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KINETIC EQUATIONS WITH REFLECTING BOUNDARY CONDITIONS*

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Abstract. A general abstract model of time-independent kinetic equations on the half-line is presented. The existence and uniqueness of the solution is proved under specified incoming flux and nonmultiplying boundary reflection processes. An iterative method is formulated for computing in principle the solution by using the solution of the analogous problem without reflection. In many concrete cases (e.g. neutron transport, BGK model in rarefied gas dynamics, etc.) the available explicit expression for the latter provides the actual solution of the general problem. Possible generalizations and open problems are briefly discussed.

Key words. kinetic theory, transport equation, reflection

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1. Introduction. In recent years substantial progress has been reported on the existence and uniqueness theory for the solution of boundary value problems of the type

$$T\psi'(x) = -A\psi(x), \qquad x \in \mathbb{R}_+, \tag{1.1}$$

$$Q_+\psi(0) = \mathscr{R}JQ_-\psi(0) + \phi_+, \tag{1.2}$$

$$\|\psi(x)\| = O(1) \qquad (x \to \infty), \tag{1.3}$$

where T is an injective self-adjoint operator, Q_+ and Q_- the orthogonal projections onto the maximal positive and negative T-invariant subspaces and A a positive self-adjoint (bounded or unbounded) Fredholm operator. The operators $\mathscr{R}$ and J as well as the precise meaning of the norm in (1.3) will be specified later. This boundary value problem models a variety of time-independent transport phenomena in semi-infinite media with boundary conditions appropriate to incoming flux specification and, if $\mathscr{R}$ is nonzero, to a (partial) reflection at the boundary. In most instances, however, it has been assumed that $\mathscr{R} = 0$ (absence of reflection), and in this case the solution ψ, whenever unique, is represented in the form

$$\psi(x) = e^{-xT^{-1}A}E\phi_+, \qquad x \in \mathbb{R}_+. \tag{1.4}$$

In this direction we note the important contributions of Hangelbroek [14], Lekkerkerker [16], Beals [1, 2], van der Mee [19] and Greenberg et al. [13]. Only recently such a theory has been developed with full account of boundary reflection processes ($\mathrm{R} \equiv 0$). Namely, Beals and Protopopescu [3], [4] obtained an existence and uniqueness theory

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for the Fokker–Planck equation

$$(1.5)\quad v\frac{\partial\psi}{\partial x}(x,v)=\frac{\partial^2\psi}{\partial v^2}(x,v)-v\frac{\partial\psi}{\partial x}(x,v),\qquad x\in\mathbb{R}_+,\quad v\in\mathbb{R},$$

$$(1.6)\quad \psi(0,v)=\alpha\psi(0,-v)+\beta\int_{-\infty}^{0}\sigma(v'\to v)\psi(0,v')\,dv'+\phi_+(v),\qquad v\in\mathbb{R}_+,$$

$$(1.7)\quad \lim_{x\to\infty}\{\psi(x,v)/x\}=b.$$

For general σ's the existence proof required a condition which will turn out to be automatically satisfied. Maslova [17], [18] published related results on the linearized Boltzmann equation with a sufficiently regular intermolecular potential. Greenberg and van der Mee [12] formulated a related radiative transfer problem in an abstract setting, but their result deals with (1.1) on a finite interval. The abstract approach was recently followed by van der Mee [20], who announced some results on this problem.

The paper is organized as follows. For the reader's convenience in §2 we provide a brief but fairly complete review of the existence and uniqueness theory for the solution of (1.1)–(1.3). Section 3 contains the procedure of *computing* the solution of the problem with reflection from the solution of the same problem without reflection ($\mathscr{R}=0$). This iterative scheme can be implemented whenever the albedo operator E in (1.4) is known explicitly, which is actually the case for a large class of problems. Namely, if A is a compact perturbation of the identity, an expression for E in terms of generalized Chandrasekhar **H**-functions [9] has been given by van der Mee [21], thereby generalizing a plethora of results obtained before for specific models (neutron transport, radiative transfer, BGK models, etc.). In some cases the iterative procedure can also be derived from a half-range completeness result involving **H**-functions (cf. [7], for instance). At present, no explicit representation is known for the albedo operator E in the case of the Fokker–Planck model (1.5)–(1.7) and more general Sturm–Liouville problems.

2. Existence and uniqueness theory. In the present section we provide a brief but fairly complete review of the existence and uniqueness theory for the solution of (1.1)–(1.3). In order to explain the later introduction of a number of concepts, we present the overall flavor of the theory by first considering T bounded and A strictly positive and neglecting reflection processes, which is relevant to radiative transfer in absorbing atmospheres [9] and neutron transport in submultiplying reactors [7]. Using semigroup theory, one may naturally write solutions to (1.1) in the form

