SUB - BAND DIFFUSION MODELS FOR QUANTUM TRANSPORT IN A STRONG FORCE REGIME *

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Abstract. We derive semi - classical approximations to quantum transport models in thin slabs with applications to SOI (Silicon Oxide on Insulator) - type semiconductor devices via a sub - band approach. In the regime considered the forces acting on the particles across the slab are much larger than the forces in the lateral direction of the slab. In a semi - classical limit the transport picture can be described on large time scales by a system of sub - band convection - diffusion equations with an inter - band collision operator, modeling the transfer of mass (charge) between the different eigenspaces and driving the system towards a local Maxwellian equilibrium.

Key words. quantum transport, Wigner functions, semi - classical limits, quantum hydrodynamics

AMS subject classifications. 65N35, 65N05

1. Introduction. Sub - band approximations to quantum mechanical transport are employed to reduce the computational complexity of the general quantum transport models. They are applicable in situations where the simulation domain exhibits a small aspect ratio. The basic starting point of sub - band models is the three dimensional Schrödinger equation of the form

$$i\hbar\partial_t\psi = \mathcal{H}\psi = -\frac{\hbar^2}{2m}\Delta_X\psi + V\psi \tag{1.1}$$

where $\psi(X,t),\ X \in \Omega \subseteq \mathbb{R}^3,\ t > 0$ is the wave function, and $V(X)$ is the potential. $\hbar$ is Planck's constant and m denotes the mass of the particle. The meaning of the term 'small aspect ratio' is that the spatial variable X and the simulation domain Ω are factored into

$$X = (x,y), \quad \Omega = \Omega_x \times \Omega_y, \quad \Omega_x \subseteq \mathbb{R}^{d_x}, \quad \Omega_y \subseteq \mathbb{R}^{d_y}, \quad d_x + d_y = 3\ , \tag{1.2}$$

i.e. a 'classical' dimension, with the variable x varying on a larger spatial scale and a 'quantum' dimension, with the variable y varying on a much smaller spatial scale. So, $|\Omega_y| << |\Omega_x|$ holds. This allows for semiclassical approximations of the transport picture, such as Boltzmann equations, hydrodynamic models, or drift - diffusion approximations, in the 'classical' $x-$ direction, while transport in the 'quantum' $y-$ direction is treated by the full Schrödinger equation. Besides reducing the computational complexity, one of the big advantages of sub - band models is, that they allow for a simple treatment of open quantum systems, since the interaction with the outside world, i.e. the boundary conditions, can be treated classically in the classical direction.

This paper is concerned with sub - band models in a regime where the force (the gradient $\nabla_y V$) in the quantum direction is much stronger than the force $\nabla_x V$ in the classical direction. As will be demonstrated, this regime is present in solid state semiconductor devices, such as SOI (=Semiconductor - Oxide - on Insulator) structures. The usual approaches to sub - band modeling [2], [14], [10] yield a decoupled system

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of semi - classical sub - band equations, which are of the same form as classical transport equations, except that the potential energy is replaced by the eigenfunction of the Hamiltonian in the quantum ($y-$) direction. Sub-band models corresponding to the regime considered in this paper, on the kinetic level, i.e. the level of the Schrödinger equation, have been studied in [3], [4]. The basic result of this paper is, that in the regime described above and using a collision mechanism relaxing the system to a local thermodynamic equilibrium, the semiclassical limit of sub - band transport models can be described by a system of drift diffusion equations of the form

$$\partial_t n_\alpha = \nabla_x \cdot [\nabla_x n_\alpha - E_\alpha n_\alpha] + \mathbf{Q}[n]_\alpha, \quad \alpha = 0, 1, \dots , \tag{1.3}$$

where n_α is the particle density in the sub - band (the eigenspace) number α, E_α is the sub - band energy (the eigenvalue number α of the Schrödinger equation) and the operator $\mathbf{Q}$ models the scattering between sub - bands (the transfer of the quantum states from one eigenspace to the other). If the forces in the quantum direction y are of moderate size, then the scattering operator $\mathbf{Q}$ can be neglected, and the theory developed in the existing literature, applies. The physical significance of the inter-band collision operator $\mathbf{Q}$ lies in the fact that it introduces a notion of equilibrium into the subband diffusion equations (1.3). As is shown in Section 5, the operator $\mathbf{Q}$ drives the system (1.3) towards an equilibrium of the form $n_\alpha = c(x)e^{-E_\alpha},\ \alpha = 0, 1, ...$ In the absence of $\mathbf{Q}$ the relative size of the sub-band densities n_α (the occupation probabilities of the different eigenspaces) has to be supplied externally through the boundary conditions.

The general framework of sub - band models

The basic idea of sub - band models is to expand the three dimensional model (1.1) into eigenfunctions of the part of the Hamiltonian acting in the quantum direction y. That is, we assume that the operator $\mathcal{H}_y = -\frac{\hbar^2}{2m}\Delta_y + V(x, y)$ has a complete set of eigenfunctions $w_\alpha(x, y)$ (which are still dependent on the classical direction x), forming an orthonormal system. They satisfy

(1.4)

$$(a)\ -\frac{\hbar^2}{2m}\Delta_y w_\alpha + V(x, y)w_\alpha = E_\alpha(x)w_\alpha, \quad (b)\ \int w_\alpha(x, y)w_{\alpha'}(x, y)\ dy = \delta_{\alpha\alpha'},\ \forall x\ .$$

For the rest of this paper, it will be important to use the self adjoint property of the Hamiltonian $\mathcal{H}$. We therefore, reformulate the Schrödinger equation (1.1) and the eigenvalue problem (1.4) weakly as

$$i\hbar \int_{\Omega_x\times\Omega_y} u\partial_t\psi\ dxdy = \tag{1.5}$$

$$\int_{\Omega_x\times\Omega_y} \frac{\hbar^2}{2m}(\nabla_x u \cdot \nabla_x\psi + \nabla_y u \cdot \nabla_y\psi) + uV\psi\ dxdy + \Gamma(\int_{\partial\Omega_x\times\Omega_y} u\mathbf{n} \cdot \nabla_x\psi\ dyd\sigma(x))$$

$$\int_{\Omega_y} \frac{\hbar^2}{2m}\nabla_y v \cdot \nabla_y w_\alpha + vV(x, y)w_\alpha\ dy = E_\alpha(x) \int_{\Omega_y} vw_\alpha\ dy, \quad \alpha = 0, 1, .. , \tag{1.6}$$

for all test functions $u(x, y)$ and $v(y)$. Note, that the weak formulation (1.5)-(1.6) implies that the system is closed in the $y-$ direction, i.e. there are no boundary

integrals over the $y-$ boundary $\partial\Omega_y$ in (1.5)-(1.6). This implies, that the boundary conditions in the $y-$ direction are such that there is no particle flux through the boundary $\partial\Omega_y$. The quantum system is open in the $x-$ direction because of the boundary term Γ in (1.5). ($\mathbf{n}$ and $\sigma(x)$ in (1.5) denote the normal vector on $\partial\Omega_x$ and the corresponding surface element.) The precise form of Γ, modeling the injection of particles into the system in the classical $x-$ direction, is a quite complicated matter, treated in [5] in detail. It is of no relevance in this paper, since we will treat the boundary terms in the $x-$ direction in a classical approximation anyway.

The wave function ψ in (1.5) is expanded into the eigenfunctions w_α, i.e. $\psi(x,y,t) = \sum_\alpha \phi_\alpha(x,t)w_\alpha(x,y)$ holds. This gives the infinite system of sub -band Schrödinger equations

$$i\hbar\partial_t\phi_\alpha = \mathcal{G}[\phi]_\alpha = \sum_{\alpha'} \mathcal{G}_{\alpha\alpha'}(x,\nabla_x)\phi_{\alpha'},\ \alpha = 0,1,\dots\ , \tag{1.7}$$

where the matrix operator $\mathcal{G}$ and the sub - band Hamiltonians $\mathcal{G}_{\alpha\alpha'}$ are given by

$$\mathcal{G}[\phi]_\alpha = \sum_{\alpha'} \mathcal{G}_{\alpha\alpha'}(x,\nabla_x)\phi_{\alpha'} = \sum_{\alpha'} \int_{\Omega_y} w_\alpha \mathcal{H}[\phi_{\alpha'}w_{\alpha'}]\ dy$$

Testing the Schrödinger equation (1.5) with $u(x,y) = r(x)w_\alpha(x,y)$, where $r(x)$ is a test function vanishing on the boundary $\partial\Omega_x$, and using (1.6) gives the operators $\mathcal{G}_{\alpha\alpha'}(x,\nabla_x)$ in their weak form as

$$\int_{\Omega_x} r(x)\mathcal{G}_{\alpha\alpha'}(x,\nabla_x)\phi(x)\ dx = \tag{1.8}$$

$$\int_{\Omega_x} \delta_{\alpha\alpha'}\left(\frac{\hbar^2}{2m}\nabla_x r\cdot\nabla_x\phi + rE_\alpha\phi\right) + \frac{\hbar^2}{2m}(ra_{\alpha\alpha'}\cdot\nabla_x\phi + \phi a_{\alpha'\alpha}\cdot\nabla_x r + rb_{\alpha\alpha'}\phi)\ dx$$

where the d_x dimensional vectors $a_{\alpha\alpha'}$ and the coefficients $b_{\alpha\alpha'}$ are given by

$$a_{\alpha\alpha'} = \int_{\Omega_y} (\nabla_x w_\alpha)w_{\alpha'}\ dy, \quad b_{\alpha\alpha'} = \int_{\Omega_y} (\nabla_x w_\alpha)\cdot(\nabla_x w_{\alpha'})\ dy \tag{1.9}$$

It is important to note that the Hamiltonian in (1.1) is a self adjoint operator, and that this property is of course preserved after expansion into any orthonormal system. That is, (1.8) is invariant under the the exchange $r \leftrightarrow \phi, \alpha \leftrightarrow \alpha'$. In their strong formulation the operators $\mathcal{G}_{\alpha\alpha'}$ are given by

$$\mathcal{G}_{\alpha\alpha'}(x,\nabla_x)\phi(x) = \delta_{\alpha\alpha'}[-\frac{\hbar^2}{2m}\Delta_x\phi + E_\alpha\phi] + \frac{\hbar^2}{2m}[2A_{\alpha\alpha'}\cdot\nabla_x\phi + B_{\alpha\alpha'}(x)\phi] \tag{1.10}$$

where the vectors $A_{\alpha\alpha'}$ and the coefficients $B_{\alpha\alpha'}$ are given in terms of $a_{\alpha\alpha'}$ and $b_{\alpha\alpha'}$ as

$$A_{\alpha\alpha'} = \frac{1}{2}(a_{\alpha\alpha'} - a_{\alpha'\alpha}), \quad B_{\alpha\alpha'} = b_{\alpha\alpha'} - \nabla_x\cdot a_{\alpha'\alpha}\ . \tag{1.11}$$

We remark that, as a consequence of the Hamiltonian being self adjoint, the coefficient vectors $A_{\alpha\alpha'}$ are antisymmetric, i.e. $A_{\alpha\alpha'} = -A_{\alpha'\alpha}$ holds. This will be important for the well posedness of the sub - band drift diffusion system (1.3).

If the coupling coefficients $A_{\alpha\alpha'}, B_{\alpha\alpha'}$ in (1.10) are neglected, the matrix operator $\mathcal{G}$ in (1.7) becomes diagonal, and allows for the separate solution of a lower dimensional Schrödinger equation for each index α (each sub - band), in which the potential energy $V(x,y)$ is replaced by the sub - band energy $E_\alpha(x)$, computed from the solution of the eigenvalue problem (1.4). The tacit, and often not explicitly stated, reason for this approach is, that the coupling coefficients $A_{\alpha\alpha'}, B_{\alpha\alpha'}$ in (1.11) depend on the derivatives of the eigenfunctions $w_\alpha(x,y)$ with respect to the classical direction x, and this dependence is assumed to be weak. As will be seen, this is the consequence of a potential energy V, whose gradients in the $y-$ direction are of moderate size. Considering strong forces in the quantum direction y, and including the coupling terms in (1.7), considerably complicates the transport picture and the involved algebra. To obtain a semi - classical approximation in the classical $x-$ direction, it will be necessary to consider self - adjoint matrices of Wigner functions instead of sequences of real Wigner functions for the diagonal terms. Indeed, the semiclassical limit on the kinetic level, i.e. the rigorous derivation of a sub - band Vlasov- or Boltzmann equation as studied [2], is still an unresolved problem in this regime. This paper is concerned with the diffusive regime, where the transport picture is augmented by a strong collision operator, driving the system towards a local thermodynamic equilibrium. A semiclassical limit, yielding the system (1.3) for the sub - band densities n_α can then be obtained in a straight forward manner - at least on a purely formal level.

