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DERIVATION OF THE HIGH FIELD SEMICONDUCTOR EQUATIONS

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Abstract. Electron and hole densities evolve in x - z phase space according to Boltzmann equations. When the mean free path of the particles is short *and* the electric force on the particles is weak, a well-known expansion (the Hilbert expansion) can be used to solve the Boltzmann equation. This asymptotic solution shows that the spatial density of electrons and holes evolves according to diffusion-drift equations. In fact, the Hilbert expansion leads directly to the Basic Semiconductor (van Roosbroeck) Equations.

As devices become smaller, electric fields become stronger, which renders the Basic Semiconductor Equations increasingly inaccurate. To remedy this problem, we use singular perturbation techniques to obtain a new asymptotic expansion for the Boltzmann equation. Like the Hilbert expansion, the new expansion requires the mean free path to be short compared to all macroscopic length scales. However, it does *not* require the electric forces to be weak. The new expansion shows that spatial densities obey diffusion-drift equations as before, but the diffusivity D and mobility μ turn out to be nonlinear functions of the electric field. In particular, our analysis determines the field-dependent mobilities $\mu(E)$ and diffusivities $D(E)$ directly from the scattering operator. By carrying out this asymptotic expansion to higher order, we obtain the high frequency corrections to the drift velocity and diffusivity, and also the corrections due to gradients in the electric field. Remarkably, we find that Einstein's relation is still satisfied, even with these corrections.

The new diffusion-drift equations, together with Poisson's equation for the electric field, form the *high-field semiconductor equations*, which can be expected to be accurate regardless of the strength of the electric fields within the semiconductor. In addition, our analysis determines the entire momentum distribution of the particles, so we derive a very accurate *first moment model* for semiconductors by substituting the asymptotically-correct distribution back into the Boltzmann equation and taking moments; this model is roughly analogous to a hydrodynamic model without an energy equation. Finally, we present the extension of the high field diffusion-drift equations to three dimensions.

1. introduction. Particle densities in *phase-space* usually evolve according to Boltzmann equations (also called transport, or kinetic equations). Here we analyze the Boltzmann equations which govern electrons and holes in semiconductors in the "short mean free path" regime.

If the mean free path is short *and* the electric force on the particles is weak, a well-known asymptotic expansion (the Hilbert expansion [1,2]) can be used to reduce Boltzmann equations to radically simpler diffusion-drift equations. When the Hilbert

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expansion is used for both the electron and hole populations, and when Poisson's equation is used to determine the electric field from the particle densities, the resulting system of equations is the *Basic Semiconductor Equations* (BSEs), or van Roosbroeck equations [3]. In the past, these equations have provided the basis for most VLSI device modeling [2-5]. As semiconductor devices become smaller, however, the strength of their internal electric fields increases dramatically. As a result, the BSEs become increasingly inaccurate as device sizes shrink, and are not useful for predicting the operating characteristics of VLSI devices much smaller than a micron. However, the Boltzmann equation is expected to be valid in VLSI structures down to $0.1\mu\text{m}$ in size [6,7].

Here we use singular perturbation techniques to analyze the Boltzmann equation in one spatial dimension. (The corresponding three dimensional analysis is done in [9].) This analysis yields a new asymptotic expansion for the Boltzmann equation which does *not* require the electric forces to be weak. As in the Hilbert expansion, we find that the *spatial densities* (as opposed to *phase-space densities*) evolve according to diffusion-drift equations to leading order. However, the diffusivity D and mobility μ turn out to be nonlinear functions of the electric force on the particles, and our analysis shows how the correct field-dependent mobilities $\mu(E)$ and diffusivities $D(E)$ can be found directly from the scattering operator. By carrying out this asymptotic expansion through $O(\epsilon)$, we also obtain the corrections to the drift velocity and diffusion coefficient due to gradients in the electric fields, as well as the high frequency corrections to the diffusion-drift equation. Remarkably, Einstein's relation [8] is still satisfied, even with these corrections.

Our analysis yields the entire phase-space distribution of the particles. So in §7 we derive a very accurate *first moment model* by substituting the asymptotically-correct momentum distribution into the Boltzmann equation, and equating the zeroeth and first-order moments. The resulting model is like a diffusion-drift model with some non-locality in the particle currents; equivalently, it is similar to a hydrodynamic model without an energy equation. However, as we shall see, the nonlinear advection term is exactly canceled by the stress tensor, so this model predicts that electron shock waves will not form. Finally, in Appendix A we apply this work to the Boltzmann equations governing both electrons and holes, and thus derive the correct *high-field semiconductor equations*. In §8 we also present the results for three spatial dimensions, which are obtained in [9].

To simplify the analysis, we assume that only electrons in a single conduction band and holes in a single valence band are important; multiple bands and valleys

are considered elsewhere [10]. Since the analysis for electrons and holes is virtually identical, we only present the analysis for electrons; the corresponding results for holes are given as part of the high field semiconductor equations in Appendix A. We use standard notation for general kinetic (transport) theory; the more specialized notation for semiconductors is also given in Appendix A. Define

$$1.1a \quad p(t, \mathbf{x}, z) = \text{density of electrons in } \mathbf{x}\text{-}z \text{ phase space ,}$$

$$1.1b \quad v(z) = \text{velocity of an electron with momentum } z .$$

Here $z \equiv \hbar k$ is the *crystal momentum* of the electron, where k is the electron's wavenumber. Thus, z is a periodic variable with a period corresponding to the first Brillouin zone. In addition, the velocity in 1.1b is given by $v(z) = \mathcal{E}'(z)$, where $\mathcal{E}(z)$ is the appropriate band energy. See Appendix A. Before continuing, let us define the usual inner product

$$1.2 \quad \langle f, g \rangle \equiv \int f^*(z) g(z) dz .$$

(Unless stated otherwise, all z integrals are to be taken over the first Brillouin zone). Let us also define the adjoint $\mathcal{L}^+$ of a linear operator $\mathcal{L}$ by

$$1.3 \quad \langle f, \mathcal{L}g \rangle \equiv \langle \mathcal{L}^+ f, g \rangle \text{ for all } f(z) , g(z) .$$

With this notation, the Boltzmann equation for electrons in a semiconductor is

$$1.4 \quad p_t + v(z)p_x + F(x)p_z = \mathcal{L}p ,$$

where $F(x) = -qE(x)$ is the force on the electrons. On the left side are the streaming terms, which account for the advection of electrons through phase-space. On the right side is the *scattering operator* $\mathcal{L}$, which accounts for “collisions” of the electrons, both among themselves and with other constituents of the environment, such as phonons and impurities. The scattering operator acts only on the z dependence of p , and determines how the momentum distribution of the electrons evolves due to collisions. In this paper we restrict ourselves to linear scattering operators, which restricts us to applications with moderate electron densities.

To ensure that the scattering operator and Boltzmann equation are physically sensible, we require them to satisfy the following properties:

A. *Symmetry*. We assume that $v(z)$ is odd in z and that $\mathcal{L}$ is even:

$$1.5 \quad v(z) = -v(-z) ; \quad f(z) = \mathcal{L}p(z) \Rightarrow f(-z) = \mathcal{L}p(-z) .$$

B. *Conservation of particles*. Scattering processes cannot create or destroy electrons, so we have

$$1.6 \quad \langle 1, \mathcal{L}p \rangle \equiv \int \mathcal{L}p \, dz = 0 \quad \text{for any } p(z) .$$

C. *Equilibrium*. In the absence of external forces and spatial gradients, the momentum distribution $p(t, z)$ must relax to equilibrium. Thus, the equation

$$1.7 \quad p_t = \mathcal{L}p$$

must have a unique (normalized) stable steady solution, namely the *equilibrium distribution* $r(z)$, which satisfies

$$1.8a \quad \mathcal{L}r = 0 , \quad \langle 1, r \rangle = 1 .$$

Since the scattering operator $\mathcal{L}$ is linear, to be physically consistent we must take $r(z)$ to be Maxwellian:

$$1.8b \quad r(z) = \frac{1}{N_0} \exp\{-\beta \mathcal{E}(z)\} ,$$

with

$$1.8c \quad v(z) = \frac{d}{dz} \mathcal{E}(z) \quad \text{and} \quad \beta = 1/k_B T .$$

Here $\mathcal{E}(z)$ is the kinetic energy (band energy) at momentum z , and the normalization constant, N_0 , is given by $\langle 1, e^{-\beta \mathcal{E}(z)} \rangle$.