$$\psi(x)=e^{-xT^{-1}A}\psi(0),\qquad 0\leqq x<\infty,$$

where $\psi(0)$ must be chosen in the subspace corresponding to the nonnegative part of the spectrum of the evolution operator $T^{-1}A$ in order that the above semigroup expression makes sense and condition (1.3) is fulfilled. On fitting the boundary condition (1.2) where $\mathscr{R}=0$, one must require $Q_+\psi(0)=\varphi_+$. If one would formulate an analogous boundary value problem for $x\in(+\infty,0)$, one should require that $\psi(0)$ be chosen in the subspace corresponding to the nonpositive part of the spectrum of $T^{-1}A$ and $Q_-\psi(0)=\varphi_-$. In a natural way one may thus express the unique solvability of both half-space problems, for $x\in(0,\infty)$ and for $x\in(-\infty,0)$, in terms of the invertibility of the operator V, which maps the nonnegative (resp. nonpositive) spectral subspace of $T^{-1}A$ into the ranges of the projections $Q_\pm$ onto forward (resp. backward) "fluxes". As a matter of fact, $V\psi(0)=\varphi_+$, $E=V^{-1}$ is called the albedo operator and formula (1.4) arises as the obvious result. Below we shall review the existence and uniqueness theory along the above set up (which originates from Hangelbroek [14]) in some detail, since the unboundedness of T, the appearance of a nonzero null space of A and the absence of compactness assumptions on A cause technical difficulties and necessitate the introduction of some novel notions.

Let us now drop the above restrictions on T and A. Let T be an injective self-adjoint operator and A a positive self-adjoint operator with closed range $\operatorname{Ran} A$ and null space $\operatorname{Ker} A$ of finite dimension, both defined on the complex Hilbert space H. For the sake of convenience we assume A to be bounded, but at the end of this work we shall discuss how to remove this restriction. We then define the zero root subspace

$$Z_0 = \{ h \in H / \exists n \in \mathbb{N} : (T^{-1}A)^n h = 0 \}, \tag{2.1}$$

and assume $Z_0 \subset D(T)$. It can then be proved (cf. [13]; the result there extends to unbounded T) that Z_0 has a finite dimension and $Z_0 = \operatorname{Ker}(T^{-1}A)^2$. Here we also assume that Z_0 is nondegenerate in the following sense:

$$\{ h \in Z_0 / (Th, k) = 0 \text{ for all } k \in Z_0 \} = \{0\}.$$

In fact, this assumption is automatically satisfied. (If T is bounded, see [13]).

PROPOSITION 2.1. *We have the following decompositions*:

$$Z_0 \oplus (T[Z_0])^{\perp} = H, \tag{2.2}$$

$$T[Z_0] \oplus Z_0^{\perp} = H, \tag{2.3}$$

$$Z_0^{\perp} = \overline{T\{(T[Z_0])^{\perp}\}} = A\{(T[Z_0])^{\perp}\}. \tag{2.4}$$

Moreover, Z_0 and $(T[Z_0])^{\perp}$ are $T^{-1}A$-invariant subspaces and there exists a unique operator S on $(T[Z_0])^{\perp}$ such that

$$T^{-1}A = (T^{-1}A|_{Z_0}) \oplus S^{-1}. \tag{2.5}$$

The operator S is self-adjoint with respect to the positive definite inner product on $(T[Z_0])^{\perp}$ given by

$$(h,k)_A = (Ah, k). \tag{2.6}$$

For isotropic neutron transport in a conservative medium, where Z_0 can be constructed explicitly, this Proposition 2.1 is due to Lekkerkerker [16]. It later appeared in more abstract form in [19], [13], [2].

Let us introduce H_T as the Hilbert space obtained by completing $D(T)$ with respect to the inner product

$$(h,k)_T = (|T|h, k).$$

Let us assume that there exists a unitary and self-adjoint operator J on H, which leaves invariant $D(T)$ and satisfies

$$TJ = -JT, \qquad AJ = JA.$$

Then J extends from $D(T)$ to a unitary and self-adjoint operator on H_T, as also do the orthogonal projections Q_+ and Q_- of H onto the maximal positive and negative T-invariant subspaces, respectively. We shall require the *reflection operator* to be a bounded operator on $Q_+[H]$, which leaves invariant $D(T)$, and satisfies the identity

$$T\mathscr{R} = \mathscr{R}^{\dagger} T \tag{2.7}$$

for some bounded operator $\mathscr{R}^+$ on H. Putting

$$\mathscr{R}h \stackrel{\text{def}}{=} J\mathscr{R}Jh, \qquad h \in Q_-[H],$$

we extend $\mathscr{R}$ to a bounded operator on H, which automatically commutes with J, leaves invariant $D(T)$ and extends from $D(T)$ to a bounded operator on H_T. In order that the operator $\mathscr{R}$ models a nonmultiplying reflection process at the boundary, we also assume that $\mathscr{R}$ extends to a contraction on H_T:

$$(|T|\mathscr{R}h, \mathscr{R}h) \leqq (|T|h, h), \qquad h \in D(T).$$

For later use we include the following result, derived by Beals [1] for injective and certain noninjective A, and generalized by Greenberg et al. [13].

THEOREM 2.2. *For every* $\phi_+ \in Q_+[H_T]$ *there exists at least one continuous function* ψ: $[0,\infty) \to H_T$, *which is continuously differentiable on* $(0,\infty)$ *and satisfies the equations*

$$T\psi'(x) = -A\psi(x), \qquad x \in \mathbb{R}_+, \tag{2.8}$$

$$Q_+\psi(0) = \phi_+, \tag{2.9}$$

$$\|\psi(x)\|_T = O(1) \qquad (x \to \infty). \tag{2.10}$$

The number of linearly independent solutions of the homogeneous ($\phi_+ = 0$) *problem coincides with the maximal number of linearly independent vectors* $h_1, \cdots, h_k \in \operatorname{Ker} A$ *satisfying* $(Th_i, h_j) = 0$ *for* $i \neq j$ *and* $(Th_i, h_i) < 0$ *for* $i = 1, 2, \cdots, k$.

