $\mathbf{s}$ and $\mathbf{r}$ shall be related to each other via $s_i = T_{ij}\, r_j$. This could be, e.g., the current $\mathbf{j}$ and the electric field $\mathbf{E}$ that are connected via the tensor of conductivity $\boldsymbol{\sigma}$, i.e. $j_i = \sigma_{ij}\, E_j$.

Such an equation only makes physical sense if it is also valid in a (any) rotated coordination system. The tensor $\mathbf{T}'$ in the rotated coordinate system must fulfill $s'_i = T'_{ij}\, r'_j$. This implies the transformation law (A.7). $s'_k = D_{ki}\, s_i = D_{ki}\, T_{ij} r_j$ and also $s'_k = T'_{km}\, r'_m = T'_{km}\, D_{mj}\, r_j$. Thus, $T'_{km}\, D_{mj} = D_{ki}\, T_{ij}$ since the previous relations are valid for arbitrary $\mathbf{r}$. Multiplication by D_{lj} yields $T'_{km}\, D_{mj}\, D_{lj} = T'_{km}\, \delta_{ml} = T'_{kl} = D_{ki}\, D_{lj}\, T_{ij}$.

The trace of a rank-2 tensor is defined as $\mathrm{tr}\,\mathbf{T} = T_{ii} = T_{11} + T_{22} + T_{33}$. It is a scalar, i.e. invariant under coordinate rotation, since $T'_{kk} = D_{ki} D_{kj} T_{ij} = \delta_{ij} T_{ij} = T_{ii}$.

A rank-2 tensor can be separated into a symmetric part $\mathbf{T}^S$ and an antisymmetric part $\mathbf{T}^A$, i.e. $T^S_{ji} = T^S_{ij}$ and $T^A_{ji} = -T^A_{ij}$ with

$$\mathbf{T} = \mathbf{T}^S + \mathbf{T}^A \tag{A.8a}$$

$$T^S_{ij} = \frac{T_{ij} + T_{ji}}{2} \tag{A.8b}$$

$$T^A_{ij} = \frac{T_{ij} - T_{ji}}{2}. \tag{A.8c}$$

A rank-2 tensor can be separated into an isotropic (spherical) part $\mathbf{T}^I$ and a deviatoric part $\mathbf{T}^D$. The isotropic part is invariant under coordinate rotation.

$$\mathbf{T} = \mathbf{T}^I + \mathbf{T}^D \tag{A.9a}$$

$$T^I_{ij} = \delta_{ij} \frac{\mathrm{tr}\,\mathbf{T}}{3} \tag{A.9b}$$

$$T^D_{ij} = T_{ij} - \delta_{ij} \frac{\mathrm{tr}\,\mathbf{T}}{3}. \tag{A.9c}$$

The trace of $\mathbf{T}$ is the same as that of $\mathbf{T}^I$. The trace of $\mathbf{T}^D$ is zero.

Rank-3 Tensors

A tensor of rank 3 transforms according to

$$T'_{ijk} = D_{il}\, D_{jm}\, D_{kn} T_{lmn}. \tag{A.10}$$

An example is the tensor $\mathbf{e}$ of piezoelectric constants that relates the rank-2 tensor of the strains with the polarization vector $\mathbf{P}$, i.e. $P_i = e_{ijk}\, \epsilon_{jk}$.

Rank-4 Tensors

A tensor of rank 4 transforms according to

$$T'_{ijkl} = D_{im}\, D_{jn}\, D_{ko}\, D_{lp}\, T_{mnop}. \tag{A.11}$$

An example is the tensor $\mathbf{C}$ of elastic constants that relates the rank 2 tensors $\boldsymbol{\epsilon}$ and $\boldsymbol{\sigma}$ of the elastic strains and stresses, i.e. $\sigma_{ij} = C_{ijkl}\, \epsilon_{kl}$.

Appendix B
Point and Space Groups

(See Tables B.1, B.2 and B.3.)

Table B.1 The 10 two-dimensional point groups in group and full and abbreviated international notation

Group	Notation		N_{sg}	Symmetry elements
	Full international	Abbrev.		
C_1	1	1	1	C_1
D_1	1m	m	3	C_1, m
C_2	2	2	1	C_2
D_2	2mm	mm	4	C_2, 2m
C_3	3	3	1	C_3
D_3	3m	3m	2	C_3, 3m
C_4	4	4	1	C_4
D_4	4mm	4m	2	C_4, 2m
C_6	6	6	1	C_6
D_6	6mm	6m	1	C_6, 6m

N_{sg} denotes the number of space groups

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Table B.2 The 32 point groups in Schönfließ and international notation

System	Class		N_{sg}	Symmetry elements
	international	Schönfließ		
Triclinic	1	C_1	1	E
	$\bar{1}$	C_i	1	$E\ i$
Monoclinic	m	C_s	3	$E\ \sigma_h$
	2	C_2	4	$E\ C_2$
	$2/m$	C_{2h}	6	$E\ C_2\ i\ \sigma_h$
Orthorhombic	$2mm$	C_{2v}	9	$E\ C_2\ \sigma_v'\ \sigma_v''$
	222	D_2	22	$E\ C_2\ C_2'\ C_2''$
	mmm	D_{2h}	28	$E\ C_2\ C_2'\ C_2''\ i\ \sigma_h\ \sigma_v'\ \sigma_v''$
Tetragonal	4	C_4	6	$E\ 2C_4\ C_2$
	$\bar{4}$	S_4	2	$E\ 2S_4\ C_2$
	$4/m$	C_{4h}	6	$E\ 2C_4\ C_2\ i\ 2S_4\ \sigma_h$
	$4mm$	C_{4v}	10	$E\ 2C_4\ C_2\ 2\sigma_v'\ 2\sigma_d$
	$\bar{4}2m$	D_{2d}	12	$E\ C_2\ C_2'\ C_2''\ 2\sigma_d\ 2S_4$
	422	D_4	12	$E\ 2C_4\ C_2\ 2C_2'\ 2C_2''$
	$4/mmm$	D_{4h}	20	$E\ 2C_4\ C_2\ 2C_2'\ 2C_2''\ i\ 2S_4\ \sigma_h\ 2\sigma_v'\ 2\sigma_h$
Trigonal (rhombohedral)	3	C_3	4	$E\ 2C_3$
	$\bar{3}$	S_6	2	$E\ 2C_3\ i\ 2S_6$
	$3m$	C_{3v}	7	$E\ 2C_3\ 3\sigma_v$
	32	D_3	6	$E\ 2C_3\ 3C_2$
	$\bar{3}m$	D_{3d}	6	$E\ 2C_3\ 3C_2\ i\ 2S_6\ 3\sigma_d$
Hexagonal	$\bar{6}$	C_{3h}	6	$E\ 2C_3\ \sigma_h\ 2S_3$
	6	C_6	1	$E\ 2C_6\ 2C_3\ C_2$
	$6/m$	C_{6h}	2	$E\ 2C_6\ 2C_3\ C_2\ i\ 2S_3\ 2S_6\ \sigma_h$
	$\bar{6}m2$	D_{3h}	6	$E\ 2C_3\ 3C_2\ \sigma_h\ 2S_3\ 3\sigma_v$
	$6mm$	C_{6v}	4	$E\ 2C_6\ 2C_3\ C_2\ 3\sigma_v\ 3\sigma_d$
	622	D_6	4	$E\ 2C_6\ 2C_3\ C_2\ 3C_2'\ 3C_2''$
	$6/mmm$	D_{6h}	4	$E\ 2C_6\ 2C_3\ C_2\ 3C_2'\ 3C_2''\ i\ 2S_3\ \ 2S_6\ \sigma_h\ 3\sigma_d\ 3\sigma_v$
Cubic	23	T	5	$E\ 4C_3\ 4C_3^2\ 3C_2$
	$m3$	T_h	7	$E\ 4C_3\ 4C_3^2\ 3C_2\ i\ 8S_6\ 3\sigma_h$
	$\bar{4}3m$	T_d	8	$E\ 8C_3\ 3C_2\ 6\sigma_d\ 6S_4$
	432	O	6	$E\ 8C_3\ 3C_2\ 6C_2'\ 6C_4$
	$m3m$	O_h	10	$E\ 8C_3\ 3C_2\ 6C_2\ 6C_4\ i\ 8S_6\ 3\sigma_h\ 6\sigma_d\ 6S_4$

N_{sg} denotes the number of space groups

Table B.3 Space group numbers and corresponding space group symbols in standard international notation

1	P1	2	$P\bar{1}$	3	P2	4	$P2_1$	5	C2
6	Pm	7	Pc	8	Cm	9	Cc	10	P2/m
11	$P2_1/m$	12	C2/m	13	P2/c	14	$P2_1/c$	15	C2/c
16	P222	17	$P222_1$	18	$P2_12_12$	19	$P2_12_12_1$	20	$C222_1$
21	C222	22	F222	23	I222	24	$I2_12_12_1$	25	Pmm2
26	$Pmc2_1$	27	Pcc2	28	Pma2	29	$Pca2_1$	30	Pnc2
31	$Pmn2_1$	32	Pba2	33	$Pna2_1$	34	Pnn2	35	Cmm2
36	$Cmc2_1$	37	Ccc2	38	Amm2	39	Abm2	40	Ama2
41	Aba2	4_2	Fmm2	43	Fdd2	44	Imm2	45	Iba2
46	Ima2	47	Pmmm	48	Pnnn	49	Pccm	50	Pban
51	Pmma	52	Pnna	53	Pmna	54	Pcca	55	Pbam
56	Pccn	57	Pbcm	58	Pnnm	59	Pmmn	60	Pbcn
61	Pbca	62	Pnma	63	Cmcm	64	Cmca	65	Cmmm
66	Cccm	67	Cmma	68	Ccca	69	Fmmm	70	Fddd
71	Immm	72	Ibam	73	Ibca	74	Imma	75	P4
76	$P4_1$	77	$P4_2$	78	$P4_3$	79	I4	80	$I4_1$
81	$P\bar{4}$	82	$I\bar{4}$	83	P4/m	84	$P4_2/m$	85	P4/n
86	$P4_2/n$	87	I4/m	88	$I4_1/a$	89	P422	90	$P42_12$
91	P4122	92	$P412_12$	93	$P4_222$	94	$P4_22_12$	95	$P4_322$
96	$P4_32_12$	97	I422	98	$I4_122$	99	P4mm	100	P4bm
101	$P4_2cm$	102	$P4_2nm$	103	P4cc	104	P4nc	105	$P4_2mc$
106	$P4_2bc$	107	I4mm	108	I4cm	109	$I4_1md$	110	$I4_1cd$
111	$P\bar{4}2m$	112	$P\bar{4}2c$	113	$P\bar{4}2_1m$	114	$P\,\bar{4}2_1c$	115	$P\bar{4}m2$
116	$P\bar{4}c2$	117	$P\bar{4}b2$	118	$P\bar{4}n2$	119	$I\bar{4}m2$	120	$I\bar{4}c2$
121	$I\bar{4}2m$	122	$I\bar{4}2d$	123	P4/mmm	124	P4/mcc	125	P4/nbm
126	P4/nnc	127	P4/mbm	128	P4/mnc	129	P4/nmm	130	P4/ncc
131	$P4_2/mmc$	132	$P4_2/mcm$	133	$P4_2/nbc$	134	$P4_2/nnm$	135	$P4_2/mbc$
136	$P4_2/mnm$	137	$P4_2/nmc$	138	$P4_2/ncm$	139	I4/mmm	140	I4/mcm
141	$I4_1/amd$	142	$I4_1/acd$	143	P3	144	$P3_1$	145	$P3_2$
146	R3	147	$P\bar{3}$	148	$R\bar{3}$	149	P312	150	P321
151	$P3_112$	152	$P3_121$	153	$P3_212$	154	$P3_221$	155	R32
156	P3m1	157	P31m	158	P3c1	159	P31c	160	R3m
161	R3c	162	$P\bar{3}1m$	163	$P\bar{3}1c$	164	$P\bar{3}m1$	165	$P\bar{3}c1$
166	$R\bar{3}m$	167	$R\bar{3}c$	168	P6	169	$P6_1$	170	$P6_5$
171	$P6_2$	172	$P6_4$	173	$P6_3$	174	$P\bar{6}$	175	P6/m
176	$P6_3/m$	177	P622	178	$P6_122$	179	$P6_522$	180	$P6_222$
181	$P6_422$	182	$P6_322$	183	P6mm	184	P6cc	185	$P6_3cm$
186	$P6_3mc$	187	$P\bar{6}m2$	188	$P\bar{6}c2$	189	$P\bar{6}2m$	190	$P\bar{6}2c$

