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ABSTRACT BOUNDARY VALUE PROBLEMS MODELING TRANSPORT PROCESSES IN SEMI-INFINITE GEOMETRY*,**

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I. Introduction

Since Hangelbroek's[11] study of non-conservative neutron transport with isotropic scattering considerable effort has been made towards the solution of abstract half-space problems of the form

$$(Tf)'(x) = -Af(x) \quad (0 \leq x < \infty) \tag{1}$$

$$Q_+ f(0) = f_+ \,, \quad ||f(x)|| = O(1) \quad (x \to \infty), \tag{2}$$

where T is an injective self-adjoint operator and A a positive self-adjoint Fredholm operator on a complex Hilbert space H and Q_+ is the orthogonal projection onto the maximal positive T-invariant subspace of H. Concrete examples abound in neutron

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transport theory[6], radiative transfer[8,23,13], rarefied gas dynamics[7], phonon transport[17] and Brownian motion in liquids[18]. Substantial contributions to the development of the abstract theory were made by Beals[2,3,4,4a], Greenberg[10,9], Hangelbroek[11,12], Lekkerkerker[12,15], Van der Mee[16,10,9], Protopopescu[4] and Zweifel[10]. In this article we review the abstract theory as presented by Greenberg et al.[10], and work out the specific example of strongly evaporating liquids. Finally, we discuss some related and open half-space problems with reflective boundary conditions.

2. Strictly dissipative models

Let us first discuss the strictly dissipative case when A is strictly positive and has zero null space. This case is relevant to c<1 neutron transport and radiative transfer with albedo of single scattering a<1. To simplify the discussion we take A and T bounded on H. Then the operator $A^{-1}T$ is self-adjoint with respect to the Hangelbroek[11] inner product

$$(h,k)_A = (Ah,k), \tag{3}$$

which turns H into the complete inner product space H_A. Let $Q_\pm$ be the (.,.)-orthogonal projection onto the maximal positive/negative T-invariant subspace of H and $P_\pm$ the $(.,.)_A$-orthogonal projection onto the maximal $(.,.)_A$-positive/-negative $A^{-1}T$-invariant subspace of H_A (= H, in this case). Then solutions to Eqs.(1) and (2) must be given by the semigroup expression

$$f(x) = e^{-xT^{-1}A}f(0) \;,\; 0\le x<\infty,$$

where $P_-f(0) = 0$ and $Q_+f(0) = f_+$. In a natural way we are bound to investigate the invertibility of the operator[12]

$$V = Q_+P_+ + Q_-P_- \;.$$

Once the invertibility of V has been established, one defines the albedo operator E by $E = V^{-1}$ and writes for the unique solution to Eqs.(1) and (2)

$$f(x) = e^{-xT^{-1}A}Ef_{+} , \ 0\leq x<\infty.$$

For neutron transport with redistribution function $p\in L_r[-1,1]$ for some $r>1$, or for radiative transfer with phase function $p\in L_r[-1,1]$ with $r>1$ the operator I-A is compact, while there exist $0<\alpha<1$ and a bounded operator D such that the regularity condition

$$I - A = |T|^{\alpha}D \qquad (4)$$

is satisfied[16]. In this case the operator V is invertible on H and thus the half-space problem (1) and (2) has a unique solution in H. For some specific cases of neutron transport theory such results were found by Hangelbroek[11]; the above general anisotropic case is due to Van der Mee[16]. The key observation in these proofs is the compactness of I-V on H. If T is unbounded, I-A compact and a generalization of (4) holds, similar results hold true, but the vectors f_+ and f(x) must belong to the domain D(T) of T.

