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Some problems in neutron transport theory

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1. Introduction. Formulation of the problem.

Today when many nuclear power stations produce a significant portion of the world's electricity, it may be assumed that most problems in reactor physics have been solved. Indeed, there are mathematical models which function well in the sense that they are in good agreement with experimental models of both qualitative and quantitative level. However, despite this fact, there remain some unsolved problems of both theoretical and practical nature. We will show this claim on two basic problems which frequently occur in reactor calculations.

Problem 1. To determine the critical value $\gamma_0 \in \mathbb{R} \subset [0, +\infty)$ of the fuel enrichment and the corresponding neutron density N in reactor body G ; to investigate the numerical aspects.

Problem 2. To examine the time behaviour of the neutron density in particular for $t \rightarrow \infty$.

By the reactor we mean a convex body G where absorption, scattering and creation of neutron take place. The neutron density N is a function of velocity $\mathbf{v} = (v_x, v_y, v_z)$, space variables $\mathbf{r} = (x, y, z)$ and time t .

Since any interaction between neutrons themselves is negligible, the models of reactor physics must be linear. Obviously, such models apply in other fields too when the particles under consideration do not interact as in the case of neutrons.

From physical point of view the most rigorous model is defined by the Boltzmann linearized operator, that is N satisfies

$$(1.1) \quad \frac{d}{dt} N = LN + SN + FN$$

and

$$(1.2) \quad N(\mathbf{r}, \mathbf{v}, t) = 0 \text{ for } \mathbf{r} \in \partial G \text{ and } (\mathbf{n}, \mathbf{v}) < 0$$

where \mathbf{n} is the outer normal, and

$$(1.3) \quad LN \equiv -\mathbf{v} \operatorname{grad} N - v \sum (\mathbf{r}, \mathbf{v}) N,$$

$$(1.4) \quad SN \equiv \int d\mathbf{v}' \mathbf{v} \sum_s (\mathbf{v}' \rightarrow \mathbf{v}, \mathbf{r}) N(\mathbf{r}, \mathbf{v}', t),$$

⁺) Delivered by the second author.

$$(1.5) \quad FN \equiv \int d\underline{y}' \nu(\underline{y}') \Sigma_f(\underline{v}') \chi(\underline{y}' \rightarrow \underline{y}) N(\underline{x}, \underline{y}, t)$$

and where Σ , Σ_s , Σ_f , ν and χ are characteristics of the reactor medium with respect to collisions with neutrons; v denotes the length of the vector \underline{y} .

Problem 1 is connected with the stationary case of (1.1) in which the characteristics Σ, Σ_s , etc. have to be arranged in such a way that the problem

$$(1.6) \quad 0 = (L + S + F)N_0, \quad N_0(\underline{x}, \underline{y}) = 0$$

$$\text{for } \underline{x} \in \partial G \text{ and } (\underline{n}, \underline{y}) < 0,$$

has a positive solution for fixed geometrical configuration of G . More precisely, the stationary state depends on some (criticality) parameter: $L = L(\gamma)$, $S = S(\gamma)$, $F = F(\gamma)$ and one has to find a γ_0 such that the problem

$$(1.7) \quad [L(\gamma) + S(\gamma) + \frac{1}{\tau(\gamma)} F(\gamma)] N_0 = 0,$$

$$N_0(\underline{x}, \underline{y}) = 0 \text{ for } \underline{x} \in \partial G, (\underline{y}, \underline{n}) < 0$$

