

Chapter 2

The Boltzmann Transport Equation and Its Projection onto Spherical Harmonics

In the framework of the semiclassical transport theory, the BTE governs the spatiotemporal evolution of the particle gas. In this chapter, the BTE in the three-dimensional wave vector space is introduced in Sect. 2.1. The PE is required for the calculation of the electric field, which enters the BTE. If only one carrier type is simulated, a drift-diffusion model is solved for the other type. The PE and drift-diffusion model are discussed in Sect. 2.2. In Sect. 2.3, basic properties of the spherical harmonics are reviewed. A generalized coordinate transform from the wavevector space to the energy space is introduced, and some important relations between transport coefficients in the energy space are explicitly derived. The spherical harmonics expansion of the BTE is shown in Sect. 2.5. Finally, noise analysis within the Langevin-Boltzmann framework is discussed in Sect. 2.6.

2.1 The Boltzmann Transport Equation

Our goal is to describe the particle kinetics based on a position-dependent band structure, which contains a few conduction (or valence) bands. However, the electronic band, which is defined in the first Brillouin zone following the reduced zone scheme [1], might not be necessarily suitable for a spherical harmonics expansion. For example, in the case of the first Si conduction band, the origin of the Brillouin zone (the Γ -point) does not coincide with the minimum of the energy.¹ Therefore, in this work, instead of the electronic bands themselves, a mathematical model called “valley” is regarded as the basis of the analysis. From its construction, the energy minimum of the valley is located at its origin in the wave vector space. The valleys are labeled with ν throughout part II. Of course, in order to obtain a meaningful physical description, a sound relationship between the original band

¹In the case of the Si valence bands, the minimum of the band energy is found at this point.

structure and the approximated valley model is required. Specific approaches to construct the band models based on the valley description are explained in Chap. 4. For the ν th valley, the relative energy at the position $\mathbf{r}$ in the real space and the wave vector $\mathbf{k}$, which is measured from the valley minimum energy, is described by the dispersion relation, $\varepsilon^\nu(\mathbf{r}, \mathbf{k})$. Since the band structure can depend on the real space, the dispersion relation of the valley also can be position dependent.

In the framework of the semiclassical transport theory, the position $\mathbf{r}$ in the real space and the momentum $\hbar\mathbf{k}$ ($\hbar$ denotes Planck's constant divided by 2π) of a particle can be measured simultaneously. Therefore, a state $(\mathbf{r}, \mathbf{k})$ in the six-dimensional phase space is required in order to specify the state of a particle. Ignoring many-particle effects except the electric field, screening and the Pauli exclusion principle, the particle ensemble can be completely characterized by the so-called one-particle one-time distribution function $f^\nu(\mathbf{r}, \mathbf{k}, t)$ for the ν th valley defined on the six-dimensional phase space [1]. The number of particles in an infinitesimal volume of the six-dimensional phase space ($d^3k d^3r$) at time t is given by

$$dN = \frac{2}{(2\pi)^3} f^\nu(\mathbf{r}, \mathbf{k}, t) d^3k d^3r, \quad (2.1)$$

where the prefactor $\frac{2}{(2\pi)^3}$ takes account of the spin degeneracy and the minimum phase space volume. The Pauli exclusion principle necessitates a distribution function smaller than one. Thus, the distribution function itself is the probability that the state $(\mathbf{r}, \mathbf{k})$ of the ν th valley is occupied [2].

A macroscopic quantity $x(\mathbf{r}, t)$ is an average of a microscopic quantity $X^\nu(\mathbf{r}, \mathbf{k})$ over the $\mathbf{k}$ space. It is an expectation of the form

$$x(\mathbf{r}, t) = \frac{2}{(2\pi)^3} \sum_\nu \int X^\nu(\mathbf{r}, \mathbf{k}) f^\nu(\mathbf{r}, \mathbf{k}, t) d^3k. \quad (2.2)$$

When the microscopic quantity is 1 ($X = 1$) and the valleys of the conduction bands (C) are considered, the corresponding macroscopic quantity is the electron density:

$$n(\mathbf{r}, t) = \frac{2}{(2\pi)^3} \sum_C \int f^C(\mathbf{r}, \mathbf{k}, t) d^3k, \quad (2.3)$$

whereas the hole density $p(\mathbf{r}, t)$ is obtained by summing over the valence band valleys (V):

$$p(\mathbf{r}, t) = \frac{2}{(2\pi)^3} \sum_V \int f^V(\mathbf{r}, \mathbf{k}, t) d^3k. \quad (2.4)$$

For the group velocity ($X = \mathbf{v}^\nu$), which is given by

$$\mathbf{v}^\nu(\mathbf{r}, \mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon^\nu(\mathbf{r}, \mathbf{k}), \quad (2.5)$$

the corresponding macroscopic quantity is the particle current density:

$$\mathbf{j}(\mathbf{r}, t) = \frac{2}{(2\pi)^3} \sum_{\nu} \int \mathbf{v}^{\nu}(\mathbf{r}, \mathbf{k}) f^{\nu}(\mathbf{r}, \mathbf{k}, t) d^3k. \quad (2.6)$$

Once the particle distribution function is known, any macroscopic quantity of interest can be calculated.

In the framework of the semiclassical transport theory, the spatiotemporal evolution of a particle gas is described by the BTE [1–4]

$$\frac{\partial f^{\nu}}{\partial t} + \frac{1}{\hbar} \mathbf{F}^{\nu} \cdot \nabla_{\mathbf{k}} f^{\nu} + \mathbf{v}^{\nu} \cdot \nabla_{\mathbf{r}} f^{\nu} = \hat{S}^{\nu}\{f\}, \quad (2.7)$$

where $\hat{S}^{\nu}\{f\}$ is the single-particle scattering integral including the Pauli exclusion principle

$$\begin{aligned} \hat{S}^{\nu}\{f\} = & \frac{\Omega_s}{(2\pi)^3} \sum_{\nu'} \int (1 - f^{\nu}(\mathbf{r}, \mathbf{k}, t)) S^{\nu, \nu'}(\mathbf{r}, \mathbf{k}|\mathbf{k}') f^{\nu'}(\mathbf{r}, \mathbf{k}', t) \\ & - (1 - f^{\nu'}(\mathbf{r}, \mathbf{k}', t)) S^{\nu', \nu}(\mathbf{r}, \mathbf{k}'|\mathbf{k}) f^{\nu}(\mathbf{r}, \mathbf{k}, t) d^3k'. \end{aligned} \quad (2.8)$$

Ω_s is the system volume and $S^{\nu, \nu'}(\mathbf{r}, \mathbf{k}|\mathbf{k}')$ the transition rate from the initial state $(\nu', \mathbf{k}')$ into the final $(\nu, \mathbf{k})$ [4]. Specific expressions for the transition rates of several scattering mechanisms are shown in Chap. 4. The total force $\mathbf{F}^{\nu}$ due to a gradient in the total energy and a magnetic field is given by

$$\mathbf{F}^{\nu}(\mathbf{r}, \mathbf{k}, t) = -\nabla_{\mathbf{r}}(\mp qV(\mathbf{r}, t) \pm E^{\nu}(\mathbf{r}) + \varepsilon^{\nu}(\mathbf{r}, \mathbf{k})) \mp q\mathbf{v}^{\nu}(\mathbf{r}, \mathbf{k}) \times \mathbf{B}, \quad (2.9)$$

where q is the positive electron charge, V the electrostatic potential, E the valley minimum in the electron picture, $\mathbf{B}$ the magnetic field, and the upper and lower signs are for electrons and holes, respectively. It is assumed that the magnetic field is time-independent and constant over the simulation domain. Components of the total force are denoted as

$$\mathbf{F}_{\text{E, pot}}^{\nu}(\mathbf{r}, t) = -\nabla_{\mathbf{r}}(\mp qV(\mathbf{r}, t) \pm E^{\nu}(\mathbf{r})), \quad (2.10)$$

$$\tilde{\mathbf{F}}_{\text{E}}^{\nu}(\mathbf{r}, \mathbf{k}) = -\nabla_{\mathbf{r}}\varepsilon^{\nu}(\mathbf{r}, \mathbf{k}), \quad (2.11)$$

$$\mathbf{F}_{\text{E}}^{\nu}(\mathbf{r}, \mathbf{k}, t) = \mathbf{F}_{\text{E, pot}}^{\nu}(\mathbf{r}, t) + \tilde{\mathbf{F}}_{\text{E}}^{\nu}(\mathbf{r}, \mathbf{k}), \quad (2.12)$$

$$\mathbf{F}_{\text{B}}^{\nu}(\mathbf{r}, \mathbf{k}) = \mp q\mathbf{v}^{\nu}(\mathbf{r}, \mathbf{k}) \times \mathbf{B}. \quad (2.13)$$

Note that when the band structure does not depend on the position, $\tilde{\mathbf{F}}_{\text{E}}^{\nu}$ vanishes. A useful relation is shown here for later use ($\nabla_{\mathbf{k}} \cdot (\mathbf{v}^{\nu} \times \mathbf{B}) = (\nabla_{\mathbf{k}} \times \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon^{\nu}) \cdot \mathbf{B} = 0$)

$$\frac{1}{\hbar} \nabla_{\mathbf{k}} \cdot \mathbf{F}^{\nu} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \cdot \mathbf{F}_{\text{E}}^{\nu} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \cdot \tilde{\mathbf{F}}_{\text{E}}^{\nu} = -\nabla_{\mathbf{r}} \cdot \mathbf{v}^{\nu}. \quad (2.14)$$

For device simulations, suitable boundary conditions at the device boundaries are required. The Neumann boundary condition is imposed on a non-contact boundary. For a contact boundary, instead of the Dirichlet boundary condition we use Neumann boundary conditions together with an interface generation rate [5, 6]

$$\gamma_s^v(\mathbf{r}, \mathbf{k}) = [f^{\text{eq}}(\mathbf{r}, \mathbf{k})\Theta(\mathbf{v}^v \cdot \mathbf{n}) + f^v(\mathbf{r}, \mathbf{k})\Theta(-\mathbf{v}^v \cdot \mathbf{n})]\mathbf{v}^v \cdot \mathbf{n}, \quad (2.15)$$

where $\mathbf{n}$ is a surface vector pointing into the device, $\Theta(x)$ the step function, and f^{eq} the equilibrium distribution specified by the particle quasi-Fermi level of the contact. When the Pauli principle is considered in the simulation, f^{eq} is given by the Fermi-Dirac distribution, otherwise by the Maxwell-Boltzmann distribution. This boundary condition corresponds to a thermal bath contact similar to the ones used in Monte Carlo simulations [7]. The injected particle flux (the first term on the RHS) is the result of an equilibrium distribution enforced by the externally applied bias, whereas the extracted particle flux (the second term) is due to the distribution within the device.

2.2 Poisson Equation and Drift-Diffusion Model

Since the driving force for particles is a function of the electrostatic potential, which is again a function of the particle density, it should be calculated in a self-consistent manner. The electrostatic potential $V(\mathbf{r}, t)$ is the solution of the Poisson equation

$$\nabla_{\mathbf{r}} \cdot (\kappa(\mathbf{r})\nabla_{\mathbf{r}}V(\mathbf{r}, t)) = -q(N_D(\mathbf{r}) - N_A(\mathbf{r}) - n(\mathbf{r}, t) + p(\mathbf{r}, t)), \quad (2.16)$$

where κ is the dielectric constant, N_A and N_D are the acceptor and donor concentrations, respectively.

The electron density $n(\mathbf{r}, t)$ and the hole density $p(\mathbf{r}, t)$ are given by (2.3) and (2.4), respectively, if the BTE is solved for the respective particle type. In many applications, only one type of particles (either electrons or holes) is treated with the BTE. In such situations, the macroscopic carrier density of the other type of particles is directly calculated based on the drift-diffusion model, where the mobility does not depend on the driving force and is calculated at equilibrium [8].

