Exact Solution of a Boundary Value Problem in Semiconductor Kinetic Theory

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Abstract

An explicit solution of the stationary one dimensional half-space boundary value problem for the linear Boltzmann equation is presented in the presence of an arbitrarily high constant external field. The collision kernel is assumed to be separable, which is also known as “relaxation time approximation”; the relaxation time may depend on the electron velocity. Our method consists in a transformation of the half-space problem into a nonnormal singular integral equation, which has an explicit solution.

I Introduction

The motion of electrons or holes in a bulk semiconductor under the action of an external field $E$ can be described by a probability density $f(t, x, p)$ for finding a charge carrier at time $t$ and point $x$ with momentum $p$. Under the assumptions of quasineutrality \[1\] and a low electron concentration, so that interactions among the electrons themselves (via collisions or PAULI’s principle) can be neglected \[4\], this probability density satisfies the linear Boltzmann equation

$$\left( \partial_t + p \partial_x - E \partial_p \right) f(t, x, p) = Qf(t, x, p)$$

where we have set the charge and effective mass of the electrons equal to unity. The linear collision operator $Q$ describes scattering of the electrons by vibrations of the host lattice and consequently strongly depends on the model for the electron-phonon interaction.
In this article we consider collision models with separable collision kernels. These models are also known as *relaxation time approximations* with momentum dependent relaxation times. Although these models do not account for some high field effects in semiconductors [3], they are widely used because of their relatively simple mathematical structure. Whilst the solution of the initial value problem is easily obtained in these models [1] [2], the boundary value problem is far more intricate. Up to now, a solution of the boundary value problem in the relaxation time approximation has been found only by Cercignani for a specific $p$-dependence of the relaxation time [6] and by Dalitz in the zero temperature limit [7].

In this article, we present a solution of the stationary one dimensional half-space problem with a constant electric field for quite general $p$-dependent relaxation times. The somewhat simpler case of a constant relaxation time is treated in the unpublished preprint [24] in great detail. In the half-space problem the semiconductor is taken semiinfinite ($x \in (0, \infty)$); at the boundary $x = 0$, electrons are shot in with a given momentum distribution $\varphi$. Thus we seek the solution of

$$\left(p\partial_x - E\partial_p\right)f(x, p) = Qf(x, p)$$

with the boundary conditions

$$f(0, p) = \varphi(p) \quad \text{for} \quad p > 0 \quad \text{and} \quad \lim_{x \to \infty} f(x, p) = 0$$

For zero electric field $E \equiv 0$ Case [8] has found a solution via an eigenfunction technique in the context of neutron diffusion in solids. Completeness theorems for these eigenfunctions have been proven by Zweifel [11] for the general equation $h(p)\partial_x f + Af = 0$ under the assumption that $A$ be a selfadjoint positive operator in some appropriate function space. In the case of a nonzero electric field however, this general result is no longer valid because the operator $A = -E\partial_p - Q$ is not selfadjoint.

Nevertheless for specific collision operators, an eigenfunction expansion of the solution might be possible also in the presence of a constant external field. In [10] a kind of half-range completeness of the eigenfunctions has been proven for a constant relaxation time in the zero temperature limit, and in [11] the same has been proven for two very specific collision kernels at arbitrary temperature of the semiconductor host lattice. In this article we show that the half-space problem in the relaxation time approximation generally can be solved via an eigenfunction expansion, provided the collision frequency is an analytic function of the momentum $p$ that increases not more than linearly in $p$ for $p \to \infty$.

We shall prove that each boundary value $\varphi$ that is a Laplace transform of any tempered distribution can be written as a superposition of “eigenfunctions”. This result (see end of section V) is in complete analogy to Case’s half-range completeness theorem for his “singular eigenfunctions”. Moreover we shall see that the eigenfunction representation of the boundary value generally contains a singular contribution of the Maxwellian of the temperature of the semiconductor lattice. This is in agreement with a conjecture of Stichel and Strothmann [12].
II The collision model

In the nondegenerate situation, the electron phonon collision operator \( Q \) in (1) has the general form \[2\]

\[
Q f(p) = M(p) \int dp' K(p', p) f(p') - f(p) \int dp' M(p') K(p, p')
\]

where \( M(p) := M_0 e^{-p^2/2\theta} \) is the Maxwellian at temperature \( \theta \) of the semiconductor lattice, which is assumed to be in equilibrium. The collision kernel \( K(p, p') \) is a symmetric and positive distribution. The second integral in (3), which gives the total scattering rate, is called collision frequency \( \nu \); its reciprocal is called relaxation time \( \tau \)

\[
\nu(p) = \frac{1}{\tau(p)} := \int dp' M(p') K(p, p')
\]

Throughout this article we assume the collision kernels to be separable, that is \( K(p, p') = \nu(p) \cdot \nu(p') = (\tau(p) \cdot \tau(p'))^{-1} \). This assumption is also known as relaxation time approximation (RTA). If we normalize the Maxwellian so that \( \int M(p) \nu(p) dp = 1 \), we obtain the RTA in its usual form

\[
Q f(p) = \frac{1}{\tau(p)} \left( M(p) \int d^3 p' \frac{f(p')}{\tau(p')} - f(p) \right)
\]

and by comparison with (4) we see that \( \tau(p) \) indeed is the relaxation time, because of our normalization \( \int M/\tau = 1 \). The relaxation time approximation (5) generally can be a good approximation for the collision operator, provided the collision kernel \( K \) is a measurable function with a finite norm \( \int dp \int dp' M(p) M(p') K^2(p, p') < \infty \). For then (5) is equivalent to keeping only the largest term in the eigenfunction representation of the symmetric and square integrable kernel \( \sqrt{M(p)} K(p, p') \sqrt{M(p')} \)