has a nonnegative nontrivial solution N_0 corresponding to $\tau(\gamma_0) = 1$ (criticality condition). From theoretical point of view the Problem 1 was more or less completely solved (see [2],[3],[5],[20]). Concerning the calculations there are difficulties connected with the fact that the data of most of the models change rapidly with respect to space variables. A real reactor situation is such that domain G consists of periodically changing subdomains G_p each of which contains cells with fuel kernel and several shells having various purposes. The cells are rather small in the sense that when any variant of the finite element method is used the majority of elements are then determined by discontinuous data. However, in practice we are not interested in the detailed behaviour of the differential neutron density; only some global characteristics of the solution are needed such as integral neutron flux, parameter of criticality etc. In order to be able to obtain such characteristics some appropriate procedures and simplifications have to be used. A very efficient procedure how to overcome difficulties with rapidly oscillating data a homogenization method has been invented. The homogenization procedure is an approximate method by which the original problem is approximated by another one (usually with respect to space variables) in which the data do not change so rapidly as the original data; the data are in a special way averaged, or, as we say homogenized.

Some mathematical and numerical aspects of the problem of criticality and homogenization will be considered in a subsequent paper. In this paper Problem 2 will be considered in detail.

2. Fundamental decay mode and asymptotic behaviour in time.

In order to investigate the asymptotic time-behaviour of any particle distribution N , we examine in more detail the Boltzmann operator $A = L + S + F$ defined by (1.2) - (1.5). We remark that $F = 0$ if the medium under consideration is nonmultiplying (a moderator). Let Y be any $L^p(G \times R^3, w)$ for $p \in (1, +\infty)$, where $w \geq 0$ is a suitable weight function.

It is known that L is an infinitesimal generator of a semigroup $T(t; L)$ of class (C_0) and that

$$\|T(t; L)\| \leq e^{-\lambda^* t},$$

where

$$\lambda^* = \inf \{ v \sum (\mathbf{x}, \mathbf{y}) : \mathbf{y} \in R^3, \mathbf{x} \in R^3, v = |\mathbf{y}| \}.$$

Since both of the operators S and F are bounded, we see that A is an infinitesimal generator of a semigroup of operators $T(t; A)$ of class (C_0) ([6, p.403, Th.13.2.1]). The semigroup $T(t; L)$ can be written explicitly by integrating the corresponding first-order differential equation, and we can conclude that $T(t; L)$ is a semigroup of positive operators, that is, $T(t; L)$ leaves invariant the cone of elements in Y with nonnegative representatives. Since the operators S and F are defined by nonnegative kernels, the semigroup $T(t; A)$ is also nonnegative ([6, p.418, Corollary 4]).

Moreover, since the kernel of S is positive almost everywhere, we may conclude that the semigroup $T(t; A)$ is primitive for sufficiently large $t > 0$, that is, for every nonnegative $u \in Y$, $u \neq 0$, there is a $\tau_u > 0$ such that $v = T(t; A)u$ is positive almost everywhere for $t > \tau_u$.

The spectrum $\sigma(A)$ has the following structure: Every λ for which $\operatorname{Re} \lambda \leq -\lambda^* \leq 0$ belongs to the continuous spectrum, i.e. $C \sigma(A) \supset \{ \lambda : \operatorname{Re} \lambda \leq -\lambda^* \}$. On the other hand, λ for which $\operatorname{Re} \lambda > -\lambda^* + \|S + F\|$ belongs to the resolvent set $\rho(A)$.

If the body G is sufficiently small, there are no further points in $\sigma(A)$ except those in $\{ \lambda : \operatorname{Re} \lambda \leq -\lambda^* \}$ ([1]). Hence, we must assume that the strip $-\lambda^* < \operatorname{Re} \lambda \leq -\lambda^* + \|S + F\|$ has

a nonempty intersection with $\sigma'(A)$. Let λ_0 be such that any λ for which $\operatorname{Re} \lambda > \lambda_0$ belongs to the resolvent set $\rho(A)$, while there exists a $\lambda_1 \in \sigma(A)$ with $\operatorname{Re} \lambda_1 = \lambda_0$.