(continued)

Table B.3 (continued)

191	P6/mmm	192	P6/mcc	193	$P6_3/mcm$	194	$P6_3/mmc$	195	P23
196	F23	197	I23	198	$P2_13$	199	$I2_13$	200	$Pm\bar{3}$
201	$Pn\bar{3}$	202	$Fm\bar{3}$	203	$Fd\bar{3}$	204	$Im\bar{3}$	205	$Pa\bar{3}$
206	$Ia\bar{3}$	207	P432	208	$P4_232$	209	F432	210	$F4_132$
211	I432	212	$P4_332$	213	$P4_132$	214	$I4_132$	215	$P\bar{4}3m$
216	$F\bar{4}3m$	217	$I\bar{4}3m$	218	$P\bar{4}3n$	219	$F\bar{4}$ 3c	220	$I\bar{4}3d$
221	$Pm\bar{3}m$	222	$Pn\bar{3}n$	223	$Pm\bar{3}n$	224	$Pn\bar{3}m$	225	$Fm\bar{3}m$
226	$Fm\bar{3}c$	227	$Fd\bar{3}m$	228	$Fd\bar{3}c$	229	$Im\bar{3}m$	230	$Ia\bar{3}d$

Appendix C
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 $f(\omega) = f_1(\omega) + \mathrm{i}f_2(\omega)$ fulfilling the following conditions[1]:

- The poles of $f(\omega)$ are below the real axis.
- The integral of $f(\omega)/\omega$ along a semicircle with infinite radius in the upper half of the complex plane vanishes.
- The function $f_1(\omega)$ is even and the function $f_2(\omega)$ is odd for real values of the argument.

The integral of $f(s)/(s-\omega)\mathrm{d}s$ 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 $s = \omega$ yields $-\pi\mathrm{i}f(\omega)$, the integral over the infinite semicircle is zero. Therefore the value of $f(\omega)$ is given by[2]

$$f(\omega) = \frac{1}{\pi\mathrm{i}} \Pr\int_{-\infty}^{\infty} \frac{f(s)}{s-\omega}\mathrm{d}s. \tag{C.1}$$

Equating the real and imaginary parts of (C.1) yields for the real part

$$f_1(\omega) = \frac{1}{\pi} \Pr\int_{-\infty}^{\infty} \frac{f_2(s)}{s-\omega}\mathrm{d}s. \tag{C.2}$$

Splitting the integral into two parts $\int_0^\infty$ and $\int_{-\infty}^0$, going from s to $-s$ in the latter and using $f_2(-\omega) = -f_2(\omega)$ and $\frac{1}{s-\omega} + \frac{1}{s+\omega} = \frac{2s}{s^2-\omega^2}$ yields (C.3a)

[1] The requirements for the function f to which the KKR apply can be interpreted as that the function must represent the Fourier transform of a linear and causal physical process.

[2] The Cauchy principal value Pr of the integral is the limit for $\delta \to 0$ of the sum of the integrals over $-\infty < s < \omega - \delta$ and $\omega + \delta < s < \infty$.

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$$f_1(\omega) = \frac{2}{\pi} \Pr \int_0^\infty \frac{s f_2(s)}{s^2 - \omega^2} \mathrm{d}s \tag{C.3a}$$

$$f_2(\omega) = -\frac{2}{\pi} \Pr \int_0^\infty \frac{f_1(s)}{s^2 - \omega^2} \mathrm{d}s. \tag{C.3b}$$

In a similar way, (C.3b) is obtained. These two relations are the Kramers–Kronig relations [1839, 1840]. They are most often applied to the dielectric function ϵ. In this case, they apply to the susceptibility, i.e. $f(\omega) = \chi(\omega) = \epsilon(\omega)/\epsilon_0 - 1$. 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 $\epsilon = \epsilon_1 + \mathrm{i}\epsilon_2$, the following KKR relations hold:

$$\epsilon_1(\omega) = \epsilon_0 + \frac{2}{\pi} \Pr \int_0^\infty \frac{s\, \epsilon_2(s)}{s^2 - \omega^2} \mathrm{d}s \tag{C.4a}$$

$$\epsilon_2(\omega) = -\frac{2\omega}{\pi} \Pr \int_0^\infty \frac{\epsilon_1(s) - \epsilon_0}{s^2 - \omega^2} \mathrm{d}s. \tag{C.4b}$$

The static dielectric constant is thus given by

$$\epsilon(0) = \epsilon_0 + \frac{2}{\pi} \Pr \int_0^\infty \frac{\epsilon_2(s)}{s} \mathrm{d}s. \tag{C.5}$$

The integral does not diverge since ϵ_2 is an odd function and zero at $\omega = 0$. Generally the jth momentum M_j of the imaginary part of the dielectric function is

$$M_j = \int_0^\infty \epsilon_2(\omega)\, \omega^j \, \mathrm{d}\omega. \tag{C.6}$$

Thus, $M_{-1} = \pi[\epsilon(0) - \epsilon_0]/2$.

Other KKRs are, e.g., the relation between the index of refraction n_r and the absorption coefficient α:

$$n_\mathrm{r}(\lambda) = \frac{1}{\pi} \Pr \int_0^\infty \frac{\alpha(s)}{1 - s^2/\lambda^2} \mathrm{d}s. \tag{C.7}$$

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 **E** is formulated with the dielectric function. The resulting polarization **P** is related to the electric field via

$$\mathbf{P} = \epsilon_0 \, \chi \, \mathbf{E}, \tag{D.1}$$

with χ being the electric susceptibility, and the displacement field **D** is given by

$$\mathbf{D} = \epsilon_0 \, \mathbf{E} + \mathbf{P} = \epsilon_0 \, \epsilon \, \mathbf{E}. \tag{D.2}$$

Thus the (relative) dielectric constant is

$$\epsilon = 1 + \chi. \tag{D.3}$$

We assume a harmonic oscillator model for an electron, i.e. an equation of motion for the amplitude $x = x_0 \exp(\mathrm{i}\omega t)$

$$m \, \ddot{x} = -C \, x. \tag{D.4}$$

The resonance frequency is $\omega_0^2 = C/m$. The presence of a harmonic electric field E of frequency ω and amplitude E_0 adds a force eE. Thus,

$$-\, m \, \omega^2 \, x = -m \, \omega_0^2 \, x + e \, E. \tag{D.5}$$

The polarization ex_0 is given by

$$ex_0 = \frac{e^2}{m} \, \frac{1}{\omega_0^2 - \omega^2} \, E_0 = \frac{e^2}{m \, \omega_0^2} \, \frac{1}{1 - \omega^2/\omega_0^2} \, E_0. \tag{D.6}$$

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

$$f = \frac{e^2}{\epsilon_0 m \omega_0^2} \tag{D.7}$$

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

$$\epsilon(\omega) = 1 + \frac{f}{1 - \omega^2/\omega_0^2}. \tag{D.8}$$

In the low-frequency limit, the dielectric function is $\epsilon(0) = 1 + f$, in the high-frequency limit $\epsilon(\infty) = 1$. The oscillator strength is the difference of ϵ for frequencies below and above the resonance.

For all systems, the high-frequency limit of ϵ is 1. This means that $\chi = 0$, 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 ω_0 and $\omega \to \infty$, these are summarized as the high-frequency dielectric constant $\epsilon_\infty > 1$. Equation (D.8) then reads

$$\epsilon(\omega) = \epsilon(\infty) + \frac{\hat{f}}{1 - \omega^2/\omega_0^2}. \tag{D.9}$$

The limit $\epsilon \to \epsilon(\infty)$ is only valid for frequencies above ω_0 but smaller than the next resonance(s) at higher frequencies.[3] Another common form is to include the background dielectric constant via

$$\epsilon(\omega) = \epsilon(\infty)\left[1 + \frac{f}{1 - \omega^2/\omega_0^2}\right]. \tag{D.10}$$

Obviously, $f = \hat{f}/\epsilon(\infty)$, making the two forms equivalent.

In order to discuss the lineshape, not only for ϵ but also for the index of refraction $n^* = n_\mathrm{r} + \mathrm{i}\kappa = \sqrt{\epsilon}$, we introduce damping to our calculation by adding a term $-m\Gamma\dot{x}$ to the left side of (D.5). This term is something like a 'friction' and would cause the oscillation amplitude to decay exponentially with a time constant $\tau = 2/\Gamma$ without external stimulus. The dielectric constant is

$$\epsilon(\omega) = \epsilon(\infty)\left[1 + \frac{f}{1 - (\omega^2 + \mathrm{i}\,\omega\Gamma)/\omega_0^2}\right] = \epsilon' + \mathrm{i}\epsilon''. \tag{D.11}$$

The real and imaginary part fulfill the Kramers–Kronig relations (C.3a) and (C.3b). For the oscillator strength, the regimes of large oscillator strength ($f \sim 1$) and small oscillator strength ($f \ll 1$) are distinguished. For the damping, two regimes

[3] For ω going to infinite values (beyond the X-ray regime), ϵ always goes towards one.

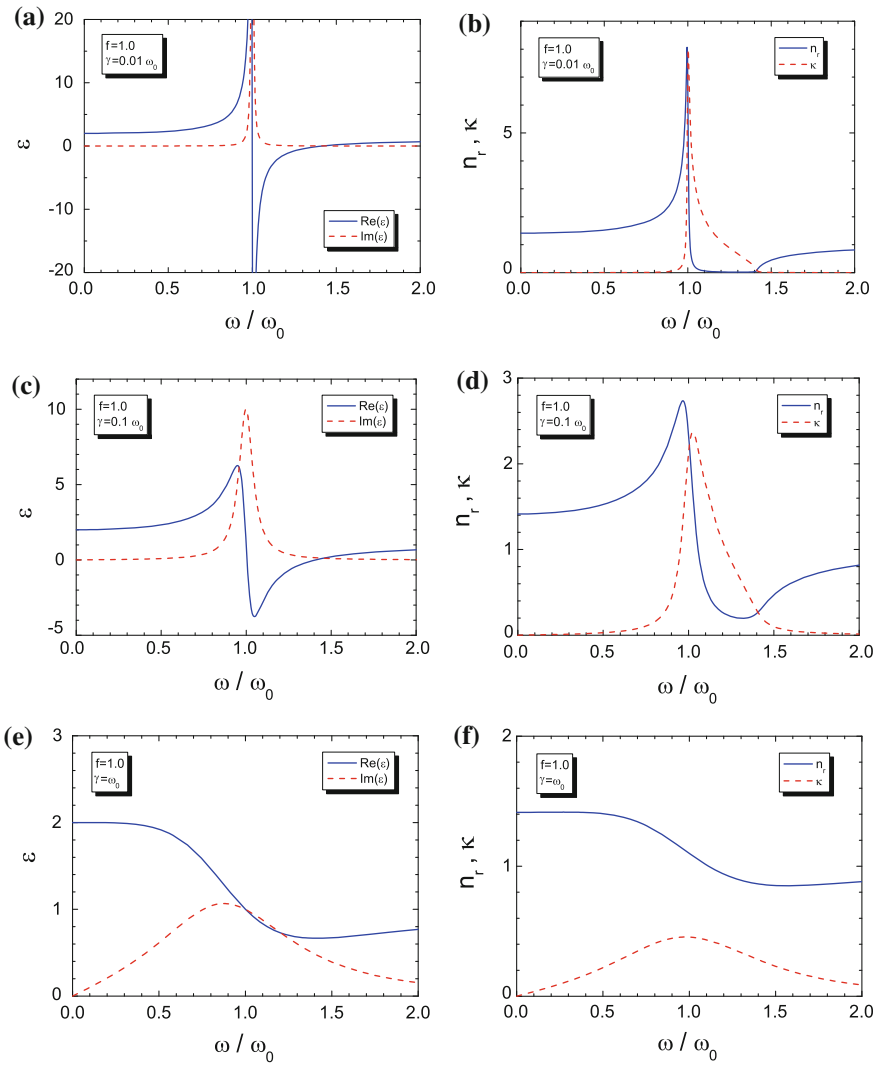

Fig. D.1 Real (*solid lines*) and imaginary (*dashed lines*) parts of the dielectric constant (**a**, **c**, **e**) and index of refraction (**b**, **d**, **f**) (D.11) for oscillator strength $f = 1$ and various values of damping: (**a**, **b**) $\Gamma = 10^{-2}\omega_0$, (**c**, **d**) $\Gamma = 10^{-1}\omega_0$, and (**e**, **f**) $\Gamma = \omega_0$

should be distinguished: Small damping ($\Gamma \ll \omega_0$) and strong damping ($\Gamma \gtrsim \omega_0$). Typical lineshapes are shown in Figs. D.1 and D.2.