For both, the Poisson equation and the drift-diffusion model the Neumann boundary condition is imposed on a non-contact boundary and the Dirichlet boundary condition on a contact boundary.

2.3 Basic Properties of Spherical Harmonics

Since the phase space has six dimensions, it is very inconvenient to discretize it in a straightforward manner with finite differences [9]. While it is possible to reduce the number of dimensions in the real space by assuming translational symmetry in

one of more dimensions, this is not possible in the $\mathbf{k}$ space. Instead of using finite differences in conjunction with cartesian coordinates, spherical coordinates are used and the dependence on the two angles is expanded with spherical harmonics. The expansion is truncated at a maximum order leading to a finite number of unknowns for the angular dependence. In the case that the SHE converges rapidly, this leads to a considerable lower number of unknowns than a finite difference approach. In this section, some useful properties of the spherical harmonics are briefly discussed and the SHE is introduced.

The spherical harmonics can be defined as either complex-valued or real-valued functions. Since the complex computation produces a lot of overhead real spherical harmonics will be used in this work

$$Y_{l,m}(\vartheta, \varphi) = \begin{cases} c_{l,m} P_l^m(\cos \vartheta) \cos(m\varphi) & \text{for } m \geq 0 \\ c_{l,m} P_l^{|m|}(\cos \vartheta) \sin(|m|\varphi) & \text{for } m < 0 \end{cases}, \quad (2.17)$$

where ϑ and φ are angles in the spherical coordinate system. The indices l and m determine the order and the sub-order of the spherical harmonics² and they have the following range:

$$l \geq 0, \quad (2.18)$$

$$-l \leq m \leq l. \quad (2.19)$$

The normalization factor $c_{l,m}$ is given as:

$$c_{l,m} = \begin{cases} \sqrt{\frac{(2l+1)}{4\pi}} & \text{for } m = 0 \\ \sqrt{\frac{(2l+1)(l-|m|)!}{2\pi(l+|m|)!}} & \text{for } m \neq 0 \end{cases}. \quad (2.20)$$

$P_l^m(x)$ is the associated Legendre polynomial

$$P_l^m(x) = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} P_l(x), \quad (2.21)$$

where $P_l(x)$ is the Legendre polynomial

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l. \quad (2.22)$$

The spherical harmonics up to the first order are

$$Y_{0,0}(\vartheta, \varphi) = \frac{1}{\sqrt{4\pi}}, \quad (2.23)$$

²In the literature, the order l and the sub-order m are usually called the degree l and the order m , respectively.

$$Y_{1,-1}(\vartheta, \varphi) = \sqrt{\frac{3}{4\pi}} \sin \vartheta \sin \varphi, \quad (2.24)$$

$$Y_{1,0}(\vartheta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos \vartheta, \quad (2.25)$$

$$Y_{1,1}(\vartheta, \varphi) = \sqrt{\frac{3}{4\pi}} \sin \vartheta \cos \varphi. \quad (2.26)$$

A quantity $X(\vartheta, \varphi)$ can be expanded with spherical harmonics by

$$X_{l,m} = \oint X(\vartheta, \varphi) Y_{l,m}(\vartheta, \varphi) d\Omega, \quad (2.27)$$

where Ω is the solid angle, $d\Omega = \sin \vartheta d\vartheta d\varphi$ and the integral extends over the whole unit sphere. The original form is recovered by

$$X(\vartheta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l X_{l,m} Y_{l,m}(\vartheta, \varphi). \quad (2.28)$$

The sums are often abbreviated by $\sum_{l,m} = \sum_{l=0}^{\infty} \sum_{m=-l}^l$.

The product of two spherical harmonics is normalized when integrated over the unit sphere

$$a_{l,m,l',m'} = \oint Y_{l,m}(\vartheta, \varphi) Y_{l',m'}(\vartheta, \varphi) d\Omega = \delta_{l,l'} \delta_{m,m'}, \quad (2.29)$$

The integral yields zero if the two spherical harmonics have different indices. In this sense the spherical harmonics are orthogonal and they form a complete set of basis functions. Other integrals related to a product of two spherical harmonics can be defined. Among many possible forms, only two frequently used quantities are shown here

$$\mathbf{a}_{l,m,l',m'} = \oint \mathbf{e}_\varepsilon Y_{l,m} Y_{l',m'} d\Omega \quad (2.30)$$

and

$$\mathbf{b}_{l,m,l',m'} = \oint \left(\mathbf{e}_\vartheta \frac{\partial Y_{l,m}}{\partial \vartheta} + \mathbf{e}_\varphi \frac{1}{\sin \vartheta} \frac{\partial Y_{l,m}}{\partial \varphi} \right) Y_{l',m'} d\Omega, \quad (2.31)$$

where $\mathbf{e}_\varepsilon$, $\mathbf{e}_\vartheta$ and $\mathbf{e}_\varphi$ are the unit vectors in the spherical coordinate system. Since $Y_{0,0}$ is constant over the solid angle, $\mathbf{b}_{l,m,l',m'}$ vanishes when the first index pair is $(0,0)$,

$$\mathbf{b}_{0,0,l',m'} = 0. \quad (2.32)$$

In the derivation and the implementation of the balance equations obtained from the projection of the BTE, products of three spherical harmonics are frequently used. They can be defined as direct extensions of the double products.

A scalar triple product $a_{l,m,l',m',l'',m''}$ is given by

$$a_{l,m,l',m',l'',m''} = \oint Y_{l,m}(\vartheta, \varphi) Y_{l',m'}(\vartheta, \varphi) Y_{l'',m''}(\vartheta, \varphi) d\Omega. \quad (2.33)$$

From its definition, $a_{l,m,l',m',l'',m''}$ is invariant under the six permutations of the three index pairs

$$\begin{aligned} a_{l,m,l',m',l'',m''} &= a_{l'',m'',l,m,l',m'} = a_{l',m',l'',m'',l,m} \\ &= a_{l,m,l'',m'',l',m'} = a_{l',m',l,m,l'',m''} = a_{l'',m'',l',m',l,m}. \end{aligned} \quad (2.34)$$

The vector triple product $\mathbf{a}_{l,m,l',m',l'',m''}$ is given by

$$\mathbf{a}_{l,m,l',m',l'',m''} = \oint \mathbf{e}_\varepsilon Y_{l,m} Y_{l',m'} Y_{l'',m''} d\Omega. \quad (2.35)$$

It is also invariant under six permutations of index pairs.

The vector triple product $\mathbf{b}_{l,m,l',m',l'',m''}$ is defined as

$$\mathbf{b}_{l,m,l',m',l'',m''} = \oint \left(\mathbf{e}_\vartheta \frac{\partial Y_{l,m}}{\partial \vartheta} + \mathbf{e}_\varphi \frac{1}{\sin \vartheta} \frac{\partial Y_{l,m}}{\partial \varphi} \right) Y_{l',m'} Y_{l'',m''} d\Omega. \quad (2.36)$$

Due to its definition, $\mathbf{b}_{l,m,l',m',l'',m''}$ is invariant only under two permutations of the index pairs

$$\mathbf{b}_{l,m,l',m',l'',m''} = \mathbf{b}_{l,m,l'',m'',l',m'}. \quad (2.37)$$

Since $Y_{0,0}$ is constant over the solid angle, $\mathbf{b}_{l,m,l',m',l'',m''}$ vanishes, when the first index pair is (0,0),

$$\mathbf{b}_{0,0,l',m',l'',m''} = 0. \quad (2.38)$$

All three triple products defined above reduce to the corresponding double products, when the second (or third) index pair is (0,0),

$$a_{l,m,l',m',0,0} = Y_{0,0} a_{l,m,l',m'} = \frac{1}{\sqrt{4\pi}} \delta_{l,l'} \delta_{m,m'}, \quad (2.39)$$

$$\mathbf{a}_{l,m,l',m',0,0} = Y_{0,0} \mathbf{a}_{l,m,l',m'}, \quad (2.40)$$

$$\mathbf{b}_{l,m,l',m',0,0} = Y_{0,0} \mathbf{b}_{l,m,l',m'}. \quad (2.41)$$

The following relation holds for an arbitrary analytic function $X(\vartheta, \varphi)$ defined on the solid angle,

$$\oint \left[\mathbf{e}_\varepsilon 2 - \mathbf{e}_\vartheta \frac{\partial}{\partial \vartheta} - \mathbf{e}_\varphi \frac{1}{\sin \vartheta} \frac{\partial}{\partial \varphi} \right] X(\vartheta, \varphi) d\Omega = 0. \quad (2.42)$$

This relation can be checked by inserting the following two equations into the original one:

$$\frac{\partial}{\partial \vartheta} \mathbf{e}_\vartheta = -\mathbf{e}_\varepsilon \quad (2.43)$$

and

$$\frac{\partial}{\partial \varphi} \mathbf{e}_\varphi = -\cos \vartheta \mathbf{e}_\vartheta - \sin \vartheta \mathbf{e}_\varepsilon. \quad (2.44)$$

This relation is quite useful to derive a relation between the two vector products, $\mathbf{a}$ and $\mathbf{b}$. By inserting $Y_{l,m}Y_{l',m'}$ or $Y_{l,m}Y_{l',m'}Y_{l'',m''}$ as $X(\vartheta, \varphi)$, it is found that

$$2\mathbf{a}_{l,m,l',m'} = \mathbf{b}_{l,m,l',m'} + \mathbf{b}_{l',m',l,m}, \quad (2.45)$$

$$2\mathbf{a}_{l,m,l',m',l'',m''} = \mathbf{b}_{l,m,l',m',l'',m''} + \mathbf{b}_{l',m',l,m,l'',m''} + \mathbf{b}_{l'',m'',l,m,l',m'}. \quad (2.46)$$

A spherical harmonic $Y_{l,m}(\vartheta, \varphi)$ has the following property

$$Y_{l,m}(\pi - \vartheta, \pi + \varphi) = (-1)^l Y_{l,m}(\vartheta, \varphi). \quad (2.47)$$

Therefore, spherical harmonics with even l 's are inversion-symmetric, while spherical harmonics with odd l 's are anti-symmetric w.r.t. inversion. In this work, we explicitly assume that the dispersion relation of the band structure is inversion-symmetric. Therefore, only the expansion coefficients with even order do not vanish. On the other hand, the group velocity of such a band structure has non-vanishing coefficients only for odd l 's.

Sometimes the spherical coordinate system for the band structure and the one for the device can be different. In order to minimize the number of the nonzero terms used for describing the band structure, each valley is usually described in its internal coordinate system [6]. However, in a simulation a global device coordinate system is used, which is shared by all valleys. Note that the device coordinate system can change according to the purpose of the simulation. For this, an algorithm for rotating the spherical harmonics with arbitrary Euler angles [10] is implemented. Up to the first (or second) order, an analytical expression can be easily used. However, since we are dealing with spherical harmonics of arbitrary order, a general scheme for the rotation is required. Rotation of spherical harmonics is performed using the ‘‘Wigner matrices’’ relative to the chosen spherical harmonics basis. Invariance of the l th spherical harmonics subspace holds. A spherical harmonic keeps its l value after the rotation. For a given l , the Wigner matrix is a $(2l + 1) \times (2l + 1)$ orthogonal matrix, which relates the spherical harmonics of order l ,

$$R \cdot Y_{l,m} = \sum_n D_{n,m}^l(R) Y_{l,n}, \quad (2.48)$$

where $R \cdot Y_{l,m}$ is the rotated spherical harmonic. Let an arbitrary function x have the spherical harmonics coefficients $x_{l,m}$, then, if $R \cdot x$ has spherical harmonics coefficients denoted as $x'_{l,m}$, the Wigner matrix connects the two coefficients via

$$x'_{l,m} = \sum_{n=-l}^l D_{m,n}^l(R) x_{l,n}. \quad (2.49)$$

Using the rotation from the global device coordinate system to the internal coordinate system, quantities calculated in the internal coordinate system can be written in the global device coordinate system.