It is known that $N(t) = T(t; A)N_0$, where $N_0 \in Y$, is a unique solution of the problem ([6, p.359, Theorem 11.5.3])

$$\frac{d}{dt} N = AN, \quad N(0) = N_0.$$

We assume that N_0 is nonnegative almost everywhere and now investigate the behaviour of N as $T \rightarrow +\infty$.

A standard procedure [19, p.210-213] consists in estimating the semigroup operator by using the resolvent inversion formula [6, Theorem 11.6.1, p.363]

$$T(t; A)N_0 = \lim_{\omega \rightarrow \infty} \frac{1}{2\pi i} \int_{\alpha - i\omega}^{\alpha + i\omega} e^{\lambda t} R(\lambda, A)N_0 d\lambda, \quad \alpha > \max(0, \lambda_0),$$

where $\lambda_0 = \operatorname{Re} \lambda_0$ is such that $\operatorname{Re} \lambda > \lambda_0$ implies $\lambda \in \rho(A)$. For such a procedure we must have complete information about that part of the spectrum of A in the region $\operatorname{Re} \lambda > -\lambda^*$.

We propose a more direct and much simpler approach. We formulate it in an abstract way.

Let Y be a real Banach space, $X = Y \oplus iY$ its complexification. Let $K \subset Y$ be a generating and normal cone. We say that a linear bounded operator $T \in B(Y) = (Y \rightarrow Y)$ is K -positive if $Tx \in K$ whenever $x \in K$. We also have a partial ordering in Y defined as follows $x \leq y \iff y - x \in K$. Similarly $T \leq S \iff (S-T)K \subset K$. We call an element $y \in K$ quasiinterior if $x'(y) > 0$ for all linear functionals $0 \neq x' \in Y'$ such that $x'(x) \geq 0$ for all $x \in K$; here Y' is the dual space of Y .

If the cone K is such that the partial ordering of Y generated by K is a lattice order, that is, $\sup\{x, y\}$ and $\inf\{x, y\}$ exist for every pair of elements x and y in Y , we call Y a Banach lattice.

In the following theorems (Theorem 1-3) we assume that Y is a Banach lattice generated by a cone K . We shall apply some deep results due to F.Niirō and I.Sawashima [16] and H.H.Schaefer [18, p.328-333].

Theorem 1. Let A be an infinitesimal generator of a semigroup of operators $T(t; A)$ of class (C_0) . Let λ_0 be such that

$$(2.1) \quad \lambda \in \sigma'(A) \implies \operatorname{Re} \lambda \leq \lambda_0 = \operatorname{Re} \lambda_0,$$

and let λ_0 be a Fredholm eigenvalue, i.e. an isolated pole of $R(\mu, A)$ to which there corresponds a finite-dimensional eigenspace

$$(2.2) \quad \mathcal{H}_0 = \{u \in Y : (A - \lambda_0 I)^k u = 0 \text{ for some } k = 1, 2, \dots\}.$$

Let the semigroup $T(t; A)$ be K -positive for $t \geq 0$.

Then

$$(2.3) \quad \sigma(A) \cap \{\lambda : \operatorname{Re} \lambda = \lambda_0\} = \{\lambda_0, \dots, \lambda_s\}$$

and

$$(2.4) \quad T(t; A) = \sum_{j=0}^s e^{\lambda_j t} [B_j + Z_j(t)] + W(t),$$

where

$$(2.5) \quad B_j B_k = B_k B_j = \delta_{jk} B_j, \quad B_j Z_j(t) = Z_j(t) B_j = Z_j(t),$$

$$(2.6) \quad B_j W(t) = W(t) B_j = \theta, \quad j, k = 0, \dots, s$$

and

$$(2.7) \quad \lim_{t \rightarrow \infty} e^{-\lambda_0 t} \|W(t)\| = 0, \quad \lim_{t \rightarrow \infty} t^{-q+1} \|Z_j(t)\| = 0,$$

where q is the order of λ_0 as a pole of $R(\mu, A)$.