III Eigenfunction expansion of the solution

In order to solve the stationary Boltzmann equation (1), we make the separation ansatz \( f_\lambda(x, p) := e^{-\lambda x} g_\lambda(p) \). We then obtain for the functions \( g_\lambda \) the ”eigenvalue” equation \( (Q + E\partial_p) g_\lambda(p) = -\lambda p g_\lambda(p) \), which reads with the collision operator (5)

\[
(E\partial_p + \lambda p - \nu(p)) g_\lambda(p) = -\nu(p) M(p) \int dp' \nu(p') g_\lambda(p')
\]

In order to get rid of the integral on the right hand side of (6), let us normalize \( \int \nu g_\lambda = 1 \). Then the general solution of (6) reads

\[
g_\lambda(p) = \frac{M_0}{E} e^{-\lambda p^2/2E+N(p)/E} \left\{ C_\lambda - \int_0^p dq \nu(q) e^{(\lambda-q^2/2E-N(q)/E)} \right\}
\]
where $C_\lambda$ is an integration constant and $N$ (read “capital $\nu$”) denotes the primitive function of the collision frequency

$$N(p) := \int_0^p dq \nu(q)$$

For general $\lambda$, (7) is integrable with respect to $p$ only if $\lim_{p \to \infty} \nu(p)/p = c < \infty$. In fact, if this condition is violated, the only $L_1$-integrable solutions of (6) are $M(p)$ with $\lambda = E/\theta$ and the homogeneous solution with $\lambda = 0$. If the condition is satisfied, the solution (7) is $L_1$-integrable for every $\lambda \cdot \text{sign}(E) > c$. For simplicity we assume that $c = 0$.

Because of the boundary condition at infinity (2), only positive values are allowed for $\lambda$. Consequently, we must assume that $E > 0$, for otherwise $g_\lambda$ would grow exponentially for $p \to \pm \infty$. This means that the field $E$ must act in such a way that the electrons are driven back to the boundary $x = 0$.

Inserting the eigenfunction (7) into the normalization condition $\int dp \nu g_\lambda = 1$, we find for the constant $C_\lambda$ after a partial integration in the numerator

$$C_\lambda = \frac{\int dp \, p \, e^{-\lambda p^2/2} e^{-\nu(p)} \int dq \nu(q) e^{\lambda q^2/2} N(q)}{\int dp \, p \, e^{-\lambda p^2/2} e^{-\nu(p)} N(p)}$$

Since equation (1) is linear, any superposition of solutions $f_\lambda(x, p)$ is a solution of (1) too. Thus we assume the solution to be of the form

$$f(x, p) = \int_0^\infty d\lambda A(\lambda) \, f_\lambda(x, p) = \int_0^\infty d\lambda A(\lambda) \, e^{-\lambda x} g_\lambda(p)$$

The expansion coefficients $A(\lambda)$ must be determined from the boundary value $\varphi$. Setting $x=0$ in (10) yields

$$f(0, p) = \varphi(p) = \int_0^\infty d\lambda A(\lambda) \, g_\lambda(p) \quad \text{for} \quad p > 0$$

If this equation can be solved for $A(\lambda)$, then the half-space problem (1) and (2) is solved by (10). Hence the task is to determine the class of boundary values $\varphi$ for which (11) has a solution $A(\lambda)$ and to determine this solution in terms of $\varphi$. We shall see that (11) indeed can be solved if the boundary value is a Laplace transform of any tempered distribution, for then (11) is equivalent to a singular integral equation which can be solved explicitly.

It is interesting to note that the representation (10) of the solution of the stationary Boltzmann equation (1) can be written in a different form which is more general than the representation via eigenfunctions. If we define

$$h(\xi) := \int_0^\infty d\lambda \, e^{-\lambda \xi/2} A(\lambda) \left( \int_{-\infty}^\infty dp \nu(p) \, e^{-\lambda p^2/2 + N(p)/E} \right)^{-1}$$

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then \( f(x, p) = \int_0^\infty d\lambda A(\lambda) e^{-\lambda x}g_\lambda(p) \) takes the form

\[
f(x, p) = e^{N(p)/E} h(p^2 + 2Ex) + \frac{e^{N(p)/E}}{E} \int_{-\infty}^{\infty} dp' \nu(p') e^{N(p')/E} \times 
\]

\[
\int_{p'} dp \nu(q) e^{-N(q)/E} M(q) h(p^2 + p'^2 - q^2 + 2Ex)
\]

The boundary condition at \( x = 0 \) leads to an integral equation for the unknown function \( h \). Maybe a solution of this equation is possible for a more general class of boundary values \( \varphi \).