This paper is organized as follows. In Section 2 we define more precisely the asymptotic regime considered in this paper and introduce an appropriate dimensionless formulation of the sub - band Schrödinger system (1.7). In section 3 we carry out the diffusive limit in the usual regime of strong collisions and large time scales. Section 4 is concerned with the actual formulation of the sub - band drift diffusion equation, i.e. the computation of the transport coefficients. In Section 5 we carry out the semiclassical limit, giving the main result of the paper, i.e. the system (1.3). Section 6 is devoted to some numerical experiments. Some of the more technical calculations are deferred to the Appendix in Section 7.

2. The asymptotic regime . The coupling coefficients $A_{\alpha\alpha'}, B_{\alpha\alpha'}$ in the sub - band Schrödinger operators $\mathcal{G}_{\alpha\alpha'}$ in (1.10) are given in terms of the eigenfunctions $w_\alpha(x,y)$. So, in order to estimate their impact, it is necessary to examine the spatial structure of these eigenfunctions. First, we define by $\varepsilon << 1$ the aspect ratio of the geometry. That is, ε is defined as the ratio of the length scales of the domains Ω_y and Ω_x in (1.2). We note, that adding a purely $x-$ dependent potential to the potential $V(x,y)$ in the eigenvalue problem (1.4) will not impact the eigenfunctions w_α, but just shift the spectrum $E_\alpha(x)$. This creates a certain ambiguity in the relation between the eigenfunctions w_α and the potential V. We resolve this ambiguity by projecting the potential onto functions with zero mean in the $y-$ direction. That is, we write $V(x,y)$ as

$$V(x,y) = V_0(x) + V_1(x,y), \quad V_0(x) = \frac{1}{|\Omega_y|}\int_{\Omega_y} V(x,y)\ dy, \quad \int V_1(x,y)\ dy = 0,\ \forall x$$

The eigenvalue problem (1.4) can now be solved by

$$(2.1) \qquad (a)\ -\frac{\hbar^2}{2m}\Delta_y w_\alpha + V_1(x,y)w_\alpha = \lambda_\alpha(x)w_\alpha, \quad (b)\ E_\alpha(x) = V_0(x) + \lambda_\alpha(x)\ .$$

Note, that $V_1(x,y)$ is uniquely determined since in mean in $y-$ direction vanishes for all x. In the presence of only moderate forces in the $y-$ direction, $V_1(x,y)$ is a

function with mean 0, varying over a domain Ω_y of order $O(\varepsilon)$, with a moderate size gradient $\nabla_y V_1(x,y)$, i.e. $V_1 = O(\varepsilon)$ has to hold. This, in turn, makes the eigenvalue problem (2.1)(a) almost independent of the classical variable x, and therefore the coupling coefficients $A_{\alpha\alpha'}, B_{\alpha\alpha'}$ in (1.9) and (1.11) will be of order $O(\varepsilon)$ as well. This corresponds to the regime where the coupling coefficients can be neglected, and the sub-band Schrödinger equations are become uncoupled in the non- self consistent case. This paper is concerned with the opposite regime, when the forces in the $y-$ direction are large, and V_1 is of the same order of magnitude as V_0.

2.1. Scaling and dimensionless formulation.

- We scale the spatial variables x and y with the characteristic length scales of their respective domains, setting $x = Lx_s, y = \varepsilon L y_s$, where $\varepsilon << 1$ is the aspect ratio of the dimensions in the quantum direction y and the classical direction x.
- We scale the potential V and the band energy E_α by the ambient temperature T of the system, setting $V(x,y) = TV_s(x_s, y_s)$ and $E_\alpha(x) = TE_{s\alpha}(x_s)$
- We scale time by the time scale corresponding to the length scale L in the classical direction and the energy scale T, setting $t = t_s L\sqrt{\frac{m}{T}}$
- We scale the eigenfunctions w_α in (1.4) by $w_\alpha(x,y) = (\varepsilon L)^{-d_y/2} w_{s\alpha}(x_s, y_s)$ and the sub - band wave functions ϕ_α by $\phi_\alpha(x,t) = L^{-d_x/2}\phi_{\alpha s}(x_s, t_s)$
- We scale the sub - band Hamiltonian $\mathcal{G}_{\alpha\alpha'}$ by the characteristic energy scale T.

This yields the scaled version of the eigenvalue problem (1.4)

$$-\frac{h_y^2}{2}\Delta_y w_{s\alpha}(x_s, y_s) + V_s w_{s\alpha} = E_{s\alpha}(x_s) w_{s\alpha}, \quad h_y = \frac{\hbar}{\varepsilon L\sqrt{mT}} \tag{2.2}$$

and the scaled sub - band system

$$(a)\ ih_x\partial_t\phi_{s\alpha} = \sum_{\alpha'} \mathcal{G}_{\alpha\alpha'}(x_s, \nabla_{x_s})\phi_{s\alpha'}, \quad h_x = \frac{\hbar}{L\sqrt{mT}} \tag{2.3}$$

$$(b)\ \mathcal{G}_{\alpha\alpha'}(x_s, \nabla_{x_s})\phi(x_s) = \delta_{\alpha\alpha'}[-\frac{h_x^2}{2}\Delta_{x_s}\phi + E_{s\alpha}\phi] + \frac{h_x^2}{2}[2A^s_{\alpha\alpha'}\cdot\nabla_{x_s}\phi + B^s_{\alpha\alpha'}\phi]$$

$$(c)\ A^s_{\alpha\alpha'}(x_s) = \frac{1}{2}\int w_{s\alpha'}(x_s, y_s)\nabla_{x_s} w_{s\alpha}(x_s, y_s) - w_{s\alpha}(x_s, y_s)\nabla_{x_s} w_{s\alpha'}(x_s, y_s)\ dy_s,$$

$$(d)\ B^s_{\alpha\alpha'}(x_s) = \int \nabla_{x_s} w_{s\alpha}(x_s, y_s)\cdot\nabla_{x_s} w_{s\alpha'}(x_s, y_s) - \nabla_x\cdot[w_{s\alpha}(x_s, y_s)\nabla_{x_s} w_{s\alpha'}(x_s, y_s)]\ dy_s\ .$$

Here $h_x = \frac{\hbar}{L\sqrt{Tm}}$ is the dimensionless Planck constant, relative to the scale of the classical direction x, and $h_y = \frac{h_x}{\varepsilon}$ is the Planck constant relative to the scales in the classical coordinate x. The original premise, that the transport picture is of a quantum mechanical nature in the $y-$ direction and classical in the $x-$ direction, means that $h_y = O(1)$ and $h_x = O(\varepsilon) << 1$ holds. We will drop the subscript s for the scaled variables from here on.

2.2. Wigner matrices. The goal of this paper is to derive a macroscopic (semi-classical) approximation to the quantum system described in the previous sections. To this end, we need to include collisions in the transport picture, i.e. some mechanism which drives the quantum system to an equilibrium. Including collision mechanisms which yield reasonably simple macroscopic equations into quantum transport equations is a complicated subject and has so far only be solved on a semi - heuristic basis. First and foremost, it requires the consideration not of a single Schrödinger equation for a single wave function as in Section 1, but the transport equations for a mixed state, using a formulation either via density matrices or Wigner functions. We recall that the density matrix $\rho(x,y,x',y',t)$ of a mixed state is given by

$$\rho(x,y,x',y',t) = \sum_n \gamma_n \psi_n(x,y,t)\psi_n(x,y,t)\psi_n(x',y',t) \tag{2.4}$$

with γ_n the occupation probability of state number n and ψ_n the wave function of the state, where each ψ_n satisfies a Schrödinger equation as in (1.1) with the same given potential V. Expanding the density matrix ρ as well as the individual wave functions ψ_n into the eigenfunctions $w_\alpha(x,y)$ in (2.2) gives.

$$\rho(x,y,x',y',t) = \sum_{\alpha\alpha'} w_\alpha(x,y) R_{\alpha\alpha'}(x,x',t) w_{\alpha'}(x',y'), \quad R_{\alpha\alpha'}(x,x',t) = \sum_n \gamma_n \phi_{n\alpha}(x,t)\phi_{n\alpha'}(x',t)^*$$

Using the fact that each of the sub - band wave functions $\phi_{n\alpha}$ satisfy the same sub - band Schrödinger equation (2.3) gives the commutator equation (or Heisenberg equation) for the expanded density matrix $R_{\alpha\alpha'}$ of the form

(2.5)

$$ih_x \partial_t R_{\alpha\alpha'} = [\mathcal{G}, R]_{\alpha\alpha'}, \quad [\mathcal{G}, R]_{\alpha\alpha'}(x,x') = \sum_\beta \mathcal{G}_{\alpha\beta}(x,\nabla_x) R_{\beta\alpha'}(x,x') - \mathcal{G}_{\alpha'\beta}(x',\nabla_{x'}) R_{\alpha\beta}(x,x') \, .$$

In this paper we are interested in a semiclassical approximation to the solution of the Heisenberg equation (2.5). To this end, it will be more convenient to consider the Wigner - Weyl transform of the Heisenberg equation (2.5) in the classical direction x only. We recall [17] that for a density matrix $r(x,x'), x \in \mathbb{R}^{d_x}$ the Wigner function $f(x,p)$ is given by the Wigner - Weyl transform $f = \mathcal{W}r$, defined by

$$f(x,p) = (\mathcal{W}r)(x,p) = (2\pi)^{-d_x} \int r(x - \frac{h_x}{2}\eta, x + \frac{h_x}{2}\eta) e^{i\eta\cdot p} \, d\eta \, , \tag{2.6}$$

where h_x denotes the (scaled) Planck constant, measuring how far away from a classical regime we are, and p is the (scaled) momentum vector. The inverse Wigner - Weyl transform is given by

$$r(x,x') = (\mathcal{W}^{-1}f)(x,x') = \int f(\frac{x+x'}{2}, p) \exp[\frac{ip}{h_x} \cdot (x - x')] \, dp \tag{2.7}$$

We define the sub-band Wigner functions $f_{\alpha\alpha'}(x,p)$ by $f_{\alpha\alpha'}(x,p) = (\mathcal{W}R_{\alpha\alpha'})(x,p)$, and transform the expanded Heisenberg equation (2.5) accordingly. This gives the system of transport equations

$$\partial_t f_{\alpha\alpha'} + \mathcal{L}[f]_{\alpha\alpha'} = 0, \quad \mathcal{L}[f]_{\alpha\alpha'} = \frac{i}{h_x} \mathcal{W}([\mathcal{G}, \mathcal{W}^{-1}f]_{\alpha\alpha'}) \, . \tag{2.8}$$

The computation of the Wigner - transformed commutator $\mathcal{L}$ is a rather tedious exercise, which is carried out in the Appendix in Section 7. The operator $\mathcal{L}$ consists

of a diagonal part $\mathcal{L}^0_{\alpha\alpha'}$ and a coupling operator $\mathcal{L}^c$, depending on the coefficients $A_{\alpha\alpha'}$, $B_{\alpha\alpha'}$ in (2.3)(c)(d). $\mathcal{L}$ is of the form

$$(a)\ \mathcal{L}[f]_{\alpha\alpha'} = \mathcal{L}^0_{\alpha\alpha'} f_{\alpha\alpha'} - \mathcal{L}^c[f]_{\alpha\alpha'} \tag{2.9}$$

$$(b)\ \mathcal{L}^0_{\alpha\alpha'} f(x,p) = p\cdot\nabla_x f(x,p) - \frac{1}{ih_x}[E_\alpha(x+\frac{ih_x}{2}\nabla_p) - E_{\alpha'}(x-\frac{ih_x}{2}\nabla_p)]f(x,p)$$

$$(c)\ \mathcal{L}^c[f]_{\alpha\alpha'} = \sum_\beta A_{\alpha\beta}(x+\frac{ih_x}{2}\nabla_p)(p-\frac{ih_x}{2}\nabla_x)f_{\beta\alpha'}(x,p) + A_{\alpha'\beta}(x-i\frac{h_x}{2}\nabla_p)(p+\frac{ih_x}{2}\nabla_x)f_{\alpha\beta}(x,p)$$

$$-\frac{ih_x}{2}B_{\alpha\beta}(x+i\frac{h_x}{2}\nabla_p)f_{\beta\alpha'}(x,p) + \frac{ih_x}{2}B_{\alpha'\beta}(x-i\frac{h_x}{2}\nabla_p)f_{\alpha\beta}(x,p)$$

The operators in (2.9) are defined via Fourier transforms in the usual sense of pseudo differential operators [16]. So, c.f.

$$E_\alpha(x+\frac{ih_x}{2}\nabla_p)f(x,p) = (2\pi)^{-d_x}\int E_\alpha(x-\frac{h_x}{2}\eta)f(x,q)e^{i\eta\cdot(p-q)}\ dqd\eta$$

holds. The particle density in the sub - band α is given by the expansion coefficient of the diagonal of the original density matrix ρ in (2.4), i.e.

