

Milne Problem for Strong Force Scaling

Irene M. Gamba

Abstract

High field kinetic semiconductor equations with a linear collision operator are considered under strong force scaling corresponding to a strong non-equilibrium regime. Boundary and interface layers are studied and a kinetic half-space problem for a slab geometry is stated and solved analytically for negative constant fields.

The solution of this problem is necessary in order to produce numerical implementations of strong-weak forcing decomposition as already implemented in the kinetic linking of Boltzmann-Stokes equation for the linking of kinetic-fluid interfaces of gas flow.

Introduction

In this lecture I will summarize recent work in collaboration with Axel Klar on kinetic high field models and their associated macroscopic models and transition regimes.

These models have been considered in [CG1], [CG2], [TT], [FV], [Pp2], based on scalings taken from the range of parameters as obtained in the computational experiments in [BW] and recently in [CGJ].

However, up to now, no analysis of the kinetic boundary layer problem to find the correct boundary conditions for the fluid approximation has been performed. Such an analysis is also required, if one wants to solve the matching problem for kinetic and macroscopic equations. Here an interface regions between the two equations has to be considered. The matching problem has to be solved, for example, for domain decomposition approaches solving simultaneously kinetic and macroscopic equations in different regions of the computational domain.

Boundary and interface regions are described by a transition layer where a stationary kinetic equation is solved as in [C1]. For semiconductor models, see, e.g. [Pp1], [Ya] [KI].

We assume this layer to have slab symmetry, that is, the particle distribution is constant on surfaces parallel to the interface. (This is generically the case whenever the curvature of the interface is small compared to the reciprocal of the mean free path). Hence, the space coordinate reduces to x , the distance to the boundary or interface. After scaling it like $\frac{x}{\varepsilon}$, where ε is the order magnitude of the mean

1991 *Mathematics Subject Classification*. Primary 35Q35, 35B30, 82C40.

free path, one has to solve a kinetic half-space problem. Existence and uniqueness results for this half-space problem have been given in [GK] for a relaxation model and negative field. However they can be easily extended to a fully linear collision operator as pointed out to us by Naoufel Ben Abdallah [BA].

In fact, one is not really interested in the full solution of the half-space problem: the only objects of interest to obtain boundary or matching conditions are the asymptotic states and the outgoing distribution.

In fact, in [GK] we have described a numerical procedure which computes just those quantities by using a Chapman-Enskog type expansion to approximate the solution. The method is seen to converge very fast numerically. For approaches to the numerical solution of the standard half-space problem in gas dynamics and semiconductor equations we refer to [AS],[Co],[GA], [ST] and for a mathematical investigation to [AC], [CGS] and [GMP].

The High Field Semiconductor Equations

We consider the semi-classical Boltzmann equation for an electron gas in a semiconductor in the parabolic band approximation in nondimensionalized form with the high field (strong force) scaling:

$$\eta \partial_t f + v \cdot \nabla_z f - \frac{\eta}{\varepsilon} E(z, t) \cdot \nabla_v f = \frac{1}{\varepsilon} Q(f)$$

with $z, v \in \mathbb{R}^3$. The collision operator reads

$$Q(f) = \int s(v, v') [M(v)f(v') - M(v')f(v)] dv' = Q^+(f) - Q^-(f),$$

where

$$0 < s_0 \leq s(v, v') \leq s_1 < +\infty \quad \text{and} \quad s(v, v') = s(v', v).$$

Here we denoted by M the centered, reduced Maxwellian $M = (2\pi)^{-\frac{3}{2}} \exp(-\frac{v^2}{2})$, $E = E(z, t) = -\nabla_z \Phi$ denotes the opposite to the electric field, which is determined by a Poisson equation for the potential Φ :

$$\nabla_z \cdot (\nabla_z \Phi) = \gamma \left(\frac{1}{\eta^d} \int_{\mathbb{R}^3} f dv - C(z) \right).$$

The function $C(z)$ denotes the ion background. The parameters η, γ are dimensionless and of order $O(1)$. The scaled mean free path ε is of order $O(\varepsilon) \ll 1$. This is the high field scaling, see [CG1].

To obtain the boundary or interface layer equations we fix a point \hat{z} on the boundary and re-scale as usual the space coordinate in the layer normal to the boundary with the mean free path ε , introducing the new coordinate x orthogonal to the boundary:

$$x = \frac{(z - \hat{z}) \cdot n}{\varepsilon}.$$

Here, n denotes the normal to the boundary or interface. This yields the new coordinates (x, \hat{z}) instead of z in the layer. To $O(1)$ one obtains from the rescaled transport equation for a bounded field E at \hat{z} :

$$v \cdot n \partial_x \varphi - \eta E \cdot \nabla_v \varphi = Q(\varphi)$$

where $x \in [0, \infty)$ and $E = E(x = 0, \hat{z}, t)$ does not depend on x . This problem has to be supplied with the in going function at the boundary, i.e. at $x = 0$: We have to prescribe $\varphi(0, v), v \cdot n > 0$.