It is possible to derive analogous results for cases when I-A is not a compact operator satisfying condition (4). The price we must pay for this generalization is that the invertibility of V, the existence of E and the solutions of Eqs.(1) and (2) must be seeked for in a larger space than D(T). The instigator of this generalization was Beals[2]. Let us define H_T as the completion of the domain D(T) of T with respect to the inner product

$$(h,\kappa)_T = (|T|h,\kappa) = (T(Q_+-Q_-)h,\kappa). \qquad (5)$$

Next let H_K be defined as the completion of the domain D(T) of $A^{-1}T$ with respect to the inner product

$$(h,\kappa)_K = (|A^{-1}T|h,\kappa)_A = (T(P_+-P_-)h,\kappa). \qquad (6)$$

Assuming A bounded, Beals[2] proved the equivalence of the inner products (5) and (6) on D(T), after which he could simply identify H_T and H_K. The operator V then is well-defined and bounded on $H_T = H_K$, has a bounded inverse and gives rise to an albedo operator $E = V^{-1}$. We obtain as a result the unique solvability of Eqs.(1) and (2) on the extension space H_T of D(T).

Next let us drop the boundedness of A but let us take T bounded. Then we could still define H_A as the completion of the domain D(A) of A with respect to the inner product (3), but for unbounded A the space H_A must be identified with a proper subspace of H. We define H_T and H_K as before. We construct the projections $Q_\pm$ on H and $P_\pm$ on H_A and consider $V = Q_+P_+ + Q_-P_-$ as an operator from H_A into H. Using the closed bilinear form associated with V (see Ref.19) we are able to prove that V is a (possibly unbounded) inverse to a bounded injective operator $E:H_T \to H_T \cap H_K$, which is the main result of Greenberg et al.[10] As a result one obtains the unique solvability of Eqs.(1) and (2) on the enlarged Hilbert space H_K. Again we must pay a price: in general, H_K is not easy to construct explicitly.

For unbounded A the equivalence of the norms (5) and (6) and therefore the natural identification of H_T and H_K may be lost, as shown by an example of Kwong[14]. In such a case E maps H_T onto a proper dense subspace of H_T (see Ref.10) and does not have a bounded inverse. On the other hand, as shown by Beals[4a], there exist unbounded A (certain differential operators), for which these norms are equivalent, H_T and H_K allow natural identification, and E has V as a bounded inverse.

Finally, if T and A are both unbounded and some minor domain assumptions are fulfilled, additional problems may arise due to the non-existence or non-unique existence of self-adjoint extensions of $A^{-1}T$ (cf.Ref.9). With the self-adjoint extension $A^{-1}T$ fixed, one recovers the results of Ref.10. Under suitable restrictions[4a], or for specific examples[4], one could again identify H_T and H_K.

3. Non-strictly dissipative models

We now discuss non-strictly dissipative cases when $\mathrm{Ker}A \neq \{0\}$. Such cases may pose additional problems. Paramount in the discussion are the zero root linear manifolds

$$Z_0 = \bigcup_{n=0}^{\infty} \mathrm{Ker}(T^{-1}A)^n \ , \ Z_0^{\dagger} = \bigcup_{n=0}^{\infty} \mathrm{Ker}(AT^{-1})^n \ ,$$

both of which are finite-dimensional. They are related by

$$T[Z_0] = Z_0^{\dagger} \ , \ \overline{T[Z_1]} = A[Z_1] = Z_1^{\dagger}, \qquad (7)$$

where

$$Z_1 = (Z_0^{\dagger})^{\perp} \ , \ Z_1^{\dagger} = Z_0^{\perp} \ . \qquad (8)$$

Moreover, we have the decompositions

$$Z_0 \oplus Z_1 = H \quad , \quad Z_0^{\dagger} \oplus Z_1^{\dagger} = H \ , \qquad (9)$$

Decompositions of the form (9) were first employed by Lekkerkerker[15] for $c = 1$ neutron transport with isotropic scattering and in some other cases by Beals[2]. Both of them considered special cases where Eqs.(1) and (2) have a unique solution. In general, as explicitly stated in Refs.16,10 and 9, these equations may sometimes have non-unique solutions.