$$n_\alpha(x,t) = R_{\alpha\alpha}(x,x,t), \quad \int \rho(x,y,x,y,t)\ dy = \sum_\alpha n_\alpha(x,t)$$

holds. The inverse formula (2.7) implies that the particle density $R_{\alpha\alpha}(x,x)$ is given in terms of the sub - band Wigner functions $f_{\alpha\alpha'}$ as

$$n_\alpha(x,t) = R_{\alpha\alpha}(x,x,t) = \int f_{\alpha\alpha}(x,p)\ dp\ .$$

2.3. Collisions. The subject of this paper is the derivation of macroscopic approximations to the sub-band Wigner equation (2.8). We therefore need to include a collision mechanism into the ballistic transport picture described by (2.8). Modeling collision mechanisms in a a fully quantum mechanical setting is a quite complicated matter (see [13] [11], [1], [15] for an overview). However, since the final result of the present paper is a drift - diffusion equation, the only information about the microscopic collision mechanism entering the macroscopic model is the form of the integral invariants of the collisions and the kernel of the operator. We therefore use a simple BGK operator. We define a Maxwellian, i.e. a notion of local thermodynamic equilibrium, at a given ambient temperature ($T = 1$ in the dimensionless formulation), which is parameterized by its sub - band densities. So, we have a sub-band density matrix $M^{(m)}_{\alpha\alpha'}(x,x')$, dependent on the parameter vector $(m_1, m_2, ..)$ with

$$M^{(m)}_{\alpha\alpha}(x,x) = m_\alpha(x),\ \forall\alpha$$

and its Wigner - transformed expansion into the sub - band basis functions $\mathcal{M}^{(m)}$

$$\mathcal{M}^{(m)}_{\alpha\alpha'}(x,p) = \mathcal{W}[M^{(m)}_{\alpha\alpha'}(x,x')], \quad \int \mathcal{M}^{(m)}_{\alpha\alpha}(x,p)\ dp = m_\alpha(x),\ \forall\alpha\ . \tag{2.10}$$

We introduce scattering into the transport picture by augmenting the ballistic transport equation (2.8) by the BGK - type collision operator

$$\partial_t f_{\alpha\alpha'} + \mathcal{L}[f]_{\alpha\alpha'} + \frac{1}{\tau}(f_{\alpha\alpha'} - \mathcal{M}^{(n)}_{\alpha\alpha'}) = 0, \quad n_\alpha = \int f_{\alpha\alpha}(x,p)\ dp\ , \tag{2.11}$$

thus conserving the particle density in each sub-band and relaxing the system towards an equilibrium of the form $f_{\alpha\alpha'} = \mathcal{M}^{(n)}_{\alpha\alpha'}$. The local equilibrium Maxwellian $M^{(m)}(x,y,x',y')$ is chosen as the maximizer of the relative Von Neumann entropy, given the particle densities in each sub-band; i.e. $M^{(m)}$ is the solution of the constrained optimization problem

$$Trace[R\cdot(I-\mathcal{G}-\ln(R))] \to max, \quad R_{\alpha\alpha}(x,x) = m_\alpha(x),\ \forall\alpha,\ \forall x\ .$$

According to the theory, developed in [8] , [9] The density matrix $M^{(m)}$ is given as the integral kernel of the operator exponential

$$M^{(m)}_{\alpha\alpha'}(x,x') = \exp[-\mathcal{G} - \delta(x-x')\delta_{\alpha\alpha'}\chi^{(m)}_\alpha(x)] \tag{2.12}$$

where the Lagrange multipliers $\chi^{(m)}_\alpha(x)$ have to be chosen such that

$$M^{(m)}_{\alpha\alpha}(x,x) = \int \mathcal{M}^{(m)}_{\alpha\alpha}(x,p)\ dp = m_\alpha(x),\ \forall\alpha,\forall x$$

holds. Here the matrix exponential in (2.12) has to be understood in terms of the spectral decomposition of the operator. Let $\psi^\nu_a(x)$ denote the eigenfunctions of the operator $\mathcal{G} + \delta(x-x')\delta_{\alpha\alpha'}\chi^{(m)}_\alpha(x)$. So, the they satisfy the problem

$$\mathcal{G}[\psi^\nu]_\alpha(x) + \chi^{(m)}_\alpha(x)\psi^\nu_\alpha(x) = \lambda_\nu\psi^\nu_\alpha(x),\ \nu = 1,2,..,\ \forall\alpha,\ \forall x$$

with λ_ν the corresponding eigenvalues, or, expanding the Hamiltonian $\mathcal{G}$,

$$\sum_\beta \mathcal{G}_{\alpha\beta}(x,\nabla_x)\psi^\nu_\beta(x) + \chi^{(m)}_\alpha(x)\psi^\nu_\alpha(x) = \lambda_\nu\psi^\nu_\alpha(x),\ \nu = 1,2,..,\ \forall\alpha,\ \forall x\ . \tag{2.13}$$

The sub-band density matrix $M^{(m)}$ is then given as

$$M^{(m)}_{\alpha\alpha'}(x,x') = \sum_\nu \psi^\nu_\alpha(x)e^{-\lambda_\nu}\psi^\nu_{\alpha'}(x')\ .$$

The matrix exponential in (2.12) makes the local entropy maximizer non-locally dependent on the macroscopic densities. Consequently, the local sub-band equilibria $\mathcal{M}^{(n)}_{\alpha\alpha'}$ will depend on the whole sequence $\{n_\alpha,\ \alpha = 1,2,..\}$ of macroscopic sub-band densities. To derive the semi-classical limit of the sub-band drift diffusion system, we will need an asymptotic expression for the sub-band Maxwellians $\mathcal{M}^{(n)}_{\alpha\alpha'}$ in powers of h_x. We refer the reader to the papers [8] , [9], [6] for the background on maximum entropy closures of the form (2.12).

Remark:

- The collision operator in (2.11) conserves the particle density n_α for each sub - band. This means that inter - band scattering due to thermodynamic effects is negligible, which is consistent with the small aspect ratio of the domain Ω. So, scattering between the sub - bands is due only to the large cross - directional fields, and the resulting coupling of the bands through the operator $\mathcal{L}_c$ in (2.9).

- In the absence of the coupling operator $\mathcal{L}_c$, it would only be necessary to consider the diagonal terms in equation (2.11), i.e. $(\mathcal{L}f)_{\alpha\alpha'}$ would depend only on $f_{\alpha\alpha'}$, and we could obtain a closed system for the diagonal Wigner functions $f_{\alpha\alpha}(x,p)$.
- In this scenario (if we neglect the coupling operator $\mathcal{L}_c$) we could immediately carry out (at least formally) the semiclassical limit, by sending $h_x \to 0$. For $h_x \to 0$, the diagonal terms in equation (2.11) would reduce to $\partial_t f_{\alpha\alpha} + p \cdot \nabla_x f_{\alpha\alpha} - \nabla_x E_\alpha \cdot \nabla_p f_{\alpha\alpha} + \frac{1}{\tau}(f_{\alpha\alpha} - \mathcal{M}^{(n)}_{\alpha\alpha}) = 0$. Standard asymptotics for a small relaxation time $\tau << 1$ would then give the standard Drift - Diffusion system for the sub - band densities n_α. This would give the standard Drift - Diffusion equations for each sub - band, where the potential energy V is replaced by the sub - band energy E_α for each α.

3. Asymptotics for small relaxation times. In this section we carry out the standard Chapman - Enskog asymptotic expansion for small relaxation times τ in (2.11), leading to a set of macroscopic transport equations for the sub - band densities n_α. Our choice of a BGK - type collision operator implies that the collision operator in (2.11) can be written as a projection operator. We define the projection operator $\mathcal{P}$ as

$$(\mathcal{P}f)_{\alpha\alpha'}(x,p) = \mathcal{M}^{(n[f])}_{\alpha\alpha'}(x,p), \quad n[f]_\alpha(x) = \int f_{\alpha\alpha}(x,p)\ dp \tag{3.1}$$

$$\Rightarrow \int (\mathcal{P}f)_{\alpha\alpha}(x,p)\ dp = \int f_{\alpha\alpha}(x,p)\ dp\ .$$

So, $\mathcal{P}$ projects onto a Maxwellian $\mathcal{M}$ preserving the density n_α for each sub - band. Using the projection operator $\mathcal{P}$, the transport equation (2.11) can be rewritten as

$$\tau[\partial_t f + (\mathcal{L}f)] + (I - \mathcal{P})f = 0, \tag{3.2}$$

with I the identity operator. We decompose f into $f = a + \tau b$ with $a = \mathcal{P}f$ and $\tau b = (I - \mathcal{P})f$. (This means we make the Ansatz that $(I - \mathcal{P})f$ is of order $O(\tau)$, which will turn out to be justified.) Using the projections $\mathcal{P}$ and $I - \mathcal{P}$ on equation (3.2) gives

$$(a)\ \partial_t a + \mathcal{P}\mathcal{L}(a + \tau b) = 0, \quad (b)\ \tau\partial_t b + (I - \mathcal{P})\mathcal{L}(a + \tau b) + b = 0, \tag{3.3}$$

Equation (3.3)(a) will yield the macroscopic transport equation, while (3.3)(b) yields the constitutive law for the fluxes in the limit $\tau \to 0$. Sending $\tau \to 0$ in (3.3)(b) gives $b = -(I - \mathcal{P})\mathcal{L}a + O(\tau)$. Inserting this into (3.3)(a) gives

$$\partial_t a + \mathcal{P}\mathcal{L}a - \tau\mathcal{P}\mathcal{L}(I - \mathcal{P})\mathcal{L}a = O(\tau^2), \tag{3.4}$$

In general, there are two possible regimes to consider. The first one is the regime where $\mathcal{P}\mathcal{L}a \neq 0$ holds. In this case the third term in (3.4) is a small perturbation of the other terms and the resulting transport equations are of a Navier - Stokes type. The second regime is valid in the case that $\mathcal{P}\mathcal{L}a = 0$ holds in (3.4). In this case, we obtain, up to higher order terms in τ, the equation

$$\partial_t a = \tau\mathcal{P}\mathcal{L}\mathcal{L}a + O(\tau^2)\ . \tag{3.5}$$

(3.5) represents a closed system of equations for the sub - band particle densities $n_\alpha(x,t)$. Integrating the diagonal terms of (3.5) with respect to p gives, using the definition (3.1) of the projection operator $\mathcal{P}$ and the definition (2.10) of the parameterized Maxwellian $\mathcal{M}$,

$$\partial_t n_\alpha(x) = \tau \int (\mathcal{L}\mathcal{L}\mathcal{M}^{(n)})_{\alpha\alpha}(x,p)\ dp\ , \tag{3.6}$$

which is a diffusion equation, since the operator $\mathcal{L}$ (the spatial derivatives) is applied twice. Note, that in this case, we are using the 'wrong' time scale, and that the macroscopic densities n_α evolve on the larger $\frac{t}{\tau}$ diffusion time scale.

4. The quantum Drift - Diffusion equation . In this section we employ the Chapman - Enskog expansion from Section 3 to the sub - band Wigner system (2.11). It turns out that, in the given regime, the long time behavior of the sub - band Wigner system is described by a diffusive equation (i.e. $\mathcal{P}\mathcal{L}a = 0$ holds in (3.4)). Therefore, the result of this section is a quantum drift - diffusion system (given by equations (4.12)-(4.14) in Section 4.3), which is still quite complicated. To derive the quantum drift diffusion system it is first necessary to compute the moments of the operator $\mathcal{L}$. This is done in Section 4.1. The quantum drift diffusion system (4.12)-(4.14) is given in terms of the moments of the parameterized subband Maxwellian $\mathcal{M}^{(n)}_{\alpha\alpha'}$. In order to compute these moments it is beneficial to express the Maxwellian as the solution of a Bloch equation in Section 4.2.