For small oscillator strength, i.e. $f \ll 1$, the index of refraction $n^* = \sqrt{\epsilon} = n_\mathrm{r} + \mathrm{i}\kappa$ is given by ($n_\infty = \sqrt{\epsilon(\infty)}$)

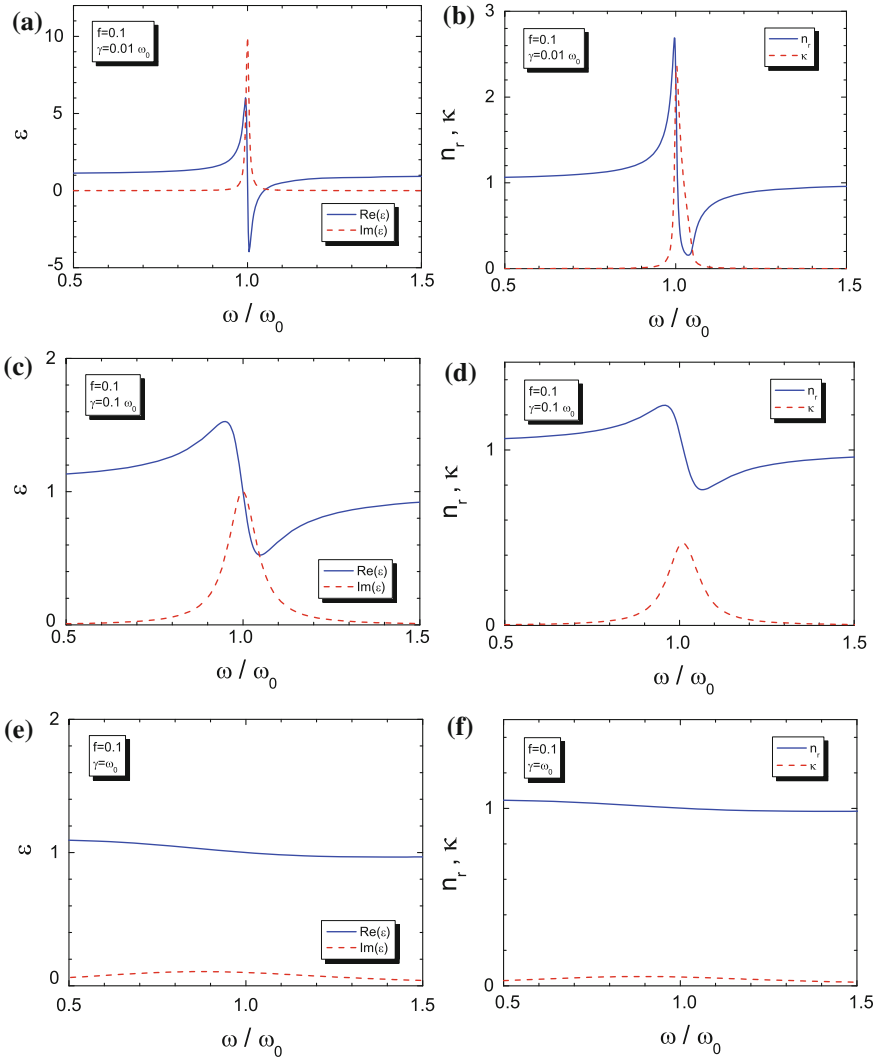

Fig. D.2 Real (*solid lines*) and imaginary (*dashed lines*) parts of the dielectric constant (**a**, **c**, **e**) and index of refraction (**b**, **d**, **f**) (D.11) for oscillator strength $f = 10^{-1}$ and various values of damping: (**a**, **b**) $\Gamma = 10^{-2}\omega_0$, (**c**, **d**) $\Gamma = 10^{-1}\omega_0$, and (**e**, **f**) $\Gamma = \omega_0$

$$n_{\mathrm{r}} = n_\infty \left[1 + \frac{f}{2}\,\frac{\omega_0^2\,(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\,\omega^2}\right] \tag{D.12a}$$

$$\kappa = n_\infty\,\frac{f}{2}\,\frac{\Gamma\,\omega_0\,(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\,\omega^2}. \tag{D.12b}$$

For small detuning from the resonance frequency, i.e. $\omega = \omega_0 + \delta\omega$ with $|\delta\omega|/\omega_0 \ll 1$, the index of refraction is given by

$$n_\mathrm{r} = n_\infty \left[1 - \frac{f}{4} \frac{\omega_0\,\delta\omega}{(\delta\omega)^2 + \Gamma^2/4}\right] \tag{D.13a}$$

$$\kappa = n_\infty \frac{f}{4} \frac{\omega_0\,\Gamma/2}{(\delta\omega)^2 + \Gamma^2/4}. \tag{D.13b}$$

The maximum absorption is given as

$$\alpha_\mathrm{m} = 2\,\frac{\omega_0}{c}\,\kappa(\omega_0) = f\,\frac{\omega_0^2}{\Gamma}\,\frac{n_\infty}{c}. \tag{D.14}$$

For zero damping, the dielectric function has a zero at

$$\omega_0' = \omega_0\,\sqrt{1+f} \approx \omega_0\,\left(1 + \frac{f}{2}\right). \tag{D.15}$$

The latter approximation is valid for $f \ll 1$. In the region between ω_0 and ω_0', the real part of the index of refraction is very small (for the physically unrealistic case of $\Gamma \equiv 0$ it is exactly zero since $\epsilon < 0$). The reflectance (for vertical incidence $R = [(1-n^*)/(1+n^*)]^2$) in this region (width: $f\omega_0/2$) is thus very high. For larger damping (and small oscillator strength), this effect is washed out.

The frequency $\omega_{\epsilon'',\mathrm{max}}$ of the maximum of the imaginary part of ϵ'' of the dielectric function ($\hat{\Gamma} = \Gamma/\omega_0$) is

$$\omega_{\epsilon'',\mathrm{max}}^2 = \omega_0^2\,\frac{2 - \hat{\Gamma}^2 + \sqrt{16 - 4\hat{\Gamma}^2 + \hat{\Gamma}^4}}{6} \approx \omega_0^2\left[1 - \left(\frac{\Gamma}{2\omega_0}\right)^2\right]. \tag{D.16}$$

The approximation is valid for small damping $\Gamma \ll \omega_0$. In this case, the detuned frequency of the maximum is close to ω_0 (Fig. D.3). The frequency position of the maximum of $\tan\delta = \epsilon''/\epsilon'$ is

$$\omega_{\tan\delta,\mathrm{max}}^2 = \omega_0^2\,\frac{2 + f - \hat{\Gamma}^2 + \Lambda^2}{6} \tag{D.17}$$

$$\Lambda^2 = \sqrt{12\,(1+f) + \left(2 + f - \hat{\Gamma}^2\right)^2}.$$

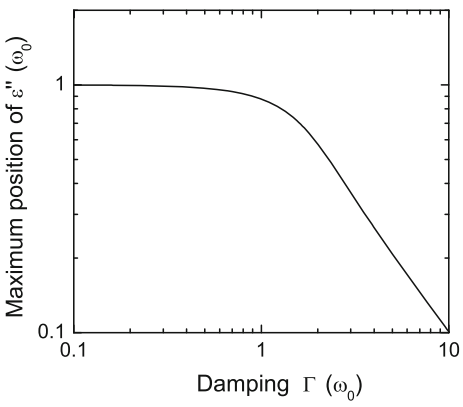

Fig. D.3 Frequency position of the maximum of ϵ'' as a function of the damping

The value of $\tan\delta$ at its maximum is (Λ has the same meaning as in (D.17))

$$(\tan\delta)_{\max} = \frac{-3\sqrt{\frac{3}{2}} f\,\hat{\Gamma}\,\sqrt{2+f-\hat{\Gamma}^2+\Lambda^2}}{-8-8f+f^2-4\,\hat{\Gamma}^2-2f\,\hat{\Gamma}^2+\hat{\Gamma}^4+\left(2+f-\hat{\Gamma}^2\right)\Lambda^2}. \quad \text{(D.18)}$$

Appendix E
Quantum Statistics

E.1 Introduction

Bosons are particles with integer spin $s = n$, fermions are particles with spin $s = n + 1/2$ 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

$$\Psi(q_1, q_2) = \Psi(q_2, q_1) \tag{E.1a}$$
$$\Psi(q_1, q_2) = -\Psi(q_2, q_1), \tag{E.1b}$$

where (E.1a) holds for bosons and (E.1b) holds for fermions. The variables q_i denote the coordinates and spin of the ith 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 ϵ_r, the number of particles in the state r is n_r.

For vanishing interaction of the particles, the total energy of the gas in the state R (with n_r particles in the state r) is

$$E_R = \sum_r n_r \, \epsilon_r. \tag{E.2}$$

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

$$N = \sum_r n_r. \tag{E.3}$$

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

$$Z = \sum_R \exp(-\beta E_R), \tag{E.4}$$

with $\beta = 1/(kT)$. The sum runs over all possible microscopic states R of the gas, i.e. all combinations of the n_r that fulfill (E.3). The probability P_S to find the system in a particular state S is given by (canonical ensemble)

$$P_S = \frac{\exp(-\beta E_S)}{Z}. \tag{E.5}$$

The average number $\bar{n}_s$ of particles in a state s is given by

$$\bar{n}_s = \frac{\sum_R n_s \exp(-\beta E_R)}{Z} = -\frac{1}{\beta Z}\frac{\partial Z}{\partial \epsilon_\mathrm{s}} = -\frac{1}{\beta}\frac{\partial \ln Z}{\partial \epsilon_\mathrm{s}}. \tag{E.6}$$

We note that the average deviation $\overline{(\Delta n_s)^2} = \overline{n_s^2 - \bar{n}_s^2} = \overline{n_s^2} - \bar{n}_s^2$ is given by

$$\overline{(\Delta n_s)^2} = \frac{1}{\beta^2}\frac{\partial^2 \ln Z}{\partial \epsilon_\mathrm{s}^2} = -\frac{1}{\beta}\frac{\partial \bar{n}_s}{\partial \epsilon_\mathrm{s}}. \tag{E.7}$$

In the Bose–Einstein statistics (for bosons), the particles are fundamentally indistinguishable. Thus, a set of $(n_1, n_2, \ldots)$ uniquely describes the system. In the case of fermions, for each state n_r is either 0 or 1. In both cases, (E.3) needs to be fulfilled.