2.4 Coordinate Transform

The particle distribution function is expanded with spherical harmonics. Before the dependence of the distribution function on the angles ϑ and φ can be expanded with spherical harmonics, it has to be decided whether the distribution function is expanded for constant energy or constant modulus of the wave vector. An expansion of the distribution function on equienergy surfaces has many advantages over an expansion w.r.t. to the modulus of the wave vector. For example, at equilibrium the distribution function is isotropic on equienergy surfaces. In many scattering models the scattering rate is a function of energy and the energy transfer during scattering is constant. Thus, the scattering integral can be easily formulated on equienergy surfaces. In addition, if a magnetic force is included in the BTE, this formulation ensures that the magnetic force term conserves energy.

In order to expand the distribution function on an equienergy surface, a coordinate transformation is required. For example, in [11], a coordinate transformation, in which the angle variables are the same as in the original $\mathbf{k}$ space, has been proposed. In this work, a generalized coordinate transform which does not necessarily preserve the angle variables is introduced. This allows us more freedom to choose the coordinate transformation. Also from this study, some relations between coefficients, which are important not only for deriving the balance equations but also for the stabilization scheme, can be obtained in a natural way. The scheme keeping the angle variables [11] is easily obtained as a special case of this generalized transformation.

Due to the position dependent band structure considered in this work, the partial derivative w.r.t. the real space is also effected by the coordinate transformation. In order to avoid confusion, subscripts $\mathbf{k}$ and ε are used for denoting the real space variables in the original space and the transformed space, respectively. All equations shown in Sect. 2.1 should be interpreted in the original space. The following mapping of the original space $(x_{\mathbf{k}}, y_{\mathbf{k}}, z_{\mathbf{k}}, k_x, k_y, k_z)$ onto the transformed space $(x_{\varepsilon}, y_{\varepsilon}, z_{\varepsilon}, \varepsilon, \vartheta, \varphi)$ is used

$$x_{\varepsilon} = x_{\mathbf{k}}, \quad (2.50)$$

$$y_{\varepsilon} = y_{\mathbf{k}}, \quad (2.51)$$

$$z_{\varepsilon} = z_{\mathbf{k}}, \quad (2.52)$$

$$\varepsilon = \varepsilon^{\nu}(\mathbf{r}_{\mathbf{k}}, \mathbf{k}), \quad (2.53)$$

$$\vartheta = \vartheta^{\nu}(\mathbf{r}_{\mathbf{k}}, \mathbf{k}), \quad (2.54)$$

$$\varphi = \varphi^{\nu}(\mathbf{r}_{\mathbf{k}}, \mathbf{k}), \quad (2.55)$$

where $\varepsilon^{\nu}(\mathbf{r}_{\mathbf{k}}, \mathbf{k})$ is the dispersion relation for the ν th valley, and the appropriate choice of $\vartheta^{\nu}(\mathbf{r}_{\mathbf{k}}, \mathbf{k})$ and $\varphi^{\nu}(\mathbf{r}_{\mathbf{k}}, \mathbf{k})$ depends on the underlying band structure. Note that they can be dependent on the real space up to this point. In the following section (Sect. 2.5), it is found that a simple form of balance equations can be obtained when ϑ^{ν} and φ^{ν} do not depend on the real space. We assume that the Jacobian determinant of the transform is nonzero. The angle-preserving transform [11] can be obtained trivially by setting ϑ and φ as follows:

$$\cos \vartheta = \frac{k_z}{k}, \quad (2.56)$$

$$\sin \vartheta \cos \varphi = \frac{k_x}{k}, \quad (2.57)$$

$$\sin \vartheta \sin \varphi = \frac{k_y}{k}, \quad (2.58)$$

where the zenith direction is aligned with the z -axis.

The del operator in the wave vector space is given by

$$\nabla_{\mathbf{k}} = \hbar \mathbf{v}^{\nu} \frac{\partial}{\partial \varepsilon} + (\nabla_{\mathbf{k}} \vartheta^{\nu}) \frac{\partial}{\partial \vartheta} + (\nabla_{\mathbf{k}} \varphi^{\nu}) \frac{\partial}{\partial \varphi}, \quad (2.59)$$

where $\mathbf{v}^{\nu}$, $\nabla_{\mathbf{k}} \vartheta^{\nu}$, and $\nabla_{\mathbf{k}} \varphi^{\nu}$ are calculated in the original space. Also the del operator in the real space is given by

$$\nabla_{\mathbf{r}_{\mathbf{k}}} = \nabla_{\mathbf{r}_{\varepsilon}} + (\nabla_{\mathbf{r}_{\mathbf{k}}} \varepsilon^{\nu}) \frac{\partial}{\partial \varepsilon} + (\nabla_{\mathbf{r}_{\mathbf{k}}} \vartheta^{\nu}) \frac{\partial}{\partial \vartheta} + (\nabla_{\mathbf{r}_{\mathbf{k}}} \varphi^{\nu}) \frac{\partial}{\partial \varphi}. \quad (2.60)$$

Note that the last three terms originate from the position dependent band structure.

The infinitesimal volume in the original $\mathbf{k}$ space is given by

$$d^3k = |\det(\hat{\mathbf{J}}^{-1})| d\varepsilon d\vartheta d\varphi, \quad (2.61)$$

where the Jacobian matrix of the transform $\hat{\mathbf{J}}$ is³

³Since the coordinate transform is applied to the six-dimensional phase space, this is only a part of the total Jacobian matrix, corresponding to the $\mathbf{k}$ space. Because the transform for the real space is just an identity transform, the entire 6×6 Jacobian matrix can be inverted blockwise.

$$\hat{\mathbf{J}} = \begin{pmatrix} \frac{\partial \varepsilon^\nu}{\partial k_x} & \frac{\partial \varepsilon^\nu}{\partial k_y} & \frac{\partial \varepsilon^\nu}{\partial k_z} \\ \frac{\partial \vartheta^\nu}{\partial k_x} & \frac{\partial \vartheta^\nu}{\partial k_y} & \frac{\partial \vartheta^\nu}{\partial k_z} \\ \frac{\partial \varphi^\nu}{\partial k_x} & \frac{\partial \varphi^\nu}{\partial k_y} & \frac{\partial \varphi^\nu}{\partial k_z} \end{pmatrix} = \begin{pmatrix} \nabla_{\mathbf{k}} \varepsilon^\nu \\ \nabla_{\mathbf{k}} \vartheta^\nu \\ \nabla_{\mathbf{k}} \varphi^\nu \end{pmatrix}, \quad (2.62)$$

where the gradients on the RHS should be understood as row vectors. Since we are working in the energy space $(\varepsilon, \vartheta, \varphi)$, it is useful to explicitly express it in terms of the Jacobian matrix of the inverse transform,

$$\hat{\mathbf{J}} = (\hat{\mathbf{J}}^{-1})^{-1} = \begin{pmatrix} \frac{\partial k_x^\nu}{\partial \varepsilon} & \frac{\partial k_x^\nu}{\partial \vartheta} & \frac{\partial k_x^\nu}{\partial \varphi} \\ \frac{\partial k_y^\nu}{\partial \varepsilon} & \frac{\partial k_y^\nu}{\partial \vartheta} & \frac{\partial k_y^\nu}{\partial \varphi} \\ \frac{\partial k_z^\nu}{\partial \varepsilon} & \frac{\partial k_z^\nu}{\partial \vartheta} & \frac{\partial k_z^\nu}{\partial \varphi} \end{pmatrix}^{-1} = \frac{1}{\det(\hat{\mathbf{J}}^{-1})} \begin{pmatrix} \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \times \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \\ \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \times \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \\ \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \times \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \end{pmatrix}, \quad (2.63)$$

where the cross products in the RHS should be understood as row vectors. The Jacobian determinant $\det(\hat{\mathbf{J}}^{-1})$ is given by

$$\det(\hat{\mathbf{J}}^{-1}) = \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \cdot \left(\frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \times \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \right). \quad (2.64)$$

Therefore, we have the following relations:

$$\nabla_{\mathbf{k}} \varepsilon^\nu = \frac{1}{\det(\hat{\mathbf{J}}^{-1})} \left(\frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \times \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \right), \quad (2.65)$$

$$\nabla_{\mathbf{k}} \vartheta^\nu = \frac{1}{\det(\hat{\mathbf{J}}^{-1})} \left(\frac{\partial \mathbf{k}^\nu}{\partial \varphi} \times \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \right), \quad (2.66)$$

$$\nabla_{\mathbf{k}} \varphi^\nu = \frac{1}{\det(\hat{\mathbf{J}}^{-1})} \left(\frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \times \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \right). \quad (2.67)$$

A similar procedure can be applied to the partial derivative w.r.t. the real space. By inspecting the inverted total Jacobian matrix, the following relation can be found

$$\begin{pmatrix} \frac{\partial k_x^\nu}{\partial x_\varepsilon} & \frac{\partial k_x^\nu}{\partial y_\varepsilon} & \frac{\partial k_x^\nu}{\partial z_\varepsilon} \\ \frac{\partial k_y^\nu}{\partial x_\varepsilon} & \frac{\partial k_y^\nu}{\partial y_\varepsilon} & \frac{\partial k_y^\nu}{\partial z_\varepsilon} \\ \frac{\partial k_z^\nu}{\partial x_\varepsilon} & \frac{\partial k_z^\nu}{\partial y_\varepsilon} & \frac{\partial k_z^\nu}{\partial z_\varepsilon} \end{pmatrix} = -\hat{\mathbf{J}}^{-1} \begin{pmatrix} \frac{\partial \varepsilon^\nu}{\partial x_{\mathbf{k}}} & \frac{\partial \varepsilon^\nu}{\partial y_{\mathbf{k}}} & \frac{\partial \varepsilon^\nu}{\partial z_{\mathbf{k}}} \\ \frac{\partial \vartheta^\nu}{\partial x_{\mathbf{k}}} & \frac{\partial \vartheta^\nu}{\partial y_{\mathbf{k}}} & \frac{\partial \vartheta^\nu}{\partial z_{\mathbf{k}}} \\ \frac{\partial \varphi^\nu}{\partial x_{\mathbf{k}}} & \frac{\partial \varphi^\nu}{\partial y_{\mathbf{k}}} & \frac{\partial \varphi^\nu}{\partial z_{\mathbf{k}}} \end{pmatrix}. \quad (2.68)$$