4.1. The moments of the operator $\mathcal{L}$. To derive the macroscopic transport picture, it is necessary to compute the moments the operator $\mathcal{L}$, given in (2.9). Given its rather complicated structure in the presence of the coupling operator $\mathcal{L}^c$, this is a quite complicated endeavor. The deeper structural reason for the fact that this will yield sufficiently simple and local diffusion equations is, that the original Hamiltonian in the Schrödinger equation (1.1) is polynomial in the momentum operator $i\nabla_x$ and, consequently, the operator $\mathcal{L}$ in (2.9) is polynomial in the momentum variable p. This allows us to express the moments of $\mathcal{L}[f]$ in terms of the moments of the Wigner function f. Before we start, we will simplify the operator $\mathcal{L}$ in (2.9). We recall that quantum mechanical density matrices have to be self adjoint operators, and that the commutator equation preserves this property. For the original density matrix to be self adjoint means that $\rho(x,y,x',y',t) = \rho(x',y',x,y,t)^*$ holds. This translates in the sub - band expansion into the relation $R_{\alpha\alpha'}(x,x') = R_{\alpha'\alpha}(x',x)^*$ for the density matrix R in (2.5) and, into the relation $f_{\alpha\alpha'}(x,p) = f_{\alpha'\alpha}(x,p)^*$ for the Wigner function f in (2.8). Note, that this relation implies that the diagonal elements $f_{\alpha\alpha}$ of the Wigner matrix, which are used to compute physically observable quantities, are real. This symmetry has to be invariant under the transport operator $\mathcal{L}$ to guarantee self adjointness, and we will use this structure to simplify the operator. In other words, if we define the adjoint of a Wigner matrix as $f^{adj}_{\alpha\alpha'}(x,p) = f_{\alpha'\alpha}(x,p)^*$, then $\mathcal{L}[f^{adj}] = \mathcal{L}[f]^{adj}$ has to hold, in order for the transport equation (2.11) to preserve the self adjoint property of the Wigner matrix f. We use this fact by writing the operator $\mathcal{L}$ in (2.9) as

$$\mathcal{L}[f] = L[f] + L[f^{adj}]^{adj}$$

where the operator L is given, according to (2.9) as

(4.1)

$$(a)\ L[f]_{\alpha\alpha'} = L^0[f]_{\alpha\alpha'} - L^c[f]_{\alpha\alpha'}, \quad (b)\ L^0[f]_{\alpha\alpha'}(x,p) = \frac{p}{2}\cdot\nabla_x f_{\alpha\alpha'}(x,p) - \frac{1}{ih_x}E_\alpha(x+i\frac{h_x}{2}\nabla_p)f_{\alpha\alpha'}(x,p)$$

$$(c)\ L^c[f]_{\alpha\alpha'} = \sum_\beta A_{\alpha\beta}(x+\frac{ih_x}{2}\nabla_p)(p-\frac{ih_x}{2}\nabla_x)f_{\beta\alpha'}(x,p) - \frac{ih_x}{2}B_{\alpha\beta}(x+i\frac{h_x}{2}\nabla_p)f_{\beta\alpha'}(x,p)$$

or, in matrix notation

$$(d)\ L^c[f] = A_(x+\frac{ih_x}{2}\nabla_p)(p-\frac{ih_x}{2}\nabla_x)f(x,p) - \frac{ih_x}{2}B(x+i\frac{h_x}{2}\nabla_p)f(x,p)$$

We note, that taking the adjoint of a Wigner matrix, does not operate on the momentum variable p, and therefore the same self - adjoint structure will be present in the moment system. We introduce the notation

$$m_j^k f_{\alpha\alpha'} = \int p_j^k f_{\alpha\alpha'}(x,p)\ dp\ ,$$

and have the following

LEMMA 4.1. *Let $C_{\alpha\alpha'}(x)$ be a matrix function and $f_{\alpha\alpha'}(x,p)$ be a Wigner matrix. Then the moment $m_\nu^k(C(x+\frac{ih_x}{2}\nabla_p)f)$ is given by*

(4.2)

$$(a)\ m^0(C(x+\frac{ih_x}{2}\nabla_p)f) = Cm^0 f, \quad (b)\ m_\nu^1(C(x+\frac{ih_x}{2}\nabla_p)f) = Cm_\nu^1 f - \frac{ih_x}{2}(\partial_{x_\nu}C)m^0 f$$

Proof:
Using the usual definition of pseudo differential operators, the $k-$ th moment for $k=0,1$ is given by

$$m_\nu^k Cf = (2\pi)^{-d_x}\int p_\nu^k C(x-\frac{h_x}{2}\eta)f(x,q)\exp[i\eta\cdot(p-q)]\ dqdpd\eta$$

Using the variable shift $p\to p+q$ in the integral and the binomial theorem gives

$$m_\nu^k Cf = (2\pi)^{-d_x}\int (p_\nu+q_\nu)^k C(x-\frac{h_x}{2}\eta)f(x,q)\exp[i\eta\cdot p]\ dqdpd\eta$$

$$= (2\pi)^{-d_x}\int \sum_j \binom{k}{j} C(x-\frac{h_x}{2}\eta)m_\nu^{k-j}f(x)(-i\partial_{\eta_\nu})^j\exp[i\eta\cdot p]\ dpd\eta$$

Integration by parts gives

$$m_\nu^k Cf = (2\pi)^{-d_x}\int \sum_j \binom{k}{j} (-\frac{ih_x}{2}\partial_{x_\nu})^j C(x-\frac{h_x}{2}\eta)m_\nu^{k-j}f(x)\exp[i\eta\cdot p]\ dpd\eta$$

$$= \sum_j \binom{k}{j}[(-\frac{ih_x}{2}\partial_{x_\nu})^j C(x)]m_\nu^{k-j}f(x)$$

The result is obtained by setting $k=0$ and $k=1$.

■

We will use Lemma 4.1 repeatedly to compute the zero and first order moments of $\mathcal{L}[f]$. To simplify the computation we will first compute only the zero and first order

moments of the operator $L[f]$ and compute the moments of $\mathcal{L}[f]$ using the symmetry relation $\mathcal{L}[f] = L[f] + L[f^{adj}]^{adj}$.

We start with the zero order moment and obtain from (4.1) and (4.2)(a)

$$(a) m^0 L^0[f]_{\alpha\alpha'} = \frac{1}{2}\sum_\nu \partial_{x_\nu} m^1_\nu f_{\alpha\alpha'} - \frac{E_\alpha}{ih_x} m^0 f_{\alpha\alpha'}, \tag{4.3}$$

$$(b)\ m^0 L^c[f]_{\alpha\alpha'} = \sum_\nu (A^\nu m^1_\nu f)_{\alpha\alpha'} - \frac{ih_x}{2}\sum_\nu (A^\nu \partial_{x_\nu} m^0 f)_{\alpha\alpha'} - \frac{ih_x}{2}(B m^0 f)_{\alpha\alpha'}$$

Similarly, we obtain for the first order moment from (4.1) and (4.2)(b)

$$(a)\ m^1_\mu L^0[f]_{\alpha\alpha'} = \frac{1}{2}\sum_\nu \partial_{x_\nu} m^2_{\mu\nu} f_{\alpha\alpha'} - \frac{1}{ih_x} E_\alpha m^1_\mu f_{\alpha\alpha'} + \frac{1}{2} m^0 f_{\alpha\alpha'} \partial_{x_\mu} E_\alpha \tag{4.4}$$

$$(b)\ m^1_\mu L^c[f]_{\alpha\alpha'} = \sum_\nu (A^\nu m^2_{\mu\nu} f)_{\alpha\alpha'} - \frac{ih_x}{2}\sum_\nu (\partial_{x_\mu} A^\nu \cdot m^1_\nu f)_{\alpha\alpha'} - \frac{ih_x}{2}\sum_\nu (A^\nu \partial_{x_\nu} m^1_\mu f)_{\alpha\alpha'}$$

$$- \frac{h_x^2}{4}\sum_\nu (\partial_{x_\mu} A^\nu \cdot \partial_{x_\nu} m^0 f)_{\alpha\alpha'} - \frac{ih_x}{2}(B m^1_\mu f)_{\alpha\alpha'} - \frac{h_x^2}{4}(\partial_{x_\mu} B \cdot m^0 f)_{\alpha\alpha'}$$

In order to compute the moments $m^j \mathcal{L}[f]$ from the moments $m^j L[f]$, given by (4.3)-(4.4), it is notationally convenient to define the matrix anti - commutator as

$$\{U, V\}_{\alpha\alpha'} = (UV)_{\alpha\alpha'} + (UV^{adj})^{adj}_{\alpha\alpha'} = (UV)_{\alpha\alpha'} + (VU^{adj})_{\alpha\alpha'} = \sum_\beta U_{\alpha\beta} V_{\beta\alpha'} + U^*_{\alpha'\beta} V_{\alpha\beta}\,. \tag{4.5}$$

Note that, for a hermitian matrix U with $U_{\alpha\beta} = U^*_{\beta\alpha}$, the definition (4.5) reduces to the usual definition of the matrix anti - commutator. Finally we remark, that for a self adjoint matrix V with $V_{\alpha\beta} = V^*_{\beta\alpha}$, the diagonal of the anti - commutator (4.5) is given by

$$\{U, V\}_{\alpha\alpha} = \sum_\beta U_{\alpha\beta} V_{\beta\alpha} + U^*_{\alpha\beta} V^*_{\beta\alpha} = 2Re(UV)_{\alpha\alpha} \tag{4.6}$$

Using the relation $\mathcal{L}[f] = L[f] + L[f^{adj}]^{adj}$, we obtain from (4.3)-(4.4)

$$(a)\ m^0 \mathcal{L}[f] = m^0 \mathcal{L}^0[f] - m^0 \mathcal{L}^c[f] \tag{4.7}$$

$$(b)\ m^0 \mathcal{L}^0[f]_{\alpha\alpha'} = \nabla_x \cdot (m^1 f) - \frac{E_\alpha - E_{\alpha'}}{ih_x}(m^0 f)_{\alpha\alpha'}$$

$$(c)\ m^0 \mathcal{L}^c[f]_{\alpha\alpha'} = \sum_\nu \{A^\nu, m^1_\nu f\}_{\alpha\alpha'} - \frac{h_x}{2}\sum_\nu \{iA^\nu, \partial_{x_\nu} m^0 f\}_{\alpha\alpha'} - \frac{h_x}{2}\{iB, m^0 f\}_{\alpha\alpha'}$$

$$(a)\ m^1_\mu \mathcal{L}[f] = m^1_\mu \mathcal{L}^0[f] - m^1_\mu \mathcal{L}^c[f] \tag{4.8}$$

$$(b) m^1_\mu \mathcal{L}^0[f]_{\alpha\alpha'} = \sum_\nu \partial_{x_\nu} m^2_{\mu\nu} f_{\alpha\alpha'} - \frac{E_\alpha - E_{\alpha'}}{ih_x} m^1_\mu f_{\alpha\alpha'} + \partial_{x_\mu}(\frac{E_\alpha + E_{\alpha'}}{2}) m^0 f_{\alpha\alpha'}$$

$$(c)\ m^1_\mu \mathcal{L}^c[f]_{\alpha\alpha'} = \sum_\nu \{A^\nu, m^2_{\mu\nu} f\}_{\alpha\alpha'} - \frac{h_x}{2} \sum_\nu \{i\partial_{x_\mu} A^\nu, m^1_\nu f\}_{\alpha\alpha'}$$

$$-\frac{h_x}{2} \sum_\nu \{iA^\nu, \partial_{x_\nu} m^1_\mu f\}_{\alpha\alpha'} - \frac{h_x^2}{4} \sum_\nu \{\partial_{x_\mu} A^\nu, \partial_{x_\nu} m^0 f\}_{\alpha\alpha'} - \frac{h_x}{2} \{iB, m^1_\mu f\}_{\alpha\alpha'} - \frac{h_x^2}{4} \{\partial_{x_\mu} B, m^0 f\}_{\alpha\alpha'}$$

4.2. The local Maxwellian $\mathcal{M}^{(n)}$. In order to formulate the macroscopic equations given in the $\tau \to 0$ limit by the Chapman - Enskog expansion of Section 3, we need to use a formulation of the local Maxwellians $\mathcal{M}^{(n)}$ in (3.1) which is more amenable to asymptotics. This is achieved by expressing the operator exponential in the definition (2.12) via the solution of a Bloch equation. The basic idea of a Bloch equation is to express the matrix exponential as the integral kernel of the semigroup solution operator of a diffusion equation. If the density matrix $M^{(n)}$ is given as the matrix exponential

$$M^{(n)} = \exp[-\mathcal{G} - \chi^{(n)}]\ ,$$

then $M^{(n)}$ can be computed as the solution of

(4.9)

$$(a)\ \partial_s R_{\alpha\alpha'}(x, x', s) = -\frac{1}{2}[(\mathcal{G}_{\alpha\beta}(x, \nabla_x) R_{\beta\alpha'} + \mathcal{G}_{\beta\alpha'}(x', \nabla_{x'}) R_{\alpha\beta}] - \frac{\chi^{(n)}_\alpha(x) + \chi^{(n)}_{\alpha'}(x')}{2} R_{\alpha\alpha'}$$

$$(b)\ R(x, x', 0) = \delta_{\alpha\alpha'} \delta(x - x')$$

evaluated at $s = 1$. So $M^{(n)}_{\alpha\alpha'}(x, x') = R_{\alpha\alpha'}(x, x', 1)$ holds. In other words, in the same way the function e^{-sz} can be expressed as the solution of the ordinary differential equation $\frac{du}{ds} = -zu,\ u(0) = 1$ the integral kernel of the operator $\exp[-\mathcal{G} - \chi^{(n)}]$ can be expressed as the solution of the evolution equation (4.9). The validity of the formulation of $\mathcal{M}^{(n)}$ via the Bloch equation (4.9) can easily be verified by expanding the density matrix R in to the eigenfunctions $\psi^\nu_\alpha(x)$ of the Hamiltonian $\mathcal{G} + \chi^{(n)}$ in (2.13) (see [12] for details). In order to compute the local Maxwellian in the sub - band Wigner picture, we have to use the Wigner transform of (4.9), and compute $\mathcal{M}^{(n)} = \mathcal{W}[M^{(n)}]$ via $\mathcal{M}^{(n)} = \mathcal{R}(x, p, s = 1),\ \mathcal{R}(x, p, s) = \mathcal{W}[R(x, x', s)]$. We have the following

THEOREM 4.2. *The local Maxwellian $\mathcal{M}^{(n)}$ can be computed as $\mathcal{M}^{(n)}(x, p) = \mathcal{R}(x, p, s = 1)$ with $\mathcal{R}$ the solution of the initial value problem*

$$\partial_s \mathcal{R} = \mathcal{K}[\mathcal{R}], \quad \mathcal{R}_{\alpha\alpha'}(x, p, s = 0) = \delta_{\alpha\alpha'}\ , \tag{4.10}$$

where the matrix operator $\mathcal{K}$ is the Wigner transformed anti - commutator in (4.9). The operator $\mathcal{K}$ is of the form $\mathcal{K}[\mathcal{R}] = K[\mathcal{R}] + K[\mathcal{R}^{adj}]^{adj}$. with K defined by

$$(a)\ K = K^0 - K^c \tag{4.11}$$

$$(b)\ K^0[\mathcal{R}]_{\alpha\alpha'} = \frac{h_x^2}{16}\Delta_x\mathcal{R}_{\alpha\alpha'} - \frac{ih_x}{4}p\cdot\nabla_x\mathcal{R}_{\alpha\alpha'} - \frac{|p|^2}{4}\mathcal{R}_{\alpha\alpha'} - \frac{1}{2}(E_\alpha + \chi_\alpha^{(n)})(x + \frac{ih_x}{2}\nabla_p)\mathcal{R}_{\alpha\alpha'}$$

$$(c)\ K^c[\mathcal{R}]_{\alpha\alpha'} = \sum_{\nu\beta} A^\nu_{\alpha\beta}(x + \frac{ih_x}{2}\nabla_p)(\frac{ih_x p_\nu}{2} + \frac{h_x^2}{4}\partial_{x_\nu})\mathcal{R}_{\beta\alpha'} + \frac{h_x^2}{4}\sum_\beta B_{\alpha\beta}(x + \frac{ih_x}{2}\nabla_p)\mathcal{R}_{\beta\alpha'}$$

The proof of Theorem 4.2 is an exercise in the use of the Wigner transform, similar to the derivation of the form of the operator $\mathcal{L}$ in (4.1). It deferred to the Appendix in Section 7.2.