E.3 Photon Statistics

This case is the Bose–Einstein statistics (cf. (E.24)) with undefined particle number. We rewrite (E.6) as

$$\bar{n}_s = \frac{\sum_{n_s} n_s \exp(-\beta n_s \epsilon_\mathrm{s}) \sum^{(s)}_{n_1,n_2,\ldots} \exp(-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \ldots))}{\sum_{n_s} \exp(-\beta n_s \epsilon_\mathrm{s}) \sum^{(s)}_{n_1,n_2,\ldots} \exp(-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \ldots))}, \tag{E.8}$$

where $\sum^{(s)}$ denotes a summation that does not include the index s. In the case of photons, the values n_r can take any value (integers including zero) without restriction and therefore the sums $\sum^{(s)}$ in the numerator and denominator of (E.8) are identical. After some calculation we find

$$\bar{n}_s = -\frac{1}{\beta}\frac{\partial}{\partial \epsilon_s} \ln\left(\sum_{n_s=0}^{\infty} \exp(-\beta n_s \epsilon_s)\right). \tag{E.9}$$

The argument of the logarithm is a geometrical series with the limit $[1- \exp(-\beta\epsilon_s)]^{-1}$. This leads to the so-called Planck distribution

$$\bar{n}_s = \frac{1}{\exp(\beta\epsilon_s) - 1}. \tag{E.10}$$

E.4 Fermi–Dirac Statistics

Now, the particle number is fixed to N. For the sum $\sum^{(s)}$ from (E.6), we introduce the term $Z_S(M)$

$$Z_s(M) = \sum_{n_1,n_2,\ldots}^{(s)} \exp(-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \ldots)), \tag{E.11}$$

when M particles are to be distributed over all states except s ($\sum_r^{(s)} n_r = M$). M is either $N-1$ if $n_s = 1$ and N if $n_s = 0$. Using Z_s, we can write

$$\bar{n}_s = \frac{1}{\frac{Z_s(N)}{Z_s(N-1)} \exp(\beta\epsilon_s) + 1}. \tag{E.12}$$

We evaluate $Z_s(N-1)$

$$\ln Z_s(N - \Delta N) = \ln Z_s(N) - \frac{\partial \ln Z_s}{\partial N}|_N \, \Delta N, \tag{E.13}$$

or

$$Z_s(N - \Delta N) = Z_s(N) \exp(-\gamma_s \Delta N), \tag{E.14}$$

with

$$\gamma_s = \frac{\partial \ln Z_s}{\partial N}. \tag{E.15}$$

Since Z_s runs over many states, the derivative is approximately equal to

$$\gamma = \frac{\partial \ln Z}{\partial N}, \tag{E.16}$$

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

$$\bar{n}_s = \frac{1}{\exp(\gamma + \beta\epsilon_s) + 1}. \tag{E.17}$$

Equation (E.3) holds also for the average values $\bar{n}_s$, i.e.

$$N = \sum_r \bar{n}_r = \sum_r \frac{1}{\exp(\gamma + \beta\epsilon_s) + 1}, \tag{E.18}$$

from which the value of γ can be calculated. Given that the free energy is given as $F = -kT \ln Z$, we find that

$$\gamma = -\frac{1}{kT}\frac{\partial F}{\partial N} = -\beta\mu\,, \tag{E.19}$$

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

$$\bar{n}_s = \frac{1}{\exp(\beta(\epsilon_s - \mu)) + 1}. \tag{E.20}$$

Now, we briefly revisit the approximation $\gamma = \gamma_s$. Exactly, γ fulfills

$$\gamma = \gamma_s - n_s \frac{\partial \gamma}{\partial N}. \tag{E.21}$$

Thus, the approximation is valid if $n_s \frac{\partial \gamma}{\partial N} \ll \gamma$. Since $n_s < 1$, this means that the chemical potential does not change significantly upon addition of another particle.

The Fermi–Dirac distribution function (E.20) for electrons is typically written as

$$f_e(E) = \frac{1}{\exp\left(\frac{E - E_F}{kT}\right) + 1}, \tag{E.22}$$

where k (or k_B) denotes the Boltzmann constant, T is the temperature, and E_F is the Fermi level, which is called the chemical potential μ in thermodynamics. The Fermi distribution is shown in Fig. E.1 for various parameters. The distribution function gives the probability that a state at energy E is populated in thermodynamic equilibrium. For $E = E_F$ the population is $1/2$ for all temperatures. At (the unrealistic case of) $T = 0$, the function makes a step from 1 (for $E < E_F$) to 0.

The high-energy tail of the Fermi distribution, i.e. for $E - E_F \gg kT$, can be approximated by the Boltzmann distribution:

$$f_e(E) \cong \exp\left(-\frac{E - E_F}{kT}\right). \tag{E.23}$$

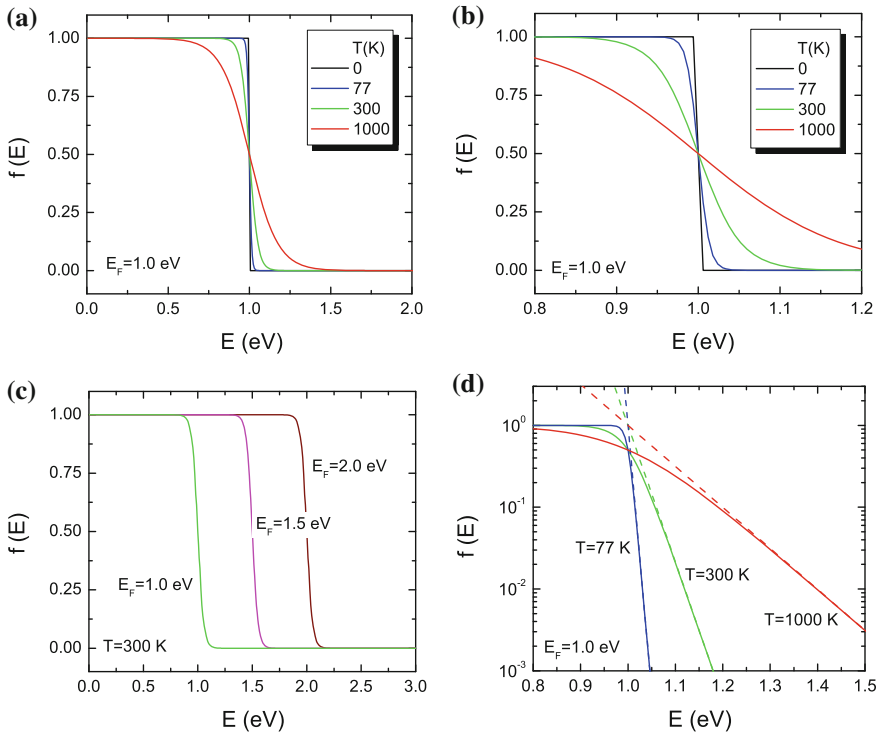

Fig. E.1 Fermi function for (**a**, **b**) different temperatures (for $E_{\mathrm{F}} = 1.0\,\mathrm{eV}$) and (**c**) for different chemical potentials (for $T = 300\,\mathrm{K}$). (**d**) Fermi function (*solid lines*) compared with Boltzmann approximation (*dashed lines*) for various temperatures and $E_{\mathrm{F}} = 1.0\,\mathrm{eV}$ on semilogarithmic plot

E.5 Bose–Einstein Distribution

Executing (E.8) with the approximation $\gamma = \gamma_s$, the Bose–Einstein distribution is found to be

$$\bar{n}_s = \frac{1}{\exp(\beta(\epsilon_{\mathrm{s}} - \mu)) - 1}. \tag{E.24}$$

Appendix F
Kronig–Penney Model

The Kronig–Penney model [64] 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.

A one-dimensional periodic hard-wall potential of finite height is assumed (Fig. F.1a). The well width is a, the barrier width b and thus the period $P = a + b$. The potential is zero in the well (regions $(0, a) + nP$) and $+U_0$ in the barrier. The Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + U(x)\,\Psi(x) = E\,\Psi(x) \tag{F.1}$$

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. $\Psi \propto \exp(\mathrm{i}kx)$ with real k. In the barrier, they have exponential character, i.e. $\Psi \propto \exp(kx)$ with real k. Thus we chose

$$\Psi(x) = A\exp(\mathrm{i}Kx) + B\exp(-\mathrm{i}Kx) \tag{F.2a}$$
$$\Psi(x) = C\exp(\kappa x) + D\exp(-\kappa x)\,. \tag{F.2b}$$

The wavefunction from (F.2a) is for the well between 0 and a with $E = \hbar^2K^2/2m$. The wavefunction from (F.2b) is for the barrier between a and $a + b$ with $U_0 - E = \hbar^2\kappa^2/2m$. From the periodicity and Bloch's theorem the wavefunction at $x = -b$ must have the form $\Psi(-b) = \exp(-\mathrm{i}kP)\,\Psi(a)$, 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 κ.

Both K and κ are real numbers. As boundary conditions, the continuity of Ψ and Ψ' are used.[4] At $x = 0$ and $x = a$ this yields

[4]Generally, Ψ'/m should be continuous, however, in the present example the mass is assumed constant throughout the structure.

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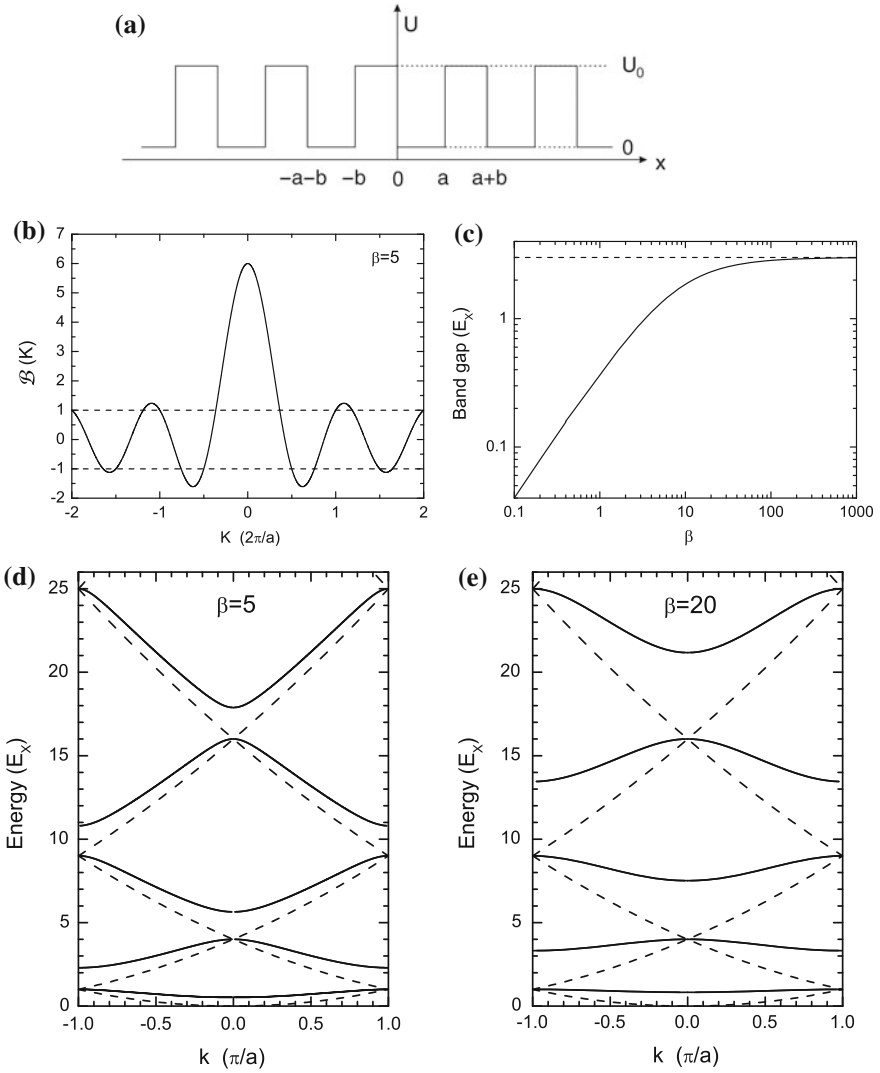

Fig. F.1 (**a**) One-dimensional periodic hard-wall potential (Kronig–Penney model). (**b**) Transcendental function $\mathcal{B}(K)$ from (F.5) for $\beta = 5$. The *dashed lines* indicate the $[-1, 1]$ interval for which solutions exist for (F.5). (**c**) Band gap between first and second subband (in units of $E_X = \hbar^2\pi^2/(2ma^2)$) as a function of β. For smaller β the band gap is $\propto \beta$. For thick barriers ($\beta \to \infty$) the band gap saturates towards $3E_X$ as expected for uncoupled wells. (**d**, **e**) The resulting energy dispersion (in units of E_X) as a function of the superlattice wavevector k for (**d**) $\beta = 5$ and (**e**) $\beta = 20$ in (F.5). The *dashed lines* are the free-electron dispersion (for $\beta = 0$) (see Fig. 6.2a)

$$A + B = C + D \tag{F.3a}$$
$$\mathrm{i}KA - \mathrm{i}KB = \kappa C - \kappa D \tag{F.3b}$$
$$A\exp(\mathrm{i}Ka) + B\exp(-\mathrm{i}Ka) = C\exp(\kappa a) + D\exp(-\kappa a) \tag{F.3c}$$
$$\mathrm{i}KA\exp(\mathrm{i}Ka) - \mathrm{i}KB\exp(-\mathrm{i}Ka) = \kappa C\exp(\kappa a) - \kappa D\exp(-\kappa a). \tag{F.3d}$$

The continuity of Ψ and Ψ' at $x = -b$ is used in the left sides of (F.3c, d).