D. *Detailed balance*. The scattering operator must satisfy detailed balance, so

$$1.9 \quad \mathcal{L}\{qr\} = r(z)\mathcal{L}^+q \quad \text{for any } q(z) .$$

E. *Fredholm Index 0*. Since $\langle 1, \mathcal{L}p \rangle = 0$ for any $p(z)$, the problem

$$1.10a \quad \mathcal{L}p = f$$

can only have a solution if

$$1.10b \quad \langle 1, f \rangle = 0 .$$

We assume that $\mathcal{L}$ is a Fredholm operator with index 0, so that $\langle 1, f \rangle = 0$ is a necessary *and* sufficient condition for $\mathcal{L}p = f$ to be solvable. Similarly, the adjoint problem $\mathcal{L}^+q = g$ is solvable if and only if the Fredholm condition $\langle g, r \rangle = 0$ is satisfied.

Note that the conservation property, 1.6, implies that

$$1.11a \quad \mathcal{L}^+1 = 0,$$

and the symmetry property implies that $r(z)$ and $\mathcal{E}(z)$ are even:

$$1.11b \quad r(z) = r(-z), \quad \mathcal{E}(z) = \mathcal{E}(-z).$$

2. Non-dimensionalization. The first step in analyzing the Boltzmann equation is non-dimensionalization. A typical momentum scale for the scattering process, z_{th} , can be obtained from the equilibrium momentum distribution $r(z)$. (See figure below.) Then $v_{th} \equiv v(z_{th})$ can be used to define a natural velocity scale. The speed at which a typical solution $p(t, z)$ of 1.7 approaches $r(z)$ can be used to define a characteristic timescale for the scattering process, the *thermalization time* τ_{th} . The *mean free length*, also called the *scattering length*, can now be defined as

$$2.1 \quad \ell = v_{th}\tau_{th} = v(z_{th})\tau_{th}.$$

Crudely speaking, the mean free length represents the typical distance a group of electrons can travel (in the absence of any applied forces) before they attain their equilibrium distribution $r(z)$. Let L be a typical macroscopic length scale, and define

$$2.2 \quad \varepsilon = \ell/L.$$

Finally, let E_{typ} be the typical size of the electric field, so that $f_{det} = qE_{typ}$ is the typical magnitude of the force $F(x)$, and define

$$2.3 \quad z_{det} = f_{det}\tau_{th}.$$

Crudely speaking, z_{det} is the typical momentum change caused by the force F between significant scattering events; clearly z_{det} represents a balance between the acceleration due to $F(x)$, and the “randomization” of z due to scattering events.

To non-dimensionalize 1.4, let

$$2.4a \quad x_{\text{new}} = x/L, \quad z_{\text{new}} = z/z_{\text{th}}, \quad v_{\text{new}} = v/v_{\text{th}}, \quad t_{\text{new}} = \varepsilon^2 t/\tau_{\text{th}}$$

$$2.4b \quad F_{\text{new}} = F/f_{\text{det}}, \quad \mathcal{L}_{\text{new}} = \tau_{\text{th}} \mathcal{L}, \quad \mathcal{E}_{\text{new}} = \mathcal{E}/(v_{\text{th}} z_{\text{th}}), \quad \beta_{\text{new}} = (v_{\text{th}} z_{\text{th}}) \beta.$$

In terms of the new variables, 1.4 becomes

$$2.5 \quad \varepsilon^2 p_t + \varepsilon v(z) p_x + \kappa F(x) p_z = \mathcal{L} p,$$

where $\kappa = z_{\text{det}}/z_{\text{th}}$.

In this paper we solve 2.5 using singular perturbation techniques based on $\varepsilon \ll 1$; that is, on the scattering length ℓ being much shorter than any macroscopic length scale. Consequently, this analysis is only valid in regions where the electric field $E(x)$ changes slowly on length scales comparable to ℓ . Similarly, if we were to allow $\mathcal{L}$ to vary with x , then we would have to require $\mathcal{L}$ to vary slowly on length scales comparable to ℓ .

There are two extremely important distinguished limits of 2.5,

$$\kappa = O(\varepsilon) \quad \text{weak force regime},$$

$$\kappa = O(1) \quad \text{strong force regime}.$$

Below we obtain the asymptotic solution of 2.5 for both regimes. For the weak force regime, this solution is just the well-known *Hilbert expansion* [1,2], which is presented below for completeness. For the strong force regime, the asymptotic solution of the Boltzmann equation was previously unknown, and represents the key advance in our work.

Both the Hilbert expansion and our new results represent *outer solutions*. Next to all material interfaces and spatial boundaries, there exist extremely thin *kinetic boundary layers*, which are only one or two scattering lengths thick. Both the Hilbert expansion and our results are not valid within such boundary layers. Even though these boundary layers are extremely thin, they can play important roles in semiconductors. We are currently developing analytical and numerical techniques for resolving such layers. Besides these boundary layers, there are usually rapidly-

decaying initial layers, which die out on the ultra-short $t \sim O(\epsilon^2)$ timescale; the results presented here are not valid during this time.

3. Weak force analysis (Hilbert expansion). Here we analyze the weak force regime. Without loss of generality, we take $\kappa = \epsilon$ and analyze

$$3.1 \quad \epsilon^2 p_t + \epsilon v(z) p_x + \epsilon F(x) p_z = \mathcal{L}p .$$

To obtain the outer solution to 3.1, we expand $p(t, x, z)$ as

$$3.2a \quad p(t, x, z) = p^0(t, x, z) + \epsilon p^1(t, x, z) + \epsilon^2 p^2(t, x, z) + \dots ,$$

where the expansion will be constructed so that

$$3.2b \quad \langle 1, p^i \rangle = 0 \quad \text{for } i = 1, 2, 3, \dots .$$

Hence the spatial density of electrons, $\langle 1, p \rangle$, will be given by the leading term $\langle 1, p^0 \rangle$.

Substituting 3.2 into 3.1, we obtain

$$3.3 \quad \mathcal{L}p^0 = 0 .$$

Thus,

$$3.4 \quad p^0(t, x, z) = n(t, x) r(z) ,$$

where the coefficient $n(t, x)$ is unknown at this stage of the expansion. Note that

$$n(t, x) = \langle 1, p^0(t, x, z) \rangle = \langle 1, p(t, x, z) \rangle ,$$

so $n(t, x)$ is the spatial density of electrons.

At $O(\epsilon)$ we have

$$3.5a \quad \mathcal{L}p^1 = v(z) p_x^0 + F(x) p_z^0 = (n_x - \beta F n) v(z) r(z) ,$$

$$3.5b \quad \langle 1, p^1 \rangle = 0 .$$

See eq. 1.8. Since $v(z)r(z)$ is odd in z , the Fredholm alternative 1.10b is satisfied, and the problem

$$3.6a \quad \mathcal{L}\tilde{r} = -v(z)r(z)$$

is solvable. We define $\tilde{r}(z)$ uniquely by requiring it to be odd,

$$3.6b \quad \tilde{r}(z) = -\tilde{r}(-z) .$$

Then $\langle 1, \tilde{r} \rangle = 0$, so the solution of 3.5 is

$$3.7 \quad p^1(t, x, z) = -(n_x - \beta F n) \tilde{r}(z) .$$

At $O(\varepsilon^2)$, eq. 3.1 yields

$$3.8 \quad \begin{aligned} \mathcal{L}p^2 &= p_t^0 + v p_x^1 + F p_z^1 \\ &= n_t r(z) - (n_x - \beta F n)_x v(z) \tilde{r}(z) - F(n_x - \beta F n) \tilde{r}'(z) . \end{aligned}$$

Since $\tilde{r}'(z)$ is a derivative, clearly $\langle 1, \tilde{r}'(z) \rangle = 0$, so applying the solvability condition to 3.8 yields the diffusion-drift equation

$$3.9a \quad n_t = D_0 n_{xx} - \mu (F n)_x + \dots \quad (\text{weak force}) ,$$

where the diffusivity D_0 and mobility μ are given by

$$3.9b \quad D_0 \equiv \langle v, \tilde{r} \rangle , \quad \mu = \beta D_0 \equiv D_0 / k_B T .$$

Thus, the phase-space density is given by

$$3.9c \quad p(t, x, z) = n \cdot r(z) - \varepsilon \{n_x - \beta F n\} \tilde{r}(z) + \dots \quad (\text{weak force}) ,$$

where the spatial density of electrons, $n(t, x)$, evolves according to 3.9a. Note that 3.9b shows that the Einstein relation, $D_0 = k_B T \mu$, is satisfied [8].

In Appendix B we carry out this expansion to higher order, and obtain the correct diffusion-drift equation through $O(\varepsilon^2)$. See eqs. B.17.

4. Strong force results. Scaling. We now investigate the strong force regime. Without loss of generality, we take $\kappa = 1$ and analyze

$$4.1 \quad \varepsilon^2 p_t + \varepsilon v(z) p_x + F(x) p_z = \mathcal{L}p \quad (\text{strong force}) .$$

To obtain the right overall scaling for this case, it is helpful to consider the weak force result 3.9a with F replaced by F/ε :

$$4.2 \quad n_t = D_0 n_{xx} - \mu (F n)_x / \varepsilon .$$

Even though this equation is *not* correct, it should still enable us to predict the scaling for the strong force regime.