The theorem actually implies that, using the BGK - type collision operator defined in (2.11), we are in the diffusion regime of the Chapman - Enskog expansion in Section 3. In addition to being self adjoint, the Wigner matrix $\mathcal{R}$, and consequently the Maxwellian $\mathcal{M}$, satisfies an anti - symmetry in the momentum vector p. From the definition (4.11) of the operator K we see that, in addition to the self adjoint relation $\mathcal{R}_{\alpha\alpha'}(x,p) = \mathcal{R}_{\alpha'\alpha}(x,p)^*$ the Wigner matrix $\mathcal{R}$ also satisfies the symmetry $\mathcal{R}_{\alpha\alpha'}(x,p) = \mathcal{R}_{\alpha\alpha'}(x,-p)^*$. (Using the definition of pseudo differential operators, it is easily verified that the transformation $\mathcal{R}_{\alpha\alpha'}(x,p) \to \mathcal{R}_{\alpha\alpha'}(x,-p)^*$ commutes with the operator K, and therefore this symmetry is preserved by the Bloch equation (4.10).) This implies for the moments of the Maxwellian $m^k\mathcal{M}^{(n)}$ that the zero order moment $m^0\mathcal{M}^{(n)}_{\alpha\alpha'}$ is purely real whereas the first order moment vector $m^1\mathcal{M}^{(n)}_{\alpha\alpha'}$ is purely imaginary. Using the formulas (4.7) for the zero order moments of the diagonal of the operator $\mathcal{L}$ we have

$$m^0\mathcal{L}^0[\mathcal{M}^{(n)}]_{\alpha\alpha} = \nabla_x\cdot(m^1\mathcal{M}^{(n)}_{\alpha\alpha})$$

$$m^0\mathcal{L}^c[\mathcal{M}^{(n)}]_{\alpha\alpha} =$$

$$\sum_\nu 2Re(A^\nu, m^1_\nu\mathcal{M}^{(n)})_{\alpha\alpha} - h_x\sum_\nu Re(iA^\nu, \partial_{x_\nu}m^0\mathcal{M}^{(n)})_{\alpha\alpha} - h_xRe(iB, m^0\mathcal{M}^{(n)})_{\alpha\alpha} = 0$$

Now the diagonal $m^1\mathcal{M}^{(n)}_{\alpha\alpha}$ has to be on one hand purely imaginary, and, on the other hand purely real because $\mathcal{M}^{(n)}$ is self adjoint. Therefore $m^1\mathcal{M}^{(n)}_{\alpha\alpha} = 0$ holds, and we obtain in sum total $m^0\mathcal{L}[\mathcal{M}^{(n)}]_{\alpha\alpha} = 0$. Therefore the projection operator $\mathcal{P}$ in Section 3 satisfies $\mathcal{P}\mathcal{L}\mathcal{M}^{(n)} = 0$ and we obtain the diffusion equation (3.6) as a result of the Chapman - Enskog expansion in Section 3.

4.3. The quantum drift diffusion system. We now turn to the actual form of the drift - diffusion equation (3.6), i.e. to the computation of the diagonal term $\int \mathcal{L}\mathcal{L}[\mathcal{M}]_{\alpha\alpha}$. Unfortunately, this involves the computation of all the moments of the off - diagonal terms of $\mathcal{L}[\mathcal{M}^{(n)}]$ as well. We define the Wigner matrix q by $q = \mathcal{L}[\mathcal{M}^{(n)}]$, and, combining (4.7) with (4.6) and setting $f = q$, we obtain, according to the previous section, the diffusion equation

$$\frac{1}{\tau}\partial_t n_\alpha = m^0\mathcal{L}\mathcal{L}[\mathcal{M}]_{\alpha\alpha} = m^0\mathcal{L}[q]_{\alpha\alpha} = \tag{4.12}$$

$$\nabla_x\cdot(m^1q)_{\alpha\alpha} + \sum_{\nu=1}^{d_x} Re[-2A^\nu m^1_\nu q + ih_xA^\nu\partial_{x_\nu}m^0q)]_{\alpha\alpha} + h_xRe[iBm^0q]_{\alpha\alpha}\ .$$

The moment matrices $m^0 q$ and $m^1_\mu q,\ \mu = 1, .., d_x$ are readily computed from (4.7)-(4.8), setting $f = \mathcal{M}^{(n)}$, as

$$(4.13) \qquad (a)\ m^0 q_{\alpha\alpha'} = m^0 \mathcal{L}[\mathcal{M}^{(n)}]_{\alpha\alpha'} = m^0 \mathcal{L}^0[\mathcal{M}^{(n)}]_{\alpha\alpha'} - m^0 \mathcal{L}^c[\mathcal{M}^{(n)}]_{\alpha\alpha'}$$

$$(b)\ m^0 \mathcal{L}^0[\mathcal{M}^{(n)}]_{\alpha\alpha'} = \nabla_x \cdot (m^1 \mathcal{M}^{(n)}) - \frac{E_\alpha - E_{\alpha'}}{i h_x} (m^0 \mathcal{M}^{(n)})_{\alpha\alpha'}$$

$$(c)\ m^0 \mathcal{L}^c[\mathcal{M}^{(n)}]_{\alpha\alpha'} = \sum_\nu \{A^\nu, m^1_\nu \mathcal{M}^{(n)}\}_{\alpha\alpha'} - \frac{h_x}{2} \sum_\nu \{iA^\nu, \partial_{x_\nu} m^0 \mathcal{M}^{(n)}\}_{\alpha\alpha'} - \frac{h_x}{2} \{iB, m^0 \mathcal{M}^{(n)}\}_{\alpha\alpha'}$$

$$(4.14) \qquad (a)\ m^1_\mu q = m^1_\mu \mathcal{L}[\mathcal{M}^{(n)}]_{\alpha\alpha'} = m^1_\mu \mathcal{L}^0[\mathcal{M}^{(n)}]_{\alpha\alpha'} - m^1_\mu \mathcal{L}^c[\mathcal{M}^{(n)}]_{\alpha\alpha'}$$

$$(b)\ m^1_\mu \mathcal{L}^0[\mathcal{M}^{(n)}]_{\alpha\alpha'} = \sum_\nu \partial_{x_\nu} m^2_{\mu\nu} \mathcal{M}^{(n)}_{\alpha\alpha'} - \frac{E_\alpha - E_{\alpha'}}{i h_x} m^1_\mu \mathcal{M}^{(n)}_{\alpha\alpha'} + \partial_{x_\mu} (\frac{E_\alpha + E_{\alpha'}}{2}) m^0 \mathcal{M}^{(n)}_{\alpha\alpha'}$$

$$(c)\ m^1_\mu \mathcal{L}^c[\mathcal{M}^{(n)}]_{\alpha\alpha'} = \sum_\nu \{A^\nu, m^2_{\mu\nu} \mathcal{M}^{(n)}\}_{\alpha\alpha'}$$

$$- \frac{h_x}{2} \sum_\nu \{i\partial_{x_\mu} A^\nu, m^1_\nu \mathcal{M}^{(n)}\}_{\alpha\alpha'} - \frac{h_x}{2} \sum_\nu \{iA^\nu, \partial_{x_\nu} m^1_\mu \mathcal{M}^{(n)}\}_{\alpha\alpha'} - \frac{h_x^2}{4} \sum_\nu \{\partial_{x_\mu} A^\nu, \partial_{x_\nu} m^0 \mathcal{M}^{(n)}\}_{\alpha\alpha'}$$

$$- \frac{h_x}{2} \{iB, m^1_\mu \mathcal{M}^{(n)}\}_{\alpha\alpha'} - \frac{h_x^2}{4} \{\partial_{x_\mu} B, m^0 \mathcal{M}^{(n)}\}_{\alpha\alpha'}$$

Equation (4.12) represents the continuity equation in the sub-band formulation, and equations (4.13) and (4.14) form the constitutive relations for the current densities and energies. The system of equations given by (4.12)- (4.14) forms a closed system for the scalar variables n_α, once the moments $m^j \mathcal{M}^{(n)}$ of the equilibrium density $\mathcal{M}^{(n)}$ are expressed in terms of the sub - band densities n_α. Unfortunately, the full sub - band quantum drift diffusion system (4.12)- (4.14) is still quite complicated, especially since the moments $m^j \mathcal{M}^{(n)}$ of the equilibrium density will depend non - locally on the sub - band densities n_α. We will therefore derive in the next section the semiclassical limit (the formal limit $h_x \to 0$). As will be seen in the next section, the local Maxwellians $\mathcal{M}^{(n)}_{\alpha\alpha'}$ reduce to their classical counterparts in this limit, i.e. $\lim_{h_x \to 0} \mathcal{M}^{(n)}_{\alpha\alpha'} = (2\pi)^{-d_x/2} \delta_{\alpha\alpha'} n_\alpha \exp(\frac{-|p|^2}{2})$ holds. This drastically reduces the complexity of the system (4.12)-(4.14). Note, however, that it is not enough to simply replace the local Maxwellian by its semiclassical limit in (4.13)-(4.14) because of the presence of the $O(h_x^{-1})$ terms in the off diagonal elements of the moment matrices $m^0 q,\ m^1 q$. We therefore need higher order asymptotic expressions for the local Maxwellians $\mathcal{M}^{(n)}_{\alpha\alpha'}$, which will be obtained from an asymptotic solution of the Bloch equation (4.10).

5. The semiclassical limit of the quantum drift - diffusion equation. In order to carry out the formal limit $h_x \to 0$ in the quantum drift diffusion system of the previous section, it is necessary to derive asymptotic expressions for the moments of the equilibrium Wigner matrices $\mathcal{M}^{(n)}$ in (4.12) (4.13) (4.14). The easiest way to derive these asymptotic expressions in the Wigner transport picture is to formally expand the solution of the Bloch equation (4.10). (This is the real reason for the formulation of the operator exponential via the Bloch formalism). This is essentially the same approach as followed in [6]. We have the following

THEOREM 5.1. *The moments of the subband Maxwellian $\mathcal{M}^{(n)}$ are given up to terms of order $O(h_x^2)$ by*

$$(5.1)\ (a)\ m^0\mathcal{M}^{(n)}_{\alpha\alpha'} = \delta_{\alpha\alpha'}n_\alpha, \quad (b)\ m^1\mathcal{M}^{(n)}_{\alpha\alpha'} = ih_x\frac{n_{\alpha'}-n_\alpha}{\ln(n_\alpha)-\ln(n_{\alpha'})}A_{\alpha\alpha'} + O(h_x^2),$$

$$(c)\ m^2_{\nu j}\mathcal{M}^{(n)}_{\alpha\alpha'} = \delta_{\alpha\alpha'}\delta_{\nu j}n_\alpha + O(h_x^2)$$

The proof of Theorem 5.1 is deferred to the Appendix in Section 7.2.