In fact, it is possible to construct at least one "albedo operator" E, which is a bounded strictly positive self-adjoint operator on H_T, such that

$$\psi(x) = e^{-xT^{-1}A}PE\phi_+ + (I-P)E\phi_+ \tag{2.11}$$

is a solution of (2.8)–(2.10). Here P is the continuous extension from $D(T)$ to H_T of the projection of H onto $(T[Z_0])^\perp$ along Z_0 (cf. (2.1)), while

$$\|I - E\|_{H_T} < 1 \tag{2.12}$$

(cf. [13], where it is shown that $\sigma(E) \subset (0,2)$). Evidently we must then have $(I-P)E\phi_+ \in \operatorname{Ker} A$ for all $\phi_+ \in Q_+[H_T]$.

The solution of the existence problem for (1.1)–(1.3) is provided by the following

THEOREM 2.3. *For every* $\phi_+ \in Q_+[H_T]$ *there exists at least one continuous function* ψ: $[0,\infty) \to H_T$, *which is continuously differentiable on* $(0,\infty)$ *and satisfies the equations*

$$T\psi'(x) = -A\psi(x), \qquad x \in \mathbb{R}_+, \tag{2.13}$$

$$Q_+\psi(0) = \mathscr{R}JQ_-\psi(0) + \phi_+, \tag{2.14}$$

$$\|\psi(x)\|_T = O(1) \qquad (x \to \infty). \tag{2.15}$$

Proof. Consider the operator

$$S_{\mathscr{R}} = I + \mathscr{R}J(I-E).$$

Because of the estimate

$$\|S_{\mathscr{R}} - I\|_{H_T} \leqq \|\mathscr{R}\|_{H_T} \|J\|_{H_T} \|I-E\|_{H_T} < 1, \tag{2.16}$$

the operator $S_{\mathscr{R}}$ is bounded and invertible on H_T. Consider the function

$$\psi(x) = e^{-xT^{-1}A}PES_{\mathscr{R}}^{-1}\phi_+ + (I-P)ES_{\mathscr{R}}^{-1}\phi_+, \qquad 0 \leqq x < \infty.$$

Then ψ is a continuous function from $[0,\infty)$ into H_T, which is bounded and continuously differentiable on $(0,\infty)$ and satisfies (2.13), since $(I-P)ES_{\mathscr{R}}^{-1}\phi_+\in\operatorname{Ker}A$. Notice that $S_{\mathscr{R}}$ maps $Q_+[H_T]$ onto itself. We now have

$$\begin{aligned}(Q_+-\mathscr{R}JQ_-)\psi(0)&=(Q_+-\mathscr{R}JQ_-)ES_{\mathscr{R}}^{-1}\phi_+\\&=(Q_+-\mathscr{R}JQ_-)EQ_+S_{\mathscr{R}}^{-1}\phi_+=(Q_+-\mathscr{R}JQ_-EQ_+)S_{\mathscr{R}}^{-1}\phi_+\\&=(Q_++\mathscr{R}JQ_-(I-E)Q_+)S_{\mathscr{R}}^{-1}\phi_+=Q_+S_{\mathscr{R}}Q_+S_{\mathscr{R}}^{-1}\phi_+=\phi_+,\end{aligned}$$

and therefore (2.14) is satisfied. □

Remark. As far as one considers only operators A which do not have negative definite parts and whose kernel is finite-dimensional, the most general boundary condition to be imposed at infinity reads

$$\exists n\geqq 0:\ \|\psi(x)\|_T=0(x^n)(x\to\infty). \tag{2.17}$$

This is the case for conservative neutron transport [16] and for the Fokker–Planck equation [4], where the root subspace as defined by (2.1) is two-dimensional and $n=1$. This implies that for large x the solution behaves as f_1+f_2x. (Here the vectors f_1 and f_2 are functions depending on the angular (for neutron transport) or velocity (for the Fokker–Planck equation) variable, but in more general cases they may contain some other variables as well, depending on the complexity of the operators T and A.) For the kinetic (transport) problems usually occurring in physical situations the solution f_1+f_2x is called normal (or Chapman–Enskog) and the vectors in the root subspace are related to the (reduced) hydrodynamical description, valid far from the boundary. Because the boundary condition (2.17) is more general than (2.15), existence of solutions is clear. For the two types of boundary condition at infinity the number of linearly independent solutions might be different if normal solutions occur.