As observed by Van d. Mee[16], the finite-dimensional subspace Z_0 is an indefinite inner product space[5] with respect to the scalar product

$$[h,\kappa] = (Th,\kappa). \qquad (10)$$

If we now choose an invertible operator β on Z_0 such that

$$[\beta h,h] = (T\beta h,h) \geq 0 \ , \ h \in Z_0,$$

then the operator

$$A_{\beta} = AP + T\beta^{-1}(I-P),$$

where P denotes the projection of H onto Z_1 along Z_0, is strictly positive self-adjoint with the same domain as A, and satisfies

$$A_\beta^{-1}T = \beta \oplus \left(T^{-1}A\Big|_{Z_1}\right)^{-1}$$

Hence, $T^{-1}A_\beta$ has the same non-zero spectrum as $T^{-1}A$. We now define H_A as the completion of $D(A) = D(A_\beta)$ with respect to the inner product

$$(h,\kappa)_{A_\beta} = (A_\beta h,\kappa),$$

$P_\pm$ as the $(.,.)_{A_\beta}$-orthogonal projection of H_A onto the maximal $(.,.)_{A_\beta}$-positive/-negative $A_\beta^{-1}T$-invariant subspace, and H_K as the completion of $D(T) = D(A_\beta^{-1}T)$ with respect to the inner product

$$(h,\kappa)_{K_\beta} = (|A^{-1}T|h,\kappa)_{A_\beta} = (T(P_+-P_-)h,\kappa).$$

The projections $Q_\pm$ and the space H_T are defined as previously, while the subscript β is suppressed in the spaces because of equivalence of inner products. We now define V as before and repeat the approach presented in Sec.2 with A_β instead of A. The crux of the matter is that $T^{-1}A_\beta$ and $T^{-1}A$ coincide on the subspace Z_1 on finite co-dimension.

The operator A_β allows us to reduce Eqs.(1) and (2) to an analogous boundary value problem with A replaced by A_β and a finite-dimensional evolution equation on Z_0, which can be trivially solved. As a result we obtain solutions to Eqs.(1) and (2) of the form

$$f(x) = e^{-xT^{-1}A}PEf_+ + (I-P)Ef_+ , \quad 0\leq x\leq\infty. \tag{11}$$

In order to establish existence, we have to prove that β can be chosen such that $(I-P)P_+[H_T]\subseteq \mathrm{Ker}A$ (or, equivalently, such that the eigenvectors of β corresponding to positive eigenvalues can all be chosen in KerA). This choice of β is, indeed, possible[10, also 9]. Uniqueness needs not always be satisfied.

The null space KerA of A is a subspace of Z_0 which allows the $[.,.]$-orthogonal decomposition

$$\text{KerA} = N_+ \oplus N_0 \oplus N_-$$

into a strictly positive subspace N_+ (i.e.,$[h,h]>0$ for $0\neq h\in N_+$), a neutral subspace N_0 (i.e.,$[h,h] = 0$ for $h\in N_0$) and a strictly negative subspace N_- (i.e.,$[h,h]<0$ for $0\neq h\in N_-$). The respective dimensions m_+, m_0 and m_- of these subspaces N_+, N_0 and N_- do not depend on the specific choice of N_+, N_0 and N_-, and thus are invariants.

<u>THEOREM 1</u>. *Equations* (1) *and* (2) *have at least one solution. The measure of non-uniqueness for the solution of* Eqs.(1) *and* (2) *equals* m_-. *Thus* Eqs.(1) *and* (2) *are uniquely solvable if and only if* $(Th,h)\geq 0$ *for all* $h\in\text{KerA}$.

In Refs.15 and 2 all problems satisfy $m_+ = m_- = 0$ and therefore the solutions must be unique. We emphasize that we seek for solutions in the manner explained in the previous section.

We also have

<u>THEOREM 2</u>. *Solutions to the boundary value problem*

$$(Tf)'(x) = -Af(x) \quad (0\leq x<\infty) \tag{12}$$

$$Q_+f(0) = f_+, \lim_{x\to\infty}\|f(x)\|=0 \tag{13}$$

are unique. The measure of non-completeness for the solution of these equations equals $m_+ + m_0$.

By the measure of non-completeness we mean the number of linearly independent $f_+\in Q_+[H_T]$, which together with all $f_+\in Q_+[H_T]$ for which Eqs.(12) and (13) have a solution span the whole space $Q_+[H_T]$. Boundary value problems of the form (12)-(13)

appear in rarefied gas dynamics to describe strong evaporation[1,20,21].