It can be written in a component-wise fashion,

$$\frac{\partial k_{d_1}^\nu}{\partial d_\varepsilon} = - \sum_{\alpha=\varepsilon, \vartheta, \varphi} \frac{\partial k_{d_1}^\nu}{\partial \alpha} \frac{\partial \alpha^\nu}{\partial d_{\mathbf{k}}}, \quad (2.69)$$

where d and d_1 are arbitrary directions, which can be x, y, z , and α represents $\varepsilon, \vartheta, \varphi$. Multiplying $\hat{\mathbf{J}}$ and using (2.63), we obtain

$$\begin{pmatrix} \nabla_{\mathbf{r}_{\mathbf{k}}} \varepsilon^\nu \\ \nabla_{\mathbf{r}_{\mathbf{k}}} \vartheta^\nu \\ \nabla_{\mathbf{r}_{\mathbf{k}}} \varphi^\nu \end{pmatrix} = - \frac{1}{\det(\hat{\mathbf{J}}^{-1})} \begin{pmatrix} \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \times \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \\ \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \times \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \\ \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \times \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \end{pmatrix} \begin{pmatrix} \frac{\partial k_x^\nu}{\partial x_\varepsilon} \frac{\partial k_x^\nu}{\partial y_\varepsilon} \frac{\partial k_x^\nu}{\partial z_\varepsilon} \\ \frac{\partial k_y^\nu}{\partial x_\varepsilon} \frac{\partial k_y^\nu}{\partial y_\varepsilon} \frac{\partial k_y^\nu}{\partial z_\varepsilon} \\ \frac{\partial k_z^\nu}{\partial x_\varepsilon} \frac{\partial k_z^\nu}{\partial y_\varepsilon} \frac{\partial k_z^\nu}{\partial z_\varepsilon} \end{pmatrix}, \quad (2.70)$$

where the cross products and the gradients should be considered as row vectors. When an arbitrary direction d is considered, three relations are derived:

$$(\nabla_{\mathbf{r}_{\mathbf{k}}} \varepsilon^\nu) \cdot \mathbf{e}_d = - \frac{1}{\det(\hat{\mathbf{J}}^{-1})} \left(\frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \times \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \right) \cdot \frac{\partial \mathbf{k}^\nu}{\partial d_\varepsilon}, \quad (2.71)$$

$$(\nabla_{\mathbf{r}_{\mathbf{k}}} \vartheta^\nu) \cdot \mathbf{e}_d = - \frac{1}{\det(\hat{\mathbf{J}}^{-1})} \left(\frac{\partial \mathbf{k}^\nu}{\partial \varphi} \times \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \right) \cdot \frac{\partial \mathbf{k}^\nu}{\partial d_\varepsilon}, \quad (2.72)$$

$$(\nabla_{\mathbf{r}_{\mathbf{k}}} \varphi^\nu) \cdot \mathbf{e}_d = - \frac{1}{\det(\hat{\mathbf{J}}^{-1})} \left(\frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \times \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \right) \cdot \frac{\partial \mathbf{k}^\nu}{\partial d_\varepsilon}, \quad (2.73)$$

where $\mathbf{e}_d$ is the d -directional unit vector.

The generalized density-of-states for a single spin direction [11]⁴ is defined as

$$Z^\nu(\mathbf{r}, \varepsilon, \vartheta, \varphi) = \frac{1}{(2\pi)^3} |\det(\hat{\mathbf{J}}^{-1})| \frac{1}{\sin \vartheta}, \quad (2.74)$$

in order for the following conventional relation to hold

$$\frac{1}{(2\pi)^3} d^3 k = Z^\nu d\varepsilon d\Omega. \quad (2.75)$$

The Jacobian determinant of the inverse transform $\det(\hat{\mathbf{J}}^{-1})$ in the above equations can be eliminated by multiplying a gradient ((2.65), (2.66), or (2.67)) and the DOS:

⁴This definition does not include the integration over the solid angle. The generalized DOS is therefore for the case that it does not depend on the angles by a factor of 4π smaller than the conventional expression.

$$(\nabla_{\mathbf{k}} \varepsilon^\nu) Z^\nu = \pm \left(\frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \times \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \right) \frac{1}{(2\pi)^3} \frac{1}{\sin \vartheta}, \quad (2.76)$$

$$(\nabla_{\mathbf{k}} \vartheta^\nu) Z^\nu = \pm \left(\frac{\partial \mathbf{k}^\nu}{\partial \varphi} \times \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \right) \frac{1}{(2\pi)^3} \frac{1}{\sin \vartheta}, \quad (2.77)$$

$$(\nabla_{\mathbf{k}} \varphi^\nu) Z^\nu = \pm \left(\frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \times \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \right) \frac{1}{(2\pi)^3} \frac{1}{\sin \vartheta}, \quad (2.78)$$

where $\pm$ appears due to the sign of the Jacobian determinant.

There might be many possible relations between the quantities shown above. However, since the density-of-states Z^ν and the group velocity $\mathbf{v}^\nu$ are the most important transport coefficients, it is expected that partial derivatives of these quantities are relevant in the derivation of the balance equations. In the remaining part of this section, only three relations will be explicitly derived, because they play important roles in the derivation of balance equations and their stabilization. The first one is related to the partial derivative w.r.t. the energy space, while the second and third ones are related to the partial derivative w.r.t. the real space. Note that the second and third ones originate from the position-dependent band structure. Therefore, in the case of a position-independent one they vanish completely.

Since the second partial derivative does not depend on the order, in which the two derivatives are taken, the following relation results

$$\frac{\partial}{\partial \varepsilon} \left(\frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \times \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \right) + \frac{\partial}{\partial \vartheta} \left(\frac{\partial \mathbf{k}^\nu}{\partial \varphi} \times \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \right) + \frac{\partial}{\partial \varphi} \left(\frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \times \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \right) = 0. \quad (2.79)$$

As an immediate result, we obtain the first relation

$$\frac{\partial}{\partial \varepsilon} (\mathbf{v}^\nu Z^\nu \sin \vartheta) + \frac{\partial}{\partial \vartheta} \left((\nabla_{\mathbf{k}} \vartheta^\nu) \frac{Z^\nu}{\hbar} \sin \vartheta \right) + \frac{\partial}{\partial \varphi} \left((\nabla_{\mathbf{k}} \varphi^\nu) \frac{Z^\nu}{\hbar} \sin \vartheta \right) = 0. \quad (2.80)$$

Expansion of the above relation with a spherical harmonic $Y_{l,m}(\vartheta, \varphi)$ yields

$$\frac{\partial}{\partial \varepsilon} \oint \mathbf{v}^\nu Z^\nu Y_{l,m} d\Omega = \oint (\nabla_{\mathbf{k}} \vartheta^\nu) \frac{Z^\nu}{\hbar} \frac{\partial Y_{l,m}}{\partial \vartheta} d\Omega + \oint (\nabla_{\mathbf{k}} \varphi^\nu) \frac{Z^\nu}{\hbar} \frac{\partial Y_{l,m}}{\partial \varphi} d\Omega, \quad (2.81)$$

which is a generalized form of a previous result [5]. In the following, this is explicitly shown.

When the angle variables are kept the same in both spaces, the gradients of the two angle variables are given by

$$\nabla_{\mathbf{k}} \vartheta^\nu = \mathbf{e}_\vartheta \frac{1}{k^\nu}, \quad (2.82)$$

$$\nabla_{\mathbf{k}} \varphi^\nu = \mathbf{e}_\varphi \frac{1}{k^\nu \sin \vartheta}, \quad (2.83)$$

which yields

$$\frac{\partial}{\partial \varepsilon} \oint \mathbf{v}^\nu Z^\nu Y_{l,m} d\Omega = \oint \frac{Z^\nu}{\hbar k^\nu} \left(\mathbf{e}_\vartheta \frac{\partial Y_{l,m}}{\partial \vartheta} + \mathbf{e}_\varphi \frac{1}{\sin \vartheta} \frac{\partial Y_{l,m}}{\partial \varphi} \right) d\Omega. \quad (2.84)$$

Expansion of $\mathbf{v}Z$ and $Z/\hbar k$ with a spherical harmonic $Y_{l',m'}(\vartheta, \varphi)$ by (2.27) [11]

$$\mathbf{v}^\nu Z^\nu = \sum_{l',m'} \{ \mathbf{v}Z \}_{l',m'}^\nu Y_{l',m'}, \quad (2.85)$$

$$\frac{Z^\nu}{\hbar k^\nu} = \sum_{l',m'} \left\{ \frac{Z}{\hbar k} \right\}_{l',m'}^\nu Y_{l',m'}, \quad (2.86)$$

yields

$$\frac{\partial}{\partial \varepsilon} \{ \mathbf{v}Z \}_{l,m}^\nu = \sum_{l',m'} \left\{ \frac{Z}{\hbar k} \right\}_{l',m'}^\nu \mathbf{b}_{l,m,l',m'}, \quad (2.87)$$

where the orthonormality of spherical harmonics was used. Similarly, we can also show that

$$\sum_{l'',m''} \frac{\partial}{\partial \varepsilon} \{ \mathbf{v}Z \}_{l'',m''}^\nu a_{l,m,l',m',l'',m''} = \sum_{l'',m''} \left\{ \frac{Z}{\hbar k} \right\}_{l'',m''}^\nu (\mathbf{b}_{l,m,l',m',l'',m''} + \mathbf{b}_{l',m',l,m,l'',m''}). \quad (2.88)$$

If an isotropic band structure with only one valley is considered, further simplifications are possible. In this case the group velocity is aligned with the radial direction,

$$\mathbf{v}Z = \mathbf{e}_\varepsilon v(\varepsilon) Z(\varepsilon), \quad (2.89)$$

and Z and k do not depend on the angle variables,

$$\frac{Z}{\hbar k} = \frac{Z(\varepsilon)}{\hbar k(\varepsilon)}. \quad (2.90)$$

From these properties and (2.80), we obtain a relation between the magnitude of the group velocity and the DOS which does not involve any spherical harmonics [5]

$$\frac{\partial v(\varepsilon) Z(\varepsilon)}{\partial \varepsilon} = 2 \frac{Z(\varepsilon)}{\hbar k(\varepsilon)}. \quad (2.91)$$

The second relation involves a gradient of the DOS. The d -directional component of the gradient of $\det(\hat{\mathbf{J}}^{-1})$, which is taken in the transformed space, evaluates to

$$\frac{\partial}{\partial d_\varepsilon} \det(\hat{\mathbf{J}}^{-1}) = \frac{\partial^2 \mathbf{k}^\nu}{\partial \varepsilon \partial d_\varepsilon} \cdot \left(\frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \times \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \right)$$

$$\begin{aligned}
& + \frac{\partial^2 \mathbf{k}^\nu}{\partial \vartheta \partial d_\varepsilon} \cdot \left(\frac{\partial \mathbf{k}^\nu}{\partial \varphi} \times \frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \right) \\
& + \frac{\partial^2 \mathbf{k}^\nu}{\partial \varphi \partial d_\varepsilon} \cdot \left(\frac{\partial \mathbf{k}^\nu}{\partial \varepsilon} \times \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \right).
\end{aligned} \tag{2.92}$$

With (2.71)–(2.73) and (2.79) we obtain

$$\begin{aligned}
\frac{\partial}{\partial d_\varepsilon} \det(\hat{\mathbf{J}}^{-1}) &= -\frac{\partial}{\partial \varepsilon} \left[(\nabla_{\mathbf{r}_k} \varepsilon^\nu) \cdot \mathbf{e}_d \det(\hat{\mathbf{J}}^{-1}) \right] \\
&\quad - \frac{\partial}{\partial \vartheta} \left[(\nabla_{\mathbf{r}_k} \vartheta^\nu) \cdot \mathbf{e}_d \det(\hat{\mathbf{J}}^{-1}) \right] \\
&\quad - \frac{\partial}{\partial \varphi} \left[(\nabla_{\mathbf{r}_k} \varphi^\nu) \cdot \mathbf{e}_d \det(\hat{\mathbf{J}}^{-1}) \right],
\end{aligned} \tag{2.93}$$

which can be expressed as a gradient of the DOS (2.74)

$$\begin{aligned}
\nabla_{\mathbf{r}_\varepsilon} (Z^\nu \sin \vartheta) &+ \frac{\partial}{\partial \varepsilon} \left((\nabla_{\mathbf{r}_k} \varepsilon^\nu) Z^\nu \sin \vartheta \right) \\
&+ \frac{\partial}{\partial \vartheta} \left((\nabla_{\mathbf{r}_k} \vartheta^\nu) Z^\nu \sin \vartheta \right) + \frac{\partial}{\partial \varphi} \left((\nabla_{\mathbf{r}_k} \varphi^\nu) Z^\nu \sin \vartheta \right) = 0.
\end{aligned} \tag{2.94}$$

This is the second relation. When ϑ^ν and φ^ν are position-independent, the last two terms vanish and the term $\sin \vartheta$ can be removed.