Eq. 4.2 shows that the density p depends on the short t/ε timescale. From the steady state of 4.2, we see that p also depends on the short $\tilde{x} = x/\varepsilon$ space scale. Now, at first sight it may appear that since p depends on the x/ε space scale, it must also depend on the very short t/ε^2 timescale. Apart from a rapid initial transient, this is not true. Consider the evolution of a packet of electrons which is initially smooth on the $O(1)$ space scale. Eq. 4.2 implies that the packet will advect rapidly with velocity $\mu F(x)/\varepsilon$ until it reaches a stagnation point, where the force $F(x)$ is zero. Near the stagnation point, the much weaker force will slowly compress the packet, while diffusion will tend to spread the packet out. It is only the long-time balance of these two effects that results in the eventual narrow spatial distribution. So after the rapid initial transient dies out, $p(t,x,z)$ will depend on timescales no shorter than t/ε . Consequently, we can drop the transient term $\varepsilon^2 p_t$ in 4.1 to leading order, and study

$$4.3 \quad \varepsilon v(z)p_x = \mathcal{L}p - F(x)p_z .$$

Since we expect p to depend on the short x/ε space scale, we cannot drop the $\varepsilon v(z)p_x$ term, and must solve the full steady transport equation. However, even though we expect the solution p to depend on the short x/ε scale, note that eq. 4.3 depends explicitly on x only through the force $F(x)$. Thus, the equation itself varies only over the $O(1)$ space scale. Our asymptotic analysis is based on exploiting the disparity between the $O(\varepsilon)$ length scale of the solution, and the $O(1)$ length scale of the equation.

The asymptotic analysis is carried out in §5 and §6. The final result can be expressed simply in terms of eigenvalues and eigenfunctions of 4.3. Separating variables,

$$4.4 \quad p = e^{\lambda x/\varepsilon} \Theta(z) ,$$

leads to an eigenvalue problem parameterized by F :

$$4.5 \quad \mathcal{M}(F)\Theta \equiv \mathcal{L}\Theta - F\Theta_z = \lambda v(z)\Theta .$$

Two eigenfunctions turn out to be crucial. First, it is easily seen that $\lambda = 0$ is an eigenvalue at each F . Indeed, the adjoint of $\mathcal{M}$ is

$$4.6 \quad \mathcal{M}^+q = \mathcal{L}^+q + Fq_z ,$$

and since $\mathcal{L}^+1 = 0$ (see 1.11a), clearly $\mathcal{M}^+1 = 0$. Therefore $\mathcal{M}^+$, and hence $\mathcal{M}$, must have a zero eigenvalue. So at each F there must be a null function $\phi(z;F)$ satisfying

$$4.7a \quad \mathcal{M}\phi \equiv \mathcal{L}\phi - F\phi_z = 0 , \quad \langle 1, \phi \rangle = 1 .$$

Also, clearly the equilibrium distribution $r(z)$ is an eigenfunction with eigenvalue $\lambda = \beta F$:

$$4.7b \quad \mathcal{M}r \equiv \mathcal{L}r - Fr_z = \beta Fv(z)r(z) , \quad \langle 1, r \rangle = 1 ,$$

since $\mathcal{L}r = 0$ and $r_z = -\beta vr$.

The asymptotic analysis in §6 shows that the solution of the Boltzmann equation 4.1 is

$$4.8a \quad p(t,x,z) = n(t,x)r(z) + \left(n - \frac{\varepsilon n_x}{\beta F} \right) (\phi(z;F) - r(z)) + \dots \quad (\text{strong force})$$

to leading order. Here $n(t,x) \equiv \langle 1, p(t,x,z) \rangle$ is the spatial density of electrons, and satisfies the diffusion-drift equation

$$4.8b \quad n_t = (Dn_x)_x - (vn)_x/\varepsilon + \dots \quad (\text{strong force})$$

to leading order, where the diffusivity $D(F)$ and the drift velocity $v(F)/\varepsilon$ are nonlinear functions of the electric force F :

$$4.8c \quad D(F) \equiv \langle v, \phi \rangle / \beta F , \quad v(F) \equiv \langle v, \phi \rangle .$$

Here $\phi(z;F)$ is defined by 4.7a. Despite the βF denominators in 4.8, none of the quantities in 4.8 are singular at $F = 0$. In fact, it turns out that 4.8 reduces exactly to the weak force result 3.9 in the limit $F \rightarrow 0$.

Also, to revert back to the original *dimensional* variables (see 2.4), one simply has to set $\varepsilon = 1$ in 4.8.

5. Eigenvalues and eigenfunctions. In this section we introduce the eigenfunctions and adjoint eigenfunctions needed to solve eq. 4.1. Consider the eigenvalue problem parameterized by F ,

$$5.1a \quad \mathcal{M}(F)p \equiv \mathcal{L}p - Fp_z = \lambda v(z)p ,$$

and its adjoint[†]

$$5.1b \quad \mathcal{M}^+(F)q \equiv \mathcal{L}^+q + Fq_z = \lambda^* v(z)q ,$$

where λ^* denotes the complex conjugate of λ . Suppose that $\Theta(z)$ is an eigenfunction with eigenvalue λ_1 , and suppose that $\chi(z)$ is an adjoint eigenfunction with eigenvalue λ_2 . Then

$$\lambda_1 \langle v\chi, \Theta \rangle = \langle \chi, \mathcal{M}\Theta \rangle = \langle \mathcal{M}^+\chi, \Theta \rangle = \lambda_2 \langle v\chi, \Theta \rangle ,$$

so clearly $\langle v\chi, \Theta \rangle = 0$ if $\lambda_1 \neq \lambda_2$. We conclude that eigenfunctions and adjoint eigenfunctions corresponding to distinct eigenvalues are co-orthogonal in the sense that $\langle v\chi, \Theta \rangle = 0$, regardless of whether $\Theta(z)$ and/or $\chi(z)$ belong to eigenvalues in the continuous or discrete spectrum of $\mathcal{L}$.

Eigenfunctions at $F = 0$. At $F = 0$ the eigenvalue equations are

$$5.2 \quad \mathcal{L}p = \lambda vp , \quad \mathcal{L}^+q = \lambda vq .$$

Clearly $\lambda = 0$ is an eigenvalue with eigenfunction $r(z)$ and adjoint eigenfunction 1:

$$5.3 \quad \mathcal{L}r = 0 , \quad \mathcal{L}^+1 = 0 .$$

To determine if this eigenvalue is simple, we differentiate 5.2 with respect to λ , and set $\lambda = 0$:

$$5.4 \quad \mathcal{L}p_\lambda = vr , \quad \mathcal{L}^+q_\lambda = v .$$

Since $v(z)$ is odd and $r(z)$ is even, clearly $\langle v, r \rangle = 0$. Hence 5.4 is solvable, and $\lambda = 0$ has a multiplicity of at least two. Define $\tilde{r}(z)$ and $\ell(z)$ as the unique solutions of

$$5.5a \quad \mathcal{L}\tilde{r} = -v(z)r(z) , \quad \mathcal{L}^+\ell = -v(z) ,$$

with

$$5.5b \quad \tilde{r}(-z) = -\tilde{r}(z) , \quad \ell(-z) = -\ell(z) ;$$

[†]At $F = 0$ the property of detailed balance (and the negative semi-definiteness of $\mathcal{L}$) guarantee that there are no complex eigenvalues λ . However, for $F \neq 0$, pairs of eigenvalues may coalesce and go into the complex plane.

then $-\tilde{r}(z)$ and $-\ell(z)$ are the generalized eigenfunctions p_λ and q_λ . Note that the property of detailed balance implies that

$$5.5.c \quad \tilde{r}(z) = r(z)\ell(z) ,$$

and that the orthogonality relations

$$5.6a \quad \langle v, r \rangle = \langle v\ell, \tilde{r} \rangle = 0$$

follow from symmetry. It is also easily shown (from the property of detailed balance and the negative semi-definiteness of $\mathcal{L}$) that

$$5.6b \quad D_0 \equiv \langle v, \tilde{r} \rangle \equiv \langle v\ell, r \rangle > 0 .$$

To determine whether the multiplicity of $\lambda = 0$ is greater than two, we differentiate 5.2 again, obtaining

$$5.7 \quad \mathcal{L}p_{\lambda\lambda} = 2vp_\lambda = -2v\tilde{r} , \quad \mathcal{L}^+q_{\lambda\lambda} = 2vq_\lambda = -2v\ell .$$

These equations are solvable, and the multiplicity of $\lambda = 0$ is greater than two, if and only if $D_0 = \langle v, \tilde{r} \rangle = \langle v\ell, r \rangle = 0$. Since $D_0 > 0$, the multiplicity of $\lambda = 0$ is exactly two.