Let us now define P as the projection onto $(T[Z_0])^\perp$ along Z_0 and PP_+ (resp. PP_-) as the projection onto the maximal positive (resp. negative) S-invariant subspace along the direct sum of Z_0 and the maximal negative (resp. positive) S-invariant subspace. Here positivity and negativity relate to the inner product (2.6) and essential use has been made of the Spectral Theorem for S (cf. Proposition 2.1). As a consequence,

$$(TPP_+h,h)=(SPP_+h,h)_A\geqq 0,\qquad (TPP_-k,k)=(SPP_-k,k)_A\leqq 0, \tag{2.18}$$

where strict positivity and negativity hold for $h\in\operatorname{Ran}PP_+$ and $k\in\operatorname{Ran}PP_-$. Then PP_+ and PP_- extend to bounded projections on H_T (cf. [1],[13]). Next put

$$M_{\mp,}=\left[\operatorname{Ran}PP_\pm\oplus\operatorname{Ker}(Q_\pm-\mathscr{R}JQ_\mp)\right]\cap Z_0 \tag{2.19}$$

for the notions concerning indefinite inner product spaces we are going to use we refer to [5].

LEMMA 2.4. *We have*

$$(Th,h)\leqq 0,\qquad h\in M_{-,\mathscr{R}}.$$

If $\|\mathscr{R}\|_{H_T}<1$, *or under the weaker assumption*

$$\operatorname{Ker}(Q_+-\mathscr{R}JQ_-)\cap Z_0=\{0\}, \tag{2.20}$$

we have

$$(Th,h)<0,\qquad 0\neq h\in M_{-,\mathscr{R}}.$$

Proof. For $h \in M_{-,\mathscr{R}}$ we first determine $g \in \operatorname{Ran} PP_+$ and $k \in \operatorname{Ker}(Q_+ - \mathscr{R}JQ_-)$ such that $h = g + k$. Since $h \in Z_0$ and $g \in (T[Z_0])^\perp$, we have $(Th, g) = 0$. Hence,

$$(Th,h)+(Tg,g)=(Tk,k)=\|Q_+k\|_T^2-\|Q_-k\|_T^2$$
$$=\|\mathscr{R}JQ_-k\|_T^2-\|Q_-k\|_T^2 \leqq -\left(I-\|\mathscr{R}\|_{H_T}^2\right)\|Q_-k\|_T^2.$$

Since $(Tg,g)=(Sg,g)_A \geqq 0$ (cf. (2.18)), we have $(Th,h) \leqq 0$. Moreover, if $(Th,h)=0$, then $g=0$ and either $\|\mathscr{R}\|_{h_T}=1$ or $Q_-k=0$; the latter would imply $k=\mathscr{R}JQ_-k+Q_-k=0$ and $h=0$. Hence, if $\|\mathscr{R}\|_{H_T}<1$, we have $(Th,h)<0$ for $0 \neq h \in M_{-,\mathscr{R}}$. The latter conclusion can also be drawn under the weaker assumption (2.20). □

In the same way we can prove that

$$(Th,h)<0, \qquad h \in M_{-,\mathscr{R}} \cap \operatorname{Ker} A,$$

provided

$$\operatorname{Ker}(Q_+ - \mathscr{R}JQ_-) \cap \operatorname{Ker} A = \{0\}. \tag{2.21}$$

THEOREM 2.5. *Under the condition* (2.21) *the number of linearly independent solutions of the homogeneous* ($\phi_+=0$) *problem* (2.13)–(2.15) *coincides with the maximal number of linearly independent vectors* $h_1, \cdots, h_k \in \operatorname{Ker} A$ *satisfying* $(Th_i, h_j)=0$ *for* $i \neq j$ *and* $(Th_i, h_i)<0$ *for* $i=1,2,\cdots,k$.

Proof. Denoting by $\mathscr{R}^*$ the adjoint of $\mathscr{R}$ in H, we easily compute

$$(T[M_{\mp,\mathscr{R}}])^\perp=\left[(T\operatorname{Ran} PP_\pm)^\perp \cap \operatorname{Ran} T^{-1}(Q_\pm - Q_\mp J\mathscr{R}^*)\right]+(T[Z_0])^\perp$$
$$=\left[(\operatorname{Ran} PP_\mp \oplus Z_0) \cap \operatorname{Ran}\left(Q_\pm + Q_\mp J(\mathscr{R}^\dagger)^*\right)T^{-1}\right]+(T[Z_0])^\perp$$
$$=\left\{\left[\operatorname{Ran} PP_\mp \oplus \operatorname{Ran}\left(Q_\pm + Q_\mp J(\mathscr{R}^\dagger)^*\right)\right] \cap Z_0\right\} \cap (T[Z_0])^\perp.$$

Here we have used the intertwining property $T\mathscr{R}=\mathscr{R}^\dagger T$ and the fact that the operator $Q_\pm + Q_\mp J(\mathscr{R}^\dagger)^*$ is a bounded projection on H and therefore has closed range. For $g \in \operatorname{Ran} PP_-$ and $k=(Q_+ + Q_-J(\mathscr{R}^\dagger)^*)l$ we obtain

$$(Th,h)+(Tg,g)=(Tk,k)=\|Q_+k\|_T^2-\|Q_-k\|_T^2=\|Q_+l\|_T^2-\left\|Q_-J(\mathscr{R}^\dagger)^*l\right\|_T^2$$
$$\geqq\left(1-\left\|(\mathscr{R}^\dagger)^*\right\|_{H_T}^2\right)\|Q_+l\|_T^2 \geqq 0,$$

because $(\mathscr{R}^\dagger)^*$ is a contraction in H_T:

$$0 \leqq \left((\mathscr{R}^\dagger)^*h,h\right)_T=((Q_+-Q_-)h,\mathscr{R}(Q_+-Q_-)h)_T \leqq \|\mathscr{R}\|_{H_T}^2\|h\|_T^2 \leqq \|h\|_T^2.$$