The third relation is obtained by the following calculation. Using (2.69) and (2.79) and taking the gradient in the real space in the transformed energy space, we can find that

$$\begin{aligned}
\nabla_{\mathbf{r}_\varepsilon} \cdot \left(\frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \times \frac{\partial \mathbf{k}^\nu}{\partial \varphi} \right) &= \sum_\alpha \frac{\partial}{\partial \vartheta} \left((\nabla_{\mathbf{r}_k} \alpha^\nu) \cdot \left(\frac{\partial \mathbf{k}^\nu}{\partial \varphi} \times \frac{\partial \mathbf{k}^\nu}{\partial \alpha} \right) \right) \\
&\quad + \frac{\partial}{\partial \varphi} \left((\nabla_{\mathbf{r}_k} \alpha^\nu) \cdot \left(\frac{\partial \mathbf{k}^\nu}{\partial \alpha} \times \frac{\partial \mathbf{k}^\nu}{\partial \vartheta} \right) \right).
\end{aligned} \tag{2.95}$$

If ϑ^ν and φ^ν are position-independent, we obtain with (2.76)–(2.78)

$$\begin{aligned}
\nabla_{\mathbf{r}_\varepsilon} \cdot (\mathbf{v}^\nu Z^\nu \sin \vartheta) &= -\frac{\partial}{\partial \vartheta} \left(\tilde{\mathbf{F}}_E^\nu \cdot (\nabla_{\mathbf{k}} \vartheta^\nu) \frac{Z^\nu}{\hbar} \sin \vartheta \right) \\
&\quad - \frac{\partial}{\partial \varphi} \left(\tilde{\mathbf{F}}_E^\nu \cdot (\nabla_{\mathbf{k}} \varphi^\nu) \frac{Z^\nu}{\hbar} \sin \vartheta \right),
\end{aligned} \tag{2.96}$$

where the definition of $\tilde{\mathbf{F}}_E$ (2.11) was used. Expansion of this equation with spherical harmonics, multiplication with two more spherical harmonics and integration over the unit sphere yields

$$\begin{aligned}
\nabla_{\mathbf{r}_\varepsilon} \cdot \sum_{l'',m''} \{ \mathbf{v} Z \}_{l'',m''}^v a_{l,m,l',m',l'',m''} \\
= \sum_{l'',m''} \left\{ \tilde{\mathbf{F}}_E \frac{Z}{\hbar k} \right\}_{l'',m''}^v (\mathbf{b}_{l,m,l',m',l'',m''} + \mathbf{b}_{l',m',l,m,l'',m''}). \quad (2.97)
\end{aligned}$$

Thus, under the coordinate transformation defined by (2.50)–(2.55), three important relations between transport coefficients, (2.80), (2.94), and (2.96), hold.

2.5 Spherical Harmonics Expansion of the Boltzmann Transport Equation

In order to obtain a projection of the BTE, which conserves the particle number, the projection onto spherical harmonics (2.27) is modified and an additional projection onto energy is performed, where both projections can be combined by integration over the $\mathbf{k}$ space [11, 12]. This projection reads for a microscopic quantity $X^v(\mathbf{r}, \mathbf{k})$

$$\begin{aligned}
\{XZ\}_{l,m}^v(\mathbf{r}, \varepsilon) &= \frac{1}{(2\pi)^3} \int \delta[\varepsilon - \varepsilon^v(\mathbf{r}, \mathbf{k})] Y_{l,m}(\vartheta^v(\mathbf{r}, \mathbf{k}), \varphi^v(\mathbf{r}, \mathbf{k})) X^v(\mathbf{r}, \mathbf{k}) d^3k \\
&= \oint Y_{l,m}(\vartheta, \varphi) X^v(\mathbf{r}, \varepsilon, \vartheta, \varphi) Z^v(\mathbf{r}, \varepsilon, \vartheta, \varphi) d\Omega. \quad (2.98)
\end{aligned}$$

The multiplication with delta function leads to the projection onto energy. Thus, the microscopic quantity $X^v(\mathbf{r}, \varepsilon, \vartheta, \varphi)$ has to be multiplied with the DOS $Z^v(\mathbf{r}, \varepsilon, \vartheta, \varphi)$ (2.74) before projection onto spherical harmonics by (2.27).

For $X^v(\mathbf{r}, \mathbf{k}) = 1$, the projection of the DOS for the v th valley is obtained

$$Z_{l,m}^v(\mathbf{r}, \varepsilon) = \frac{1}{(2\pi)^3} \int \delta[\varepsilon - \varepsilon^v(\mathbf{r}, \mathbf{k})] Y_{l,m}(\vartheta^v(\mathbf{r}, \mathbf{k}), \varphi^v(\mathbf{r}, \mathbf{k})) d^3k. \quad (2.99)$$

The conventional DOS is given by

$$\frac{1}{(2\pi)^3} \int \delta[\varepsilon - \varepsilon^v(\mathbf{r}, \mathbf{k})] d^3k = \oint Z^v(\mathbf{r}, \varepsilon, \vartheta, \varphi) d\Omega = Z_{0,0}^v(\mathbf{r}, \varepsilon) \frac{1}{Y_{0,0}} \quad (2.100)$$

With (2.33) a DOS with two index pairs can be defined

$$Z_{l,m,l',m'}^v(\mathbf{r}, \varepsilon) = \sum_{l'',m''} Z_{l'',m''}^v(\mathbf{r}, \varepsilon) a_{l,m,l',m',l'',m''}. \quad (2.101)$$

and the projection of the $X^v(\mathbf{r}, \varepsilon, \vartheta, \varphi) Z^v(\mathbf{r}, \varepsilon, \vartheta, \varphi)$ can be directly calculated with the individually projected quantities

$$\{XZ\}_{l,m}^v(\mathbf{r}, \varepsilon) = \sum_{l',m'} X_{l',m'}^v(\mathbf{r}, \varepsilon) Z_{l,m,l',m'}^v(\mathbf{r}, \varepsilon). \quad (2.102)$$

With $X^v(\mathbf{r}, \mathbf{k}, t) = f^v(\mathbf{r}, \mathbf{k}, t)$, the generalized energy distribution is obtained

$$\begin{aligned} g_{l,m}^v(\mathbf{r}, \varepsilon, t) &= \frac{1}{(2\pi)^3} \sum_v \int_{BZ^v} \delta[\varepsilon - \varepsilon^v(\mathbf{r}, \mathbf{k})] Y_{l,m}(\vartheta^v(\mathbf{r}, \mathbf{k}), \varphi^v(\mathbf{r}, \mathbf{k})) f^v(\mathbf{r}, \mathbf{k}, t) d^3k \\ &= \oint Y_{l,m}(\vartheta, \varphi) g^v(\mathbf{r}, \varepsilon, \vartheta, \varphi, t) d\Omega, \end{aligned} \quad (2.103)$$

where the generalized energy distribution is defined as

$$g^v(\mathbf{r}, \varepsilon, \vartheta, \varphi, t) = Z^v(\mathbf{r}, \varepsilon, \vartheta, \varphi) f^v(\mathbf{r}, \varepsilon, \vartheta, \varphi, t). \quad (2.104)$$

Similar to (2.102) one obtains

$$g_{l,m}^v(\mathbf{r}, \varepsilon, t) = \sum_{l',m'} Z_{l,m,l',m'}^v(\mathbf{r}, \varepsilon) f_{l',m'}^v(\mathbf{r}, \varepsilon, t). \quad (2.105)$$

The BTE is projected in the same way as the microscopic quantity (2.98) [11]

$$\frac{1}{(2\pi)^3} \int \delta[\varepsilon - \varepsilon^v(\mathbf{r}, \mathbf{k})] Y_{l,m}(\vartheta^v(\mathbf{r}, \mathbf{k}), \varphi^v(\mathbf{r}, \mathbf{k})) \{BTE\} d^3k. \quad (2.106)$$

In the next subsections, the spherical harmonics expansion of the three individual terms of the BTE – the time derivative, free-streaming operator, and scattering integral – is discussed.

2.5.1 Time Derivative

The partial derivative w.r.t. time yields

$$\begin{aligned} \frac{\partial}{\partial t} f^v(\mathbf{r}, \mathbf{k}, t) &\rightarrow \frac{1}{(2\pi)^3} \sum_v \int_{BZ^v} \delta[\varepsilon - \varepsilon^v(\mathbf{r}, \mathbf{k})] Y_{l,m}(\vartheta^v(\mathbf{r}, \mathbf{k}), \varphi^v(\mathbf{r}, \mathbf{k})) \frac{\partial f^v(\mathbf{r}, \mathbf{k}, t)}{\partial t} d^3k \\ &= \frac{\partial}{\partial t} g_{l,m}^v(\mathbf{r}, \varepsilon, t) = \frac{\partial}{\partial t} \sum_{l',m'} Z_{l,m,l',m'}^v(\mathbf{r}, \varepsilon) f_{l',m'}^v(\mathbf{r}, \varepsilon, t). \end{aligned} \quad (2.107)$$

by interchanging integration and differentiation.

2.5.2 Free-Streaming Operator

Two terms of the free-streaming operator can be recognized. They are the drift term by the total force and the diffusion term.

The drift term evaluates with (2.59) and integration by parts to

$$\begin{aligned}
\frac{1}{\hbar} \mathbf{F}^\nu \cdot \nabla_{\mathbf{k}} f^\nu &\rightarrow \oint Y_{l,m} \mathbf{F}^\nu \cdot \left[\mathbf{v}^\nu Z^\nu \frac{\partial}{\partial \varepsilon} + \frac{Z^\nu}{\hbar} (\nabla_{\mathbf{k}} \vartheta^\nu) \frac{\partial}{\partial \vartheta} + \frac{Z^\nu}{\hbar} (\nabla_{\mathbf{k}} \varphi^\nu) \frac{\partial}{\partial \varphi} \right] f^\nu d\Omega \\
&= \oint Y_{l,m} \mathbf{F}^\nu \cdot \mathbf{v}^\nu Z^\nu \frac{\partial f^\nu}{\partial \varepsilon} d\Omega \\
&\quad - \int_0^{2\pi} \int_0^\pi \frac{\partial}{\partial \vartheta} \left[Y_{l,m} \mathbf{F}^\nu \cdot \frac{Z^\nu}{\hbar} (\nabla_{\mathbf{k}} \vartheta^\nu) \sin \vartheta \right] f^\nu d\vartheta d\varphi \\
&\quad - \int_0^{2\pi} \int_0^\pi \frac{\partial}{\partial \varphi} \left[Y_{l,m} \mathbf{F}^\nu \cdot \frac{Z^\nu}{\hbar} (\nabla_{\mathbf{k}} \varphi^\nu) \sin \vartheta \right] f^\nu d\vartheta d\varphi \\
&= \oint \mathbf{F}^\nu \cdot \frac{\partial}{\partial \varepsilon} [Y_{l,m} \mathbf{v}^\nu Z^\nu f^\nu] d\Omega \\
&\quad - \oint \frac{\partial}{\partial \vartheta} [Y_{l,m} \mathbf{F}^\nu] \cdot \frac{Z^\nu}{\hbar} (\nabla_{\mathbf{k}} \vartheta^\nu) f^\nu d\Omega \\
&\quad - \oint \frac{\partial}{\partial \varphi} [Y_{l,m} \mathbf{F}^\nu] \cdot \frac{Z^\nu}{\hbar} (\nabla_{\mathbf{k}} \varphi^\nu) f^\nu d\Omega, \tag{2.108}
\end{aligned}$$

where the first relation (2.80) was used. With (2.59) and (2.14), this yields

$$\begin{aligned}
\frac{1}{\hbar} \mathbf{F}^\nu \cdot \nabla_{\mathbf{k}} f^\nu &\rightarrow \oint \frac{\partial}{\partial \varepsilon} [\mathbf{F}^\nu \cdot Y_{l,m} \mathbf{v}^\nu Z^\nu f^\nu] d\Omega \\
&\quad - \oint \frac{\partial Y_{l,m}}{\partial \vartheta} \mathbf{F}^\nu \cdot \frac{Z^\nu}{\hbar} (\nabla_{\mathbf{k}} \vartheta^\nu) f^\nu d\Omega \\
&\quad - \oint \frac{\partial Y_{l,m}}{\partial \varphi} \mathbf{F}^\nu \cdot \frac{Z^\nu}{\hbar} (\nabla_{\mathbf{k}} \varphi^\nu) f^\nu d\Omega \\
&\quad + \oint Y_{l,m} (\nabla_{\mathbf{r}_{\mathbf{k}}} \cdot \mathbf{v}^\nu) Z^\nu f^\nu d\Omega. \tag{2.109}
\end{aligned}$$

Note that the gradient in the above equation is taken in the original space ($\nabla_{\mathbf{r}_{\mathbf{k}}}$).