Besides the double eigenvalue at $\lambda = 0$, $\mathcal{L}$ will have other discrete eigenvalues and/or a continuous spectrum. In particular, if $\Theta(z)$ is an eigenfunction with eigenvalue λ , then $\Theta(-z)$ is an eigenfunction with eigenvalue $-\lambda$. So the spectrum of $\mathcal{L}$ is symmetric about $\lambda = 0$, and contains both positive and negative eigenvalues. In addition, the adjoint eigenfunction with eigenvalue λ is $\chi(z) = \Theta(z)/r(z)$. Finally, since the eigenfunctions at $\lambda = 0$ must be orthogonal to all other eigenfunctions, we have

$$5.8 \quad \langle v, \Theta \rangle = 0 , \quad \langle v\ell, \Theta \rangle = 0 , \quad \langle v\chi, r \rangle = 0 , \quad \langle v\chi, \tilde{r} \rangle = 0 .$$

Eigenfunctions at $F \neq 0$. Now consider eigenvalues and eigenfunctions for $F \neq 0$. As mentioned earlier, one eigenvalue is zero for all F . Moreover, the eigenvalue $\lambda = 0$ has multiplicity two at $F = 0$, so there must be exactly one other eigenvalue which goes through zero at $F = 0$. (See figure below). Clearly this other eigenvalue is $\lambda = \beta F$. Let $\phi(z; F)$ and $r(z)$ be the eigenfunctions corresponding to these eigenvalues, and let 1 and $\psi(z; F)$ be the adjoint eigenfunctions:

$$5.9a \quad \mathcal{M}\phi \equiv \mathcal{L}\phi - F\phi_z = 0 ,$$

$$5.9b \quad \mathcal{M}^+1 = 0 ,$$

$$5.9c \quad \mathcal{M}r \equiv \mathcal{L}r - Fr_z = \beta Fvr ,$$

$$5.9d \quad \mathcal{M}^+\psi \equiv \mathcal{L}^+\psi + F\psi_z = \beta Fv\psi .$$

We normalize ϕ and ψ so that

$$5.10 \quad \langle 1, \phi \rangle = 1, \quad \langle 1, r \rangle = 1, \quad \langle \psi, r \rangle = 1.$$

Note that these eigenfunctions satisfy the symmetry relations

$$5.11a \quad \phi(z; -F) = \phi(-z; F) ,$$

$$5.11b \quad \psi(z; -F) = \psi(-z; F) ,$$

and that the property of detailed balance yields

$$5.11c \quad \phi(z; F) = r(z)\psi(z; -F) = r(z)\psi(-z; F) .$$

Together, 5.11a and 5.11b imply that these functions satisfy the orthogonality relations

$$5.12a \quad \langle v, r \rangle = \langle v\psi, \phi \rangle = 0 .$$

In addition, we define $v(F) = \langle v, \phi \rangle$, and note that

$$5.12b \quad v(F) = \langle v, \phi \rangle , \quad v(-F) = -v(F) = \langle v\psi, r \rangle .$$

Besides the eigenvalues $\lambda = 0$ and $\lambda = \beta F$, $\mathcal{M}(F)$ will have other discrete eigenvalues and/or a continuous spectrum. In particular, the property of detailed balance shows that if $\Theta(z)$ is an eigenfunction of $\mathcal{M}(F)$ with eigenvalue λ , then $\chi(z) \equiv \Theta(-z)/r(z)$ is an adjoint eigenfunction of $\mathcal{M}(F)$ with eigenvalue $-(\lambda - \beta F)$. Thus, if λ belongs to the spectrum, then $-(\lambda - \beta F)$ does also, so the spectrum of $\mathcal{M}(F)$ is symmetric about $\lambda = \beta F/2$ and contains both positive and negative eigenvalues. Moreover, suppose that λ belongs to the spectrum of $\mathcal{M}(F)$, and let $\Theta(z)$ and $\chi(z)$ be the

corresponding eigenfunction and adjoint eigenfunction. Then if $\lambda \neq 0$ and $\lambda \neq \beta F$, the orthogonality conditions yield

$$5.13 \quad \langle v, \Theta \rangle = 0, \quad \langle v\psi, \Theta \rangle = 0, \quad \langle v\chi, \phi \rangle = 0, \quad \langle v\chi, r \rangle = 0.$$

Eigenfunctions near $F = 0$. Analogous to “passage through resonance” phenomena, special care must be taken when F is near zero: Because of the nearness of the eigenvalues $\lambda = \beta F$ and $\lambda = 0$, the two eigenspaces $\phi(z; F)$ and $r(z)$ interact very strongly as F goes through zero. To help understand this interaction, $\phi(z; F)$ and $\psi(z; F)$ are expanded in powers of F in Appendix D. In particular, these expansions show that

$$5.14 \quad v(F) \equiv \langle v, \phi \rangle = \beta F \langle v, \tilde{r} \rangle + O(\beta^3 F^3) \text{ for } F \text{ small.}$$

6. Analysis of the strong force case. Since the density p evolves on the t/ε time scale, let

$$6.1 \quad t^{\text{new}} \equiv t/\varepsilon.$$

Then the Boltzmann equation 4.1 becomes

$$6.2 \quad \varepsilon p_t + \varepsilon v(z) p_x = \mathcal{M}(F)p \quad (\text{strong force}).$$

To motivate our asymptotic solution, note that 6.2 is

$$6.3 \quad \varepsilon v(z) p_x = \mathcal{M}(F)p \equiv \mathcal{L}p - F(x)p_z$$

to leading order. Now, we can easily construct the solution to 6.3 corresponding to the eigenvalue $\lambda(F) = 0$,

$$6.4a \quad h^0(x, z) = \frac{1}{v(F)} \left\{ \phi(z; F) + \varepsilon h_1^0(x, z) + \varepsilon^2 h_2^0(x, z) + \dots \right\},$$

via a power series. Corresponding to the eigenvalue $\lambda = \beta F$, we have the exact solution

$$6.4b \quad h^1(x, z) = \exp\left\{ \frac{\beta}{\varepsilon} \int_0^x F(x) dx \right\} r(z)$$

to 6.3. Moreover, suppose that $\Theta(z; F)$ is an eigenfunction whose eigenvalue $\lambda(F)$ is part of the continuous or discrete spectrum of $\mathcal{M}(F)$, and suppose that $\lambda \neq 0$ and

$\lambda \neq \beta F$. Then we can easily construct the solution of 6.3 corresponding to the eigenvalue $\lambda(F)$,

$$6.4c \quad h(\lambda, x, z) = \exp\left\{\frac{1}{\varepsilon} \int_0^x \{\lambda(F) + \dots\} dx\right\} \left\{ \theta(z; F) + \varepsilon h_1(\lambda, x, z) + \dots \right\},$$

by using geometrical optics.

The general solution of 6.3 can be obtained as a superposition of 6.4a, 6.4b, and components of the form 6.4c. However, suppose that the solution contained components of the form 6.4c at leading order. Then the solution would become transcendently large, either as x increased (if $\lambda > 0$) or as x decreased (if $\lambda < 0$). Thus, such components *can not be part of the leading order solution* except very near to spatial boundaries, where either x cannot increase or x cannot decrease. That is, components of the form 6.4c can only exist at leading order in the *kinetic boundary layers* adjacent to spatial boundaries and material interfaces. Beyond these boundary layers, in the *outer region*, the solution can only contain components of the form 6.4a and 6.4b[†]. Thus we conclude that the *outer solution* of 6.3 must be of the form

$$6.5a \quad p(t, x, z) = a(t, x) \phi(z; F) + b(t, x) r(z) + \varepsilon R(t, x, z),$$

where, without loss of generality, we can take $R(t, x, z)$ to be orthogonal to both $\phi(z; F)$ and $r(z)$:

$$6.5b \quad \langle v, R \rangle = 0, \quad \langle v \psi, R \rangle = 0.$$

Since the full Boltzmann equation 6.2 only differs from 6.3 by $O(\varepsilon)$, clearly the outer solution of 6.2 is also of the form 6.5. Thus, the outer solution to eq. 6.2 can be obtained by assuming that $p(t, x, z)$ is of the form 6.5, and by carefully treating

$$6.5c \quad \varepsilon a_x = O(1), \quad \varepsilon b_x = O(1), \quad \varepsilon R_x = O(1), \quad a_t = O(1), \quad b_t = O(1), \quad R_t = O(1)$$

See the scaling discussion in §4.

Substituting 6.5 into 6.2 yields the exact equation

$$6.6 \quad \mathcal{M}(F)R - \varepsilon v R_x = \frac{1}{\varepsilon} (\varepsilon b_x - \beta F b) v r + a_x v \phi + a F_x v \phi_F + a_t \phi + b_t r + \varepsilon R_t.$$

[†]The same reasoning allows us to eliminate terms of the form 6.4b at leading order *only* if $F(x)$ has one sign. In general, $F(x)$ will be positive in some regions and negative in others, so we expect the solution to contain a term of the form 6.4b.