**IV A singular integral equation for the expansion coefficients**

If we insert the eigenfunctions (7) into the boundary condition \( f(0, p) = \varphi(p) \) for \( p > 0 \) and make the substitutions \( t = p^2/2E \) and \( s = q^2/2E \), the integral equation (11) for the expansion coefficients \( A(\lambda) \) reads

\[
E M_0 e^{-N(\sqrt{2E}t)/E} \varphi(\sqrt{2Et}) = \int_0^{\infty} d\lambda A(\lambda) C_\lambda e^{-\lambda t} - \int_0^{\infty} d\lambda A(\lambda) e^{-\lambda t} \int_0^t ds e^{\lambda s} \sqrt{E/2s} \nu(\sqrt{2Es}) e^{-N(\sqrt{2Es})-sE/\theta}
\]

Now let us make the assumption that the left hand side of (12) can be written as a Laplace transform of any tempered distribution \( \Psi \)

\[
E M_0 e^{-N(\sqrt{2Et})/E} \varphi(\sqrt{2Et}) = \int_0^{\infty} d\lambda e^{-\lambda t} \Psi(\lambda)
\]

Additionally let us assume that there is a continuous function \( N \) with \( N(\mu) > 0 \) for \( \mu > 0 \) and

\[
\sqrt{E/2s} e^{-N(\sqrt{2Es})/E} \nu(\sqrt{2Es}) = \int_0^{\infty} d\mu e^{-\mu s} N(\mu)
\]

Examples for which this holds are \( \nu(p) = ap^\alpha \) with \(-1 < \alpha \leq 1\) and sums of these powers. If we integrate (14) from \( s \) to infinity, we find

\[
E e^{-N(\sqrt{2Es})/E} = \int_0^{\infty} d\mu e^{-\mu s} N(\mu) / \mu
\]

Therefore \( N/\mu \) is locally integrable at \( \mu = 0 \) and consequently \( N(0) = 0 \). Integrating a second time from \( s \) to infinity, we find

\[
\lim_{\mu \to 0} N(\mu) = 0, \text{ so that } \beta(\lambda) \text{ defined below}
\]

\[
\beta(\lambda) = \int_0^{\infty} d\mu e^{-\mu \beta(\lambda)}/\mu
\]
(see (19)) is a continuous function of $\lambda$. Insertion of (13) and (14) into (12) and usage of the shifting theorem of the Laplace transform leads to (remember uniqueness of the Laplace transform)

\[
\Psi(\lambda) = \left\{ C_\lambda + \mathcal{P} \int_0^\infty \frac{\mathcal{N}(\mu)}{\lambda - E/\theta - \mu} \right\} A(\lambda) \\
- \Theta(\lambda - E/\theta) \mathcal{N}(\lambda - E/\theta) \mathcal{P} \int_0^\infty \frac{A(\mu)}{\mu - \lambda}
\]

where the symbol “$\mathcal{P}$” means Cauchy’s principal value and $\Theta$ denotes Heaviside’s step function. This equation is a singular integral equation for the expansion coefficients $A(\lambda)$. In the limit $\theta \to 0$, the $\Theta$-function in front of the singular integral over $A$ vanishes, which simplifies the situation considerably and allows the treatment described in [7], section 6.

In contrast to “normal” singular equations however, the right hand side of (16) has a zero at $\lambda = E/\theta$. Thus we are dealing with a “nonnormal” problem. This zero is easily split off by a partial integration using $-E \partial_q e^{N/q/E} = \nu e^{-N/E}$ in the numerator of $C_\lambda$ (see (9)) and usage of $E = \int_0^\infty d\mu N/\mu$ (see (15)). The result is

\[
\Psi(\lambda) = (\lambda - E/\theta) \left\{ \alpha(\lambda) A(\lambda) + \beta(\lambda) \mathcal{P} \int_0^\infty \frac{A(\mu)}{\mu - \lambda} \right\}
\]

with the notations

\[
\alpha(\lambda) = \mathcal{P} \int_0^\infty \frac{\mathcal{N}(\mu)}{\mu(\lambda - \mu - E/\theta)} \\
= \int_{-\infty}^\infty dp \int_{-\infty}^\infty dq \ e^{-\lambda p^2/2E + N(p)/E} \ e^{(\lambda - E/\theta) q^2/2E - N(q)/E} \\
+ \int_{-\infty}^\infty dp \int_0^p dq \ e^{-\lambda p^2/2E + N(p)/E}
\]

\[
\beta(\lambda) = -\Theta(\lambda - E/\theta) \frac{\mathcal{N}(\lambda - E/\theta)}{\lambda - E/\theta}
\]

V Solution of the singular integral equation

In appendix A.I we will prove that $\alpha(\lambda) < 0$ for $\lambda \leq E/\theta$. Therefore $\alpha(\lambda) \pm i\pi \beta(\lambda)$ has no zeroes for $\lambda \in \mathbb{R}^+$, and we can transform the nonnormal problem (17) into a normal problem simply by dividing both sides by $(\lambda - E/\theta)$.

However, if we divide the left hand side of (17) by $(\lambda - E/\theta)$, we obtain a distribution, even if $\Psi$ is a smooth function. Although the standard theory of singular
integral equations [14] only deals with Hölder-continuous functions, physicists have for a long time been applying the same methods to distributions as well (see [15] for a comprehensive but heuristic treatment); meanwhile ESTRADA and KANWAL have presented a rigorous theory [16]. Recently the semiinfinite Hilbert transform of distributions has been discussed in a more general framework [18].

If we divide (17) by \((\lambda - E/\theta)\), we obtain the normal singular integral equation

\[
\Upsilon(\lambda) = \alpha(\lambda) A(\lambda) + \beta(\lambda) \mathcal{P} \int_0^\infty d\mu \frac{A(\mu)}{\mu - \lambda}
\]

The tempered distribution \(\Upsilon\) is the most general solution of the (distributional) equation \(\Upsilon \cdot (\lambda - E/\theta) = \Psi\). Thus we can write

\[
\Upsilon(\lambda) = \mathcal{P} \frac{\Psi(\lambda)}{\lambda - E/\theta} + c_E \delta(\lambda - E/\theta)
\]

where \(c_E\) is an arbitrary constant which will be essential later on. The symbol \(\mathcal{P}\) stands for “particular solution”, which is known to exist from HÖRMANDER’s theorem [17]. If we define principal value integrals in the more general sense of [16] or [18], we may read this symbol as “principal value”.