To simplify the problem, we assume from now on that the z_1 -coordinate points in the direction of the normal, that $E = (E_1, 0, 0)$ and that $\eta = 1$. Then the above reduces to the following one dimensional problem

$$v_1 \partial_x \varphi - E_1 \partial_{v_1} \varphi = Q(\varphi)$$

with $x \in [0, \infty), v_1 \in \mathbb{R}, \varphi = \varphi(x, v_1)$. M is now the one-dimensional Maxwellian $M(v) = (2\pi)^{-\frac{1}{2}} \exp(-\frac{v^2}{2}), v \in \mathbb{R}$ and we have used the definition $\langle f \rangle := \int_{\mathbb{R}} f(v) dv$.

One observes that

$$\partial_x \langle v\varphi \rangle = 0,$$

which means $\langle v\varphi \rangle$ is constant in x .

We shall pose the half-space problem for strong forcing and sketch the proof presented in [GK].

The Milne Problem for Strong Negative Field E

For given $-E$ a positive constant, let $P = P(E, v)$ be the unique distribution that solves the problem

$$(1) \quad E \frac{\partial P}{\partial v} = Q(P), \quad \int P dv = 1.$$

We shall call P the space homogeneous stationary solution. In fact, P is the leading term of the the renormalized distribution function obtained by the Chapman-Enskog expansion under a strong force scaling, given the higher order term to a distribution corresponding to strong non-equilibrium states.

The solvability of (1) in L^∞ can be found in Trugman and Taylor [TT] for the relaxation type operator in one dimension, has also been discussed in Frosali, Van der Mee and Pavari Fontana [FV] and Poupaud [P1] for the general linear collision operators (in L^1).

In the case of the relaxation operator with relaxation parameter τ (that is when $s(v, v') = \text{constant} = \tau^{-1}$), the distribution solution P satisfies the following explicit formula for $u = -\tau E$ given by

$$(2) \quad P_u = \frac{1}{u} \exp\left(-\frac{\lambda}{u}\right) \text{erf}\left(\frac{\lambda}{\sqrt{2\theta}}\right),$$

with $u > 0, \lambda = v - \frac{2\theta}{u}$ and $\text{erf}(x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^x e^{-t^2} dt$.

For $u < 0$, the solution is given by $P_u(v) = P_{-u}(-v)$.

In this case P satisfies

$$\langle vP \rangle = u \quad \text{and} \quad \langle v^2 P \rangle = 1 + 2u^2.$$

Clearly, P yields distributions that are small perturbations of strong non-equilibrium states.

Hence, in the general linear case, we consider the following problem

$$(3) \quad \begin{cases} v \frac{\partial f}{\partial x} + E \frac{\partial f}{\partial v} = Q(f) \\ f(0, v) = k(v) \quad \text{on } v > 0, \quad 0 \leq k(v) \leq KP(v). \end{cases}$$

The following theorem shows that the solution of problem (3) is unique and relaxes to a multiple of P when the space variable tends to infinity.

THEOREM. (Strong forcing Milne problem) *If $-E > 0$, then problem (3) has a **unique** solution φ with $0 \leq \varphi \leq KP(E, v)$, K a positive constant, $P(E, v)$ the space-homogeneous solution of the stationary equation (1). Moreover,*

$$(4) \quad \lim_{x \rightarrow \infty} \varphi(x, v) = \lambda_{\infty} P(v), \quad \text{with } 0 \leq \lambda_{\infty} \leq K .$$

The proof of this theorem, contained in [GK] for the relaxation case, requires several intermediate steps. The extension to the linear case follows the same strategy as in the relaxation case.

1. The first step consists in making a construction of a solution for the half space problem (3). This is done by the construction of minimal and maximal solutions that control any possible solution of (3) by a constant factor of the homogeneous solution P .
2. The second step is to study the asymptotic behavior of the solutions as the space variable x goes to infinite, i.e the limiting behavior in (4). This step requires several estimates:
 - The control the gain operator (or the average of f in the relaxation case) by a factor μ_0 of the gain operator acting on P . The multiplicative factor μ_0 depends on λ given by the quotient of the first moments of f by P .
 - The construction of a decreasing sequence μ_k and an increasing unbounded one x_k , such that an upper estimate for f by a factor μ_k of P is obtained whenever the gain operator acting on f is bounded above by a factor μ_k of the gain operator acting on P , in a set depending on the characteristic surfaces of the equation (3) that passes through x_k , that is

$$Q^+(f) \leq \mu_k Q^+(P) \quad \text{for } (x, v) \in D_k = \left\{ (x, v), x \geq x_k, v \leq \sqrt{2E(x - x_k)} \right\},$$

then $f \leq \mu_k P$ on D_k . In addition the sequence μ_k is telescoping and bounded below by λ .