Defining $n(t, \mathbf{x})$ to be the spatial density of electrons,

$$6.7 \quad n(t, \mathbf{x}) \equiv \langle 1, \mathbf{p} \rangle = a + b + \varepsilon \langle 1, \mathbf{R} \rangle ,$$

and taking the inner product of 6.6 with 1, we obtain

$$6.8a \quad n_t = -\{a v(\mathbf{F})\}_x .$$

Here we have used $\langle 1, \mathcal{M}\mathbf{R} \rangle = \langle v, \mathbf{R} \rangle = 0$ and $v(\mathbf{F}) \equiv \langle v, \phi \rangle$. Similarly, taking the inner product of 6.6 with $\psi(z, \mathbf{F})$ yields

$$6.8b \quad (\varepsilon b_x - \beta F b) v(\mathbf{F}) = \varepsilon a F_x \langle v \psi, \phi_F \rangle + \varepsilon a_t \langle \psi, \phi \rangle + \varepsilon b_t - \varepsilon^2 F_x \langle v \psi_F, \mathbf{R} \rangle + \varepsilon^2 \langle \psi, \mathbf{R}_t \rangle .$$

Finally, from 6.8a, 6.8b, and 6.6 we obtain

$$6.8c \quad \mathcal{M}(\mathbf{F})\mathbf{R} - \varepsilon v \mathbf{R}_x = a F_x \left\{ v \phi_F - \frac{v'(\mathbf{F})}{v(\mathbf{F})} v \phi + \frac{\langle v \psi, \phi_F \rangle}{v(\mathbf{F})} v \mathbf{r} \right\} - \varepsilon F_x \frac{\langle v \psi_F, \mathbf{R} \rangle}{v(\mathbf{F})} v \mathbf{r} \\ + a_t \left\{ \phi - \frac{v \phi}{v(\mathbf{F})} + \frac{\langle \psi, \phi \rangle}{v(\mathbf{F})} v \mathbf{r} \right\} + b_t \left\{ \mathbf{r} - \frac{v(\phi - \mathbf{r})}{v(\mathbf{F})} \right\} \\ + \varepsilon \left\{ \mathbf{R}_t - \frac{\langle 1, \mathbf{R}_t \rangle}{v(\mathbf{F})} v \phi + \frac{\langle \psi, \mathbf{R}_t \rangle}{v(\mathbf{F})} v \mathbf{r} \right\} .$$

Note that 6.8a-6.8c are exact.

6.1. Leading order solution. At leading order, 6.7 and 6.8 yield

$$6.9 \quad n = a + b , \quad n_t = -\{a v(\mathbf{F})\}_x , \quad \varepsilon b_x = \beta F b .$$

The second equation implies that $a_x = O(1)$, so we can re-write the last equation as $\varepsilon n_x = \beta F(n - a)$ to leading order. Consequently,

$$6.10 \quad a = n - \frac{\varepsilon n_x}{\beta F} + O(\varepsilon) , \quad b = \frac{\varepsilon n_x}{\beta F} + O(\varepsilon) .$$

The second equation now shows that the spatial density evolves according to the diffusion-drift equation

$$6.11a \quad n_t = (\varepsilon D n_x - v n)_x + O(\varepsilon) \quad (\text{strong force}) ,$$

to leading order, where the drift velocity $v(\mathbf{F})$ and the diffusivity $D(\mathbf{F})$ are given by

$$6.11b \quad v(\mathbf{F}) = \langle v, \phi \rangle , \quad D = v(\mathbf{F})/\beta F \quad (\text{strong force}) .$$

Once eqs. 6.11 have been solved for the spatial density $n(t, \mathbf{x})$, then eqs. 6.5 and 6.10 provide the leading order phase-space distribution:

$$6.11c \quad p(t, \mathbf{x}, z) = nr(z) + \left(n - \frac{\varepsilon n_x}{\beta F} \right) (\phi(z; F) - r(z)) + \dots$$

6.2. Higher order analysis. In Appendix C we carry out the asymptotic analysis of the strong force regime to higher order. There we find that the spatial density of electrons evolves according to

$$6.12a \quad \frac{\partial n}{\partial t} = \frac{\partial}{\partial \mathbf{x}} \left\{ \left(1 - \varepsilon \gamma(F) \frac{\partial}{\partial t} \right) \left(\varepsilon \tilde{D} \frac{\partial n}{\partial \mathbf{x}} - \tilde{v} n \right) \right\} + O(\varepsilon^2)$$

where the drift velocity $\tilde{v}$ and diffusivity $\tilde{D}$ are now given by

$$6.12b \quad \tilde{v} = \langle v, \phi \rangle \{ 1 - \varepsilon \alpha(F) F_x + \dots \}, \quad \tilde{D} = \tilde{v} / \beta F = k_B T \tilde{v} / F.$$

Here $\alpha(F)$ and $\gamma(F)$ are defined by

$$6.13a \quad \alpha(F) = \langle 1, S^1 \rangle, \quad \gamma(F) = \langle 1, S^2 \rangle,$$

where $S^1(z; F)$ and $S^2(z; F)$ are defined as the solutions of

$$6.13b \quad \mathcal{M}S^1 = v\phi_F - \frac{v'(F)}{v(F)} v(\phi - r), \quad \langle v, S^1 \rangle = 0,$$

$$6.13c \quad \mathcal{M}S^2 = \phi - \frac{v(\phi - r)}{v(F)}, \quad \langle v, S^2 \rangle = 0.$$

Remarkably, 6.12b shows that Einstein's relation is still satisfied, even though the drift velocity and diffusion coefficient depend on gradients of the force at this order.

Appendix C demonstrates that, with sufficient patience, we can analyze the strong force case to as high of order as we wish. However, the asymptotic analysis is valid *only* in regions where the electric field changes gradually over a single mean free path, and the domain-of-validity of higher order results is usually more restricted than that of lower order results [14]. One often expects there to be thin layers (e.g., next to the source and drain, as well as other junctions) in which the electric field changes too rapidly for asymptotic solutions to be very accurate. In these regions non-local effects should be significant, since the electron will experience significantly different environments before scattering. Below we account for such effects in the simplest possible way, by using a Karman-Pohlhausen procedure to derive a first moment model.

7. First moment model. Whenever the electric field varies gradually over a mean free path, the momentum distribution of the electrons is of the form

$$7.1 \quad p(t, x, z) = a(t, x) \phi(z; F) + b(t, x) r(z)$$

to leading order. See eq. 6.5. This distribution should also be fairly realistic in any thin layers where the electric field varies more rapidly. So consider the following procedure: Suppose we demand that the momentum distribution always be of the form 7.1; then we cannot satisfy the Boltzmann equation

$$7.2 \quad \varepsilon p_t + \varepsilon v(z) p_x + F(x) p_z = \mathcal{L}p$$

exactly, so instead we demand that the zeroeth and first-order moments of 7.2 be satisfied exactly; this then gives us two equations to determine $a(t, x)$ and $b(t, x)$.

The upshot of this Karman-Pohlhausen procedure is a *first moment model* for semiconductors. In regions where the electric field *does* vary gradually over a mean free path, this model automatically reduces to the asymptotically correct solution, 6.11. In any thin regions where the electric field changes more rapidly, at least the first moments of the Boltzmann equation are satisfied exactly. Consequently, we expect the first moment model to be very accurate, although we have not yet made extensive comparisons between the first moment model and direct (numerical) solutions of the Boltzmann equation.

To make the derivation more transparent, let us re-write 7.1 as

$$7.3a \quad p(t, x, z) = n(t, x) r(z) + J(t, x) \frac{\phi(z; F) - r(z)}{v(F)} .$$

Then

$$7.3b \quad n(t, x) \equiv \langle 1, p \rangle , \quad J(t, x) \equiv \langle v, p \rangle ,$$

so $n(t, x)$ is the spatial density and $J(t, x)$ is the flux of electrons. Taking the inner product of 7.2 with respect to 1 yields

$$7.4a \quad n_t + J_x = 0 ,$$

and taking the inner product of 7.2 with respect to $v(z)$ yields

$$7.4b \quad \varepsilon J_t + \varepsilon \langle v^2, p \rangle_x + F \langle v, p_z \rangle = \langle v, \mathcal{L}p \rangle .$$

Substituting the presumed distribution 7.3a into 7.4b, and using

$$7.5 \quad \mathcal{L}r = 0, \quad \mathcal{L}\phi = F\phi_z, \quad r_z = -\beta vr,$$

we obtain the *first moment model*

$$7.6a \quad n_t + J_x = 0,$$

$$7.6b \quad J_t + \{c(F)J\}_x = \frac{\sigma}{\epsilon D} \left(v(F)n - \epsilon D(F)n_x - J \right),$$

where

$$7.6c \quad c(F) = \frac{\langle v^2, \phi - r \rangle}{v(F)}, \quad \sigma = \langle v^2, r \rangle,$$

and where the drift velocity and diffusivity are defined by

$$7.6d \quad v(F) = \langle v, \phi \rangle, \quad D(F) = v(F)/\beta F,$$

as before. Note that whenever the force F changes slowly on the x/ϵ space scale, eq. 7.6b yields

$$7.7 \quad J \sim v(F)n - \epsilon D(F)n_x.$$

So whenever the electric field *does* vary gradually, the first moment model reduces to the asymptotically-correct diffusion-drift model 6.11, as expected.