A nontrivial solution arises only if the determinant of the coefficient matrix is zero. This leads (after some tedious algebra) to

$$\cos(kP) = \left[\frac{\kappa^2 - K^2}{2\kappa K}\right] \sinh(\kappa b)\ \sin(Ka) + \cosh(\kappa b)\ \cos(Ka). \tag{F.4}$$

Further simplification can be reached by letting the barrier thickness $b \to 0$ and $U_0 \to \infty$. Then $P \to a$. The limit, however, is performed in such a way that the barrier 'strength' $U_0 b \propto \kappa^2 b$ remains constant and finite. Equation (F.4) then reads (for $\kappa b \to 0$: $\sinh(\kappa b) \to \kappa b$ and $\coth(\kappa b) \to 1$):

$$\cos(ka) = \beta \frac{\sin(Ka)}{Ka} + \cos(Ka) = \mathcal{B}(K). \tag{F.5}$$

The coupling strength $\beta = \kappa^2 ba/2$ represents the strength of the barrier. Equation (F.5) only has a solution if the right side is in the interval $[-1, 1]$ (Fig. F.1b). The function $\sin(x)/x$ 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.1c. The dispersion is different from the free-electron dispersion and has several separated bands. The band gaps are related to the K values, i.e. energies for which (F.5) cannot be fulfilled. At the zone boundary ($k = \pi/a$) the bands are split and the tangent is horizontal ($\mathrm{d}E/\mathrm{d}k = 0$). The form of the dispersion is similar to the arccos function.

For large coupling between the potential wells (small β, $\beta \lesssim 1$) the band gap E_{12} between the first and the second subband at the X-point is $E_{12} = 4\beta/\pi^2 E_\mathrm{X}$ with $E_\mathrm{X} = \hbar^2\pi^2/(2ma^2)$. In this case, the width of the subbands is wide. For small coupling (large β) the band gap E_{12} converges towards $3E_\mathrm{X}$ as expected for decoupled potential wells with energy levels $E_n = E_\mathrm{X} n^2$ and the width of the bands is small.

Appendix G
The k · p Perturbation Theory

The solutions of the Schrödinger equation (cf. Sect. 6.2.1)

$$H\,\Psi_{n\mathbf{k}}(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right)\Psi_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\,\Psi_{\mathrm{n}\mathbf{k}}(\mathbf{r}), \tag{G.1}$$

with a lattice periodic potential U, i.e. $U(\mathbf{r}) = U(\mathbf{r}+\mathbf{R})$ for direct lattice vectors $\mathbf{R}$, are Bloch waves of the form

$$\Psi_{n\mathbf{k}}(\mathbf{r}) = \exp(\mathrm{i}\,\mathbf{k}\,\mathbf{r})\,u_{n\mathbf{k}}(\mathbf{r}), \tag{G.2}$$

with the lattice periodic Bloch function $u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R})$.

Inserting the Bloch wave into (G.1), the following equation is obtained for the periodic Bloch function:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + \frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}\right)u_{n\mathbf{k}}(\mathbf{r}) = \left(E_n(\mathbf{k}) - \frac{\hbar^2k^2}{2m}\right)u_{\mathrm{n}\mathbf{k}}(\mathbf{r}). \tag{G.3}$$

For simplicity, we assume a band edge $E_n(0)$ at $\mathbf{k} = 0$. In its vicinity, the $\mathbf{k}\cdot\mathbf{p}$ term can be treated as a perturbation. The dispersion for a nondegenerate band[5] is given up to second order in k

$$E_n(\mathbf{k}) = E_n(0) + \sum_{i,j=1}^{3}\left(\frac{\hbar^2}{2m}\,\delta_{ij} + \frac{\hbar^2}{m}\sum_{l\neq n}\frac{p^i_{nl}\,p^j_{ln}}{E_n(0) - E_l(0)}\right)k_i\,k_j, \tag{G.4}$$

with l running over other, so-called *remote* bands. The momentum matrix element is given by $p^i_{nl} = \langle u_{n0}|p_i|u_{l0}\rangle$ (cf. (6.35)). The coefficients in front of the quadratic

[5] Apart from the spin degeneracy.

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terms are the components of the dimensionless inverse effective-mass tensor (cf. (6.39))

$$\left(\frac{m}{m^*}\right)_{ij} = \delta_{ij} + \frac{2}{m}\sum_{l\neq n}\frac{p^i_{nl}\,p^j_{ln}}{E_n(0) - E_l(0)}. \tag{G.5}$$

For degenerate bands, the $p^i_{nn'}$ vanish when n and n' belong to the degenerate set and also the first-order correction is zero. In the Löwdin perturbation theory [1841], 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

$$\mathbf{k}\cdot\mathbf{p} + \mathbf{k}\cdot\mathbf{p}\sum_{l\neq n}\frac{|l\rangle\langle l|}{E_n(0) - E_l(0)}\,\mathbf{k}\cdot\mathbf{p}, \tag{G.6}$$

with the index l running over all bands not being in the degenerate set. The dispersion relation is obtained by diagonalization of the Hamiltonian (G.3) in the degenerate basis but with the perturbation given by (G.6).

The spin-orbit interaction [1244] adds an additional term

$$H_{\mathrm{so}} = \frac{\hbar}{4\,m^2\,c^2}\,(\boldsymbol{\sigma}\times\nabla U)\;\mathbf{p} \tag{G.7}$$

to the Hamiltonian, where $\boldsymbol{\sigma}$ are the Pauli spin matrices and c the vacuum speed of light. In the Schrödinger equation for the Bloch functions two new terms arise:

$$\begin{aligned}\Bigg(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + \frac{\hbar}{4m^2c^2}\,(\boldsymbol{\sigma}\times\nabla U)\;\mathbf{p}\\ + \frac{\hbar}{m}\mathbf{k}\left[\mathbf{p} + \frac{\hbar}{4m^2c^2}\,(\boldsymbol{\sigma}\times\nabla U)\right]\Bigg)u_{n\mathbf{k}}(\mathbf{r}) = \left(E_n(\mathbf{k}) - \frac{\hbar^2k^2}{2m}\right)u_{n\mathbf{k}}(\mathbf{r}).\end{aligned} \tag{G.8}$$

The linear term in $\mathbf{k}$ is again treated as a perturbation. The first spin-orbit term in (G.8) is lattice periodic, thus the solutions at $\mathbf{k} = 0$ are still periodic Bloch functions, however, different ones from previously. If the band edge is not degenerate, the momentum operator in (G.3) is simply replaced by

$$\boldsymbol{\pi} = \mathbf{p} + \frac{\hbar}{4\,m^2\,c^2}\,(\boldsymbol{\sigma}\times\nabla U)\,, \tag{G.9}$$

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.

In the 8-band Kane model [441], 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 Δ_0 as parameter. The band- edge Bloch functions are denoted as $|i\uparrow\rangle$, where the index $i = s, x, y, z$ labels the symmetry of the different

Table G.1 Basis set that diagonalizes the spin-orbit interaction

$\lvert J, m_j\rangle$	Wavefunction	Symmetry
$\lvert\frac{1}{2}, \frac{1}{2}\rangle$	$\mathrm{i}\lvert s\uparrow\rangle$	Γ_6
$\lvert\frac{1}{2}, -\frac{1}{2}\rangle$	$\mathrm{i}\lvert s\downarrow\rangle$	Γ_6
$\lvert\frac{3}{2}, \frac{3}{2}\rangle$	$\frac{1}{\sqrt{2}}\lvert(x+\mathrm{i}y)\uparrow\rangle$	Γ_8
$\lvert\frac{3}{2}, \frac{1}{2}\rangle$	$\frac{1}{\sqrt{6}}\lvert(x+\mathrm{i}y)\downarrow\rangle - \sqrt{\frac{2}{3}}\lvert z\uparrow\rangle$	Γ_8
$\lvert\frac{3}{2}, -\frac{1}{2}\rangle$	$-\frac{1}{\sqrt{6}}\lvert(x-\mathrm{i}y)\uparrow\rangle - \sqrt{\frac{2}{3}}\lvert z\downarrow\rangle$	Γ_8
$\lvert\frac{3}{2}, -\frac{3}{2}\rangle$	$\frac{1}{\sqrt{2}}\lvert(x-\mathrm{i}y)\uparrow\rangle$	Γ_8
$\lvert\frac{1}{2}, \frac{1}{2}\rangle$	$\frac{1}{\sqrt{3}}\lvert(x+\mathrm{i}y)\downarrow\rangle + \sqrt{\frac{1}{3}}\lvert z\uparrow\rangle$	Γ_7
$\lvert\frac{1}{2}, -\frac{1}{2}\rangle$	$-\frac{1}{\sqrt{3}}\lvert(x-\mathrm{i}y)\uparrow\rangle + \sqrt{\frac{1}{3}}\lvert z\downarrow\rangle$	Γ_7

bands. The linear combinations that diagonalize the spin-orbit interaction are given in Table G.1. The band gap and the spin-orbit interaction are given by

$$E_{\mathrm{g}} = E_{\Gamma_6} - E_{\Gamma_8} \tag{G.10a}$$

$$\Delta_0 = E_{\Gamma_8} - E_{\Gamma_7}. \tag{G.10b}$$

The Hamiltonian in the basis states of Table G.1 is given by

$$\begin{bmatrix}
k^2+E_{\mathrm{g}} & 0 & \sqrt{2}Pk_+ & -\sqrt{\frac{2}{3}}Pk_z & -\sqrt{\frac{2}{3}}Pk_- & 0 & \sqrt{\frac{1}{3}}Pk_z & -\sqrt{\frac{4}{3}}Pk_- \\
0 & k^2+E_{\mathrm{g}} & 0 & \sqrt{\frac{2}{3}}Pk_+ & -\sqrt{\frac{2}{3}}Pk_z & \sqrt{2}Pk_- & \sqrt{\frac{4}{3}}Pk_+ & \sqrt{\frac{1}{3}}Pk_z \\
\sqrt{2}Pk_- & 0 & k^2 & 0 & 0 & 0 & 0 & 0 \\
-\sqrt{\frac{2}{3}}Pk_z & \sqrt{\frac{2}{3}}Pk_- & 0 & k^2 & 0 & 0 & 0 & 0 \\
-\sqrt{\frac{2}{3}}Pk_+ & -\sqrt{\frac{2}{3}}Pk_z & 0 & 0 & k^2 & 0 & 0 & 0 \\
0 & \sqrt{2}Pk_+ & 0 & 0 & 0 & k^2 & 0 & 0 \\
\sqrt{\frac{1}{3}}Pk_z & \sqrt{\frac{4}{3}}Pk_- & 0 & 0 & 0 & 0 & k^2-\Delta_0 & 0 \\
-\sqrt{\frac{4}{3}}Pk_+ & \sqrt{\frac{1}{3}}Pk_z & 0 & 0 & 0 & 0 & 0 & k^2-\Delta_0
\end{bmatrix} \tag{G.11}$$

with the energy measured from the valence-band edge in units of $\hbar^2/(2m)$ and

$$\frac{1}{2}\,\mathrm{i}\,\hbar P = \langle s|\pi_x|x\rangle = \langle s|\pi_y|y\rangle = \langle s|\pi_z|z\rangle \tag{G.12a}$$