We now obtain

$$(Th,h) \geqq 0, \qquad h \in (T[M_{-,\mathscr{R}}])^\perp \cap Z_0.$$

Since Z_0 is nondegenerate with respect to the indefinite inner product

$$[h,k]=(Th,k), \tag{2.22}$$

$M_{-,\mathscr{R}}$ is negative and $(T[M_{-,\mathscr{R}}])^\perp \cap Z_0$ is positive, the subspace $M_{-,\mathscr{R}}$ is maximal negative with respect to this inner product. Under the condition (2.21) the subspace $M_{-,\mathscr{R}} \cap \operatorname{Ker} A$ then is strictly negative and maximal in this respect among the subspaces of Ker$A$. Because the linear span of the vectors $h_1,\cdots,h_k$ in the statement of this theorem is also a maximal strictly negative subspace of Ker$A$ and the dimension of such a subspace does not depend on its specific choice, we must have $\dim(M_{-,\mathscr{R}}\cap \operatorname{Ker}A)=k$. Finally, if ψ is a solution of (2.13)–(2.15) with $\phi_+=0$, then necessarily $(I-P)\psi(0)\in M_{-,\mathscr{R}}\cap \operatorname{Ker}A$. □

Under the condition (2.21) we find the same existence and uniqueness result as for $\mathscr{R}=0$, which we easily see on comparing Theorems 2.2 and 2.5. If one would drop condition (2.21), the homogeneous ($\phi_+=0$) problem (2.13)–(2.15) in general has more linearly independent solutions than is to be expected from the above theorem. As an example, consider the case $\mathscr{R}=I$, which describes *purely specular reflection*. First we observe that every $k\in H_T$, which satisfies $Q_+k\text{-}\mathscr{R}JQ_-k$ for $\mathscr{R}=I$, has the property

$$(Tk,k)=\|Q_+k\|_T^2-\|Q_-k\|_T^2=\|JQ_-k\|_T^2-\|Q_-k\|_T^2=0,$$

since J is a unitary operator on H_T. If such a vector k would belong to the space $\operatorname{Ran}PP_+\oplus\operatorname{Ker}A$, as it should be if it were the initial value of a solution ψ, then $k=-g+h$ for some $g\in\operatorname{Ran}PP_+$ and $h\in\operatorname{Ker}A$. Since $Q_+k=JQ_-k$ implies

$$Jk=JQ_+k+JQ_-k=J(JQ_-k)+Q_+k=k,$$

and therefore $Jg=g$ and $Jh=h$, the property $g=Jg\in\operatorname{Ran}PP_-$ would give rise to $g=0$ and thus $k\in\operatorname{Ker}A$, whence $k\in\operatorname{Ker}A\cap\operatorname{Ker}(I-J)$. Conversely, every such k would fulfill the condition $JQ_-k=Q_+Jk=Q_+k$ and therefore be an initial value of some solution ψ. Thus the constant functions $\psi(x)=k$, where $k=Jk\in\operatorname{Ker}A$, are the solutions of the homogeneous ($\phi_+=0$) problem (2.13)–(2.15) with $\mathscr{R}=I$.

Remark. The analogue of Theorem 2.5 for the kinetic equation (2.13) with boundary conditions (2.14) and (2.17) can easily be obtained by repeating the arguments with Z_0 instead of Ker$A$. It then appears that under the assumption (2.20) the number of linearly independent solutions of the homogeneous ($\phi_+=0$) problem coincides with the maximal number of linearly independent vectors $h_1,\cdots,h_k\in Z_0$ satisfying $(Th_i,h_j)=0$ for $i\neq j$ and $(Th_i,h_i)<0$ for $i=1,2,\cdots,k$, which is the same result as for $\mathscr{R}=0$. In the case of purely specular reflection ($\mathscr{R}=I$) this number generally is larger and in fact equals the dimension of the subspace $Z_0\cap\operatorname{Ker}(I-J)$ of "even" root subspace vectors. In general, for $Z_0\neq\operatorname{Ker}A$ one will find a larger measure of nonuniqueness of the solution than for the problem (2.13)–(2.15), which can be accounted for by considering the normal solutions f_1+f_2x.

3. An iteration procedure. Let us consider a suitable bounded strictly positive albedo operator E on H_T, such that $\psi(0)=E\phi_+$ yields a solution of (2.8)–(2.10). Such an operator always exists and satisfies (2.12). It is unique, if and only if $(Th,h)\geq 0$ for all $h\in\operatorname{Ker}A$ (cf. Theorem 2.2). Using the norm estimate (2.16), we may write a solution of (2.13)–(2.15) as follows:

$$\psi(x)=e^{-xT^{-1}A}PEg_++(I-P)Eg_+,\qquad x\in\mathbb{R}_+,$$

where

$$g_+=S_{\mathscr{R}}^{-1}\phi_+=\sum_{n=0}^{\infty}(-1)^n[\mathscr{R}j(I-E)]^n\phi_+; \tag{3.1}$$