Surprisingly, there is no nonlinear advection term in 7.6b. Unlike the hydrodynamic model, the first moment model predicts that there will *not* be any electron shock waves. Further investigation shows that the nonlinear advection term is missing because the stress-tensor cancels it out exactly.

8. Three dimensions. Future work. The new field-dependent diffusion-drift equation 6.11, and the first moment model 7.6, are the key results of our analysis. Along with the equivalent results for holes and Poisson's equation, they constitute the high field semiconductor equations in Appendix A.

We are currently analyzing the Boltzmann equation in three dimensions [9,10]. Although this analysis is substantially more difficult [15], arguments similar to the ones presented here show that the spatial density $n(t, \mathbf{x})$ satisfies

$$8.1a \quad n_t = \nabla \cdot (\varepsilon D \nabla n - \nu n) + \varepsilon^2 \nabla \cdot \mathbf{M} \cdot \nabla \left(\frac{\nu \cdot \nabla n}{\beta \mathbf{F} \cdot \nu} \right) + \dots$$

to leading order, where the drift velocity $\nu(\mathbf{F})$, diffusivity tensor D , and dispersion tensor $\mathbf{M}$ are defined by

$$8.1b \quad \nu(\mathbf{F}) \equiv \langle \mathbf{v}(\mathbf{z}), \phi \rangle, \quad D \equiv \frac{\nu \otimes \nu}{\beta \mathbf{F} \cdot \nu} + \langle 1, \nu \otimes \Phi \rangle, \quad \mathbf{M} = \langle 1, \mathbf{w} \otimes (\tilde{\Phi} - \Phi) \rangle.$$

Here $\mathbf{w}(\mathbf{z}; \mathbf{F})$ is orthogonal to the force $\mathbf{F}$, and is related to the velocity $\mathbf{v}(\mathbf{z})$ by

$$8.1c \quad \mathbf{w}(\mathbf{z}; \mathbf{F}) = \mathbf{v}(\mathbf{z}) - \frac{\mathbf{v} \cdot \mathbf{F}}{\nu \cdot \mathbf{F}} \nu(\mathbf{F}),$$

and $\phi(\mathbf{z}; \mathbf{F})$, $\Phi(\mathbf{z}; \mathbf{F})$, and $\tilde{\Phi}(\mathbf{z}; \mathbf{F})$ are defined by

$$8.1d \quad \mathcal{M}(\mathbf{F})\phi \equiv \mathcal{L}\phi - \mathbf{F} \cdot \nabla_{\mathbf{z}} \phi = 0, \quad \text{with } \langle 1, \phi \rangle = 1,$$

$$8.1e \quad \mathcal{M}(\mathbf{F})\Phi = -\mathbf{w}\phi, \quad \text{with } \langle 1, \Phi \rangle = 0,$$

$$8.1f \quad \mathcal{M}(\mathbf{F})\tilde{\Phi} - \beta \mathbf{F} \cdot \nu \tilde{\Phi} = -\mathbf{w}r, \quad \text{with } \langle 1, \tilde{\Phi} \rangle = 0.$$

Since $\Phi \cdot \mathbf{F} \equiv 0$, we see that $\beta D_{\mathbf{M}} \mathbf{F} \equiv \nu(\mathbf{F})$. Thus, Einstein's relation is once again satisfied, at least if we disregard the dispersion term. (The dispersion term does not arise in one dimension because $\mathbf{M}\mathbf{F} = 0$; in 1-d this implies that $\mathbf{M} = 0$.) We are currently using this asymptotic analysis to develop a three dimensional first moment model analogous to the one in §7.

In the immediate future, we intend to compare direct (numerical) solutions of the Boltzmann equation to the high-field diffusion-drift equations 6.11 and 6.12, and to the first moment model 7.4. Preliminary results show very good agreement between the analytical predictions and the numerical solutions. We also intend to evaluate our results with realistic scattering operators for semiconductors, and then compare the theoretically-predicted drift velocities and diffusivity tensors with experimental values. This work should be completed shortly.

Next to all material interfaces and spatial boundaries, there exist extremely thin *kinetic boundary layers*, which are only one or two mean free lengths thick. The high-field diffusion-drift equations represent *outer solutions*, which are not valid within such boundary layers, while the first moment model is only approximately correct in these boundary layers. Even though these boundary layers are extremely thin, they can play critical roles in semiconductors. We are currently developing analytical and numerical techniques analogous to the ones in [15-17] for resolving such layers.

Appendix A. Other notation. The high field semiconductor equations. Let $\mathcal{E}_n(\mathbf{k})$ be the energy of the relevant conduction band, where $\mathbf{k}$ is the electronic wave-number, and recall that $\mathcal{E}_n(\mathbf{k})$ is periodic with a period corresponding to the first Brillouin zone. Also recall that the velocity of an electron with wavenumber $\mathbf{k}$ is

$$\text{A.1} \quad \mathbf{v}^e(\mathbf{k}) \equiv \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}_n(\mathbf{k}) .$$

Let $f^e(t, \mathbf{x}, \mathbf{k})$ be the probability density that state $\mathbf{k}$ in band n is occupied at position $\mathbf{x}$. Then, neglecting inter-band transitions, the Boltzmann equation for the electrons in band n is

$$\text{A.2} \quad f_t^e + \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}_n(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f^e - \frac{q\mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f^e = \mathcal{L}^{(e)} f^e .$$

Here we are assuming that all nonlinear scattering terms can be omitted; this implies that the scattering operator $\mathcal{L}^{(e)}$ has a Maxwellian equilibrium distribution [2,5,13],

$$\text{A.3} \quad r^e(\mathbf{k}) = \frac{1}{N_e} \exp\{-\beta \mathcal{E}_n(\mathbf{k})\}, \text{ with } \beta = k_B T ,$$

where the normalization N_e will be chosen later.

Before continuing, let us connect this notation with the notation used previously. Recall that $\mathbf{z} \equiv \hbar \mathbf{k}$ is the crystal momentum of an electron, and that

$$\text{A.4} \quad p(t, \mathbf{x}, \mathbf{z}) d^3z = \frac{1}{4\pi^3} f^e(t, \mathbf{x}, \mathbf{k}) d^3k$$

is the phase-space density for electrons in a single band [5,13]. Using $\mathcal{E}(\mathbf{z})$ to denote $\mathcal{E}_n(\mathbf{z}/\hbar)$, the Boltzmann equation A.2 can be written as

$$\text{A.5} \quad p_t + \mathbf{v}(\mathbf{z}) \cdot \nabla_{\mathbf{x}} p + \mathbf{F}(\mathbf{x}) \cdot \nabla_{\mathbf{z}} p = \mathcal{L}^{(e)} p .$$

Here $\mathbf{v}(\mathbf{z}) = \nabla_{\mathbf{z}} \mathcal{E}(\mathbf{z})$, and $\mathbf{F} = -q\mathbf{E}$ is the force on the electrons.

For holes, we let $\mathcal{E}_m(\mathbf{k})$ be the energy of the relevant valence band, and let $f^h(t, \mathbf{x}, \mathbf{k})$ be the probability density that state $\mathbf{k}$ in band m is *unoccupied* at position $\mathbf{x}$. Since the deterministic orbits of electrons and holes are exactly the same, the Boltzmann equation for holes is

$$\text{A.6} \quad f_t^h + \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}_m(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f^h - \frac{q\mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f^h = \mathcal{L}^{(h)} f^h .$$

As before, we are assuming that the density of holes is not so large that the nonlinear scattering terms need to be included; this implies that the scattering operator $\mathcal{L}^{(h)}$ has the equilibrium distribution

$$\text{A.7} \quad r^h(\mathbf{k}) = \frac{1}{N_h} \exp\{+\beta \mathcal{E}_m(\mathbf{k})\}.$$

High field equations. In one spatial dimension, the phase-space densities are

$$\text{A.8} \quad p^e(t, x, z) dz = \frac{1}{\pi} f^e(t, x, k) dk, \quad p^h(t, x, z) dz = \frac{1}{\pi} f^h(t, x, k) dk,$$

so the spatial density of electrons and holes is

$$\text{A.9} \quad n(t, x) = \langle 1, f^e \rangle, \quad p(t, x) = \langle 1, f^h \rangle,$$

where the inner product is defined as

$$\text{A.10} \quad \langle f, g \rangle \equiv \frac{1}{\pi} \int f^*(k) g(k) dk.$$

Accordingly, we normalize r^e and r^h so that $\langle 1, r^e \rangle = \langle 1, r^h \rangle = 1$.