The zero on the right hand side of (17) has introduced an arbitrary constant into our problem. This is in agreement with Prössdorf’s result in a nondistributional framework [19] that such a zero increases the index of the equation by one.

Although the problem of “nonnormality” is solved, there is still a problem with eq. (20). The standard theory of singular integral equations is only applicable to equations on a finite interval, but our equation lives on a semiinfinite interval. We can circumvent this difficulty with the transformation

\[
\mu = \frac{1 + y}{1 - y} \quad \text{and} \quad \lambda = \frac{1 + x}{1 - x}
\]

which maps the interval \(0 < \lambda < \infty\) monotonously onto the interval \(-1 < x < 1\). This transformation does not seem to be well known. For instance Paveri-Fontana and Zweifel [20] recently presented an ab initio derivation of an inversion formula for the half-Hilbert transform which turns out to be equivalent to the well known inversion formula on a finite interval [21] if the transformation (22) is made.

With this transformation, equation (20) transforms into

\[
\hat{\Upsilon}(x) = \hat{\alpha}(x) \hat{A}(x) + \hat{\beta}(x) \mathcal{P} \int_{-1}^{1} dy \frac{\hat{A}(y)}{y - x}
\]

with the definitions

\[
\hat{\Upsilon}(x) := \frac{\Upsilon\left(\frac{1 + x}{1 - x}\right)}{1 - x} \quad \text{and} \quad \hat{A}(x) := \frac{A\left(\frac{1 + x}{1 - x}\right)}{1 - x}
\]

\[
\hat{\alpha}(x) := \alpha\left(\frac{1 + x}{1 - x}\right) \quad \text{and} \quad \hat{\beta}(x) := \beta\left(\frac{1 + x}{1 - x}\right)
\]
Although the theory of singular integral equations on a finite interval is well-developed (see [13] or [22] for a comprehensive summary), we will sketch the solution of (23) in some detail. Let us start with the definition of the analytic function $F$ associated with the distribution $\hat{A}$:

$$F(z) := \frac{1}{2\pi i} \int_{-1}^{1} dx' \frac{\hat{A}(x')}{x' - z} \quad \text{for} \quad z \in \mathbb{C} \setminus [-1, 1]$$

which is a holomorphic function in $\mathbb{C} \setminus [-1, 1]$. If $z$ approaches the cut $[-1, 1]$ from above or below, its boundary values are given by the Plemelj formula

$$\lim_{\epsilon \to 0} F(x \pm i\epsilon) = F^\pm(x) = \frac{1}{2\pi i} \mathcal{P} \int_{-1}^{1} dx' \frac{\hat{A}(x')}{x' - x} \pm \frac{1}{2} \hat{A}(x)$$

Hence our integral equation (23) can be written as a relation between these two boundary values (remember that $\alpha \pm \pi i \beta \neq 0$)

$$\frac{\hat{Y}(x)}{\hat{\alpha}(x) - \pi i \hat{\beta}(x)} = \frac{\hat{\alpha}(x) + \pi i \hat{\beta}(x)}{\hat{\alpha}(x) - \pi i \hat{\beta}(x)} F^+(x) - F^-(x)$$

which is known as a Riemann-Hilbert problem in the literature. Now we are looking for a function $\chi$ which is holomorphic in the complex plane cut at $[-1, 1]$ and satisfies the boundary condition

$$\frac{\hat{\alpha}(x) + \pi i \hat{\beta}(x)}{\hat{\alpha}(x) - \pi i \hat{\beta}(x)} = \frac{\chi^+(x)}{\chi^-(x)}$$

If we find such a function, we can determine $\chi F$ from (24) and therefore also $F$, and from $\hat{A} = F^+ - F^-$ we can obtain $\hat{A}$. A function with this property is

$$\chi(z) = (z + 1)^m (z - 1)^n e^{\Gamma(z)} \quad \text{with}$$

$$\Gamma(z) := \frac{1}{\pi} \int_{-1}^{1} dx' \frac{\gamma(x')}{x' - z} \quad \text{and}$$

$$\gamma(x) := \frac{1}{2i} \ln \left( \frac{\hat{\alpha}(x) + \pi i \hat{\beta}(x)}{\hat{\alpha}(x) - \pi i \hat{\beta}(x)} \right) = \arccot \left( \frac{\hat{\alpha}(x)}{\pi \hat{\beta}(x)} \right)$$

In (27) we are choosing the main branch of the arcus cotangens (see appendix A.II). The exponents $m$ and $n$ must be chosen in such a way that $\chi$ and $F$ are integrable near the end points $z = \pm 1$ (see [22] for details; this is the crucial point where the interval must be finite):

$$-1 < m - \lim_{x \to -1} \gamma(x)/\pi < 1$$

$$-1 < n + \lim_{x \to +1} \gamma(x)/\pi < 1$$

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In appendix A.II it is proven that \(\gamma(-1) = 0\) and \(\gamma(+1) = \pi\). Therefore we must choose \(m = 0\) and \(n = -1\). Thus the index of the integral equation, which is defined by \(m + n\), is \(-1\). Consequently, (23) has a solution \(\hat{A}\) only if the inhomogeneity \(\hat{Y}\) satisfies the orthogonality relation [14]

\[
\int_{-1}^{1} dx \frac{\hat{Y}(x) \chi^{-}(x)}{\hat{\alpha}(x) - \pi i \hat{\beta}(x)} = 0
\]  