the series is absolutely convergent in the norm of H_T, uniformly in ϕ_+ on bounded subsets of $Q_+[H_T]$. We may therefore compute g_+ by iterating the vector equation

$$g_++\mathscr{R}J(I-E)g_+=\phi_+ \tag{3.2}$$

on $Q_+[H_T]$. Depending on the choice of the albedo operator E—unique if and only if $(Th,h)\geqq 0$ for $h\in \operatorname{Ker} A$—, different solutions are generated. In order to find all solutions, especially in the cases where they are nonunique, one should still solve the homogeneous ($\phi_+=0$) problem (2.13)–(2.15). For instance, if $\operatorname{Ker} A\neq\{0\}$ and $Jh=h$ for all $h\in\operatorname{Ker} A$, which occurs for the Fokker–Planck example (1.5)–(1.7) (disregarding for the moment that this model does not satisfy the boundedness assumption on A), we would have $(Th,h)=(TJh,Jh)=-(JTh,Jh)=-(Th,h)=0$ for all $h\in\operatorname{Ker} A$. This would imply existence of a unique albedo operator and therefore the generation by iteration of one solution only. Nevertheless the problem is nonuniquely solvable and the homogeneous problem should be solved as well. A similar remark applies to the solution of (2.13) with boundary conditions (2.14) and (2.17).

Let us consider the case when A is a compact perturbation of the identity satisfying

$$(3.3)\qquad \exists 0<\alpha<1:\operatorname{Ran}(I-A)\subset\operatorname{Ran}|T|^{\alpha},\qquad Z_0\subset D\left(|T|^{2+\alpha}\right),$$

which occurs in one-speed and symmetric multigroup neutron transport (cf. [19]), and several BGK models in rarefied gas dynamics. If we choose a closed subspace $\mathbb{B}\supset\operatorname{Ran}(I-A)$, which may be chosen finite-dimensional if $I-A$ has finite rank, and operators $\pi:H\to\mathbb{B}$ and $j:\mathbb{B}\to H$ such that πj is the identity on $\mathbb{B}$ and $j\pi$ the orthogonal projection of H onto $\mathbb{B}$, a representation for E can be found in terms of generalized Chandrasekhar **H**-functions. More precisely, if $\sigma(\cdot)$ denotes the resolution of the identity of the self-adjoint operator T, we have (see [21])

$$(3.4)\qquad E\phi_+=\phi_++\int_{-\infty}^{0}\int_0^{\infty}\frac{\nu}{\nu-\mu}\sigma(d\mu)(I-A)j\mathbf{H}_l(-\mu)\mathbf{H}_r(\nu)\pi\sigma(d\nu)\phi_+,$$

where $\mathbf{H}_l(-\mu)$ and $\mathbf{H}_r(\nu)$ are solutions of the nonlinear integral equations

$$(3.5)\qquad \mathbf{H}_l(z)^{-1}=I-z\int_0^{\infty}(z+t)^{-1}\mathbf{H}_r(t)\pi\sigma(dt)(I-A)j,$$

$$(3.6)\qquad \mathbf{H}_r(z)^{-1}=I-z\int_0^{\infty}(z+t)^{-1}\pi\sigma(-dt)(I-A)j\mathbf{H}_l(t).$$

The solutions and their inverses must be analytic for $\operatorname{Re} z>0$ and continuous for $\operatorname{Re} z\geqq 0$. If $\operatorname{Ker} A\neq\{0\}$, the continuity of $\mathbf{H}_l$ and $\mathbf{H}_r$ at infinity must be replaced by a weaker requirement. (The precise description of such requirements was not given in [21].) Equation (3.2) then has the form

$$(3.7)\qquad g_+-\int_{-\infty\,(\mu)}^{0}\int_{0\,(\nu)}^{\infty}\frac{\nu}{\nu-\mu}\mathscr{R}J\sigma(d\mu)(I-A)j\mathbf{H}_l(-\mu)\mathbf{H}_r(\nu)\pi\sigma(d\nu)g_+=\phi_+.$$

On solving the **H**-equations (3.5)–(3.6) we may compute g_+ by iteration. It should be noted that the above expression (3.4) for E was formulated for $\phi_+\in Q_+[H]$, but allows continuous extension to $\phi_+\in Q_+[H_T]$.

Let us consider the specific example of the scalar BGK model. The existence and uniqueness theory for this example without reflection is immediate from [1], and has also been published by Kaper [15]. For a combination of specular and diffuse reflection (no absorption) solutions were obtained before by Cercignani [8], using expansion with respect to increasing powers of the accommodation coefficient α. Let $L_2(\mathbb{R})_\delta$ be the Hilbert space of complex measurable functions on $\mathbb{R}$ with inner product

$$(h,k)=\int_{-\infty}^{\infty}h(v)\overline{k(v)}\,d\delta(v),\qquad d\delta(v)=\pi^{-1/2}e^{-v^2}dv,$$

and define T, Q_+, Q_-, A, $\mathscr{R}$ and J as follows:

$$(Th)(v)=vh(v), \qquad (Ah)(v)=h(v)-\pi^{-1/2}\int_{-\infty}^{\infty} h(v')e^{-(v')^2}dv',$$