To express the high field equations, define $\phi^e(k; E)$ and $\phi^h(k; E)$ by

$$\text{A.11a} \quad \mathcal{L}^{(e)} \phi^e = -\frac{qE}{\hbar} \phi_k^e, \quad \langle 1, \phi^e \rangle = 1,$$

$$\text{A.11b} \quad \mathcal{L}^{(h)} \phi^h = -\frac{qE}{\hbar} \phi_k^h, \quad \langle 1, \phi^h \rangle = 1,$$

and define the drift velocities and diffusivities

$$\text{A.12a} \quad v_e(E) = -\langle v^e, \phi^e \rangle, \quad D_e(E) = k_B T v_e(E)/qE,$$

$$\text{A.12b} \quad v_h(E) = +\langle v^h, \phi^h \rangle, \quad D_h(E) = k_B T v_h(E)/qE,$$

where $v^e(k)$ and $v^h(k)$ are the electron and hole velocities:

$$\text{A.13} \quad v^e(k) = \frac{1}{\hbar} \mathcal{E}'_n(k), \quad v^h(k) = \frac{1}{\hbar} \mathcal{E}'_m(k).$$

Adapting the moment model of §7 to the Boltzmann equations A.2 and A.6, we find that the spatial densities of electrons and holes evolve according to

$$\text{A.14a} \quad n_t + J_x^e = 0, \quad p_t + J_x^h = 0,$$

where the electron and hole particle fluxes are given by

$$\text{A.14b} \quad J_t^e - \{c^e(E) J^e\}_x = \frac{\alpha^e}{D_e(E)} (-v_e(E) n - D_e(E) n_x - J^e),$$

$$\text{A.14c} \quad J_t^h + \{c^h(E) J^h\}_x = \frac{\alpha^h}{D_h(E)} (v_h(E) p - D_h(E) p_x - J^h).$$

Here the electric field is determined by Poisson's equation,

$$\text{A.14d} \quad E = -\Phi_x, \quad -(\epsilon\Phi_x)_x = q(p - n + C),$$

where C is the charge concentration of ionized impurities, and

$$\text{A.15a} \quad c^e(E) = \langle (v^e)^2, (\phi^e - r^e) \rangle / v_e(E), \quad \alpha^e = \langle (v^e)^2, r^e \rangle,$$

$$\text{A.15b} \quad c^h(E) = \langle (v^h)^2, (\phi^h - r^h) \rangle / v_h(E), \quad \alpha^h = \langle (v^h)^2, r^h \rangle,$$

Eqs. A.14a-A.14d form the high field semiconductor equations. Note that wherever the electric field varies slowly over a mean free path, we can replace A.14b and A.14c by their "local equilibrium values"

$$\text{A.16} \quad J^e = -v_e(E)n - D_e(E)n_x, \quad J^h = v_h(E)p - D_h(E)p_x,$$

and obtain the asymptotically-correct field-dependent diffusion-drift model.

Appendix B. Higher order solution for the weak force regime. Here we carry out the asymptotic expansion

$$\text{B.1a} \quad p(t, x, z) = p^0(t, x, z) + \epsilon p^1(t, x, z) + \epsilon^2 p^2(t, x, z) + \dots,$$

$$\text{B.1b} \quad \langle 1, p^i \rangle = 0 \quad \text{for } i = 1, 2, 3, \dots$$

for the solution of the weak force Boltzmann equation

$$\text{B.2} \quad \epsilon^2 p_t + \epsilon v(z) p_x + \epsilon F(x) p_z = \mathcal{L}p$$

through $O(\epsilon^2)$. In §3 we found that

$$\text{B.3a} \quad p^0(t, x, z) = n(t, x) r(z), \quad p^1(t, x, z) = -(n_x - \beta F n) \tilde{r}(z),$$

where the spatial density $n(t, x)$ satisfies

$$\text{B.3b} \quad n_t = \langle v, \tilde{r} \rangle (n_x - \beta F n)_x + \dots$$

to leading order. Define $\alpha_1(t, x)$ and $\alpha_2(t, x)$ by

$$\text{B.4} \quad n_t = \langle v, \tilde{r} \rangle (n_x - \beta F n)_x + \epsilon \alpha_1 + \epsilon^2 \alpha_2 + \dots$$

Then expanding the Boltzmann equation yields

$$\text{B.5a} \quad \mathcal{L}p^2 = vp_x^1 + Fp_z^1 + \langle v, \tilde{r} \rangle (n_x - \beta F n)_x r(z), \quad \langle 1, p^2 \rangle = 0$$

$$\text{B.5b} \quad \mathcal{L}p^3 = vp_x^2 + Fp_z^2 + p_t^1 + \alpha_1 r(z), \quad \langle 1, p^3 \rangle = 0$$

$$\text{B.5c} \quad \mathcal{L}p^4 = vp_x^3 + Fp_z^3 + p_t^2 + \alpha_2 r(z), \quad \langle 1, p^4 \rangle = 0$$

through $O(\varepsilon^4)$.

Substituting B.3a into B.5a, we obtain

$$\text{B.5} \quad \mathcal{L}p^2 = -(n_x - \beta F n)_x [v\tilde{r} - \langle v, \tilde{r} \rangle r] - F(n_x - \beta F n)\tilde{r}_z, \quad \langle 1, p^2 \rangle = 0.$$

Define $\Phi(z)$ and $\chi(z)$ to be the unique solutions of

$$\text{B.6a} \quad \mathcal{L}\Phi = r - v\tilde{r}/\langle v, \tilde{r} \rangle, \quad \langle 1, \Phi \rangle = 0,$$

$$\text{B.6b} \quad \mathcal{L}\chi = \tilde{r}_z, \quad \langle 1, \chi \rangle = 0;$$

then the solution of B.5 is

$$\text{B.7} \quad p^2 = \langle v, \tilde{r} \rangle (n_x - \beta F n)_x \Phi(z) - F(n_x - \beta F n)\chi(z).$$

Since

$$\text{B.8} \quad \Phi(z) = \Phi(-z), \quad \chi(z) = \chi(-z),$$

p^0 is even in z , p^1 is odd in z , and p^2 is even in z . Consequently, integrating B.5b and B.5c over z yields the solvability conditions

$$\text{B.9a} \quad \alpha_1 = 0,$$

$$\text{B.9b} \quad \alpha_2 \langle 1, r \rangle + F \langle 1, p_z^3 \rangle + \langle v, p^3 \rangle_x + \langle 1, p^2 \rangle_t = 0.$$

Since $\langle 1, r \rangle = 1$ and $\langle 1, p^2 \rangle = 0$, we obtain

$$\text{B.10} \quad \alpha_1 = 0, \quad \alpha_2 = -\langle v, p^3 \rangle_x.$$

To simplify B.10, define ℓ by

$$\text{B.11a} \quad \mathcal{L}^+ \ell = -v, \quad \ell(z) = -\ell(-z),$$

and note that

$$\text{B.11b} \quad \tilde{r}(z) = r(z)\ell(z).$$

Then

$$\text{B.12} \quad \alpha_2 = \langle \mathcal{L}^+ \ell, p^3 \rangle_x = \langle \ell, p^1 \rangle_{tx} + \langle v\ell, p^2 \rangle_{xx} + (F\langle \ell, p_z^2 \rangle)_x ,$$

and since

$$\text{B.13} \quad p^1 = -(n_x - \beta F n) \tilde{r}(z) , \quad p^2 = n_t \Phi(z) - F(n_x - \beta F n) \chi(z) + O(\varepsilon^2) ,$$

we have

$$\begin{aligned} \text{B.14} \quad \alpha_2 = & -\langle \ell, \tilde{r} \rangle (n_x - \beta F n)_{xt} + [\langle v\ell, \Phi \rangle n_x + \langle \ell, \Phi_z \rangle F n]_{xt} \\ & - \langle v\ell, \chi \rangle [F(n_x - \beta F n)]_{xx} - \langle \ell, \chi_z \rangle [F^2(n_x - \beta F n)]_x . \end{aligned}$$

Eq. B.14 is the $O(\varepsilon^2)$ correction to the diffusion drift equation, eq. B.3b. It can be simplified by using the property of detailed balance to derive the identity

$$\text{B.15} \quad \langle \ell, \Phi_z \rangle = -\beta \langle v\ell, \Phi \rangle + \langle v\ell, \chi \rangle / \langle v, \tilde{r} \rangle .$$