- From the two previous estimates, as k goes to infinity, $\mu_k \rightarrow \lambda$, $x_k \rightarrow \infty$ and (4) holds with $\lambda_{\infty} = \lambda$.
3. The third and final step consists into proving uniqueness in within the class of functions that satisfy the data and the homogeneous behavior at infinity.

References

- [AS] K. Aoki and Y. Sone, *Gas Flows Around the Condensed Phase with Strong Evaporation or Condensation*, Advances in Kinetic Theory and Continuum Mechanics, Proceedings of a Symposium in Honor of H. Cabannes (1991).
- [AC] M.D. Arthur and C. Cercignani, *Nonexistence of a Steady Rarefied Supersonic Flow in a Half Space*, ZAMP, Vol 31, (1980).
- [BW2] H.U. Barenger and J.W. Wilkins, *Ballistic structure in the electron distribution function of small semiconducting structures: General features and specific trends*, Physical Review B **36** No 3 (1987), 1487–1502.
- [BA] N. Ben Abdallah, *Personal communication* (1998).
- [C1] C. Cercignani, "Half-space problems in the Kinetic Theory of Gases", *Trends in Applications of Pure Mathematics to Mechanics*, Edited by E. Kröner and K. Kirchgässner, Springer, Berlin (1986).
- [CG1] C. Cercignani, I.M. Gamba, and C.D. Levermore, *High field approximations to a Boltzmann-Poisson system boundary conditions in a semiconductor*, Applied Math Letters, Vol 10 (4), pp.111-118, (1997).
- [CG2] C. Cercignani, I.M. Gamba, and C.L. Levermore, *A High Field Approximation to a Boltzmann-Poisson System in Bounded Domains*, TICAM report 97-20, submitted for publication (1998).
http://www.ma.utexas.edu/mp_arc/e/98-69.ps.
- [CGJ] C. Cercignani, I.M. Gamba, J. Jerome, and C.W. Shu, *Device Benchmark Comparisons via Kinetic, Hydrodynamic and High-Field Models*, to appear in CMAME (1999).
- [Co] F. Coron, *Computation of the Asymptotic States for Linear Halfspace Problems*, TTSP, 19 (1990).
- [CGS] F. Coron, F. Golse and C. Sulem, *a classification of well posed Kinetic problems*, Communications in Pure and Applied Mathematics, vol. 41, 4, pp.409–436, (1988).
- [FV] G. Frosali, C.V.M. van der Mee and S.L. Pavari Fontana, *Conditions for run-away phenomena in the kinetic theory of particle swarms*, J. Math. Physics, **30**(5), 1177–1186 (1989).
- [GK] I.M. Gamba and A. Klar, *The Milne problem for high field kinetic semiconductor equations*, preprint, submitted for publication (1998).
- [GA] F. Golse and A. Klar, *A Numerical Methods for Computing Asymptotic States and Outgoing Distributions for Kinetic Linear Half Space Problems* J. Statist. Phys. **80** no. 5–6, 1033–1061 (1995).
- [GMP] W. Greenberg, C. van der Mee and V. Protopopescu, *Boundary Value Problems in Abstract Kinetic Theory*, Birkhäuser, (1987).
- [Kl] A. Klar, *A Numerical Method for Kinetic Semiconductor Equations in the Drift Diffusion Limit*, to appear in SIAM J. Sci. Comp. (1998).
- [Pp1] F. Poupaud, *Diffusion Approximation of the Linear Semiconductor Equation*, J. Asympt. Anal., **4**:293 (1991).
- [Pp2] F. Poupaud, *Runaway Phenomena and Fluid Approximation Under High Fields in Semiconductor Kinetic Theory* ZAMM. Z. angew. Math. Mech. **72** 8, 359-372, (1992).
- [ST] C.E. Siewert and J.R. Thomas, *Strong Evaporation into a Half Space II*, Z. Angew. Math. Physik, **33**:202, (1982).

- [TT] S. A. Trugman and A. J. Taylor, *Analytic solution of the Boltzmann equation with applications to electron transport in inhomogeneous semiconductors*. *Phys. Rev. B* **33**, 5575–5584 (1986).
- [Ya] A. Yamnahakki, *Second order boundary conditions of Drift Diffusion Equations of Semiconductors*, *Math. Meth. Appl. Sci.*, **5**:429, (1995).

DEPARTMENT OF MATHEMATICS, THE UNIVERSITY OF TEXAS AT AUSTIN, AUSTIN, TX 78712-1082