Fortunately \(\Upsilon\) contains an arbitrary constant, which we will choose in such a way that this orthogonality relation holds. If (28) is satisfied, the solution of our integral equation (23) is unique and reads

\[
\hat{A}(x) = F^{+}(x) - F^{-}(x) \quad \text{with}
\]

\[
F(z) = \frac{1}{\chi(z) 2\pi i} \int_{-1}^{1} dx' \frac{\chi^{-}(x') \hat{Y}(x')}{[\hat{\alpha}(x') - \pi i \hat{\beta}(x')] (x' - z)}
\]

By application of the Plemelj formula to (25)-(27) we can express \(\chi^{\pm}\) in terms of principal value integrals. Moreover, the solution of the original equation on the semiinfinite interval \((0, \infty)\) is easily obtained via the transformation inverse to (22).

If we set \(x = (\lambda - 1)/(\lambda + 1)\) and \(x' = (\mu - 1)/(\mu + 1)\), we obtain

\[
A(\lambda) = \frac{\alpha(\lambda)}{\alpha^{2}(\lambda) + \pi^{2} \beta^{2}(\lambda)} \Upsilon(\lambda)
\]

\[
- \frac{\beta(\lambda) e^{-G(\lambda)}}{\sqrt{\alpha^{2}(\lambda) + \pi^{2} \beta^{2}(\lambda)}} \mathcal{P} \int_{0}^{\infty} d\mu \frac{(\mu + 1) e^{G(\mu)} \Upsilon(\mu)}{(\lambda + 1) \sqrt{\alpha^{2}(\mu) + \pi^{2} \beta^{2}(\mu)} (\mu - \lambda)}
\]

with the notations

\[
G(\lambda) := \frac{\lambda + 1}{\pi} \mathcal{P} \int_{0}^{\infty} d\mu \frac{g(\mu)}{(\mu + 1)(\mu - \lambda)}
\]

\[
g(\mu) := \frac{1}{2i} \ln \left( \frac{\alpha + \pi i \beta}{\alpha - \pi i \beta} \right) = \arccot \left( \frac{\alpha(\mu)}{\pi \beta(\mu)} \right)
\]

The orthogonality relation for the inhomogeneity \(\Upsilon\) becomes

\[
\int_{0}^{\infty} d\mu \frac{\Upsilon(\mu) e^{G(\mu)}}{\sqrt{\alpha^{2}(\mu) + \pi^{2} \beta^{2}(\mu)}} = 0
\]

According to Noether’s theorem on singular integral equations [23], a necessary and sufficient condition for the solvability of the inhomogeneous equation (20) is the
orthogonality of the inhomogeneity $\mathcal{Y}$ to all solutions $B(\lambda)$ of the adjoint homogeneous equation

\begin{equation}
\alpha(\lambda) B(\lambda) - \mathcal{P} \int_0^\infty d\mu \frac{\beta(\mu) B(\mu)}{\mu - \lambda} = 0
\end{equation}

In our situation, this equation only has one solution. Comparison of Noether’s orthogonality condition $\int \mathcal{Y} B = 0$ with (32) shows (the same result is obtained, of course, by direct solution of (33))

\begin{equation}
B(\lambda) = \frac{e^{G(\lambda)}}{\sqrt{\alpha^2(\lambda) + \pi^2 \beta^2(\lambda)}}
\end{equation}

Because of $\frac{\mu + 1}{(\mu - \lambda)(\mu + 1)} = \frac{1}{\mu - \lambda} + \frac{1}{\lambda + 1}$ and (32), we may write (29) as

\begin{equation}
A(\lambda) = \frac{1}{\alpha^2(\lambda) + \pi^2 \beta^2(\lambda)} \left\{ \alpha(\lambda) \mathcal{Y}(\lambda) - \frac{\beta(\lambda)}{B(\lambda)} \mathcal{P} \int_0^\infty d\mu \frac{B(\mu) \mathcal{Y}(\mu)}{\mu - \lambda} \right\}
\end{equation}

Now let us insert $\mathcal{Y}$ according to (21). The constant $c_E$ must be chosen

\begin{equation}
c_E = -\frac{1}{B(E/\theta)} \int_0^\infty d\mu B(\mu) \mathcal{P} \frac{\Psi(\mu)}{\mu - E/\theta}
\end{equation}

so that the orthogonality relation (32) is satisfied. Finally we arrive at the solution of the singular integral equation for the expansion coefficients:

\begin{equation}
A(\lambda) = \frac{1}{\alpha^2(\lambda) + \pi^2 \beta^2(\lambda)} \left\{ \alpha(\lambda) \mathcal{P} \frac{\Psi(\lambda)}{\lambda - E/\theta} \\
+ \alpha(\lambda) c_E \delta(\lambda - E/\theta) - \frac{\beta(\lambda)}{B(\lambda)(\lambda - E/\theta)} \mathcal{P} \int_0^\infty d\mu \frac{B(\mu) \Psi(\mu)}{\mu - \lambda} \right\}
\end{equation}

where $B(\lambda)$ is given by (34).