The result (5.1) appears somewhat unusual at first glance, since the asymptotic expression for the first order moments contains an $O(h_x)$ term, whereas asymptotic expansions to thermal equilibrium solutions are usually expansions in $\hbar^2$ [6]. The reason for this is the presence of first order derivatives in the Hamiltonian $\mathcal{G}$. A term of the form $h_x^2\nabla_x$ in the Hamiltonian results in a term $h_x p$ under the Wigner transform, yielding an $O(h_x)$ term in the corresponding matrix exponential. Note, that the moment matrices $m^0\mathcal{M}^{(n)}_{\alpha\alpha'}$ and $m^2\mathcal{M}^{(n)}_{\alpha\alpha'}$ are real and symmetric in the indices α, α' while the first order moment matrices $m^1\mathcal{M}^{(n)}_{\alpha\alpha'}$ are purely imaginary and antisymmetric in α, α'. Thus the $O(h_x)$ term does not appear in the diagonal of $\mathcal{M}^{(n)}$, and therefore does not contribute to any physical observables.

From (4.13) we can conclude that the zero order moment $m^0 q$ is (at least formally) of order $O(h_x)$, since $m_1\mathcal{M}^{(n)} = O(h_x)$ holds and $\mathcal{M}^0(n)$ is up to $O(h_x^2)$ a diagonal matrix. Thus, the terms involving $m^0 q$ in the continuity equation (4.12) constitute an order $O(h_x^2)$ perturbation, and in the semiclassical limit $h_x \to 0$ the continuity equation becomes

$$(5.2)\qquad \frac{1}{\tau}\partial_t n_\alpha = \nabla_x \cdot (m^1 q)_{\alpha\alpha} - 2\sum_\mu Re(A^\mu m^1_\mu q)_{\alpha\alpha}$$

Using the asymptotic expressions (5.1)(a)(c) in the formula (4.14) for $m^1 q$, we obtain

$$m^1_\mu q_{\alpha\alpha'} = m^1_\mu \mathcal{L}[\mathcal{M}^{(n)}]_{\alpha\alpha'} =$$

$$\delta_{\alpha\alpha'}\partial_{x_\mu}n_\alpha - (E_\alpha - E_{\alpha'})A^\mu_{\alpha\alpha'}\frac{n_{\alpha'}-n_\alpha}{\ln(n_\alpha)-\ln(n_{\alpha'})} + \delta_{\alpha\alpha'}n_\alpha\partial_{x_\mu}E_\alpha - (A^\mu_{\alpha\alpha'}n_{\alpha'} + A^\mu_{\alpha'\alpha}n_\alpha) + O(h_x^2)$$

or, using the anti - symmetry of the matrices A^μ,

$$(5.3)\qquad m^1_\mu q_{\alpha\alpha'} =$$

$$\delta_{\alpha\alpha'}(\partial_{x_\mu} n_\alpha + n_\alpha \partial_{x_\mu} E_\alpha) + A^\mu_{\alpha\alpha'}(n_\alpha - n_{\alpha'})(1 + \frac{E_\alpha - E_{\alpha'}}{\ln(n_\alpha) - \ln(n_{\alpha'})}) + O(h_x^2)$$

Inserting (5.3) into (5.2), we observe first that, because of the antisymmetry of the matrices A^μ, the diagonal term $m^1 q_{\alpha\alpha}$ is simply given by $m^1 q_{\alpha\alpha} = \nabla_x n_\alpha + n_\alpha \nabla_x E_\alpha$. Also, because of this antisymmetry, the diagonal term $m^1 q_{\alpha\alpha}$ does not contribute to the diagonal of the matrix product $A^\mu m^1_\mu q$. Thus, inserting (5.3) into (5.2), we obtain

$$\frac{1}{\tau}\partial_t n_\alpha = \nabla_x \cdot (\nabla_x n_\alpha + n_\alpha \nabla_x E_\alpha) + Q[n]_\alpha \tag{5.4}$$

$$Q[n]_\alpha = -2 \sum_{\mu\beta} A^\mu_{\alpha\beta} A^\mu_{\beta\alpha} (n_\beta - n_\alpha)(1 + \frac{E_\beta - E_\alpha}{\ln(n_\beta) - \ln(n_\alpha)})$$

or

$$Q[n]_\alpha = \sum_\beta \kappa_{\alpha\beta}(n_\beta - n_\alpha)(1 + \frac{E_\beta - E_\alpha}{\ln(n_\beta) - \ln(n_\alpha)}), \quad \kappa_{\alpha\beta} = 2\sum_\mu (A^\mu_{\alpha\beta})^2 \geq 0 \tag{5.5}$$

Equation (5.4) represents the sub-band drift diffusion equation in the formal semi-classical limit. Note, that the sub-band densities n_α will evolve on a slower $O(\frac{1}{\tau})$, or diffusion - , time scale than the solution of the underlying kinetic equation. The collision operator Q in (5.5) models the scattering, i.e. the transfer of mass, from one eigenspace or sub-band to the other. We point out that this scattering mechanism is not due to the collisions introduced in Section 2.2, which conserve mass in each sub-band, but to the strong forces in the quantum direction. (The scattering coefficients are proportional to the coefficients $(A^\mu_{\alpha\alpha'})^2$, and they in turn depend on the variation of the potential in the $y-$ direction in Section 2). The inter-band collision operator Q is of a somewhat unusual form since, due to its nonlinear structure and the dependence on the eigenvalues E_α, it cannot be separated into the usual in- and outscattering terms. It does, however, exhibit the usual desired properties of a collision operator, namely its kernel is given by the physically correct equilibrium distribution and it dissipates a relative entropy. We summarize these properties in

THEOREM 5.2. *The inter sub-band collision operator $Q[n]$ in (5.5) has the following properties.*

1. *$Q[n]$ conserves the total mass* independently of how many sub-bands are used in the expansion, *i.e. if N terms are used in the eigenfunction expansion ($\alpha = 1, .., N$) then $\sum_{\alpha=1}^N Q[n]_\alpha = 0$ holds for any N.*
2. *The kernel of Q is given by multiples of the Maxwell distribution e^{-E_α}, i.e. the kernel of Q consists of densities $n_\alpha = ce^{-E_\alpha}$, $\alpha = 1, .., N$ with an arbitrary function $c(x)$.*
3. *Q dissipates locally the relative entropy $\mathcal{E} = \sum_\alpha n_\alpha(\ln(n_\alpha) + E_\alpha - 1)$, i.e. $\sum_{\alpha=1}^N (\ln(n_\alpha) + E_\alpha) Q[n]_\alpha \leq 0$ holds.*

Proof:

The statements 1-3 are most easily proven by introducing chemical potentials and writing the collision operator Q in a weak form. We define the chemical potentials ϕ_α, $\alpha = 1, .., N$ by the relation $n_\alpha = \exp(\phi_\alpha - E_\alpha)$. In terms of the chemical potentials Q in (5.5) can be written as

$$Q[n]_\alpha = \sum_\beta \kappa_{\alpha\beta} \frac{n_\beta - n_\alpha}{\ln(n_\beta) - \ln(n_\alpha)} (\phi_\beta - \phi_\alpha)$$

In order to write Q in weak form we test against the vector $u_\alpha,\ \alpha = 1,..,N$ and form the sum

$$\sum_{\alpha=1}^{N} u_\alpha Q[n]_\alpha = \sum_{\alpha,\beta=1}^{N} u_\alpha \kappa_{\alpha\beta} \frac{n_\beta - n_\alpha}{\ln(n_\beta) - \ln(n_\alpha)} (\phi_\beta - \phi_\alpha) = \sum_{\alpha,\beta=1}^{N} u_\beta \kappa_{\alpha\beta} \frac{n_\beta - n_\alpha}{\ln(n_\beta) - \ln(n_\alpha)} (\phi_\alpha - \phi_\beta)\,.$$

For the second equality we have used the fact that the matrix elements $\kappa_{\alpha\beta}$ are symmetric because of the anti-symmetry of the coefficients $A_{\alpha\beta}$ in (5.5). Thus we can express the sum as

$$\sum_{\alpha=1}^{N} u_\alpha Q[n]_\alpha = -\frac{1}{2} \sum_{\alpha,\beta=1}^{N} \kappa_{\alpha\beta} \frac{n_\beta - n_\alpha}{\ln(n_\beta) - \ln(n_\alpha)} (u_\beta - u_\alpha)(\phi_\beta - \phi_\alpha) \tag{5.6}$$

Setting $u_\alpha = 1,\ \alpha = 1,..,N$ in (5.6) gives $\sum_\alpha Q[n]_\alpha = 0$, proving the first statement.

Setting $\phi_\alpha = \ln(c),\ n_\alpha = ce^{-E_\alpha},\ \alpha = 1,..,N$ in (5.6) gives $\sum_{\alpha=1}^{N} u_\alpha Q[n]_\alpha = 0,\ \forall u$, and therefore $Q[n]_\alpha = 0,\ \forall \alpha$, proving the second statement.

Finally, setting $u_\alpha = \phi_\alpha,\ \alpha = 1,..,N$ gives $\sum_{\alpha=1}^{N} \phi_\alpha Q[n]_\alpha = \sum_{\alpha=1}^{N} [\ln(n_\alpha) + E_\alpha] Q[n]_\alpha \le 0$, since the coefficients $\kappa_{\alpha\beta}$ non - negative and the logarithm is a monotonically increasing function. This proves the third statement.

∎

We conclude this section by reversing the scaling of Section 2.1 and formulating the resulting quantum drift diffusion system in the original dimensional variables. Recalling the original scaling in Section 2.1 we re-scale

$$n_\alpha(x,t) \to \frac{1}{n^{tot}} n_\alpha(Lx, t_0 L\sqrt{\frac{m}{T}}), \quad E_\alpha(x) \to \frac{1}{T} E_\alpha(Lx), \quad Q[n] \to \frac{L^2}{n^{tot} T} Q[n], \quad \tau \to \frac{\tau}{t_0}$$

with the original time scale t_0 in Section 2.1 given by $t_0 = L\sqrt{\frac{m}{T}}$, L the characteristic length in $x-$ direction, T the ambient temperature and m the mass of the particle. The scaling factor n^{tot} for the sub-band particle densities will not appear in the unscaled equations and has to be determined by initial conditions and the boundary conditions in the $x-$ direction. This gives the unscaled diffusion equation

$$\frac{m}{\tau} \partial_t n_\alpha = \nabla_x \cdot (T \nabla_x n_\alpha + n_\alpha \nabla_x E_\alpha) + Q[n]_\alpha$$

We recall that the coupling coefficients $A_{\alpha\beta}$ are given in terms of the eigenfunctions $w_\alpha(x,y)$ by (1.9) and (1.11) and (2.3)(c). Re-scaling

$$w_\alpha(x,y) \to (\varepsilon L)^{d_y/2} w_\alpha(Lx, \varepsilon L y), \quad A^\mu_{\alpha\beta}(x) \to L A^\mu_{\alpha\beta}(Lx), \quad \kappa_{\alpha\beta}(x) \to L^2 \kappa_{\alpha\beta}(Lx),$$

gives

$$\kappa_{\alpha\beta} = 2 \sum_\mu (A^\mu_{\alpha\beta})^2, \quad A^\mu_{\alpha\beta} = \frac{1}{2} \int_{\Omega_y} w_\beta(x,y) \partial_{x_\mu} w_\alpha(x,y) - w_\alpha(x,y) \partial_{x_\mu} w_\beta(x,y)\ dy$$

where the w_α are now the solutions of the unscaled eigenvalue problem (1.6), nomalized to $\int_{\Omega_y} w_\alpha w_\beta\ dy = \delta_{\alpha\beta}$. Finally, the unscaled collision operator Q is now of the form

$$Q[n]_\alpha = \sum_\beta \kappa_{\alpha\beta} (n_\beta - n_\alpha)(T + \frac{E_\beta - E_\alpha}{\ln(n_\beta) - \ln(n_\alpha)})\,.$$

The asymptotics used in this paper were based on the assumptions that the relaxation time τ is smaller then the kinetic time scale t_0 and that the scaled Planck constant h_x for the transport in $x-$ direction is small, i.e. that $\frac{\tau}{L}\sqrt{\frac{T}{m}} << 1$ and $\frac{\hbar}{L\sqrt{mT}} << 1$ holds.

6. Numerical Results. In this section we present some numerical results, elucidating the asymptotic theory derived in the previous sections. Ideally, one would like to numerically compare solutions of the original Schrödinger equations to the sub - band approximations derived in this paper. This would involve a solution of the fully three dimensional Schrödinger equation for a mixed state (i.e. a solution for the six dimensional density matrix) including the non - local collision mechanisms used here, which is beyond the scope of this paper. So, the purpose of this section is threefold, namely

- To demonstrate the conditions under which the regime discussed in this paper is valid.
- To study the effect of the inter - band collision operator on solutions of the resulting drift diffusion equations.
- To study the convergence of the sub - band expansion, i.e. how many terms are necessary in a simple example.