$$k_\pm = k_x \pm \mathrm{i}k_y. \tag{G.12b}$$

The inclusion of remote bands renormalizes the above Hamiltonian to

$$\begin{bmatrix}
Dk^2+E_\mathrm{g} & 0 & \sqrt{2}Pk_+ & -\sqrt{\frac{2}{3}}Pk_z & -\sqrt{\frac{2}{3}}Pk_- & 0 & \sqrt{\frac{1}{3}}Pk_z & -\sqrt{\frac{4}{3}}Pk_- \\
0 & Dk^2+E_\mathrm{g} & 0 & \sqrt{\frac{2}{3}}Pk_+ & -\sqrt{\frac{2}{3}}Pk_z & \sqrt{2}Pk_- & \sqrt{\frac{4}{3}}Pk_+ & \sqrt{\frac{1}{3}}Pk_z \\
\sqrt{2}Pk_- & 0 & H_\mathrm{h} & R & S & 0 & \frac{\mathrm{i}}{\sqrt{2}}R & -\mathrm{i}\sqrt{2}S \\
-\sqrt{\frac{2}{3}}Pk_z & \sqrt{\frac{2}{3}}Pk_- & R^* & H_\mathrm{l} & 0 & S & \frac{H_\mathrm{h}-H_\mathrm{l}}{\sqrt{2}\mathrm{i}} & \mathrm{i}\sqrt{\frac{3}{2}}R \\
-\sqrt{\frac{2}{3}}Pk_+ & -\sqrt{\frac{2}{3}}Pk_z & S^* & 0 & H_\mathrm{l} & -R & -\mathrm{i}\sqrt{\frac{3}{2}}R^* & \frac{H_\mathrm{h}-H_\mathrm{l}}{\sqrt{2}\mathrm{i}} \\
0 & \sqrt{2}Pk_+ & 0 & S^* & -R^* & H_\mathrm{h} & -\mathrm{i}\sqrt{2}S^* & -\frac{\mathrm{i}}{\sqrt{2}}R^* \\
\sqrt{\frac{1}{3}}Pk_z & \sqrt{\frac{4}{3}}Pk_- & -\frac{\mathrm{i}}{\sqrt{2}}R^* & -\frac{H_\mathrm{h}-H_\mathrm{l}}{\sqrt{2}\mathrm{i}} & \mathrm{i}\sqrt{\frac{3}{2}}R & \mathrm{i}\sqrt{2}S & \frac{H_\mathrm{h}+H_\mathrm{l}}{\sqrt{2}}-\Delta_0 & 0 \\
-\sqrt{\frac{4}{3}}Pk_+ & \sqrt{\frac{1}{3}}Pk_z & \mathrm{i}\sqrt{2}S^* & -\mathrm{i}\sqrt{\frac{3}{2}}R^* & -\frac{H_\mathrm{h}-H_\mathrm{l}}{\sqrt{2}\mathrm{i}} & \frac{\mathrm{i}}{\sqrt{2}}R & 0 & \frac{H_\mathrm{h}+H_\mathrm{l}}{\sqrt{2}}-\Delta_0
\end{bmatrix} \tag{G.13}$$

with

$$D = 1 + \frac{2}{m}\sum_{l\neq n}\frac{|\langle s|\pi_x|l\rangle|^2}{E_\mathrm{g}-E_l(0)} \tag{G.14a}$$

$$\gamma_1' = \left[1 + \frac{2}{m}\sum_{l\neq n}\frac{|p_{xl}^x|^2}{E_n(0)-E_l(0)}\right] - \frac{2P^2}{3E_\mathrm{g}} \tag{G.14b}$$

$$\gamma_2' = \left[1 + \frac{2}{m}\sum_{l\neq n}\frac{|p_{xl}^y|^2}{E_n(0)-E_l(0)}\right] - \frac{P^2}{3E_\mathrm{g}} \tag{G.14c}$$

$$\gamma_3' = \left[\frac{2}{m}\sum_{l\neq n}\frac{p_{xl}^x p_{ly}^y + p_{xl}^y p_{ly}^x}{E_n(0)-E_l(0)}\right] - \frac{P^2}{3E_\mathrm{g}} \tag{G.14d}$$

$$H_\mathrm{h} = (\gamma_1'+\gamma_2')(k_x^2+k_y^2) + (\gamma_1'-2\gamma_2')k_z^2 \tag{G.14e}$$

$$H_\mathrm{l} = (\gamma_1'-\gamma_2')(k_x^2+k_y^2) + (\gamma_1'+2\gamma_2')k_z^2 \tag{G.14f}$$

$$R = -2\sqrt{3}\gamma_3' k_- k_z \tag{G.14g}$$

$$S = \sqrt{3}\gamma_2'(k_x^2-k_y^2) + 2\sqrt{3}\gamma_3'\mathrm{i}k_x k_y. \tag{G.14h}$$

The Hamiltonian in the presence of inhomogeneous strain is given in [463]. The hole bands decouple from the conduction band for $E_\mathrm{g}\to\infty$ (six-band model [1082]). The heavy and light holes can be treated separately for $\Delta_0\to\infty$ (Luttinger Hamiltonian). For the Γ_8 states, the Hamiltonian is then given by

$$\begin{bmatrix}
H_\mathrm{h} & R & S & 0 \\
R^* & H_\mathrm{l} & 0 & S \\
S^* & 0 & H_\mathrm{l} & -R \\
0 & S^* & -R^* & H_\mathrm{h}
\end{bmatrix}. \tag{G.15}$$

Appendix H
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 m^*_{ij}. The effective-mass theory is a useful approximation for the treatment of shallow impurities (Sect. 7.5) or quantum wells (Sect. 12.3.2) with a potential that is slowly varying with respect to the scale of the lattice constant.

For the lattice-periodic potential, the Schrödinger equation

$$H_0\, \Psi_{n\mathbf{k}} = E_n(\mathbf{k})\, \Psi_{n\mathbf{k}} \tag{H.1}$$

is solved by the Bloch wave $\Psi_{n\mathbf{k}}$. With a perturbing potential V, the Schrödinger equation reads

$$(H_0 + V)\ \Psi_{n\mathbf{k}} = E_n(\mathbf{k})\, \Psi_{n\mathbf{k}}. \tag{H.2}$$

According to Wannier's theorem [1842], the solution is approximated by the solution of the

$$(E_n(-\mathrm{i}\nabla) + V)\, \Phi_n = E\, \Phi_n. \tag{H.3}$$

The dispersion relation is expanded to second order as described in Appendix G. The function Φ_n is termed the *envelope function* since it varies slowly compared to the lattice constant and the exact wavefunction is approximated (in lowest order) by

$$\Psi(\mathbf{r}) = \Phi_n(\mathbf{r})\ \exp(\mathrm{i}\,\mathbf{k}\,\mathbf{r})\, u_{n0}(\mathbf{r}). \tag{H.4}$$

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Appendix I
Boltzmann Transport Theory

I.1 Boltzmann Transport Equation

The Boltzmann treatment of transport in semiconductors goes beyond the relaxation time approximation (cmp. Sect.sec:cond) and contains this approach as its simplest approximation. The distribution function of carriers $f(\mathbf{r}, \mathbf{p}, t)$ is considered with regard to their momentum $\mathbf{p} = (p_x, p_y, p_z)$, their position $(r) = (x, y, z)$ 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 $f_0(\mathbf{p})$. 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 δt the change δf is zero,

$$\frac{\delta f}{\delta t} = 0. \tag{I.1}$$

Within the time interval δt the momenta change as $\mathbf{p} \to \mathbf{p} + \mathbf{F}\,\delta t$ and the coordinates as $\mathbf{r} \to \mathbf{r} + \mathbf{p}/m^*\,\delta t$. We assume here for simplicity an isotropic mass and also the particle energy given by $E = \mathbf{p}^2/(2\,m^*)$. The condition (I.1) written in partial derivatives reads

$$\left(\frac{\partial}{\partial t} + \frac{1}{m^*}\,\mathbf{p}\cdot\nabla_{\mathbf{r}} + \mathbf{F}\cdot\nabla_{\mathbf{p}}\right) f(\mathbf{p}, \mathbf{r}, t) = 0. \tag{I.2}$$

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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

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}}. \tag{I.3}$$

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

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \iiint [f(\mathbf{p}', \mathbf{r}, t)\, P(\mathbf{p}', \mathbf{p}) - f(\mathbf{p}, \mathbf{r}, t)\, P(\mathbf{p}, \mathbf{p}')]\, \mathrm{d}\mathbf{p}'. \tag{I.4}$$

with $P(\mathbf{p}, \mathbf{p}')$ being the transition probability per time that a momentum $\mathbf{p}$ is changed into $\mathbf{p}'$ by collisions. The collision integral must be calculated explicitly using microscopic and eventually quantum mechanical models. This leads now to the Boltzmann transport equation

$$\left(\frac{\partial}{\partial t} + \frac{1}{m^*}\mathbf{p} \cdot \nabla_{\mathbf{r}} + \mathbf{F} \cdot \nabla_{\mathbf{p}}\right) f(\mathbf{p}, \mathbf{r}, t) = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}. \tag{I.5}$$

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

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{f(\mathbf{p}) - f_0}{\tau(\mathbf{p})}. \tag{I.6}$$

Compared to the relaxation time approximation, the major difference on the level of (I.6) here is the consideration of the momentum (and energy) dependence of the distribution function and the relaxation time.

I.2 Conductivity

In thermodynamical equilibrium the number of electronic states per unit volume associated with an element $\mathrm{d}\mathbf{p} = \mathrm{d}p_x\, \mathrm{d}p_y\, \mathrm{d}p_z$, including spin degeneracy of 2 is

$$\frac{2}{h^3} f_0(\mathbf{p})\, \mathrm{d}\mathbf{p}. \tag{I.7}$$

In the presence of an electric field $\mathbf{E}$, which we assume here in x-direction, a steady-state current will arise and the number of electronic states changes to

$$\frac{2}{h^3} f(\mathbf{p})\, \mathrm{d}\mathbf{p}, \tag{I.8}$$

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

$$j_x = -\frac{2\,e}{h^3} \iiint v_x \,[f(\mathbf{p}) - f_0(\mathbf{p})]\,\mathrm{d}\mathbf{p}. \tag{I.9}$$

This is a generalization of (8.4). The Boltzmann transport equation (I.5) with (I.6) simplifies to

$$-\frac{f(\mathbf{p}) - f_0}{\tau(\mathbf{p})} = -e\,E_x\,\frac{\partial f}{\partial p_x} \approx -e\,E_x\,\frac{\partial f_0}{\partial p_x}. \tag{I.10}$$

The last approximation is valid for small fields and makes j_x proportional to E_x (ohmic regime). The derivative with respect to p_x is converted to a derivative with respect to energy, yielding

$$\frac{f(\mathbf{p}) - f_0}{\tau(\mathbf{p})} = e\,v_x\,E_x\,\frac{\partial f_0}{\partial E}. \tag{I.11}$$

We note that for the Fermi–Dirac distribution (E.22) $f_0(E)$:

$$\frac{\partial f_0}{\partial E} = -\frac{1}{kT} f_0\,[1 - f_0]\,, \tag{I.12}$$

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

$$\frac{\partial f_0}{\partial E} \approx -\frac{1}{kT} f_0 = -\frac{1}{kT}\,\exp\left(-\frac{E - E_\mathrm{F}}{kT}\right), \tag{I.13}$$

Now the current density is given as

$$j_x = -\frac{2\,e^2}{h^3}\,E_x \iiint v_x^2\,\tau(\mathbf{p})\,\frac{\partial f_0}{\partial E}\,\mathrm{d}\mathbf{p}. \tag{I.14}$$

If we assume that τ depends only on the momentum and not its direction,[6] and replace v_x^2 by $v^2/3$ assuming isotropy, the integral reads[7]

$$j_x = -\frac{8\pi\,e^2}{3\,h^3}\,E_x \int_0^\infty v^2\,\tau(p)\,\frac{\partial f_0}{\partial E}\,p^2\,\mathrm{d}p. \tag{I.15}$$

The quantity $8\pi\,p^2\mathrm{d}p\,f_0/h^3$ (cmp. I.7) denotes the number $\mathrm{d}n$ of electrons with momentum in the range $\mathrm{d}p$. Thus the integral can also be written as (in Boltzmann approximation)

[6] This might be incorrect e.g. for piezoelectric scattering.