Obviously, our solution $f(x, p) = \int d\lambda A(\lambda) e^{-\lambda x} g_\lambda(p)$ is well defined only if $\Psi/\alpha$ is locally integrable at $\lambda = 0$. From eq. (A.1) in the appendix we conclude that for $\lambda \to 0$

$$1/\alpha(\lambda) \sim \text{const} \cdot \int_{-\infty}^{\infty} dp p e^{-\lambda p^2/2E + N(p)/E} \to \infty$$

Thus, if we demand

\begin{equation}\int_0^\infty dp p \varphi(p) = \int_0^\infty dp p \varphi(p) e^{-N(p)/E} e^{N(p)/E}
\end{equation}

(4.44) $\frac{M_0}{E} \int_0^\infty d\lambda \Psi(\lambda) \int_0^\infty dp p e^{-\lambda p^2/2E + N(p)/E}$
the solution of the half-space problem is given by the eigenfunction expansion (10) with expansion coefficients (36).

Let us repeat this result in the form of a half-range completeness theorem for the eigenfunctions $g_\lambda$.

**Theorem:** The integral $N$ over the collision frequency be such that

$$E e^{N(p)/E} = \int_0^\infty d\mu \ e^{\mu p^2/2E} N(\mu)/\mu$$

for some continuous function $N$ with $N(\mu) > 0$ for $\mu > 0$. Then each function $\varphi : \mathbb{R}^+ \rightarrow \mathbb{R}$ with $\int_0^\infty dp \varphi < \infty$, that is a Laplace transform of any tempered distribution $\Phi$

$$\varphi(p) = \int_0^\infty d\mu \Phi(\mu) \ e^{-\mu p^2/2E}$$

is a superposition of eigenfunctions

$$\varphi(p) = \int_\lambda^\infty d\lambda A(\lambda) \ g_\lambda(p)$$

where the expansion coefficients are given by (36) with

$$\Psi(\lambda) = \frac{1}{M_0} \int_0^\lambda d\mu \frac{N(\mu)}{\mu} \Phi(\lambda - \mu)$$

**Remarks:** a) Relation (38) between $\Psi$ and $\Phi$ is an immediate consequence of (14) and the convolution theorem of the Laplace transform.

b) According to (36), the expansion coefficients $A(\lambda)$ generally contain a singular contribution from the eigenvalue $\lambda = E/\theta$, the corresponding eigenfunction of which is the Maxwellian $M(p)$ at temperature $\theta$. This confirms a conjecture of Stichel and Strothmann [12], who took this as a starting point for an asymptotic analysis of the boundary value problem.

**VI Examples**

**VI.I Maxwellian as boundary value**

If the boundary value is a Maxwellian of the temperature $\theta$ of the host medium, that is $\varphi(p) = M(p) = M_0 e^{-p^2/2\theta}$, the solution of the half-space problem reads $f(x, p) = e^{-Ex/\theta} M(p)$, as can be deduced from (1) with the use of $QM \equiv 0$. Hence we should obtain $A(\lambda) = \delta(\lambda - E/\theta)$, so that this situation provides a nice test of our solution.

Indeed, for $\varphi = M$ the inverse Laplace transform $\Psi$ defined in (13) reads

$$\Psi(\lambda) = \Theta(\lambda - E/\theta) \frac{N(\lambda - E/\theta)}{\lambda - E/\theta} = -\beta(\lambda)$$
Thus the expansion coefficients (36) read in this case

\[
A(\lambda) = \frac{1}{\alpha^2(\lambda) + \pi^2 \beta^2(\lambda)} \left\{ \alpha(\lambda) c_E \delta(\lambda - E/\theta) \\
- \frac{\alpha(\lambda) \beta(\lambda)}{\lambda - E/\theta} + \frac{\beta(\lambda)}{B(\lambda) (\lambda - E/\theta)} \mathcal{P} \int_0^\infty d\mu \frac{B(\mu) \beta(\mu)}{\mu - \lambda} \right\}
\]

and the constant \(c_E\) is given by (note that the symbol \(\mathcal{P}\) can be omitted because of \(\beta(\lambda) \equiv 0\) for \(\lambda \leq E/\theta\))

\[
c_E = \frac{1}{B(E/\theta)} \int_0^\infty d\mu \frac{B(\mu) \beta(\mu)}{\mu - E/\theta}
\]

Because of relation (33), the integrals over \(B\beta\) can be replaced by \(\alpha(\lambda) B(\lambda)\) and \(\alpha(E/\theta) B(E/\theta)\). If we take care of \(\beta(E/\theta) = 0\), we obtain indeed \(A(\lambda) = \delta(\lambda - E/\theta)\).

VI.II Constant relaxation time

In case of a constant relaxation time \(\nu(p) = \text{const.} = 1/\tau\), the quantities \(\alpha\), \(\beta\) and \(B\) in the formula (36) for the expansion coefficients can be calculated explicitly. Moreover there is a relation between \(\alpha\) and \(\beta\) that allows a simplification of some expressions. For details of the calculation we refer the interested reader to [24].

Without loss of generality we can set \(\tau\) and \(\theta\) equal unity [25]. Then the function \(\mathcal{N}\) that is necessary for the calculation of \(\Psi\) via (38) reads

\[
\mathcal{N}(\mu) = \left(\frac{E}{2\pi \mu}\right)^{1/2} e^{-1/2E\mu} \int_0^\infty dx \frac{x^{-3/2} e^{-1/x}}{2(\lambda - E)}
\]

where the principal value integral in \(\alpha\) allows for an explicit evaluation

\[
\mathcal{P} \int_0^\infty dx \frac{x^{-3/2} e^{-1/x}}{y - x} = \begin{cases} 
  y\sqrt{\pi} \left(1 - \sqrt{-y} e^{-y} \int_0^\infty e^{-t^2} dt\right) & \text{for } y \leq 0 \\
  y\sqrt{\pi} \left(1 - 2\sqrt{y} e^{-y} \int_0^{\sqrt{y}} e^t dt\right) & \text{for } y \geq 0
\end{cases}
\]