From this identity and B.3b, we obtain

$$\text{B.16} \quad \alpha_2 = \frac{\langle v\ell, \Phi \rangle - \langle \ell, \tilde{r} \rangle}{\langle v, \tilde{r} \rangle} n_{tt} - \{ (\langle v\ell, \chi \rangle F_x + \langle \ell, \chi_z \rangle F^2)(n_x - \beta F n) \}_x .$$

Hence, the spatial density $n(t, x)$ evolves according to the equation

$$\text{B.17a} \quad n_t + \varepsilon^2 \gamma n_{tt} = (\bar{D} n_x - \bar{\mu} F n)_x$$

through $O(\varepsilon^2)$, where the diffusion coefficient $\bar{D}$ and mobility $\bar{\mu}$ are given by

$$\text{B.17b} \quad \bar{D} = \langle v, \tilde{r} \rangle - \varepsilon^2 F_x \langle v\ell, \chi \rangle - \varepsilon^2 F^2 \langle \ell, \chi_z \rangle + \dots ,$$

$$\text{B.17c} \quad \bar{\mu} = \beta \bar{D} = \bar{D} / k_B T ,$$

and

$$\text{B.17d} \quad \gamma = \langle \ell, \tilde{r} - v\Phi \rangle / \langle v, \tilde{r} \rangle .$$

Moreover, the phase-space density is

$$\text{B.18} \quad p(t, x, z) = n(t, x) r(z) - \varepsilon (n_x - \beta F n) \tilde{r}(z) + \varepsilon^2 n_t \Phi(z) - \varepsilon^2 F (n_x - \beta F n) \chi(z) + \dots$$

Appendix C. Higher order analysis of the strong force regime. Here we carry out the strong force expansion to higher order. At leading order, 6.8c is

$$\begin{aligned} \text{C.1} \quad \mathcal{M}(F)R - \varepsilon v R_x &= a F_x \left\{ v \phi_F - \frac{v'(F)}{v(F)} v \phi + \frac{\langle v \psi, \phi_F \rangle}{v(F)} v r \right\} \\ &\quad + a_t \left\{ \phi - \frac{v \phi}{v(F)} + \frac{\langle \psi, \phi \rangle}{v(F)} v r \right\} + b_t \left\{ r - \frac{v(\phi - r)}{v(F)} \right\}. \end{aligned}$$

To solve C.1, define $R^1(z;F)$, $R^2(z;F)$, and $R^3(z;F)$ as the unique solutions to

$$\text{C.2a} \quad \mathcal{M}R^1 = v \phi_F - \frac{v'(F)}{v(F)} v \phi + \frac{\langle v \psi, \phi_F \rangle}{v(F)} v r, \quad \langle v, R^1 \rangle = 0,$$

$$\text{C.2b} \quad \mathcal{M}R^2 = \phi - \frac{v \phi}{v(F)} + \frac{\langle \psi, \phi \rangle}{v(F)} v r, \quad \langle v, R^2 \rangle = 0,$$

$$\text{C.2c} \quad \mathcal{M}R^3 - \beta F v R^3 = r - \frac{v(\phi - r)}{v(F)}, \quad \langle v \psi, R^3 \rangle = 0.$$

Then

$$\text{C.3} \quad R(t, x, z) = a F_x R^1 + a_t R^2 + b_t R^3 + O(\varepsilon),$$

and so

$$\text{C.4a} \quad n = a + b + \varepsilon a F_x \langle 1, R^1 \rangle + \varepsilon a_t \langle 1, R^2 \rangle + \varepsilon b_t \langle 1, R^3 \rangle + \dots,$$

$$\text{C.4b} \quad n_t = -(a v(F))_x,$$

$$\text{C.4c} \quad b - \frac{\varepsilon}{\beta F} b_x = -\varepsilon a F_x \frac{\langle v \psi, \phi_F \rangle}{\beta F v} - \varepsilon a_t \frac{\langle \psi, \phi \rangle}{\beta F v} - \frac{\varepsilon b_t}{\beta F v} + \dots,$$

through $O(\varepsilon)$. From C.4a and C.4b, we now obtain

$$\text{C.5a} \quad b = n - a - \varepsilon a F_x \langle 1, R^1 \rangle - \varepsilon a_t \langle 1, R^2 \rangle - \varepsilon b_t \langle 1, R^3 \rangle + O(\varepsilon^2),$$

and

$$\text{C.5b} \quad a_x = -(n_t + v' a F_x)/v, \quad b - \frac{\varepsilon}{\beta F} b_x = O(\varepsilon),$$

which yields

$$\text{C.6} \quad n - \frac{\varepsilon n_x}{\beta F} - \varepsilon a_t \left(\langle 1, R^2 \rangle - \frac{\langle (\psi - 1), \phi \rangle}{\beta F v} \right) = a \left(1 + \varepsilon F_x \langle 1, R^1 \rangle - \varepsilon F_x \frac{\langle v(\psi - 1), \phi_F \rangle}{\beta F v} \right)$$

through $O(\varepsilon)$. That is,

$$\text{C.7} \quad n - \frac{\varepsilon n_x}{\beta F} - \varepsilon a_t \langle 1, S^2 \rangle = a \left(1 + \varepsilon F_x \langle 1, S^1 \rangle \right),$$

where $S^1(z; F)$ and $S^2(z; F)$ are the solutions of

$$\text{C.8a} \quad \mathcal{M}S^1 = v\phi_F - \frac{v'(F)}{v(F)}v(\phi - r), \quad \langle v, S^1 \rangle = 0,$$

$$\text{C.8b} \quad \mathcal{M}S^2 = \phi - \frac{v(\phi - r)}{v(F)}, \quad \langle v, S^2 \rangle = 0.$$

From C.4b and C.7, we now discover that the spatial density satisfies

$$\text{C.9a} \quad \frac{\partial n}{\partial t} = \frac{\partial}{\partial x} \left\{ \left(1 - \varepsilon \langle 1, S^2 \rangle \frac{\partial}{\partial t} \right) \left(\varepsilon \tilde{D} \frac{\partial n}{\partial x} - \tilde{v} n \right) \right\} + O(\varepsilon^2),$$

where the drift velocity $\tilde{v}$ and diffusivity $\tilde{D}$ are given by

$$\text{C.9b} \quad \tilde{v} = \langle v, \phi \rangle [1 - \varepsilon F_x \langle 1, S^1 \rangle + \dots], \quad \tilde{D} = \tilde{v} / \beta F = k_B T \tilde{v} / F.$$

Once C.9 has been solved for $n(t, x)$, the phase space distribution is given by

$$\begin{aligned} \text{C.9c} \quad p(t, x, z) = & nr + \left(n - \frac{\varepsilon n_x}{\beta F} \right) \left(\phi - r + \varepsilon F_x [S^1 - \langle 1, S^1 \rangle \phi] \right) \\ & + \varepsilon \frac{\partial}{\partial t} \left(n - \frac{\varepsilon n_x}{\beta F} \right) \left(S^2 - \langle 1, S^2 \rangle \phi \right) + \frac{\varepsilon^2}{\beta F} n_{xt} (R^3 - \langle 1, R^3 \rangle r) + O(\varepsilon^2). \end{aligned}$$

Appendix D. Eigenfunctions near $F = 0$. Here we expand $\phi(z; F)$ and $\psi(z; F)$ in powers of F to help understand the interaction of the two eigenspaces $\phi(z; F)$ and $r(z)$ as F goes through zero. Define

$$\text{D.1a} \quad \mathcal{L}r^{(k)} = \frac{1}{\beta} r_z^{(k-1)}, \quad \langle 1, r^{(k)} \rangle = 0, \quad k = 2, 3, \dots,$$

$$\text{D.1b} \quad \mathcal{L}^+ \ell^{(k)} = \frac{1}{\beta} \ell_z^{(k-1)} - v \ell^{(k-1)}, \quad \langle \ell^{(k)}, r \rangle = 0, \quad k = 2, 3, \dots,$$

with

$$\text{D.1c} \quad r^{(0)} = r(z), \quad \ell^{(0)} = 1, \quad r^{(1)} = \tilde{r}(z), \quad \ell^{(1)} = \ell,$$

and note that $r^{(k)}(z) = r(z) \ell^{(k)}(z)$. Clearly,

$$\text{D.3a} \quad \phi(z;F) = r(z) + \beta F \tilde{r}(z) + \beta^2 F^2 r^{(2)}(z) + \dots ,$$

$$\text{D.3b} \quad \psi(z;F) = 1 - \beta F \ell(z) + \beta^2 F^2 \ell^{(2)}(z) - \dots ,$$

so $v(F)$ can be expanded as

$$\text{D.4} \quad v(F) \equiv \langle v, \phi \rangle = \beta F \langle v, \tilde{r} \rangle + \beta^3 F^3 \langle v, r^{(3)} \rangle + \dots .$$

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