4. Applications to strong evaporation

Arthur and Cercignani[1] considered the boundary value problem (12) and (13) for the Hilbert space H of functions $h,\kappa: \mathbb{R} \to \mathbb{C}$ with inner product

$$(h,\kappa) = \pi^{-\frac{1}{2}} \int_{-\infty}^{\infty} h(c_x)\overline{\kappa(c_x)} e^{-c_x^2} dc_x .$$

Their operators T, Q_+ and A are defined by

$$(Th)(c_x) = (c_x+d)h(c_x); (Q_+h)(c_x) = \begin{cases} h(c_x) & \text{for } c_x>-d \\ 0 & \text{for } c_x<-d \end{cases} \tag{14}$$

$$(Ah)(c_x)=h(c_x)-\pi^{-\frac{1}{2}} \int_{\infty}^{\infty} \left\{1+2c_x c_x'+2(c_x^2-\tfrac{1}{2})(c_x'^2-\tfrac{1}{2})\right\} e^{-c_x'^2} h(c_x')dc_x' . \tag{15}$$

This boundary value problem describes the strong evaporation of a liquid into a half-space vacuum with drift velocity d>0 in the x-direction, where transverse effects are neglected. Two papers of Siewert and Thomas[20,21] followed: the first one covered the same problem, but the second one considered a two group half-space problem where both longitudinal and transverse effects were accounted for.

For the operator A in Eq.(15) we find

$$\text{Ker } A = \text{span}\{1,c_x,c_x^2-\tfrac{1}{2}\}.$$

The indefinite scalar product (10) has the form

$$[h,\kappa] = \pi^{-\frac{1}{2}} \int_{-\infty}^{\infty} (c_x+d)h(c_x)\overline{\kappa(c_x)}\, e^{-c_x^2} dc_x . \tag{16}$$

Therefore, $\{1,c_x^2-\tfrac{1}{2},dc_x-c_x^2\}$ is an $[.,.]$-orthogonal set, which spans KerA. Further,

$$[1,1] = d,[c_x^2-\tfrac{1}{2},c_x^2-\tfrac{1}{2}] = \tfrac{1}{2}d,[dc_x-c_x^2,dc_x-c_x^2] = \tfrac{1}{2}d(d^2-\tfrac{3}{2}).$$

Using the definitions for m_+, m_0 and m_- in the previous section we find

$$\begin{cases} m_+=2, m_0=0, m_-=1 & \text{for } 0<d<\tfrac{1}{2}\sqrt{6} \\ m_+=2, m_0=1, m_-=0 & \text{for } d=\tfrac{1}{2}\sqrt{6} \\ m_+=3, m_0=0, m_-=0 & \text{for } d>\tfrac{1}{2}\sqrt{6}\ . \end{cases}$$

Theorem 2 yields a measure of non-completeness 2 for $d<\frac{1}{2}\sqrt{6}$ and 3 for $d\geq\frac{1}{2}\sqrt{6}$. In Refs.1 and 20, however, one always takes the incoming flux $f_+\in Q_+[\mathrm{Ker}A]$. A close inspection now gives that, with $f_+\in Q_+[\mathrm{Ker}A]$, no non-trivial solutions of Eqs.(12) and (13) exist for $d\geq\frac{1}{2}\sqrt{6}$. If $d<\frac{1}{2}\sqrt{6}$, the subspace of $f_+\in Q_+[\mathrm{Ker}A]$ for which a solution to Eqs.(12) and (13) exists has dimension 1 and is strictly negative with respect to the inner product (16). This can be physically interpreted by stating that, if $d<\frac{1}{2}\sqrt{6}$, for every value of the drift velocity at the surface there exist unique values for density and temperature at the surface for which Eqs.(12) and (13) have a solution.

5. Some related and open half-space problems

The development of abstract half-space theory sofar has been predominantly oriented towards partial-range boundary conditions, where $Q_+f(0)$ is given and a growth condition at infinity is imposed. This bias towards non-reflective boundary conditions is a severe restriction in applications to rarefied gas dynamics, Brownian motion in fluids and radiative transfer, because reflection by the surface of the medium is neglected this way. For a specific Fokker-Planck equation Beals and Protopopescu[4] recently supplied half-space theory with reflective boundary conditions.