The diffusion term of the free-streaming operator evaluates to

$$\mathbf{v}^\nu \cdot \nabla_{\mathbf{r}_{\mathbf{k}}} f^\nu \rightarrow \oint Y_{l,m} \mathbf{v}^\nu Z^\nu \cdot \nabla_{\mathbf{r}_{\mathbf{k}}} f^\nu d\Omega, \tag{2.110}$$

where the gradient in the real space is also taken in the original space.

The total free-streaming operator can be split into two parts w.r.t. the derivatives in the $\mathbf{k}$ - and real space

$$\frac{1}{\hbar} \mathbf{F}^\nu \cdot \nabla_{\mathbf{k}} f^\nu + \mathbf{v} \cdot \nabla_{\mathbf{r}_{\mathbf{k}}} f^\nu \rightarrow D_{\mathbf{k}} + D_{\mathbf{r}}, \tag{2.111}$$

where

$$\begin{aligned}
 D_{\mathbf{k}} = & \oint \frac{\partial}{\partial \varepsilon} \left[(\mathbf{F}_{\text{E,pot}}^{\nu} + \tilde{\mathbf{F}}_{\text{E}}^{\nu}) \cdot Y_{l,m} \mathbf{v}^{\nu} Z^{\nu} f^{\nu} \right] d\Omega \\
 & - \oint \frac{\partial Y_{l,m}}{\partial \vartheta} \mathbf{F}^{\nu} \cdot \frac{Z^{\nu}}{\hbar} (\nabla_{\mathbf{k}} \vartheta^{\nu}) f^{\nu} d\Omega \\
 & - \oint \frac{\partial Y_{l,m}}{\partial \varphi} \mathbf{F}^{\nu} \cdot \frac{Z^{\nu}}{\hbar} (\nabla_{\mathbf{k}} \varphi^{\nu}) f^{\nu} d\Omega, \tag{2.112}
 \end{aligned}$$

and

$$D_{\mathbf{r}} = \oint Y_{l,m} Z^{\nu} \cdot \nabla_{\mathbf{r}_{\mathbf{k}}} (\mathbf{v}^{\nu} f^{\nu}) d\Omega. \tag{2.113}$$

Using the expression for the gradient in the real space (2.60), $D_{\mathbf{r}}$ can be rearranged,

$$\begin{aligned}
 D_{\mathbf{r}} = & \nabla_{\mathbf{r}_{\varepsilon}} \cdot \oint Y_{l,m} Z^{\nu} \mathbf{v}^{\nu} f^{\nu} d\Omega - \oint \nabla_{\mathbf{r}_{\varepsilon}} [Y_{l,m} Z^{\nu}] \cdot \mathbf{v}^{\nu} f^{\nu} d\Omega \\
 & + \frac{\partial}{\partial \varepsilon} \oint Y_{l,m} Z^{\nu} (\nabla_{\mathbf{r}_{\mathbf{k}}} \varepsilon^{\nu}) \cdot (\mathbf{v}^{\nu} f^{\nu}) d\Omega - \oint \frac{\partial}{\partial \varepsilon} [(\nabla_{\mathbf{r}_{\mathbf{k}}} \varepsilon^{\nu}) Y_{l,m} Z^{\nu}] \cdot \mathbf{v}^{\nu} f^{\nu} d\Omega \\
 & - \int_0^{2\pi} \int_0^{\pi} \frac{\partial}{\partial \vartheta} [(\nabla_{\mathbf{r}_{\mathbf{k}}} \vartheta^{\nu}) Y_{l,m} Z^{\nu} \sin \vartheta] \cdot \mathbf{v}^{\nu} f^{\nu} d\vartheta d\varphi \\
 & - \int_0^{2\pi} \int_0^{\pi} \frac{\partial}{\partial \varphi} [(\nabla_{\mathbf{r}_{\mathbf{k}}} \vartheta^{\nu}) Y_{l,m} Z^{\nu} \sin \vartheta] \cdot \mathbf{v}^{\nu} f^{\nu} d\vartheta d\varphi \\
 = & \nabla_{\mathbf{r}_{\varepsilon}} \cdot \oint Y_{l,m} Z^{\nu} \mathbf{v}^{\nu} f^{\nu} d\Omega + \frac{\partial}{\partial \varepsilon} \oint Y_{l,m} Z^{\nu} (\nabla_{\mathbf{r}_{\mathbf{k}}} \varepsilon^{\nu}) \cdot (\mathbf{v}^{\nu} f^{\nu}) d\Omega \\
 & - \oint \frac{\partial Y_{l,m}}{\partial \vartheta} (\nabla_{\mathbf{r}_{\mathbf{k}}} \vartheta^{\nu}) Z^{\nu} \cdot \mathbf{v}^{\nu} f^{\nu} d\Omega - \oint \frac{\partial Y_{l,m}}{\partial \varphi} (\nabla_{\mathbf{r}_{\mathbf{k}}} \vartheta^{\nu}) Z^{\nu} \cdot \mathbf{v}^{\nu} f^{\nu} d\Omega, \tag{2.114}
 \end{aligned}$$

where the second relation (2.94) was used.

When ϑ^{ν} and φ^{ν} are position-independent, the last two terms in the above equation vanish. Then, the projected free-streaming operator can be written as

$$\begin{aligned}
 D_{\mathbf{k}} + D_{\mathbf{r}} = & \oint \frac{\partial}{\partial \varepsilon} \left[\mathbf{F}_{\text{E,pot}}^{\nu} \cdot Y_{l,m} \mathbf{v}^{\nu} Z^{\nu} f^{\nu} \right] d\Omega \\
 & - \oint \frac{\partial Y_{l,m}}{\partial \vartheta} \mathbf{F}^{\nu} \cdot \frac{Z^{\nu}}{\hbar} (\nabla_{\mathbf{k}} \vartheta^{\nu}) f^{\nu} d\Omega \\
 & - \oint \frac{\partial Y_{l,m}}{\partial \varphi} \mathbf{F}^{\nu} \cdot \frac{Z^{\nu}}{\hbar} (\nabla_{\mathbf{k}} \varphi^{\nu}) f^{\nu} d\Omega \\
 & + \nabla_{\mathbf{r}_{\varepsilon}} \cdot \oint Y_{l,m} \mathbf{v}^{\nu} Z^{\nu} f^{\nu} d\Omega. \tag{2.115}
 \end{aligned}$$

With the coupling coefficients

$$\mathbf{A}_{l,m,l',m'}^v = \oint Y_{l,m} \mathbf{v}^v Z^v Y_{l',m'} d\Omega, \quad (2.116)$$

$$B_{E,l,m,l',m'}^v = \oint \mathbf{F}_E^v \cdot \left[\frac{\partial Y_{l,m}}{\partial \vartheta} \frac{Z^v}{\hbar} (\nabla_{\mathbf{k}} \vartheta^v) + \frac{\partial Y_{l,m}}{\partial \varphi} \frac{Z^v}{\hbar} (\nabla_{\mathbf{k}} \varphi^v) \right] Y_{l',m'} d\Omega, \quad (2.117)$$

$$B_{B,l,m,l',m'}^v = \oint \mathbf{F}_B^v \cdot \left[\frac{\partial Y_{l,m}}{\partial \vartheta} \frac{Z^v}{\hbar} (\nabla_{\mathbf{k}} \vartheta^v) + \frac{\partial Y_{l,m}}{\partial \varphi} \frac{Z^v}{\hbar} (\nabla_{\mathbf{k}} \varphi^v) \right] Y_{l',m'} d\Omega, \quad (2.118)$$

$D_{\mathbf{k}} + D_{\mathbf{r}}$ finally reads

$$\begin{aligned} D_{\mathbf{k}} + D_{\mathbf{r}} = \sum_{l',m'} \frac{\partial}{\partial \varepsilon} \left[\mathbf{F}_{E,\text{pot}}^v \cdot \mathbf{A}_{l,m,l',m'}^v f_{l',m'}^v \right] + \nabla_{\mathbf{r}_\varepsilon} \cdot \left[\mathbf{A}_{l,m,l',m'}^v f_{l',m'}^v \right] \\ - B_{E,l,m,l',m'}^v f_{l',m'}^v - B_{B,l,m,l',m'}^v f_{l',m'}^v. \end{aligned} \quad (2.119)$$

Actual values of the coupling coefficients $\mathbf{A}_{l,m,l',m'}^v$, $B_{E,l,m,l',m'}^v$, and $B_{B,l,m,l',m'}^v$ depend on the underlying band structure. However, from the definitions, (2.116) and (2.117), and the first and third relations, (2.80) and (2.96), we can readily find the following relations valid for the general case with a position-dependent band structure and the generalized coordinate transform:

$$\mathbf{A}_{l,m,l',m'}^v = \mathbf{A}_{l',m',l,m}^v, \quad (2.120)$$

$$\nabla_{\mathbf{r}_\varepsilon} \cdot \mathbf{A}_{l,m,l',m'}^v + \mathbf{F}_{E,\text{pot}}^v \cdot \frac{\partial}{\partial \varepsilon} \mathbf{A}_{l,m,l',m'}^v = B_{E,l,m,l',m'}^v + B_{E,l',m',l,m}^v, \quad (2.121)$$

$$B_{E,0,0,l',m'}^v = B_{B,0,0,l',m'}^v = 0. \quad (2.122)$$

Note that the above (2.120)–(2.122) are generalized versions of (15)–(17) in [6], respectively, which were derived under the assumption of a position-independent band structure and an angle-preserving coordinate transform.