$$(Q_+h)(v)=\begin{cases} h(v), & v>0,\\ 0, & v<0,\end{cases} \qquad (Q_-h)(v)=\begin{cases} 0, & v>0,\\ h(v), & v<0,\end{cases}$$

$$(Jh)(v)=h(-v), \qquad (\mathscr{R}h)(v)=\alpha h(v)+2\beta\pi^{-1/2}\int_0^{\infty} v'h(v')e^{-(v')^2}dv',$$

where $\mathscr{R}$ is defined on $\operatorname{Ran} Q_+$ and $\alpha,\beta\geqq 0$ with $\alpha+\beta\leqq 1$. This model satisfies the assumptions of the previous section and existence is assured. First we solve the **H**-equation (i.e., (3.5)–(3.6) with $\mathbf{H}_l=\mathbf{H}_r$ and $\mathbb{B}=\{\text{constant functions}\}$)

$$\mathbf{H}(z)^{-1}=1-\frac{z}{\sqrt{\pi}}\int_0^{\infty}(z+t)^{-1}\mathbf{H}(t)e^{-t^2}dt,$$

requiring a solution such that $\mathbf{H}$ and $\mathbf{H}^{-1}$ are analytic for $\operatorname{Re} z>0$, continuous for $\operatorname{Re} z\geqq 0$ and satisfying $\mathbf{H}(z)=O(z)$ for $z\to\infty$ with $\operatorname{Re} z\geqq 0$. We find

$$(E\phi_+)(v)=\begin{cases} \phi_+(v), & v>0,\\ \dfrac{1}{\sqrt{\pi}}\displaystyle\int_0^{\infty}\frac{v'}{b'-v}\mathbf{H}(-v)\mathbf{H}(v')\phi_+(v')e^{-(v')^2}dv', & v<0.\end{cases}$$

Therefore, we write (3.2) in the form

$$g_+(v)-\frac{\alpha}{\sqrt{\pi}}\int_0^{\infty}\frac{v'}{v'+v}\mathbf{H}(v)\mathbf{H}(v')g_+(v')e^{-(v')^2}dv'$$
$$-\frac{2\beta}{\pi}\int_0^{\infty}\int_0^{\infty}\frac{vv'}{v'+v}\mathbf{H}(v)\mathbf{H}(v')g_+(v')e^{-[v^2+(v')^2]}dv'\,dv=\phi_+(v),$$

which has to be solved by iteration. The initial value of the solution is then given by $\psi(0,v)=g_+(v)$ for $v>0$ and by

$$\psi(0,v)=\frac{1}{\sqrt{\pi}}\int_0^{\infty}\frac{v'}{v'-v}\mathbf{H}(-v)\mathbf{H}(v')g_+(v')e^{-(v')^2}dv'$$

for $v<0$.

For the isotropic Lorentz gas (neutron transport) the calculation has been carried out for various combinations of selective, specular and diffuse boundary conditions (cf. [10], [11]) yielding interesting and sometimes striking conclusions about their influence on the boundary layer structure, density profile at the wall, validity of Fick's law, etc. For instance, the selective reflection of slow particles and absorption of fast ones leads to an accumulation of particles near the wall and a reversal of the density gradient (interpreted in terms of Fick's law, as equivalent to a negative diffusion coefficient [11]). For the Fokker–Planck equation such selective boundary conditions have been investigated numerically by Burschka and Titulaer [6]. We remark that in general (e.g. for so-called selective boundary conditions [6], [11]) the operator $\mathscr{R}$ is not self-adjoint in H_T. Since only the contraction property of $\mathscr{R}$ plays a role in all derivations and not whether it is self-adjoint, our existence, uniqueness and iteration results also apply to selective boundary conditions.

4. Discussion.

4.1. Generalization to unbounded A. Hitherto we have assumed that A is a bounded operator. For many applications, especially the ones involving BGK models in rarefied gas dynamics, this is sufficient. The Fokker–Planck model (1.5)–(1.7), however, does not satisfy these assumptions. We shall therefore point out what type of hypotheses on T and A, with A unbounded, would entail a repetition of the previous arguments.

Let us assume that T is (bounded or unbounded) injective self-adjoint on H, and let us define Q_+, Q_- and H_T as before. Suppose A is a positive self-adjoint operator with closed range and finite-dimensional kernel, possibly unbounded, such that $D(T) \cap D(A)$ is dense in H. On defining Z_0 as before and repeating the previous hypotheses on Z_0, we may derive Proposition 2.1. It should be noted that $T^{-1}A$, with $D(T^{-1}A) = \{h \in D(A)/Ah \in \operatorname{Ran} T\}$, is closable, but not necessarily closed. Still we may derive the decompositions (2.2) and (2.3) where $T^{-1}A|_{Z_0}$ is closed (and even bounded) and $T^{-1}A$ and S^{-1} should be replaced by their respective closures. As a result, S will be a closed *symmetric* operator with respect to the inner product (2.6). We shall assume that S is, in fact, self-adjoint on the completion of $(T[Z_0])^{\perp} \cap D(A)$ (which is dense in H, due to the density of $D(T) \cap D(A)$) with respect to (2.6). By H_A we shall denote the direct sum of this completion and Z_0. Since A has a closed range and a finite-dimensional kernel, H_A is densely imbedded in H. We define H_K as the direct sum of Z_0 and the completion of $D(T) \cap H_A (\supset D(T) \cap D(A))$ with respect to the inner product

$$(h,k)_K = (|S|h,k)_A,$$

where the absolute value of S is taken in H_A. As before, we define the projections P, PP_+ and PP_- on H_A (and not on H) and extend them continuously to projections on H_K (and not on H_T).