In order to address the first point, we generate a potential which roughly describes the actual physical situation in a SOI (Silicon Oxide on Insulator) semiconductor device, and compute the coupling coefficients $A_{\alpha\alpha'}$ corresponding to this example. In a self - consistent calculation, the potential would have to be computed from a self consistent solution of Poisson's equation using the densities $n(x,t) = \sum_\alpha n_\alpha(x,t)$. The present paper is concerned with the non - self consistent case. So, we compute an approximate potential V, obtained from a simple classical Boltzmann model of the form

$$-\nabla_x \cdot (e_{di}\nabla_x V) + n_i \exp(V-\phi) - D = 0 \ , \tag{6.1}$$

where e_{di} is the dielectric constant, ϕ is a a simple approximate chemical potential, satisfying $\Delta_x \phi = 0$, n_i is the intrinsic particle density and D is some background concentration (the doping concentration of the device). The simulation domain is depicted in the left panel of Figure 6.1, where the green area denotes the actual simulation domain, in the yellow areas (the oxide) V satisfies the Laplace equation. The bias applied to the device is modeled by applying Drichlet boundary conditions to the Laplace equation for the chemical potential ϕ at the interfaces between the oxide (yellow) and the simulation domain (green). The corresponding potential (as the solution of equation (6.1) is depicted in the right panel of Figure 6.1. Computing the eigenfunctions $w_\alpha(x,y)$, according to (1.4), yields the coupling coefficients $A_{\alpha\alpha'}$, defined in (1.11). They are depicted for the case of three sub - bands, in dimensionless form in the left panel of Figure 6.2. Note, that they are antisymmetric $A_{\alpha\beta} = -A_{\beta\alpha}$ holds. The size of the coupling coefficients $A_{\alpha\beta}$ in dimensionless variables verifies that, under the given biasing conditions, the coupling terms in the Hamiltonian $\mathcal{G}$ in Section 1 cannot be neglected. In the right panel of Figure 6.2 we show the densities n_α computed from the diffusion equation (5.4)-(5.5) in logarithmic scale, using three terms in the sub - band expansion. To investigate the effect of the coupling operator on the sub-band drift diffusion system, we solve the system with and without the coupling operator Q, using the potential depicted in Figure 6.1. Figure 6.3 shows the particle and current densities (on a linear scale) for each sub-band as well as the total particle and current densities. Note that, in the one dimensional steady state

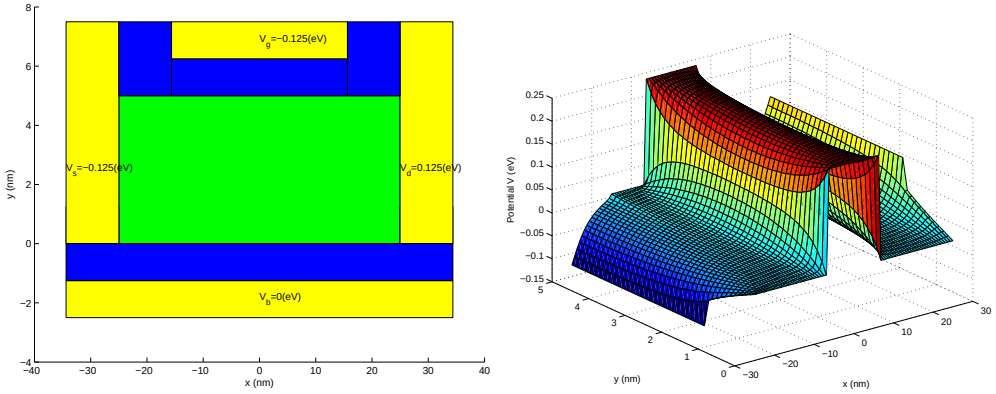

FIG. 6.1. *Left Panel: Schematic, green=simulation domain, blue= metal contacts, yellow=insulaing oxide. Right Panel: Potential V from the Boltzmann model (6.1).*

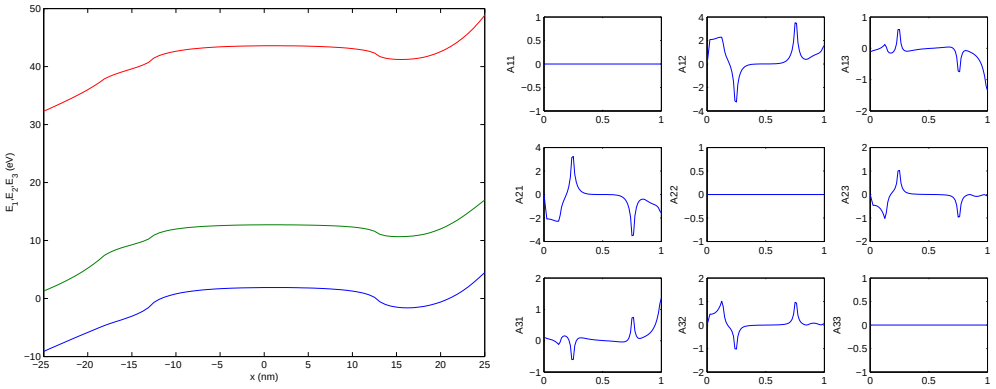

FIG. 6.2. *Left Panel: Band energies $E_\alpha(x)$. Right Panel: Coupling coefficients $A_{\alpha\beta}(x)$ for the first three terms in the sub-band expansion.*

case, without the coupling operator Q the current densities are constant in space. We see that the scattering between the different eigenspaces produces a significant (30%) reduction in the total current. Finally, we solve the same problem using 8 terms in the sub-band expansion. Figure 6.4 shows the corresponding particle densities on a logarithmic scale. We see, that the last 4 expansion terms do not contribute significantly to the over all solution any more.

7. Appendix.

7.1. The sub-band Hamiltonian in the Wigner picture . To write the commutator $[\mathcal{G}, R]$ in Section 2 in the Wigner transformed variables, i.e. to compute the operators $\mathcal{L}^0_{\alpha\alpha'}$, $\mathcal{L}^c$ in (2.9), it is necessary to express general linear differential operators acting on the $x-$ and $x'-$ variables in terms of the Wigner - Weyl transform and its inverse (2.6)-(2.7). We have the following

PROPOSITION 7.1. *Let the linear differential operator $D(x, \nabla_x)$ be given by $D(x, \nabla_x) = C(x)\nabla_x^k$ then, under the Wigner - Weyl transform (2.6), the differen-*

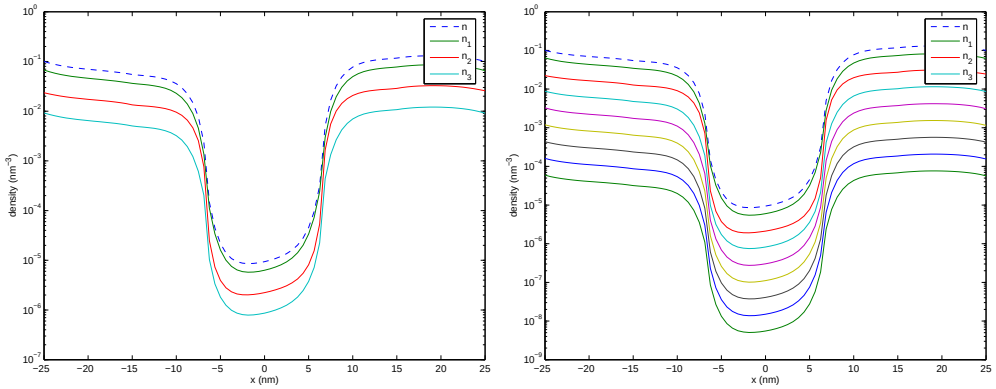

FIG. 6.3. *Sub-band densities $n_\alpha(x)$ and total particle density (dashed line) using three (left panel) and eight (right panel) expansion terms.*

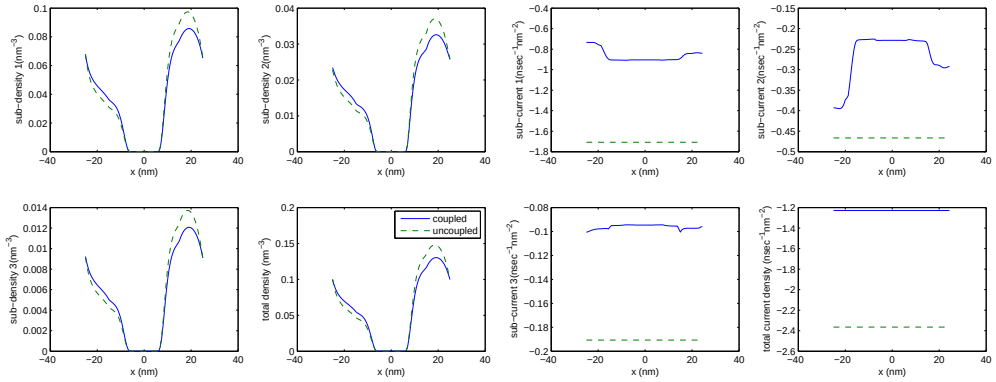

FIG. 6.4. *Comparison between the coupled and uncoupled case for three sub-bands. Left 4 Panels: particle densities. Right 4 panels: current densities. Solid lines: with coupling, Dashed lines: without coupling. Second bottom panel from left: total particle density. Fourth bottom panel from left: total current density.*

tial operator D, acting on the variable x, becomes

$$(7.1)\ \ (a)\ \mathcal{W}[D(x,\nabla_x)r(x,x')](x,p) = C(x+\frac{ih_x}{2}\nabla_p)\sum_j 2^{-j}\binom{k}{j}(\frac{ip}{h_x})^{k-j}\cdot\nabla_x^j f(x,p)$$

and the same differential operator D, acting on the variable x', becomes

$$(b)\ \mathcal{W}[D(x',\nabla_{x'})r(x,x')](x,p) = C(x-\frac{ih_x}{2}\nabla_p)\sum_j 2^{-j}\binom{k}{j}(-\frac{ip}{h_x})^{k-j}\cdot\nabla_x^j f(x,p)$$

Proof: We first use the inverse Wigner - Weyl transform, given by (2.7) and obtain

$$D(x,\nabla_x)r(x,x') = C(x)\nabla_x^k\int f(\frac{x+x'}{2},q)\exp[\frac{iq}{h_x}\cdot(x-x')]\ dq$$

$$= C(x)\int\sum_j\binom{k}{j}2^{-j}(\frac{iq}{h_x})^{k-j}\cdot\nabla_x^j f(\frac{x+x'}{2},q)\exp[\frac{iq}{h_x}\cdot(x-x')]\ dq\ .$$

Using the Wigner - Weyl transform (2.6) on this expression gives

$$\mathcal{W}[D(x,\nabla_x)r](x,p) = (2\pi)^{-d_x}\int C(x-\frac{h_x}{2}\eta)\sum_j \binom{k}{j} 2^{-j}(\frac{iq}{h_x})^{k-j}\cdot\nabla_x^j f(x,q)\exp[i\eta\cdot(p-q)]\,dqd\eta\,,$$

which is the usual definition of (7.1)(a) in pseudo differential operator notation. (7.1)(b) is obtained in a similar manner.

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Remark: In general the expressions $p^{k-j}\cdot\nabla_x^j$ in (7.1) have to be understood in tensor notation. We will only use Proposition 7.1 with $k=0,1,2$, i.e. for $1,\nabla_x,|\nabla_x|^2$, where the meaning of these terms is quite self -evident.

As a consequence of Proposition 7.1, a part of the Hamiltonian $\mathcal{G}_{\alpha\alpha'}$ in (2.3)(b) of the form $C_{\alpha\alpha'}(x)\nabla_x^k$ yields a contribution of the form

$$\frac{i}{h_x}\sum_{j\beta} 2^{-j}(\frac{i}{h_x})^{k-j}\binom{k}{j}[C_{\alpha\beta}(x+i\frac{h_x}{2}\nabla_p)p^{k-j}\cdot\nabla_x^j f_{\beta\alpha'}(x,p)-(-1)^{k-j}C_{\alpha'\beta}(x-i\frac{h_x}{2}\nabla_p)p^{k-j}\cdot\nabla_x^j f_{\alpha\beta}(x,p)]$$

to the Wigner transformed commutator $\mathcal{L}[f]=\frac{i}{h_x}\mathcal{W}[\mathcal{G},\mathcal{W}^{-1}f]$ in (2.8).