[7] Using $\mathrm{d}\mathbf{p} = 4\pi\,p^2\,\mathrm{d}p$.

$$j_x = \frac{e^2}{3\,kT}\,E_x \int_0^\infty v^2\,\tau\,\mathrm{d}n. \tag{I.16}$$

Denoting the average of a quantity a over the electron distribution with $\langle a\rangle$ according to

$$\langle a\rangle = \frac{\int a\,\mathrm{d}n}{n}, \tag{I.17}$$

the equation (I.16) can be written as

$$j_x = \frac{n\,e^2}{3\,kT}\,E_x\,\langle v^2\tau\rangle. \tag{I.18}$$

Using $m^*\langle v^2\rangle = 3\,kT$, we thus have obtained

$$\sigma = \frac{n\,e^2}{m^*}\,\frac{\langle v^2\tau\rangle}{\langle v^2\rangle}, \tag{I.19}$$

and with $\sigma = n\,(-e)\,\mu$ (for electrons), the mobility

$$\mu = -\frac{e}{m^*}\,\frac{\langle v^2\tau\rangle}{\langle v^2\rangle}. \tag{I.20}$$

For degenerate semiconductors, similar as for metals, the derivative of f_0 in (I.15) has a significant value only in the few-kT vicinity of the Fermi level. In an approximation we can evaluate the integral by replacing $E^{3/2}$ and τ by their values at the Fermi level and find[8] (using (6.66))

$$\sigma = \frac{j_x}{E_x} = \frac{n\,e^2\,\tau_\mathrm{F}}{m^*}. \tag{I.21}$$

Starting again with (I.15), using the density of states (6.67) in the form (per volume)

$$D(E) = m^*\,\frac{8\,\pi}{h^3}\,\sqrt{2\,m^*E}, \tag{I.22}$$

and $\mathrm{d}p/\mathrm{d}E = \sqrt{2m^*/E}$ we write

$$j_x = -\frac{e^2}{3}\,E_x \int_0^\infty D(E)\,v^2\,\tau(E)\,\frac{\partial f_0}{\partial E}\,\mathrm{d}E. \tag{I.23}$$

[8] $\int_0^\infty \frac{\partial f_0}{\partial E}\,\mathrm{d}E = -1 + [1 + \exp(E_\mathrm{F}/kT)]^{-1} \approx -1$ for $E_\mathrm{F} \gg kT$.

Using an energy-dependent mobility, in the spirit of (I.20) defined as

$$\mu(E) = -e\,\frac{v^2\,\tau(E)}{3\,kT}, \tag{I.24}$$

the conductivity can be written in a generalized form integrating over single electron states [1843] (neglecting correlation effects):

$$\begin{aligned}\sigma &= e\int D(E)\,\mu(E)\,kT\,\frac{\partial f_0}{\partial E}\,\mathrm{d}E \\ &= -e\int D(E)\,\mu(E) f_0(E)\,[1-f_0(E)]\,\mathrm{d}E.\end{aligned} \tag{I.25}$$

I.3 Hall Effect

Treating the Hall effect with the Boltzmann transport equation and making the assumptions of isotropy, one obtains (cmp. (13.12) and (13.21))

$$R_\mathrm{H} = \frac{1}{q\,n}\,\frac{\langle v^2\tau^2\rangle\,\langle v^2\rangle}{\langle v^2\tau\rangle^2}. \tag{I.26}$$

The Hall mobility determined from the Hall coefficient is

$$\mu_\mathrm{H} = \sigma\,R_\mathrm{H} = \frac{e}{m^*}\,\frac{\langle v^2\tau^2\rangle}{\langle v^2\tau\rangle^2}, \tag{I.27}$$

and thus different from the field mobility (I.20).

I.4 Thermopower

The electronic energy transported per electron is $E - E_\mathrm{F}$. Writing (I.25) as $\sigma = \int \sigma(E)\,\mathrm{d}E$, the weighing factor for electrons at energy E contributing to conduction is $\sigma(E)\,\mathrm{d}E/\sigma$. Therefore the Seebeck coefficient (thermopower) can be written [721]

$$S = -\frac{k}{e}\int\left(\frac{E-E_\mathrm{F}}{kT}\right)\frac{\sigma(E)}{\sigma}\,\mathrm{d}E. \tag{I.28}$$

or

$$S = -\frac{k}{e}\,\frac{\int D(E)\,\mu(E)\,[(E-E_\mathrm{F})/kT]f\,(1-f)\,\mathrm{d}E}{\int D(E)\,\mu(E) f\,(1-f)\,\mathrm{d}E}. \tag{I.29}$$

For band conduction the thermopower is obtained by integrating (I.29) for electrons (S_n) and holes (S_p) (using the Boltzmann approximation) as [721]

$$S_n = -\frac{k}{e}\left(\frac{E_C - E_F}{kT} + A_C\right) \tag{I.30a}$$

$$S_p = \frac{k}{e}\left(\frac{E_F - E_V}{kT} + A_V\right), \tag{I.30b}$$

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

$$A_C = \frac{\int_0^\infty (E'/kT)\,\sigma(E')\,\mathrm{d}E'}{\int_0^\infty \sigma(E')\,\mathrm{d}E'}, E' = E - E_C \tag{I.31a}$$

$$A_V = \frac{\int_{-\infty}^0 (E'/kT)\,\sigma(E')\,\mathrm{d}E'}{\int_{-\infty}^0 \sigma(E')\,\mathrm{d}E'}, E' = E_V - E. \tag{I.31b}$$

If the product of the density of states and the mobility $D\mu$ depends on the energy like E^γ, the constant is $A = 1 + \gamma$ (for $\gamma > -1$). For a parabolic band ($D \propto E^{1/2}$) and acoustic deformation potential scattering $\mu \propto E^{-1/2}$ (Sect. 8.3.4), A=1; for moderate ionized impurity scattering $\mu \propto E^{3/2}$ (Sect. 8.3.3) and $A = 3$.

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

$$S = \frac{S_n\,\sigma_n + S_p\,\sigma_p}{\sigma_n + \sigma_p}. \tag{I.32}$$

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 [723, 1844–1846].

Appendix J
Noise

Noise is a general phenomenon effecting every measurement process and the performance of semiconductor devices [1847–1852]. 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 [1850].

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.

J.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 $2T$ (symmetric around $t = 0$) is defined as

$$\langle A \rangle_T = \frac{1}{2\,T} \int_{-T}^{T} A(t)\,\mathrm{d}t. \tag{J.1}$$

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The time average of the signal $\langle A\rangle$ in general is the limit for large times,

$$\langle A\rangle = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} A(t)\,\mathrm{d}t. \tag{J.2}$$

Two identical experiments will (should) share the same limits, i.e. $\langle A\rangle = \langle B\rangle$. The fluctuation or noise of A is defined as $a(t)$ via

$$a(t) = A(t) - \langle A\rangle, \tag{J.3}$$

thus evidently $\langle a\rangle = 0$. For an identical but different experiment, $a(t) \neq b(t)$ as stated before.

The *variance* σ^2 (or second moment) of the signal is the average of the squared fluctuation,

$$\sigma^2 = \langle a^2\rangle = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} a(t)^2\,\mathrm{d}t = \langle A^2\rangle - \langle A\rangle^2. \tag{J.4}$$

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

$$\sigma = \langle a^2\rangle^{1/2} = \sqrt{\langle A^2\rangle - \langle A\rangle^2}. \tag{J.5}$$

The quantity σ^2 is a measure of the noise power, where $\langle A\rangle^2$ is a measure of the dc power.[9]

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 T_0, the measured signals A_{T_0} in a series of such subsequent identical measurements will still exhibit a fluctuation. How large this remaining fluctuation is depends on the choice of T_0 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 $N(t_i)$ aggregated at times t_i, $i = 0, 1, \ldots, m$. The average is then defined as

$$\langle N\rangle = \lim_{m\to\infty} \frac{1}{m} \sum_{i=0}^{m} N(t_i). \tag{J.6}$$

[9]Imagine a fluctuating current $I(t) = \langle I\rangle + i(t)$ leading to Joule heating ($\propto I^2$) at a resistor. Comparing the heating from I and $\langle I\rangle = \langle I\rangle$ (from a low noise current source) can yield the noise power. Also $\langle i^2\rangle$ could be determined by first compensating I with $\langle I\rangle$ (from a low noise current source) and then measuring the temperature increase at the resistor.

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 $\sigma^2 = \langle N \rangle = \bar{N}$.

J.2 Correlations

If a measurable quantity is subject to two fluctuating quantities $a_1(t)$ and $a_2(t)$, the time average of $a_1 + a_2$ is

$$\langle (a_1 + a_2)^2 \rangle = \langle a_1^2 \rangle + \langle a_2^2 \rangle + 2\langle a_1\, a_2 \rangle. \tag{J.7}$$

The third term is the decisive one; the correlation coefficient of noise quantities a_1 and a_2 is defined as

$$c_{12} = \frac{\langle a_1\, a_2 \rangle}{\sqrt{a_1^2\, a_2^2}} = \frac{\langle a_1\, a_2 \rangle}{\sigma_1\, \sigma_2}. \tag{J.8}$$

If the two noise quantities are independent of each other they are termed *uncorrelated* and $c_{12} = 0$. 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 $c_{12} = 0$, the noise powers of the two processes are simply added,

$$\langle (a_1 + a_2)^2 \rangle = \langle a_1^2 \rangle + \langle a_2^2 \rangle. \tag{J.9}$$

This concept can be generalized to several noise sources.

A more general concept to determine correlation of two functions a_1 and a_2 is the *cross correlation* function, defined by

$$\rho_{12}(\tau) = \langle a_1(t)\, a_2(t + \tau) \rangle, \tag{J.10}$$

which is the average of function a_1 and time-shifted function a_2. Often $t = 0$ is used when the nature of the fluctuations does not change with time. An important time-shift is $\tau = 0$, and it follows that

$$c_{12} = \frac{\rho_{12}(0)}{\sigma_1\, \sigma_2}, \tag{J.11}$$

Two noise quantities a_1 and a_2 are uncorrelated if $\rho_{12}(\tau) = 0$ holds for all times τ; thus $c_{12} = 0$ is a special but important case.[10]

[10] A simply example of correlated noise sources with $c_{12} = 0$ are the voltages at a resistor and a capacitance in series; the fact that they are 90° out of phase makes $c_{12} = 0$ although the fluctuations of the voltages, due to fluctuations of the driving current, are obviously correlated.

If a_1 and a_2 are the same function, i.e. $a = a_1 = a_2$, (J.10) becomes the *auto correlation* function,

$$\rho(\tau) = \langle a(t)\, a(t+\tau)\rangle, \tag{J.12}$$

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

$$\rho(\tau) = \rho(-\tau). \tag{J.13}$$

The value at $\tau = 0$ is

$$\rho(0) = \langle a^2\rangle = \sigma^2. \tag{J.14}$$

Typically, $\rho(\tau \to \infty) = 0$ 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.

J.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 $W(\nu)$, with

$$\int_0^\infty W(\nu)\,\mathrm{d}\nu = \langle a^2\rangle. \tag{J.15}$$

Since the quantity $\langle a^2\rangle$ is finite and the spectral power density $W(\nu)$ is positive, for high frequencies, $W(\nu)$ must decrease to zero. Starting from the auto correlation function ρ, its Fourier transform shall be denoted w,

$$w(\nu) = \int_{-\infty}^\infty \rho(\tau)\ \exp(-2\pi\,\mathrm{i}\,\nu\,\tau)\,\mathrm{d}\tau. \tag{J.16}$$

Also,

$$\rho(\tau) = \int_{-\infty}^\infty w(\nu)\ \exp(2\pi\,\mathrm{i}\,\nu\,\tau)\,\mathrm{d}\nu. \tag{J.17}$$

Using $\tau = 0$ in this equation, we have obtained an equation similar to (J.15). With (J.12) $w(\nu)$ can be identified as a spectral power density. Due to (J.13), w is a real and even function and we find for the noise power spectrum W in (J.15) $W = 2\,w$ (Wiener-Khintchine theorem),

$$W(\nu) = 2\int_{-\infty}^\infty \rho(\tau)\ \exp(-2\pi\,\mathrm{i}\,\nu\,\tau)\,\mathrm{d}\tau = 4\int_0^\infty \rho(\tau)\ \cos(-2\pi\,\nu\,\tau)\,\mathrm{d}\tau. \tag{J.18}$$

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 ν_0, the variance is given by

$$\langle a^2 \rangle(\nu_0, B) = \int_{\nu_0 - B/2}^{\nu_0 + B/2} W(\nu)\, \mathrm{d}\nu \approx W(\nu_0)\, B. \tag{J.19}$$

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

J.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 [1529, 1530] and theoretically derived by Nyquist [1531].