Moreover, $B_{0,q} = \lim_{\rho \rightarrow \lambda_0} (\rho - \lambda_0)^q R(\rho, A)$ is K -positive and hence, if $u_0 \in K$, then $v_0 = B_{0,q} u_0 \neq 0$ is an eigenvector of A in $K : Av_0 = \lambda_0 v_0$.

Theorem 2. If the semigroup $T(t; A)$ in Theorem 1 is such that for every $u \in K$, $u \neq 0$, there exists $\tau_0(u) > 0$ and a positive integer $p = p(u)$ such that $[T(t; A)]^p u$ is quasi-interior with respect to K for $t > \tau_0(u)$, then

$$(a) \quad s = 0 \text{ in (2.3)}, \quad B_{0,q} = B_0;$$

$$(b) \quad \mathcal{H}_0 = B_0 Y \text{ with } \dim \mathcal{H}_0 = 1,$$

and $B_0 v$ is quasi-interior whenever $v \in K$, $v \neq 0$; if $y \in K$ is any eigenvector of A then $y = cu_0 = B_0 v_0$, $v_0 \in K$, $v_0 \neq 0$. Furthermore,

$$(c) \quad T(t; A) = e^{\lambda_0 t} B_0 + W(t)$$

with

$$(2.8) \quad \lim_{t \rightarrow \infty} e^{-\lambda_0 t} \|W(t)\| = 0.$$

Under the hypotheses of Theorem 2, we consider the Cauchy problem

$$(2.9) \quad \frac{d}{dt} u(t) = Au, \quad u(0) = u_0 \in K.$$

By Theorem 2 we have the following representation of the solution

$$\begin{aligned} u(t) &= T(t;A)u_0 = \\ &= e^{\lambda_0 t} B_0 u_0 + W(t)u_0. \end{aligned}$$

It follows from (2.8) that

$$(2.10) \quad \lim_{t \rightarrow \infty} e^{-\lambda_0 t} u(t) = B_0 u_0.$$

Thus we have

Theorem 3. The asymptotic behaviour of any solution $u(t)$ of (2.9) is non-oscillatory.

Remark. Let μ_0 be an eigenvalue of A , and M_0 the corresponding eigenvector. We see that any $M(t)$ of the form $e^{\lambda_0 t} M_0$ is always a solution of (2.9) with $u(0) = M_0$. Such a solution is called a decay mode; a decay mode is called fundamental if $M_0 \in K$, $M_0 \neq 0$.

It is easy to see that the normalized fundamental decay mode is unique if $T(t;A)$ fulfils the hypotheses of Theorem 2.

To apply our previous theory we have to show only that the point λ_0 , the bound of the spectrum $\sigma(A)$, is an isolated pole of the resolvent operator $R(\mu, A)$. We emphasize this fact because a complete analysis of the existence of decay modes and the uniqueness of the fundamental decay mode can be made without any further information about the spectrum of the operator A . This makes our approach different from the sort of analysis proposed by others. On the other hand, we describe only the peripheral part of the spectrum of the semigroup $T(t;A)$. If we make assumptions involving compactness about $ST(t;L)S$ [22] or other closely related assumptions, we can give a complete description of $\sigma(A)$. Actually, under certain assumptions concerning compactness of $T(t_1;L)S \dots T(t_k;L)S$ it has been shown that every $\mu \in \sigma(T(t;A))$ for which $|\mu| > e^{-\lambda^* t}$ has the form $\mu = e^{\lambda t}$, where λ is an isolated pole of $R(\mu, A)$ with finite-dimensional invariant subspace $\mathcal{H}(\lambda) = \{ u : (A - \lambda I)^k u = 0 \text{ for some } k = 1, 2, \dots \}$, [21], [22], [19]. However, these assumptions are not fulfilled in general, e.g. for some models including the case of inelastic scattering in the

high-energy range [11].