For the free Hamiltonian $-\frac{h_x^2}{2}\delta_{\alpha\alpha'}\Delta_x$ we have $k=2,\ C_{\alpha\alpha'}=-\frac{h_x^2}{2}\delta_{\alpha\alpha'}$, and the corresponding contribution to $\mathcal{L}$ is

$$p\cdot\nabla_x f_{\alpha\alpha'}(x,p)$$

For the term involving the sub - band energy E_α in (2.3) we have $k=0,\ C_{\alpha\alpha'}(x)=\delta_{\alpha\alpha'}E_\alpha(x)$, and consequently a contribution of the form

$$\frac{i}{h_x}[E_\alpha(x+\frac{ih_x}{2})-E_{\alpha'}(x-\frac{ih_x}{2}\nabla_p)]f_{\alpha\alpha'}(x,p)$$

Note, that the these first two terms are diagonal in the index α, and yield the usual uncoupled sub-band equations. This gives the operator $\mathcal{L}^0_{\alpha\alpha'}$ in (2.9)(b). We now turn to the coupling terms. For the first coupling term of the form $h_x^2 A_{\alpha\alpha'}\phi$ in (2.3)(b) we have $k=1,\ C_{\alpha\alpha'}=h_x^2A_{\alpha\alpha'}$, and consequently a contribution of the form

$$ih_x\sum_{j=0}^{1}\sum_\beta 2^{-j}(\frac{i}{h_x})^{1-j}[A_{\alpha\beta}(x+i\frac{h_x}{2}\nabla_p)p^{1-j}\nabla_x^j f_{\beta\alpha'}(x,p)-(-1)^{1-j}A_{\alpha'\beta}(x-i\frac{h_x}{2}\nabla_p)p^{1-j}\nabla_x^j f_{\alpha\beta}(x,p)]$$

$$=-\sum_\beta A_{\alpha\beta}(x+i\frac{h_x}{2}\nabla_p)\cdot p f_{\beta\alpha'}(x,p)+A_{\alpha'\beta}(x-i\frac{h_x}{2}\nabla_p)\cdot p f_{\alpha\beta}(x,p)$$

$$+\frac{ih_x}{2}\sum_\beta A_{\alpha\beta}(x+i\frac{h_x}{2}\nabla_p)\nabla_x f_{\beta\alpha'}(x,p)-A_{\alpha'\beta}(x-i\frac{h_x}{2}\nabla_p)\nabla_x f_{\alpha\beta}(x,p)$$

For the second coupling term in (2.3), involving the coefficient B, we have $k=0,\ C_{\alpha\alpha'}=\frac{h_x^2}{2}B_{\alpha\alpha'}$, and consequently a contribution of the form

$$\frac{ih_x}{2}\sum_\beta[B_{\alpha\beta}(x+i\frac{h_x}{2}\nabla_p)f_{\beta\alpha'}(x,p)-B_{\alpha'\beta}(x-i\frac{h_x}{2}\nabla_p)f_{\alpha\beta}(x,p)]$$

This gives the operator $\mathcal{L}^c$ in (2.9)(c).

7.2. The asymptotic form of the local thermal equilibrium. Proof of Theorem 4.2: The operator K in (4.11) is the Wigner transform of $\mathcal{G}+\chi$. So

$$K[f] = -\frac{1}{2}\mathcal{W}[(\mathcal{G}+\chi^{(m)})[R]], \quad f = \mathcal{W}[R]$$

holds. Again we use Proposition 7.1 together with the form (2.3) of the sub-band Hamiltonian $\mathcal{G}$. Setting $C = \frac{h_x^2}{4}\delta_{\alpha\alpha'},\ k=2$ in (7.1) gives

$$\mathcal{W}[\frac{h_x^2}{4}\delta_{\alpha\alpha'}\Delta_x R] = \delta_{\alpha\alpha'}[\frac{h_x^2}{16}\Delta_x f + \frac{ih_x}{4}p\cdot\nabla_x f - \frac{|p|^2}{4}f]$$

Setting $C = -\frac{1}{2}(E_\alpha(x)+\chi_\alpha^{(m)}(x)),\ k=0$ in (7.1) gives

$$\mathcal{W}[-\frac{1}{2}(E_\alpha(x)+\chi_\alpha^{(m)}(x))R] = -\frac{1}{2}(E_\alpha+\chi_\alpha^{(m)})(x+\frac{ih_x}{2}\nabla_p)f$$

This establishes the operator K_0 in (4.11)(b). To compute K^c we set $C = \frac{h_x^2}{2}A_{\alpha\alpha'},\ k=1$ in (7.1) and obtain

$$\mathcal{W}[\frac{h_x^2}{2}A_{\alpha\beta}R_{\beta\alpha'}] = A_{\alpha\beta}(x+\frac{ih_x}{2}\nabla_p)(\frac{ih_x}{2}pf_{\beta\alpha'} + \frac{h_x^2}{4}\nabla_x f_{\beta\alpha'})$$

∎

Proof of Theorem 5.1: In order to prove the result it is sufficient to expand the operators K^0, K^c in the Bloch equation (4.11) up to (inclusively) terms of order h_x. That is we consider the system

$$\partial_s\mathcal{R}_{\alpha\alpha'}(x,p,s) = \mathcal{K}[\mathcal{R}] = K[\mathcal{R}] + K[\mathcal{R}^{adj}]^{adj}$$

$$K[\mathcal{R}] = K^0[\mathcal{R}] - K^c[\mathcal{R}] = -\frac{ih_x}{4}p\cdot\nabla_x\mathcal{R}_{\alpha\alpha'} - \frac{|p|^2}{4}\mathcal{R}_{\alpha\alpha'} - \frac{1}{2}(E_\alpha+\chi_\alpha^{(n)})\mathcal{R}_{\alpha\alpha'} - \frac{ih_x}{4}\nabla_x(E_\alpha+\chi_\alpha^{(n)})\cdot\nabla_p\mathcal{R}_{\alpha\alpha'}$$

$$-\frac{ih_x}{2}\sum_{\nu\beta}A^\nu_{\alpha\beta}p_\nu\mathcal{R}_{\beta\alpha'} + O(h_x^2)$$

We note that the sub-band energy E_α can be absorbed into the Lagrange multiplier $\chi_\alpha^{(n)}$ which has to be determined by the sub-band densities n_α anyway. Using the definition of the operator $\mathcal{K}$ via the adjoint we obtain

$$\partial_s\mathcal{R}_{\alpha\alpha'}(x,p,s) = \mathcal{K}[\mathcal{R}]_{\alpha\alpha'} = -\frac{|p|^2}{2}\mathcal{R}_{\alpha\alpha'} - \frac{\chi_\alpha^{(n)}+\chi_{\alpha'}^{(n)}}{2}\mathcal{R}_{\alpha\alpha'} - \frac{ih_x}{4}(\nabla_x\chi_\alpha^{(n)} - \nabla_x\chi_{\alpha'}^{(n)})\cdot\nabla_p\mathcal{R}_{\alpha\alpha'}$$

$$-\frac{ih_x}{2}\sum_{\nu\beta}[A^\nu_{\alpha\beta}p_\nu\mathcal{R}_{\beta\alpha'} - A^\nu_{\alpha'\beta}p_\nu\mathcal{R}_{\alpha\beta}] + O(h_x^2), \quad \mathcal{R}_{\alpha\alpha'}(x,p,0) = \delta_{\alpha\alpha'}$$

We use the integrating factor $\Lambda_{\alpha\alpha'}(x,p,s) = \exp[-\frac{s|p|^2}{2} - \frac{s}{2}(\chi_\alpha^{(n)} + \chi_{\alpha'}^{(n)})]$ an set $\mathcal{R}_{\alpha\alpha'} = \Lambda_{\alpha\alpha'}U_{\alpha\alpha'}$, giving

$$\Lambda_{\alpha\alpha'}\partial_s U_{\alpha\alpha'} = -\frac{ih_x}{4}(\nabla_x\chi_\alpha^{(n)} - \nabla_x\chi_{\alpha'}^{(n)})\cdot\nabla_p(\Lambda_{\alpha\alpha'}U_{\alpha\alpha'}) - \frac{ih_x}{2}\sum_{\nu\beta}[A^\nu_{\alpha\beta}p_\nu\Lambda_{\beta\alpha'}U_{\beta\alpha'} - A^\nu_{\alpha'\beta}p_\nu\Lambda_{\alpha\beta}U_{\alpha\beta}] + O(h_x^2)$$

subject to the initial condition $U_{\alpha\alpha'}(x,p,s=0) = \delta_{\alpha\alpha'}$. Expanding $U_{\alpha\alpha'}$ into $U^0_{\alpha\alpha'} + h_xU^1_{\alpha\alpha'} + ...$ gives for the zero order term $U^0_{\alpha\alpha'}(x,p,s) = \delta_{\alpha\alpha'}$. The first order term satisfies the initial value problem

$$\Lambda_{\alpha\alpha'}\partial_s U^1_{\alpha\alpha'} = -\frac{i}{4}(\nabla_x\chi_\alpha^{(n)} - \nabla_x\chi_{\alpha'}^{(n)})\cdot\nabla_p(\Lambda_{\alpha\alpha'}\delta_{\alpha\alpha'}) - \frac{i}{2}\sum_{\nu\beta}[A^\nu_{\alpha\beta}p_\nu\Lambda_{\beta\alpha'}\delta_{\beta\alpha'} - A^\nu_{\alpha'\beta}p_\nu\Lambda_{\alpha\beta}\delta_{\alpha\beta}]$$

subject to homogeneous initial conditions. This gives, using the anti - symmetry of the matrices A^ν

$$\Lambda_{\alpha\alpha'}\partial_s U^1_{\alpha\alpha'} = -\frac{i}{2}\sum_\nu A^\nu_{\alpha\alpha'}p_\nu(\Lambda_{\alpha'\alpha'} + \Lambda_{\alpha\alpha}), \quad U^1_{\alpha\alpha'}(x,p,s=0) = 0$$

or, using the expression for the integrating factor $\Lambda_{\alpha\alpha'}$

$$\partial_s U^1_{\alpha\alpha'} = -i\cosh(\frac{s}{2}(\chi_\alpha^{(n)} - \chi_{\alpha'}^{(n)}))\sum_\nu A^\nu_{\alpha\alpha'}p_\nu, \quad U^1_{\alpha\alpha'}(x,p,s=0) = 0$$

$$\Rightarrow\ U^1_{\alpha\alpha'}(x,p,s) = -2i\frac{\sinh(\frac{s}{2}(\chi_\alpha^{(n)} - \chi_{\alpha'}^{(n)}))}{\chi_\alpha^{(n)} - \chi_{\alpha'}^{(n)}}\sum_\nu A^\nu_{\alpha\alpha'}p_\nu,$$

Consequently, the sub-band Maxwellian $\mathcal{M}^{(n)}$ is then given by

$$\mathcal{M}^{(n)}_{\alpha\alpha'} = \mathcal{R}_{\alpha\alpha'}|_{s=1} = \Lambda_{\alpha\alpha'}(U^0_{\alpha\alpha'} + h_xU^1_{\alpha\alpha'})|_{s=1} + O(h_x^2)\ \Rightarrow$$

$$\mathcal{M}^{(n)}_{\alpha\alpha'}(x,p) = \exp[-\frac{|p|^2}{2} - \frac{1}{2}(\chi_\alpha^{(n)} + \chi_{\alpha'}^{(n)})][\delta_{\alpha\alpha'} - 2ih_x\frac{\sinh(\frac{1}{2}(\chi_\alpha^{(n)} - \chi_{\alpha'}^{(n)}))}{\chi_\alpha^{(n)} - \chi_{\alpha'}^{(n)}}\sum_\nu A^\nu_{\alpha\alpha'}p_\nu] + O(h_x^2)$$

or

$$\mathcal{M}^{(n)}_{\alpha\alpha'}(x,p) = \exp(-\frac{|p|^2}{2})[\delta_{\alpha\alpha'}e^{-\chi_\alpha^{(n)}} - ih_x\frac{e^{-\chi_{\alpha'}^{(n)}} - e^{-\chi_\alpha^{(n)}}}{\chi_\alpha^{(n)} - \chi_{\alpha'}^{(n)}}\sum_\nu A^\nu_{\alpha\alpha'}p_\nu] + O(h_x^2)$$

Computing the moments of the sub-band Maxwellian up to order $O(h_x^2)$ gives

$$m^0\mathcal{M}^{(n)}_{\alpha\alpha'}(x) = (2\pi)^{d_x}\delta_{\alpha\alpha'}e^{-\chi_\alpha^{(n)}}, \quad m^1_\mu\mathcal{M}^{(n)}_{\alpha\alpha'}(x) = -(2\pi)^{d_x}ih_x\frac{e^{-\chi_{\alpha'}^{(n)}} - e^{-\chi_\alpha^{(n)}}}{\chi_\alpha^{(n)} - \chi_{\alpha'}^{(n)}}A^\mu_{\alpha\alpha'},$$

$$m^2_{\mu\nu}\mathcal{M}^{(n)}_{\alpha\alpha'}(x) = (2\pi)^{d_x}\delta_{\mu\nu}\delta_{\alpha\alpha'}e^{-\chi_\alpha^{(n)}}\ .$$

The Lagrange multipliers $\chi_\alpha^{(n)}$ have to be chosen such that on the diagonal $m^0\mathcal{M}^{(n)}_{\alpha\alpha} = n_\alpha$ holds. Therefore we obtain the relation $n_\alpha = (2\pi)^{d_x}e^{-\chi_\alpha^{(n)}}$ and, up to terms of order $O(h_x^2)$,

$$m^0\mathcal{M}^{(n)}_{\alpha\alpha'}(x) = \delta_{\alpha\alpha'}n_\alpha, \quad m^1_\mu\mathcal{M}^{(n)}_{\alpha\alpha'}(x) = ih_x\frac{n_{\alpha'} - n_\alpha}{\ln n_\alpha - \ln n_{\alpha'}}A^\mu_{\alpha\alpha'}$$

$$m^2_{\mu\nu}\mathcal{M}^{(n)}_{\alpha\alpha'}(x) = \delta_{\mu\nu}\delta_{\alpha\alpha'}n_\alpha \ .$$

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