Let us pose the problem in an abstract way. We first need an operation representing the reversal of the direction of propagation. By an inversion symmetry we mean a unitary and self-adjoint operator J (i.e., $J = J^*$ and $J^2 = I$) leaving invariant the domains of T and A and satisfying

$$JT = -TJ \ , \ JA = AJ. \tag{17}$$

In actual kinetic models we usually have $(Jh)(\mu) = h(-\mu)$ and Eqs. (17) are caused by the principle of reciprocity (cf. Ref.8 for radiative transfer; Ref.6 for neutron physics). We also need a surface reflection operator $R:Q_+[H]\to Q_+[H]$, which leaves invariant the domain of T and describes the dissipativity of the surface reflection if it satisfies

$$0\leq(TRh,h)\leq(Th,h) \ , \ h\in Q_+[H]\cap D(T). \tag{18}$$

In a straightforward way one shows that R extends to a positive contraction operator on the Hilbert space $Q_+[H_T]$. We may extend R to H (or, via restriction to D(T), to H_T) by putting

$$Rh \overset{\text{def.}}{=} RQ_+h + JRJQ_-h.$$

The positivity and contractivity of R on H_T are retained this way. We may now write down the boundary value problem

$$(Tf)'(x) = -Af(x) \quad (0\leq x<\infty) \tag{19}$$

$$Q_+f(0) = RJQ_-f(0)+f_+ \ , \ ||f(x)|| = O(1)(x\to\infty). \tag{20}$$

Of course, the problem can be posed on H as well as on H_T. We observe that $R = I$ in case of specular reflection, $R = 0$ in case of total absorption in the radiative transfer case and for diffuse reflection R is an integral operator. One could, in the radiative transfer case, take a dissipative combination of specular and diffuse reflection[22]:

$$(Rh)(\mu) = \rho_s h(\mu)+2\rho_d \int_0^1 \nu h(\nu)d\nu \quad (0\leq\mu\leq 1, h\in L_2[0,1]),$$

where $\rho_s+\rho_d\leq 1$, $\rho_s\geq 0$ and $\rho_d\geq 0$.

Let us perform the construction of Section 3 for KerA = (0) and obtain an albedo operator E which maps $Q_+[H_T]$ into $PP_+[H_T]$. Then, for a solution of the form (11), we find the equation

$$(Q_+-\mathcal{R}JQ_-)f(0) = f_+.$$

Take g with $P_+g = f(0)$ and recall V. Then we have the equation

$$[V-\mathcal{R}J(I-V)]g = f_+$$

on H_T. For models where V has a bounded inverse $E = V^{-1}$ on H_T we thus have to investigate the invertibility on H_T of the $\mathcal{R}$-scattering operator

$$S_{\mathcal{R}} = I+\mathcal{R}J(I-E),$$

which is immediate from the dissipativity condition (18) and the estimate $||I-E||<1$ in H_T-norm (see Refs.10 and 9 for cases when $H_T = H_K$). We obtain the particular solution

$$f(x) = e^{-xT^{-1}A}\, ES_{\mathcal{R}}^{-1}f_+, \quad 0\leq x<\infty. \tag{21}$$

Uniqueness of solutions to Eqs.(19)-(20) is more difficult to establish. We present the following results for KerA = (0):

(i) If KerA = {0}, the function (21) is the only solution to Eqs.(19)-(20).

(ii) If KerA ≠ {0}, the measure of non-uniqueness is finite and bounded above by m_- if $||\mathcal{R}||<1$ in H_T-norm, and by m_-+m_0 if $||\mathcal{R}|| = 1$ in H_T-norm.

(iii) For specular reflection ($\mathcal{R}$=I) the solutions to the homogeneous $f_+ = 0$ problem (19)-(20) are the constant functions

$$f(x) \equiv h = Jh \in \mathrm{Ker}A.$$

In particular, for the Beals-Protopopescu example ($m_0=1, m_+=m_-=0$) we find uniqueness if $||R||<1$ in H_T-norm and non-uniqueness if $R = I$. Herewith we recover their results for $R = \alpha I$, $0\leq\alpha\leq 1$. At this moment the general uniqueness problem is open.

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