On the other hand, our theory does not cover the model excluding the up-scattering. With some minor modifications this case can also be considered by our method and the main results, such as the final Theorem, remain valid in general.

We already know that the semigroup $T(t;A)$ is K -positive in Y , where K is the cone of elements of $Y = L^p(G \times R^3, w)$, $1 < p < +\infty$, with nonnegative representatives, $w \geq 0$. It follows that $R(a,A)$ is also K -positive, where $a > \max(0, \lambda_0)$ ([6, Theorem 11.7.2]).

Let us write A in the form $A = L + S_1 + S_2 + F$, in which S_1 includes the elastic scattering and the inelastic scattering in high-energy range and S_2 the inelastic scattering in low-energy range. Since S_1 is bounded and S_2 and F are compact operators, we have that

$$R(a,A) = R(a,L+S_1) + R(a,A)(S_2+F)R(a,L+S_1).$$

A crucial assumption for the applicability of our theory is the fulfilment of the strict inequality

$$(2.11) \quad r = r(R(a,A)) > r(R(a,L+S_1)) = r_1,$$

the relation $r \geq r_1$ being trivial.

Actually, we have

Lemma. Under the assumption (3.11) for some $a > \max(0, -\lambda^* + \|S+F\|)$ the point λ_0 is a pole of the resolvent operator $R(\mu, A)$.

Remark. We note that the validity of (2.11) follows from the compactness of $(S+F)T(t;L)(S+F)$ and similar other assumptions, as we have mentioned above. The converse is obviously not necessarily true, as we have mentioned, in the case of inelastic scattering in the high-energy range.

Proof of the Lemma. The operator $R(a,A)$ is an operator of Radon-Nikolskii type [14] whence it follows that its peripheral spectrum consists of a finite set of Fredholm eigenvalues ν_0, \dots, ν_s . Obviously,

$$\nu_j = \frac{1}{a - \lambda_j}, \text{ where } \lambda_j \in \sigma(A), j = 0, \dots, s,$$

$$|\nu_j| = r(R(a,A)). \text{ We identify } \lambda_0 \text{ by setting } r(R(a,A)) = \frac{1}{a - \lambda_0}.$$

Let $R(a,A)y_j = \nu_j y_j$, $y_j \neq 0$ and let $b > a$. We see that

$$R(b,A)y_j = \frac{1}{b-\lambda_j} y_j.$$

Thus, for all $b > a$ we have that

$$\left| \frac{1}{b-\lambda} \right| \leq \left| \frac{1}{b-\lambda_0} \right|$$

for every $\lambda \in \sigma(A)$. Since b can be arbitrarily large, we conclude that $\lambda \in \sigma(A)$ implies that $\operatorname{Re} \lambda \leq \lambda_0$. Because $r = r(R(a,A)) \in \sigma(R(a,A))$, the spectral mapping theorem shows that λ_0 is a Fredholm eigenvalue of A since r has this property with respect to $R(a,A)$. This completes the proof of the Lemma.

The conclusion of the Lemma implies that Theorems 1-3 apply to those cases of neutron transport where the assumption (3.11) holds. In our opinion, this is the case in most of the models used until now.

As a consequence we have the following final result.

Theorem. If $\sigma(A) \cap \{\lambda : \operatorname{Re} \lambda > -\lambda^*\} \neq \emptyset$, then there exists exactly one normalized fundamental decay mode (λ_0, M_0) and we have that for every solution N of

$$\frac{d}{dt} N = AN, \quad N(0) = N_0 \geq 0,$$

$$\lim_{t \rightarrow \infty} \| e^{-\lambda_0 t} N(t) - cM_0 \| = 0,$$

where $c > 0$ is a constant independent of t .

More precisely, $cM_0 = PN_0$, where P is the residue of the Laurent expansion of $R(\mu, A)$ about the point λ_0 .

We remark that this last theorem gives a solution to Problem 10 of Kaper's Collection of problems in [7].

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