Moreover in this situation the function \(B(\lambda)\), which generally contains a principal value integral (see (34) and (30)), can be expressed in terms of a regular integral. We find (apart from an irrelevant constant which cancels out in (36))

\[
B(\lambda) \propto \lambda^{-3/2} e^{1/2E\lambda} \xi(\lambda) \quad \text{with}
\]

\[
\xi(\lambda) = \exp \left\{ \frac{E}{2\pi} \int_E^\infty d\mu \frac{g(\mu)}{\mu + \lambda - E} \frac{2\lambda - E}{2\mu - E} \right\}
\]
where \( g(\mu) = \arccot(\alpha/\pi\beta) \) is the function defined in (31). The function \( \xi \) is a smooth function of \( \lambda \) which is very close to a straight line; it is sketched in figure 1 for different values of the field \( E \).

At first glance, the divergence of \( B(\lambda) \) for \( \lambda \to 0 \) might cause trouble in the integrals in (36). However, it follows from (37) that \( \Psi(\lambda)\lambda^{-3/2}e^{1/2E\lambda} \) is locally integrable at \( \lambda = 0 \). Hence all integrals in (36) are well defined.

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A Appendix

A.I Negativity of $\alpha(\lambda)$ for $\lambda \leq E/\theta$

For $\lambda \leq E/\theta$, the first integral in the definition of $\alpha(\lambda)$ (18) is a regular integral instead of a singular integral. Hence we may write this integral with the use of (15)

$$\begin{align*}
\int_0^\infty d\mu \frac{\mathcal{N}(\mu)}{\mu(\lambda - \mu - E/\theta)} &= -\int_0^\infty d\mu \frac{\mathcal{N}(\mu)}{\mu} \int_0^p \frac{p}{E} e^{(\lambda - \mu - E/\theta)q^2/2E} \\
&= -\int_0^\infty dp \, p \, e^{(\lambda - E/\theta)q^2/2E - N(p)/E}
\end{align*}$$

Thus, combining terms in (18), we obtain for $\lambda \leq E/\theta$

$$(A.1) \quad \alpha(\lambda) = -\frac{\int_0^\infty dp \, e^{-\lambda p^2/2E + N(p)/E} \int_p^\infty dq \, q \, e^{(\lambda - E/\theta)q^2/2E - N(q)/E}}{-\int_0^\infty dp \, e^{-\lambda p^2/2E + N(p)/E}}$$

Since $N(p)$ is an increasing function, the denominator of (A.1) is always positive. Now we will prove that the numerator is positive too. For this purpose, let us convert all integrals over regions with negative values of $p$ and $q$ into integrals over positive values. If we do so, we can write for the numerator of (A.1)

$$\begin{align*}
&\int_0^\infty dp \, e^{-\lambda p^2/2E + N(p)/E} \int_p^\infty dq \, q \, e^{(\lambda - E/\theta)q^2/2E - N(q)/E} \\
- &\int_0^\infty dp \, e^{-\lambda p^2/2E + N(-p)/E} \int_0^\infty dq \, q \, e^{(\lambda - E/\theta)q^2/2E - N(q)/E} \\
+ &\int_0^\infty dp \, e^{-\lambda p^2/2E + N(-p)/E} \int_0^p dq \, q \, e^{(\lambda - E/\theta)q^2/2E - N(-q)/E}
\end{align*}$$

In the first term we write $\int_p^\infty dq = \int_0^\infty dq - \int_0^p dq$. Collecting terms with $\int_0^\infty dq$ and $\int_0^p dq$, the numerator of (A.1) reads

$$(A.2) \quad \int_0^\infty dp \, e^{-\lambda p^2/2E} \left\{ \int_0^\infty dq \, q \, e^{(\lambda - E/\theta)q^2/2E} \left( e^{N(p)/E - N(q)/E} - e^{N(-p)/E - N(q)/E} \right) \right\} > 0 \text{ for } p > 0$$

$$+ \int_0^p dq \, q \, e^{(\lambda - E/\theta)q^2/2E} \left( e^{N(-p)/E - N(-q)/E} - e^{N(p)/E - N(q)/E} \right) < 0 \text{ for } p > q$$
We can estimate the positive first term in the curly braces via $\int_0^\infty dq > \int_0^p dq$. Thus we arrive at the following lower estimate for (A.2):

$$\int_0^\infty dp p e^{-\lambda p^2/2E} \int_0^p dq q e^{(\lambda-E/\theta)q^2/2E} \left( e^{N(-p)/E-N(-q)/E} - e^{N(-p)/E-N(q)/E} \right) > 0 \text{ for } q > 0$$

Since this lower estimate is positive, the numerator in (A.1) is positive, and consequently $\alpha(\lambda)$ is negative for $\lambda \leq E/\theta$.

### A.II Behaviour of $\alpha$ and $\beta$ for large $\lambda$

The index of our singular integral equation depends crucially on the values of

$$g(\lambda) = \frac{1}{2i} \ln \left( \frac{\alpha(\lambda) + \pi i \beta(\lambda)}{\alpha(\lambda) - \pi i \beta(\lambda)} \right)$$

for $\lambda \to 0$ and $\lambda \to \infty$. Thus we need to determine the behaviour of the argument of the logarithm as $\lambda$ varies from zero to infinity.