Using the general result from Langevin theory of motion under a fluctuating force, the mobility[11] is given as

$$\mu(\omega) = \frac{e}{kT} \int_0^\infty \langle v(t)\, v(0) \rangle \, \exp(\mathrm{i}\omega t)\, \mathrm{d}t. \tag{J.20}$$

Now we restrict ourselves to times much longer than the relaxation time constant, and subsequently to frequencies much smaller than $1/\tau$. In this case the conductivity $\sigma(\omega) = e\, n\, \mu(\omega)$ does not depend on frequency and can be taken as its low frequency limit σ_0 (cmp. Sect. 8.5). In a conductor (resistor) of length L and cross section A shall be N electrons ($n = N\,(A\,L)$). With the electron velocities $v_i(t)$, the current is

$$I(t) = \frac{e}{L} \sum_i v_i(t). \tag{J.21}$$

Without external field, $\langle v_i(t) \rangle = 0$ and $\langle I(t) \rangle = 0$ and we name this fluctuating current $i(t)$. If all electrons move independently of each other,

$$\langle i(\tau)\, i(0) \rangle = N\, \frac{e^2}{L^2}\, \langle v(\tau)\, v(0) \rangle. \tag{J.22}$$

The power spectrum of $i(t)$ is according to (J.18),

[11] In the Langevin theory the mobility is the ratio of velocity v and the force K, here the mobility is the ratio of v and the field E with $K = -e\,E$.

$$W(\omega) = 2\int_{-\infty}^{\infty} \langle i(\tau)\, i(0)\rangle \, \exp(\mathrm{i}\omega\tau)\, \mathrm{d}\tau = 4N\,\frac{e^2}{L^2}\int_0^{\infty} \langle v(\tau)\, v(0)\rangle \, \exp(\mathrm{i}\omega\tau)\, \mathrm{d}\tau$$
$$= 4\,\frac{N\,e^2}{L^2}\,\frac{\mu\, kT}{e} = 4\,\frac{N\,e^2}{L^2}\,\frac{\sigma_0\, kT\, A\, L}{e^2\, N} = 4\,\sigma_0\,\frac{A}{L}\,kT. \tag{J.23}$$

Then, using the conductance $G = R^{-1} = \sigma_0\, A/L$, we find the frequency independent spectral power

$$W = 4\,kT\,G. \tag{J.24}$$

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

$$\langle i^2\rangle = 4\,kT\,G\,B, \tag{J.25}$$

and the variance of the fluctuating voltage at a resistor with resistance R in a frequency range B is ($i = u/R$)

$$\langle u^2\rangle = 4\,kT\,R\,B. \tag{J.26}$$

At room temperature ($T_0 = 293\,\mathrm{K}$), the quantity $k\,T_0$ is about 26 meV; in the context here, the unit W s = W/Hz is the appropriate one, and $k\,T_0 = 4.04 \times 10^{-21}$ 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 (J.26) and (J.25) are valid for frequencies $h\,\nu \ll kT$; for larger frequencies the quantum nature of electromagnetic radiation and photon statistics play a role. For practical purposes even cooled devices at $T = 4\,\mathrm{K}$ 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 lattice temperature must be replaced by the temperature of the carrier gas.

For a RC low pass, the power spectrum $W_i = 4\,kT\,G$ at the resistor is converted using $u^2 = |Z|^2\, i^2$ to $W_u = 4\,kT\,R/[1 + (\omega\, R\, C)^2]$.

J.3.2 1/f Noise

For many processes a frequency dependent noise spectral power following a ν^{α}-law is found with α close to -1. 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 [1853, 1854]. As an example the noise spectrum of a RuO_2 thick film resistor is depicted in Fig. J.1a; 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. J.1b 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 3×10^{-6} Hz [1855].

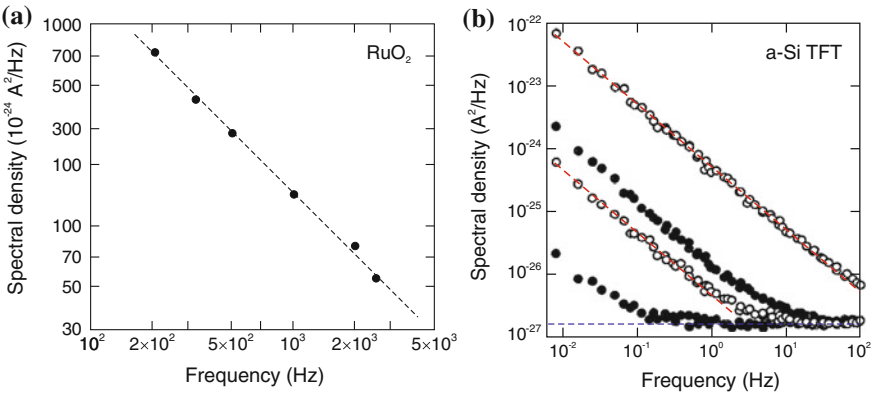

Fig. J.1 (**a**) Noise current density spectrum of a ruthenium oxide resistor (at $T = 300$ K and current of $I = 1$ mA), experimental data (*symbols*) and $1/f$-dependency (*dashed line*). Adapted from [1856]. (**b**) Noise current density spectrum of an amorphous silicon thin film transistor, experimental data (*symbols*) for various source-drain voltages, thermal noise (*horizontal blue dashed line*) and $1/f$-dependency (*red dashed lines*). Adapted from [1857]

J.3.3 Shot Noise

A dc current $\langle i \rangle = I_0$ through a resistor is a sequence of electron transfers from one contact to the other. The transit time $t_{\rm tr}$ is given by the length L and the drift velocity $v_{\rm D}$ as $t_{\rm tr} = L/v_{\rm D} = L^2/(\mu\, V)$. 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 ($f \ll t_{\rm tr}^{-1}$), the noise power is

$$W = 2\, e\, I_0, \tag{J.27}$$

and the current noise thus is given by

$$\langle i^2 \rangle = 2\, e\, I_0\, B, \tag{J.28}$$

This noise term has been first found for vacuum diodes in the saturation regime which also serve as noise normals according to (J.28). It is important for the validity of (J.28) 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 (J.28).

The maximal noise level (J.28) 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 [1858] and in the limit of large

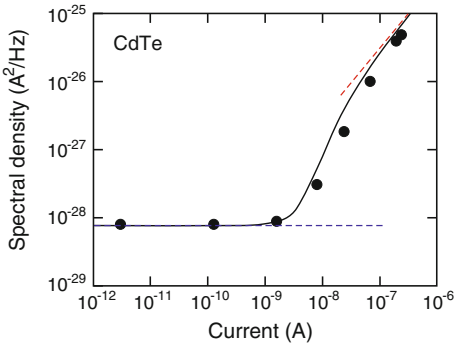

Fig. J.2 Noise of semi-insulating (dark) CdTe detector at $T = 323\,\mathrm{K}$ (at a frequency of about 1–2 kHz when $1/f$-noise plays no role). Experimental data (*symbols*) and detailed theory (*black line*). The *dashed blue line* represents the thermal noise (J.25), the *dashed red line* the shot noise (J.28). Adapted from [1859]

currents for CdTe detectors [1859] (Fig. J.2). 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 [1860]. The modification in non-degenerate semiconductors on length scales intermediate between the elastic and inelastic mean free paths is discussed in [1861]. The case of shot noise in semiconductors in the presence of transport of electrons and holes has been treated in [1858–1862].

J.3.4 Generation-Recombination Noise

It is a semiconductor specific property that the carrier density is subject to fluctuations due to generation and recombination.[12] 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 [1863, 1864].

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 $T = 78\,\mathrm{K}$ (Fig. J.3a) with the plateau at 10^6–$10^7\,\mathrm{Hz}$ on top of the $1/f$ noise [1865] (The plateau at 10^8–$10^9\,\mathrm{Hz}$ is due to velocity fluctuations). The spectral power of the generation-recombination noise contribution is given by

$$W = I_0^2 \, \frac{\langle \delta n^2 \rangle}{\langle n \rangle^2} \, \frac{4\,\tau_0}{1 + (\omega\,\tau_0)^2}, \tag{J.29}$$

[12] A metal exhibits a constant carrier density.

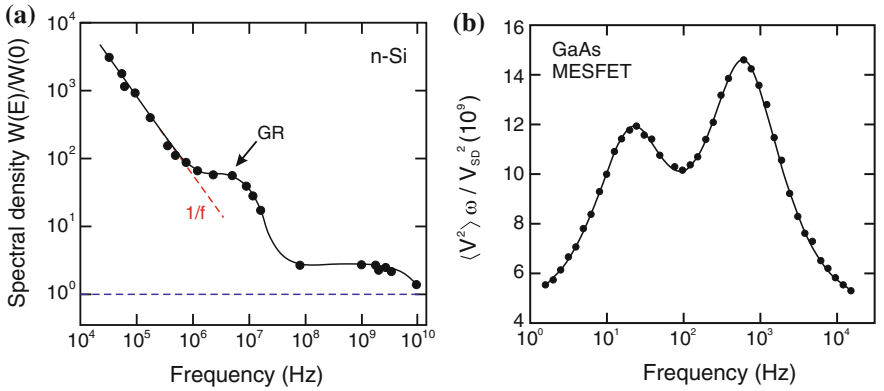

Fig. J.3 (**a**) Current noise spectrum of n-type Si ($T = 78\,\mathrm{K}$, $n = 3 \times 10^{13}\,\mathrm{cm}^{-3}$) for an electric field of $E = 200\,\mathrm{V/cm}$ along the $\langle 100 \rangle$ direction, in relative units to the noise spectrum for $E = 0$. The *dashed blue line* indicates the level of thermal noise, The *arrow* labeled 'GR' denotes the contribution of generation-recombination noise. Adapted from [1865]. (**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 (J.29) (times ω) for two different traps. Adapted from [1866]

where τ_0 is the characteristic relaxation time, $\langle n \rangle = \bar{n}$ is the average carrier density (average carrier number per given volume) and $\langle \delta n^2 \rangle = \langle (n - \bar{n})^2 \rangle$ 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 $W \times \omega$ can be plotted (Fig. J.3b) which takes the shape of a peak (for logarithmic frequency axis) [1866].

For a partially compensated semiconductor with $N_\mathrm{D} > N_\mathrm{A}$ it is found (if holes can be neglected) [1864]

$$\frac{\langle \delta n^2 \rangle}{\langle n \rangle} = \left[1 + \frac{\bar{n}\, N_\mathrm{D}}{(\bar{n} + N_\mathrm{A})\,(N_\mathrm{D} - N_\mathrm{A} - \bar{n})} \right]^{-1} \leq 1. \tag{J.30}$$

The fluctuation $\langle \delta n^2 \rangle / \langle n \rangle^2$ is typically smaller than the Poisson value of 1; such sub-Poissonian statistics is typical of a repulsive correlation. For the case $N_\mathrm{D} \gg N_\mathrm{A}$ [1864], (J.30) simplifies to

$$\frac{\langle \delta n^2 \rangle}{\langle n \rangle^2} = \left[1 + \frac{N_\mathrm{D}}{N_\mathrm{D} - \bar{n}} \right]^{-1} = \frac{N_\mathrm{D} - \bar{n}}{2\,N_\mathrm{D} - \bar{n}}. \tag{J.31}$$

In the ambipolar regime, typically close to intrinsic conditions, when only free electrons and holes are important, it is found [1864] ($\mu_\mathrm{n} < 0$)

$$\frac{\langle \delta n^2 \rangle}{\langle n \rangle^2} = \frac{\bar{n}^2\, \bar{p}\, (\mu_\mathrm{p} - \mu_\mathrm{n})^2}{(\bar{n} + \bar{p})\,(\bar{p}\,\mu_\mathrm{p} - \bar{n}\,\mu_\mathrm{n})^2}. \tag{J.32}$$

which simplifies to

$$\frac{\langle \delta n^2 \rangle}{\langle n \rangle^2} = \frac{1}{2}. \tag{J.33}$$

in the intrinsic case ($\bar{n} = \bar{p}$).

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