If A is bounded, we may identify H_A and H (which is a trivial observation) as well as H_K and H_T (see [1]; cf. [13] for a different proof). The existence and uniqueness theory has then been developed in §2. For a large class of models on $L_2(a,b)$, where T is a multiplication by an indefinite weight function and A is a Sturm–Liouville type differential operator, it has been proved by Beals [2] that the Hilbert spaces H_T and H_K are completions of $D(T) \cap D(A)$ with respect to equivalent inner products and can be identified. Moreover, for the models Beals considered the previous assumptions on T and A, including the self-adjointness assumption on S, are satisfied. As for bounded A, we may then develop the theory of §2 and the first paragraph of §3 for these indefinite Sturm–Liouville problems and essentially the same results are found. Moreover, for these cases the operator S is bounded self-adjoint on $H_A \cap (T[Z_0])^{\perp}$ (which is due to more specific assumptions on T and A) and even compact. A specific example of such a model is the Fokker–Planck equation (1.5)–(1.7). For this example the equivalence proof of H_T and H_K is contained in [3]. It should be noticed that Theorem 2.3 answers in the affirmative the existence issue raised in [4], thereby making redundant the condition imposed there to enforce existence of solutions (namely, the condition $Bl \in \operatorname{cls}\{Bu_n : n > 0\}$ in [4]).

4.2. The albedo operator for indefinite Sturm–Liouville problems. It is by no means clear how to proceed finding the albedo operator E for (1.5)–(1.7) and other Sturm–Liouville type models. One way, suggested by the approach in [4], is to use the completeness of the eigenfunctions $(u_n)_{0 \neq n \in \mathbf{Z}}$ of $T^{-1}A$ at the nonzero eigenvalues $(\lambda_n)_{0 \neq n \in \mathbf{Z}}$, where we order these by $\ldots \leq \lambda_{-2} \leq \lambda_{-1} < 0 < \lambda_1 \leq \lambda_2 \leq \ldots$ and take account of multiplicities. (It should be noted that under weak oscillation conditions on A these eigenvalues are simple). We add an orthogonal basis $u_{0,1}, \cdots, u_{0,l}$ of a given maximal positive subspace N_+ of Ker$A$ (i.e., $(Tu_{0,i}, u_{0,i}) \geqq 0$). The full-range completeness property implies that every vector $h \in PP_+[H_K] \oplus N_+$ can be expanded as the series

$$h = \sum_{i=1}^{l} \xi_{0,i} u_{0,i} + \sum_{n=1}^{\infty} \xi_n u_n. \tag{4.1}$$

Half-range completeness (for the problem without reflection) amounts to the possibility of expanding every vector $g_+ \in Q_+[H_T]$ (where $H_K \simeq H_T$) as

$$g_+ = \sum_{i=1}^{l} \eta_{0,i} Q_+ u_{0,i} + \sum_{n=1}^{\infty} \eta_n Q_+ u_n;$$

here Q_+ is the restriction to the interval I_+ where the indefinite weight is positive. (For (1.5)–(1.7) we have $I_+ = \mathbb{R}_+$). *Assuming* the existence of a nonnegative weight function $\mathbf{H}$ on I_+ satisfying

$$\int_{I_+} u_{0,i}(v) u_{0,j}(v) \mathbf{H}(v)\, dv = \delta_{i,j} \theta_{0,i} \qquad \theta_{0,i} > 0, \tag{4.2}$$

$$\int_{I_+} u_n(v) u_m(v) \mathbf{H}(v)\, dv = \delta_{n,m} \theta_n, \qquad \theta_n > 0, \tag{4.3}$$

$$\int_{I_+} u_{0,i}(v) u_n(v) \mathbf{H}(v)\, dv = 0, \tag{4.4}$$

we can easily evaluate the (unique) albedo operator E such that

$$EQ_+[H_T] = PP_+[H_K] \oplus N_+.$$

Indeed, on expanding $h = Eg_+$ with $g_+ \in Q_+[H_T]$ as the series (4.1) we obtain

$$g_+ = Q_+ E g_+ = \sum_{i=1}^{l} \xi_{0,i} Q_+ u_{0,i} + \sum_{n=1}^{\infty} \xi_n Q_+ u_n. \tag{4.5}$$

Using (4.2)–(4.4), we then easily derive

$$Eg_+ = \sum_{i=1}^{l} \theta_{0,i}^{-1} \left(\int_{I_+} u_{0,i}(v) g_+(v) \mathbf{H}(v)\, dv \right) u_{0,i} + \sum_{n=1}^{\infty} \theta_n^{-1} \left(\int_{I_+} u_n(v) g_+(v) \mathbf{H}(v)\, dv \right) u_n.$$

If the weight function $\mathbf{H}$ on I_+ is known, the boundary value problem with reflection can again be solved by iterating (3.2), using (4.6). At present even the existence (let alone the computation) of such a weight function is an open problem.

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