2.5.3 Scattering Operator

The scattering integral also has to be expanded with spherical harmonics. A constant energy transfer is considered. The transition rate can then be expressed as

$$S_{\eta}^{v,v'}(\mathbf{r}, \mathbf{k}|\mathbf{k}') = \frac{1}{\Omega_s} c_{\eta}^{v,v'}[\mathbf{r}, \mathbf{k}|\mathbf{k}'] \delta(\varepsilon^v(\mathbf{k}) - \varepsilon^{v'}(\mathbf{k}') - \hbar\omega_{\eta}), \quad (2.123)$$

where $\mathbf{k}$ and $\mathbf{k}'$ are the initial and final wave vectors, respectively, $\hbar\omega_{\eta}$ the constant energy transfer, and Ω_s the system volume. (Emission and absorption are treated

as separate processes.) The scattering integral is split into in-scattering and out-scattering terms,

$$\hat{S}\{f\} = \hat{S}^{\text{in}}\{f\} - \hat{S}^{\text{out}}\{f\}, \quad (2.124)$$

with

$$\begin{aligned} \hat{S}^{\text{in}}\{f\} &= \sum_{\eta} \hat{S}_{\eta}^{\text{in}}\{f\} \\ &= \sum_{\eta} \frac{\Omega_s}{(2\pi)^3} \sum_{\nu'} \int_{BZ} (1 - f^{\nu}(\mathbf{r}, \mathbf{k})) S_{\eta}^{\nu, \nu'}(\mathbf{r}, \mathbf{k}|\mathbf{k}') f^{\nu'}(\mathbf{r}, \mathbf{k}') d^3 k', \end{aligned} \quad (2.125)$$

$$\begin{aligned} \hat{S}^{\text{out}}\{f\} &= \sum_{\eta} \hat{S}_{\eta}^{\text{out}}\{f\} \\ &= \sum_{\eta} \frac{\Omega_s}{(2\pi)^3} \sum_{\nu'} \int_{BZ} (1 - f^{\nu'}(\mathbf{r}, \mathbf{k}')) S_{\eta}^{\nu', \nu}(\mathbf{r}, \mathbf{k}'|\mathbf{k}) f^{\nu}(\mathbf{r}, \mathbf{k}) d^3 k'. \end{aligned} \quad (2.126)$$

Projection of the scattering term is given by

$$\hat{S}_{\eta}\{f\} \rightarrow \hat{S}_{\eta, l, m}^{\nu}(\mathbf{r}, \varepsilon) = \hat{S}_{\eta, l, m}^{\nu, \text{in}}(\mathbf{r}, \varepsilon) - \hat{S}_{\eta, l, m}^{\nu, \text{out}}(\mathbf{r}, \varepsilon). \quad (2.127)$$

Projection of the in-scattering term yields

$$\begin{aligned} \hat{S}_{\eta, l, m}^{\nu, \text{in}}(\mathbf{r}, \varepsilon) &= \sum_{\nu'} \sum_{l', m'} \sum_{l'', m''} [Z_{l'', m''}^{\nu}(\mathbf{r}, \varepsilon) - g_{l'', m''}^{\nu}(\mathbf{r}, \varepsilon)] g_{l', m'}^{\nu'}(\mathbf{r}, \varepsilon - \hbar\omega_{\eta}) \\ &\quad \{ \oint \oint Y_{l, m}(\vartheta, \varphi) Y_{l'', m''}(\vartheta, \varphi) \\ &\quad \times c_{\eta}^{\nu, \nu'}(\mathbf{r}, \varepsilon, \vartheta, \varphi | \varepsilon - \hbar\omega_{\eta}, \vartheta', \varphi') \\ &\quad \times Y_{l', m'}(\vartheta', \varphi') d\Omega' d\Omega \}. \end{aligned} \quad (2.128)$$

Projection of the out-scattering term yields

$$\begin{aligned} \hat{S}_{\eta, l, m}^{\nu, \text{out}}(\mathbf{r}, \varepsilon) &= \sum_{\nu'} \sum_{l', m'} \sum_{l'', m''} [Z_{l'', m''}^{\nu'}(\mathbf{r}, \varepsilon + \hbar\omega_{\eta}) - g_{l'', m''}^{\nu'}(\mathbf{r}, \varepsilon + \hbar\omega_{\eta})] g_{l', m'}^{\nu}(\mathbf{r}, \varepsilon) \\ &\quad \{ \oint \oint Y_{l, m}(\vartheta, \varphi) Y_{l'', m''}(\vartheta', \varphi') \\ &\quad \times c_{\eta}^{\nu', \nu}(\mathbf{r}, \varepsilon + \hbar\omega_{\eta}, \vartheta', \varphi' | \varepsilon, \vartheta, \varphi) \\ &\quad \times Y_{l', m'}(\vartheta, \varphi) d\Omega' d\Omega \}. \end{aligned} \quad (2.129)$$

When the transition rate depends only on the relative angle between the initial and final wave vectors, it can be easily projected onto spherical harmonics with the addition theorem [13]

$$c_{\eta}^{v,v'}(\mathbf{r}, \varepsilon, \vartheta, \varphi | \varepsilon - \hbar\omega_{\eta}, \vartheta', \varphi') = \sum_{l'''=0}^{\infty} c_{\eta,l'''}^{v,v'}(\mathbf{r}, \varepsilon^v(\mathbf{k})) \sum_{m'''=-l'''}^{l'''} Y_{l''',m'''}(\vartheta, \varphi) Y_{l''',m'''}(\vartheta', \varphi') \quad (2.130)$$

Projection of the in-scattering term yields

$$\begin{aligned} \hat{S}_{\eta,l,m}^{v,\text{in}}(\mathbf{r}, \varepsilon) &= \sum_{v'} \sum_{l',m'} \sum_{l'',m''} [Z_{l'',m''}^v(\mathbf{r}, \varepsilon) - g_{l'',m''}^v(\mathbf{r}, \varepsilon)] g_{l',m'}^{v'}(\mathbf{r}, \varepsilon - \hbar\omega_{\eta}) \\ &\quad \times c_{\eta,l'}^{v,v'}(\mathbf{r}, \varepsilon) a_{l,m,l',m',l'',m''}. \end{aligned} \quad (2.131)$$

Projection of the out-scattering term yields

$$\begin{aligned} \hat{S}_{\eta,l,m}^{v,\text{out}}(\mathbf{r}, \varepsilon) &= \sum_{v'} \sum_{l',m'} \sum_{l'',m''} [Z_{l'',m''}^{v'}(\mathbf{r}, \varepsilon + \hbar\omega_{\eta}) - g_{l'',m''}^{v'}(\mathbf{r}, \varepsilon + \hbar\omega_{\eta})] g_{l',m'}^v(\mathbf{r}, \varepsilon) \\ &\quad \times c_{\eta,l''}^{v',v}(\mathbf{r}, \varepsilon + \hbar\omega_{\eta}) a_{l,m,l',m',l'',m''}. \end{aligned} \quad (2.132)$$

Significant simplification can be obtained when the transition rate does not depend on the scattering angle at all

$$c_{\eta,l}^{v,v'}(\mathbf{r}, \varepsilon) = 4\pi c_{\eta}^{v,v'}(\mathbf{r}, \varepsilon) \delta_{l,0}. \quad (2.133)$$

Projection of the in-scattering term yields

$$\begin{aligned} \hat{S}_{\eta,l,m}^{v,\text{in}}(\mathbf{r}, \varepsilon) &= \sum_{v'} [Z_{l,m}^v(\mathbf{r}, \varepsilon) - g_{l,m}^v(\mathbf{r}, \varepsilon)] g_{0,0}^{v'}(\mathbf{r}, \varepsilon - \hbar\omega_{\eta}) \\ &\quad \times c_{\eta,0}^{v,v'}(\mathbf{r}, \varepsilon) Y_{0,0}. \end{aligned} \quad (2.134)$$

Projection of the out-scattering term yields

$$\begin{aligned} \hat{S}_{\eta,l,m}^{v,\text{out}}(\mathbf{r}, \varepsilon) &= \sum_{v'} [Z_{0,0}^{v'}(\mathbf{r}, \varepsilon + \hbar\omega_{\eta}) - g_{0,0}^{v'}(\mathbf{r}, \varepsilon + \hbar\omega_{\eta})] g_{l,m}^v(\mathbf{r}, \varepsilon) \\ &\quad \times c_{\eta,0}^{v',v}(\mathbf{r}, \varepsilon + \hbar\omega_{\eta}) Y_{0,0}. \end{aligned} \quad (2.135)$$

Note that this is a velocity-randomizing scattering mechanism (for example, phonon scattering with constant matrix element). Moreover, in the case of impurity scattering, an approximation by an isotropic-elastic process [7, 14] can be used.⁵

More information about the scattering mechanisms used in this work can be found in Chap. 4.

2.5.4 Boundary Condition

The interface generation rate shown in (2.15) is projected onto spherical harmonics

$$\gamma_s^v \rightarrow \gamma_{s,l,m}^v(\mathbf{r}, \varepsilon) = \sum_{l',m'} D_{l,m,l',m'}^v f_{l',m'}^v + E_{l,m,0,0}^v f_{0,0}^{\text{eq}}, \quad (2.136)$$

with

$$D_{l,m,l',m'}^v = \oint \Theta(-\mathbf{v}^v Z^v \cdot \mathbf{n}) \mathbf{v}^v Z^v \cdot \mathbf{n} Y_{l,m} Y_{l',m'} d\Omega, \quad (2.137)$$

and

$$E_{l,m,l',m'}^v = \oint \Theta(\mathbf{v}^v Z^v \cdot \mathbf{n}) \mathbf{v}^v Z^v \cdot \mathbf{n} Y_{l,m} Y_{l',m'} d\Omega. \quad (2.138)$$

The interface generation rate is implemented as a volume generation rate within the box of the terminal [5].

2.5.5 Balance Equations

Collecting the previous results, the balance equation for $f_{l,m}^v$, which is the projection of the BTE onto spherical harmonics, can be formulated

$$\begin{aligned} & \sum_{l',m'} \frac{\partial}{\partial t} [Z_{l,m,l',m'}^v f_{l',m'}^v] + \frac{\partial}{\partial \varepsilon} [\mathbf{F}_E^v \cdot \mathbf{A}_{l,m,l',m'}^v f_{l',m'}^v] \\ & + \nabla_{\mathbf{r}_\varepsilon} \cdot [\mathbf{A}_{l,m,l',m'}^v f_{l',m'}^v] \\ & - B_{E,l,m,l',m'}^v f_{l',m'}^v - B_{B,l,m,l',m'}^v f_{l',m'}^v \\ & = \sum_{\eta} \hat{S}_{\eta,l,m}^{v,\text{in}} - \hat{S}_{\eta,l,m}^{v,\text{out}}, \end{aligned} \quad (2.139)$$

⁵The polar optical phonon, which is important for III–V materials, cannot be properly treated as a velocity-randomizing one. In this case, higher-order expansions of the transition rate should be considered, as shown in [15].

where $\gamma_{s,l,m}^\nu$ has to be considered on a contact surface.

In order to simulate realistic semiconductor devices, a stabilization scheme is required, which is discussed in Chap. 3.

2.6 Noise Analysis

In this work, only noise analysis under small-signal operation [16] is treated, and we assume that only DC signals are applied to the contacts of the semiconductor device.⁶

Realization of the stochastic process underlying the BTE yields stochastic variables which fluctuate around their expected value [16, 18, 19]. Under stationary conditions the fluctuation of a stochastic variable is defined as the difference between the variable and its expected value.⁷

The fluctuations are characterized by their spectral intensities. The cross-spectrum of two fluctuations $\delta X(t)$ and $\delta Y(t)$ is given by Fourier transformation of the corresponding correlation function [19, 20]

$$S_{XY}(\omega) = 2 \int_{-\infty}^{\infty} E\{\delta X(t)\delta Y(0)\} \exp(-i\omega t) dt, \quad (2.140)$$

where $E\{\}$ is the expectation. Instead of evaluating the correlation function and Fourier transform it, the spectral intensity can be directly evaluated based on a stochastic differential equation, the Langevin-Boltzmann equation, which can be formulated directly in the frequency domain.

Scattering results in fluctuations of the distribution function, which in turn lead to fluctuations of the expected values. When stationary bias conditions are assumed, noise can be calculated directly in the frequency domain. The deviation of the particle distribution function at angular frequency ω is denoted as $\delta f^\nu(\mathbf{r}, \mathbf{k})e^{i\omega t}$. The fluctuations are assumed to be so small that they can be calculated based on the linearization of the BTE. The linearized BTE reads in the frequency domain

$$L_{\text{BTE}}(\delta f, \delta V) = i\omega \delta f^\nu + \frac{1}{\hbar} \mathbf{F}_s^\nu \cdot \nabla_{\mathbf{k}} \delta f^\nu + \frac{1}{\hbar} \delta \mathbf{F}^\nu \cdot \nabla_{\mathbf{k}} f_s^\nu + \mathbf{v}^\nu \cdot \nabla_{\mathbf{r}} \delta f - \delta \hat{S}\{\delta f\}, \quad (2.141)$$

where i is the imaginary unit number, ω the angular frequency, $\mathbf{F}_s^\nu$ the steady-state solution of the total force, δf^ν a fluctuation of the distribution function, $\delta \mathbf{F}^\nu$ a fluctuation of the total force defined in (2.9)

$$\delta \mathbf{F}^\nu = -\nabla_{\mathbf{r}}(\mp q \delta V), \quad (2.142)$$

⁶Noise analysis under large-signal conditions has been demonstrated for bulk simulations within the framework of the deterministic BTE solver in [17].