First note that the absolute value of this argument is equal to unity for any value of $\lambda$, because numerator and denominator are complex conjugates. Moreover, because of $\beta \equiv 0$ for $\lambda \leq E/\theta$, the argument is +1 for $\lambda \leq E/\theta$ and with the choice $\ln(1) = 0$ we have

$$g(\lambda) \equiv 0 \quad \text{for } \lambda \leq E/\theta$$

Now let us consider real and imaginary part of the argument of the logarithm

$$\text{Re} \left( \frac{\alpha + \pi i \beta}{\alpha - \pi i \beta} \right) = \frac{\alpha^2 - \pi^2 \beta^2}{\alpha^2 + \pi^2 \beta^2} \quad \text{and} \quad \text{Im} \left( \frac{\alpha + \pi i \beta}{\alpha - \pi i \beta} \right) = \frac{2\pi \alpha \beta}{\alpha^2 + \pi^2 \beta^2}$$

We know from the previous section that $\alpha(E/\theta)$ is negative, and from the definition (19) we know that $\beta(\lambda) < 0$ for $\lambda > E/\theta$. In consequence the imaginary part is positive if $\lambda$ is slightly greater than $E/\theta$.

Moreover, from (A.4) we see that the real part cannot be positive whilst the imaginary part is zero. In other words the positive real axis cannot be crossed for finite $\lambda$.

In order to determine the behaviour for $\lambda \to \infty$, we use the lemma on the asymptotic behaviour of $\alpha$ and $\beta$ (see below). An immediate consequence of the lemma is that $\lim_{\lambda \to \infty} \beta/\alpha = 0$ and $\alpha(\lambda) > 0$ for large values of $\lambda$. Hence $(\alpha + \pi i \beta)/(\alpha - \pi i \beta)$ approaches +1 with a negative imaginary part for $\lambda \to \infty$.

Applying this result to our function $g(\lambda)$ defined in (A.3), we obtain the limiting values

$$\lim_{\lambda \to \infty} g(\lambda) = 0 \quad \text{and} \quad \lim_{\lambda \to \infty} g(\lambda) = \pi$$
The logarithm may be expressed in terms of the arcus tangens function

\[ g(\lambda) = \arctan \left( \frac{\pi \beta(\lambda)}{\alpha(\lambda)} \right) = \arccot \left( \frac{\alpha(\lambda)}{\pi \beta(\lambda)} \right) \]

We must choose the branch of the arcus tangens, or arcus cotangens respectively, in such a way that (A.6) is a continuous function of \( \lambda \) and (A.5) is satisfied. The resulting branches are sketched in figure 2.

**Lemma:** As \( \lambda \) approaches infinity, the asymptotic behaviour of \( \alpha \) and \( \beta \) is given by

\[ \beta(\lambda) \sim \sqrt{E/2\pi \nu(0)} \lambda^{-3/2} \]

\[ \alpha(\lambda) \sim \sqrt{E/2\pi \lambda} \int_{-\infty}^{\infty} dp e^{-\nu(p)} \nu(0) = \frac{\sqrt{E/2\pi \lambda}}{M_0 \nu(0)} \]

**Proof:** (A.7) is a consequence of (14) and the Tauberian theorems on the Laplace transform (see \[29\], part 1), which may be applied because of \( \mathcal{N} \geq 0 \). If we remember the definition \( \beta(\lambda + E/\theta) = \Theta(\lambda) \mathcal{N}(\lambda)/\lambda \), we see that (A.7) holds.

The asymptotic evaluation of \( \alpha(\lambda) \) is a bit more intricate. Let us examine each term in the definition (18) separately:

The first term on the right hand side of (18) behaves like

\[ \lambda \to \infty, \quad \frac{1}{\lambda - E/\theta} \int_{0}^{\infty} d\mu \frac{\mathcal{N}(\mu)}{\mu} = \frac{E}{\lambda - E/\theta} \]

The denominator of the second term in (18) can be written as an integral over the positive real axis, which is easily evaluated asymptotically with LAPLACE’s method (see \[27\], chapter 3)

\[ \int_{0}^{\infty} dp e^{-\lambda p^2/2E} \left( e^{N(p)/E} - e^{N(-p)/E} \right) \lambda \to \infty, \nu(0) \sqrt{2\pi E} \lambda^{-3/2} \]

The numerator of the second term on the right hand side of (18) can be evaluated as follows: after conversion of all integrals over the negative real axis into integrals over the positive axis, we substitute \( t = q^2/2E \) and \( s' = p^2/2E \). If we then transform \( s = s' - t \) and change the order of integrations, we obtain

\[ E^2 \int_{0}^{\infty} ds e^{-\lambda s} \int_{0}^{\infty} dt e^{-Et/\theta} \left\{ e^{N(\sqrt{2E(s+t)}/E-N(\sqrt{2Et})/E)} - e^{N(-\sqrt{2E(s+t)}/E-N(-\sqrt{2Et})/E)} \right\} \]
Again we may apply Laplace’s method [27]; we only need to determine the behaviour of the inner integral for $s \to 0$. The term in curly braces behaves like

$$\{...\} \sim s \left( \frac{s}{\sqrt{2Et}} \nu \left( \sqrt{2Et} \right) + \nu \left( \sqrt{-2Et} \right) \right)$$

Thus the inner integral behaves like $s \int_{-\infty}^{\infty} dp \, e^{p^2/2\theta} \nu(p)/E$, and consequently the numerator in (18) behaves like

(A.11) \quad \lambda \to \infty \quad \frac{E}{\lambda^2} \int_{-\infty}^{\infty} dp \, e^{-p^2/2\theta} \nu(p)$

Collecting (A.9) - (A.11) and insertion into $\alpha(\lambda)$ according to (18) yields (A.8).
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