⁷From this definition, the expectation of a fluctuation is always zero.

$\delta \hat{S}\{\delta f\}$ the linearized scattering integral

$$\begin{aligned} \delta \hat{S}\{\delta f\} = & \frac{\Omega_s}{(2\pi)^3} \sum_{v'} \int_{BZ} (1 - f_s^v(\mathbf{r}, \mathbf{k})) S^{v,v'}(\mathbf{r}, \mathbf{k}|\mathbf{k}') \delta f^{v'}(\mathbf{r}, \mathbf{k}', \omega) \\ & - \delta f^v(\mathbf{r}, \mathbf{k}, \omega) S^{v,v'}(\mathbf{r}, \mathbf{k}|\mathbf{k}') f_s^{v'}(\mathbf{r}, \mathbf{k}') \\ & - (1 - f_s^{v'}(\mathbf{r}, \mathbf{k}')) S^{v',v}(\mathbf{r}, \mathbf{k}'|\mathbf{k}) \delta f^v(\mathbf{r}, \mathbf{k}, \omega) \\ & + \delta f^{v'}(\mathbf{r}, \mathbf{k}', \omega) S^{v',v}(\mathbf{r}, \mathbf{k}'|\mathbf{k}) f_s^v(\mathbf{r}, \mathbf{k}) d^3k'. \end{aligned} \quad (2.143)$$

f_s^v is the noiseless solution of the stationary BTE. When the transition rate depends on the particle distribution function or the electrostatic potential, such a dependency should be also considered.

For the calculation of noise, Green's functions are required, which are the solution of the linearized equations for a single particle source term [19]. When the electron is generated in the conduction band, the corresponding Green's functions are defined by

$$L_{\text{BTE}}(G_f, G_V) = (2\pi)^3 \delta(\mathbf{r} - \mathbf{r}') \delta(\mathbf{k} - \mathbf{k}') \delta_{v,v'}. \quad (2.144)$$

$G_f^{v,v'}(\mathbf{r}, \mathbf{r}', \mathbf{k}, \mathbf{k}', \omega)$ is the linear response in the frequency domain of the particle distribution function to the generation of a single particle of arbitrary spin.⁸ $G_V^{v'}(\mathbf{r}, \mathbf{r}', \mathbf{k}', \omega)$ is the response of the potential.

With the Green's functions the response of an expectation to the generation of a particle can be calculated. The response of an expectation to the generation of a particle is given by

$$G_X^{v'}(\mathbf{r}, \mathbf{r}', \mathbf{k}', \omega) = \frac{1}{(2\pi)^3} \sum_v \int_{BZ} X^v(\mathbf{r}, \mathbf{k}) G_f^{v,v'}(\mathbf{r}, \mathbf{r}', \mathbf{k}, \mathbf{k}', \omega) d^3k. \quad (2.145)$$

For example, the current response of the k th terminal to the source term is given by the integral of the total current response over the contact area (∂G_k)

$$G_{I_k}^{v'}(\mathbf{r}', \mathbf{k}', \omega) = \int_{\partial G_k} [\mp q G_j^{v'}(\mathbf{r}, \mathbf{r}', \mathbf{k}', \omega) - i\omega\kappa \nabla_{\mathbf{r}} G_V^{v'}(\mathbf{r}, \mathbf{r}', \mathbf{k}', \omega)] d\mathbf{A}, \quad (2.146)$$

where $G_j^{v'}$ is the response of the particle flux and the total current response is the sum of the particle and displacement current responses [22]. Only a single carrier type is assumed. If electrons and holes are presented, particle currents for both carrier types have to be included.

⁸ A formulation which keeps the spin variable can be found in [21].

Noise is quantified by the corresponding power spectral densities (PSD) of the fluctuations [20]. The fundamental PSD is the one of the distribution function, with which the PSDs of all expectations of the distribution function can be calculated [19, 23]

$$S_{ff}^{v_1, v_2}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{k}_1, \mathbf{k}_2, \omega) = \int K_{ff}^{v_1, v_2}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}, \mathbf{k}_1, \mathbf{k}_2, \omega) d^3r, \quad (2.147)$$

with the local noise contribution

$$\begin{aligned} & K_{ff}^{v_1, v_2}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}, \mathbf{k}_1, \mathbf{k}_2, \omega) \\ &= \frac{4\Omega_s}{(2\pi)^3} \sum_v \sum_{v'} \int_{BZ} \int_{BZ} \left[G_f^{v_1, v}(\mathbf{r}_1, \mathbf{r}, \mathbf{k}_1, \mathbf{k}, \omega) - G_f^{v_1, v'}(\mathbf{r}_1, \mathbf{r}, \mathbf{k}_1, \mathbf{k}', \omega) \right] \\ & \quad \times \left[G_f^{v_2, v}(\mathbf{r}_2, \mathbf{r}, \mathbf{k}_2, \mathbf{k}, \omega) - G_f^{v_2, v'}(\mathbf{r}_2, \mathbf{r}, \mathbf{k}_2, \mathbf{k}', \omega) \right]^* \\ & \quad \times \left[1 - f_s^v(\mathbf{r}, \mathbf{k}) \right] S^{v, v'}(\mathbf{r}, \mathbf{k} | \mathbf{k}') f_s^{v'}(\mathbf{r}, \mathbf{k}') d^3k d^3k'. \end{aligned} \quad (2.148)$$

The factor of four stems from spin degeneracy and the fact that particle scattering is a Poisson process. Its single-sided white PSD is given by two times the transition rate probability [20]. The PSD is white, because scattering is treated as instantaneous in the framework of the BTE [4]. For the same reason scattering is local in the real space. The scattering process can be viewed as the annihilation of a particle in the initial state and generation of a particle in the final state. The response of the distribution function to the generation of a particle is described by the corresponding Green's function. Annihilation simply requires a negative sign. Thus, the response of the distribution function at $(\mathbf{r}, \mathbf{k})$ is given by the difference of the Green's functions for the initial and final states. Correlation with a fluctuation for the state 2, integration over all initial and final wave vectors and summation over all initial and final bands yields (2.148).

The PSD for expectations of two microscopic variables X and Y can be calculated

$$\begin{aligned} S_{XY}(\mathbf{r}_1, \mathbf{r}_2, \omega) &= \frac{1}{(2\pi)^6} \sum_{v_1} \sum_{v_2} \int_{BZ} \int_{BZ} X^{v_1}(\mathbf{r}_1, \mathbf{k}_1) \\ & \quad \times S_{ff}^{v_1, v_2}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{k}_1, \mathbf{k}_2, \omega) Y^{v_2}(\mathbf{r}_2, \mathbf{k}_2) d^3k_1 d^3k_2. \end{aligned} \quad (2.149)$$

For device simulations, in addition to the linearized BTE, the linearized PE should be considered in order to obtain the fluctuations of electrostatic potential,

$$L_{PE}(\delta f, \delta V) = \nabla_{\mathbf{k}} \cdot (\kappa \nabla_{\mathbf{k}} \delta V) + q(-\delta n + \delta p) = 0, \quad (2.150)$$

where no inhomogeneous term for the Poisson equation is imposed. Expressions for δn and δp can be easily obtained with the corresponding Green's functions.

Although evaluation of (2.149) is straightforward in principle, it is extremely CPU intensive. Therefore, (2.147)–(2.149) are replaced by

$$S_{XY}(\mathbf{r}_1, \mathbf{r}_2, \omega) = \int K_{XY}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}, \omega) d^3r, \quad (2.151)$$

with the local noise contribution

$$\begin{aligned} K_{XY}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}, \omega) &= \frac{4\Omega_s}{(2\pi)^6} \sum_v \sum_{v'} \int \int \left[G_X^v(\mathbf{r}_1, \mathbf{r}, \mathbf{k}, \omega) - G_X^{v'}(\mathbf{r}_1, \mathbf{r}, \mathbf{k}', \omega) \right] \\ &\quad \times \left[G_Y^v(\mathbf{r}_2, \mathbf{r}, \mathbf{k}, \omega) - G_Y^{v'}(\mathbf{r}_2, \mathbf{r}, \mathbf{k}', \omega) \right]^* \\ &\quad \times [1 - f^v(\mathbf{r}, \mathbf{k})] S^{v,v'}(\mathbf{r}, \mathbf{k}|\mathbf{k}') f^{v'} d^3k d^3k' \end{aligned} \quad (2.152)$$

The Green's function of the expectation for the microscopic quantity X is expanded with spherical harmonics

$$G_{X,l,m}^v(\mathbf{r}, \mathbf{r}', \varepsilon', \omega) = \oint G_X^v(\mathbf{r}, \mathbf{r}', \mathbf{k}(\varepsilon', \vartheta', \varphi'), \omega) Y_{l,m}(\vartheta', \varphi') d\Omega'. \quad (2.153)$$

The Green's function $G_{X,l,m}$ can be directly calculated with the generalized adjoint method [24]. This is standard procedure in numerical noise calculations [25]. Due to the stabilization scheme required for reliable device simulation, the actual construction of L_{BTE} needs more efforts. This point is explained in detail in Chap. 3.

The spherical harmonics expansion of the local contribution to the noise yields an expression related with an integral over the product of four spherical harmonics [26]. Again, significant simplification is obtained when the transition rate does not depend on the scattering angle. In this case, we obtain

$$\begin{aligned} K_{XY}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}, \omega) &= \sum_v \sum_{v'} \sum_{\eta} \sum_{l_1, m_1} \sum_{l_2, m_2} \sum_{l_3, m_3} \int_0^\infty G_{X,l_1,m_1}^v G_{Y,l_2,m_2}^{v*} a_{l_1, m_1, l_2, m_2, l_3, m_3} \\ &\quad \times (Z_{l_3, m_3}(\mathbf{r}, \varepsilon) - g_{l_3, m_3}(\mathbf{r}, \varepsilon)) g_{0,0}(\mathbf{r}, \varepsilon - \hbar\omega_\eta) \\ &\quad - G_{X,l_1,m_1}^v G_{Y,l_2,m_2}^{v*} \delta_{l_1, l_3} \delta_{m_1, m_3} Y_{0,0} \\ &\quad \times (Z_{l_1, m_1}(\mathbf{r}, \varepsilon) - g_{l_1, m_1}(\mathbf{r}, \varepsilon)) g_{l_2, m_2}(\mathbf{r}, \varepsilon - \hbar\omega_\eta) \\ &\quad - G_{X,l_1,m_1}^{v'} G_{Y,l_2,m_2}^{v*} \delta_{l_2, l_3} \delta_{m_2, m_3} Y_{0,0} \\ &\quad \times (Z_{l_2, m_2}(\mathbf{r}, \varepsilon) - g_{l_2, m_2}(\mathbf{r}, \varepsilon)) g_{l_1, m_1}(\mathbf{r}, \varepsilon - \hbar\omega_\eta) \\ &\quad + G_{X,l_1,m_1}^{v'} G_{Y,l_2,m_2}^{v*} a_{l_1, m_1, l_2, m_2, l_3, m_3} \\ &\quad \times (Z_{0,0}(\mathbf{r}, \varepsilon) - g_{0,0}(\mathbf{r}, \varepsilon)) g_{l_3, m_3}(\mathbf{r}, \varepsilon - \hbar\omega_\eta) \\ &\quad Y_{0,0} c_{\eta,0}[\mathbf{r}, \varepsilon] d\varepsilon. \end{aligned} \quad (2.154)$$

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2011, XVIII, 227 p., Hardcover

ISBN: 978-3-7091-0777-5