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Letters to the Editors

Note on the Use of Generalized Functions and the Poincaré-Bertrand Formula in Neutron Transport Theory

INTRODUCTION

Recently there has been some confusion about the proper use of the Poincaré-Bertrand formula in neutron transport theory[1,2,3].

In this note we intend to demonstrate that the angular Green's functions, which appear in the literature, do not require any prescription that is in conflict with the usual Cauchy principle value integration procedure, as has been stated in Refs. 1 and 2, nor that the Poincaré-Bertrand formula admits any ambiguity in its interpretation, as has been stated in Ref. 3.

We shall stress the proper use of the concept of a generalized function and of a direct product of two generalized functions. We refer to Ref. 4 for the mathematical background.

THEORY

We introduce the following definitions:

Definition 1 - D_1 is the one-dimensional space of real test-functions $\phi(\nu)$ that vanish identically outside the interval $-1 \leq \nu \leq 1$.

Definition 2 - D_1^* is the space of generalized functions $T(\nu)$ defined as continuous linear functionals on D_1 by

$$\Big\langle T(\nu),\ \phi(\nu)\Big\rangle_1 \equiv \int_{-1}^{+1} T(\nu)\phi(\nu)d\nu$$

for every $\phi \epsilon D_1$.

In Case's method the homogeneous, mono-energetic neutron transport equation for a medium with plane symmetry and isotropic scattering gives rise to an equation of the form

$$\left[1 - \left(\frac{\mu}{\nu}\right)\right] T_\mu(\nu) = \frac{1}{2}\, c \int_{-1}^{+1} T_\mu(\nu)d\mu\ . \tag{1}$$

One looks for solutions of (1) that belongs to D_1^*. Here μ must be considered as a real parameter, $-1 \leq \mu \leq 1$. Since (1) is homogeneous a normalization condition is imposed:

$$\left\langle \int_{-1}^{+1} T_\mu(\nu)d\mu,\ \phi(\nu)\right\rangle_1 \equiv \int_{-1}^{+1} \phi(\nu)d\nu \tag{2}$$

for every $\phi \epsilon D_1$.

Theorem 1 - The solution of equation (1) that satisfies the condition (2) is

$$T_\mu(\nu) = \frac{\frac{1}{2}c\nu}{\nu-\mu} + \lambda(\nu)\,\delta(\nu-\mu), \tag{3}$$

with

$$\lambda(\nu) = 1 - \frac{1}{2}c\nu\ \ln\frac{1+\nu}{1-\nu}\ ,$$

where $(\nu-\mu)^{-1}$ and $\delta(\nu-\mu)$ are defined by

$$\left\langle \frac{1}{\nu-\mu},\ \phi(\nu)\right\rangle_1 \equiv ⨍_{-1}^{+1} \frac{\phi(\nu)}{\nu-\mu}\,d\nu \equiv \lim_{\epsilon \to 0} \int_{|\nu-\mu|>\epsilon} \frac{\phi(\nu)}{\nu-\mu}\,d\nu, \tag{4}$$

$$\Big\langle \delta(\nu-\mu), \phi(\nu)\Big\rangle_1 \equiv \phi(\mu)\ ,$$

for every $\phi \epsilon D_1$.

The theorem states that for every $\phi \epsilon D_1$ one has

$$\left\langle \left[1 - \left(\frac{\mu}{\nu}\right)\right] T_\mu(\nu),\ \phi(\nu)\right\rangle_1 = \left\langle \frac{1}{2}\, c \int_{-1}^{+1} T_\mu(\nu), d\mu,\ \phi(\nu)\right\rangle_1$$

$$= \frac{1}{2}\, c \int_{-1}^{+1} \phi(\nu)d\nu\ ,$$

where $T_\mu(\nu)$ is defined by (3).

Note that the generalized function $(\nu-\mu)^{-1}$ is defined in (4) as the principal value of a Cauchy-integral over ν.

In (4) the roles of μ and ν are interchangeable, so that $(\nu-\mu)^{-1}$ considered as a generalized function of μ corresponds to the functional

$$\left\langle \frac{1}{\nu-\mu},\ \phi(\mu)\right\rangle_1 = ⨍_{-1}^{+1} \frac{\phi(\mu)}{\nu-\mu}\,d\mu\ .$$

In order to establish the usual orthogonality relations we need the concept of the product of two generalized functions.

Definition 3 - D_2 is the two-dimensional space of real test-functions $\phi(\nu,\nu')$ that vanish identically outside the square $S\{-1 \leq \nu \leq 1,\ -1 \leq \nu' \leq 1\}$.

Definition 4 - D_2^* is the space of generalized functions $T(\nu,\nu')$ defined as continuous linear functionals on D_2 by

$$\Big\langle T(\nu,\nu'),\ \phi(\nu,\nu')\Big\rangle_2 \equiv \iint_S T(\nu,\nu')\phi(\nu,\nu')d\nu\, d\nu'$$

for every $\phi \epsilon D_2$.

Definition 5 - The direct product $T(\nu) \times T(\nu')$ of two generalized functions $T(\nu)$ and $T(\nu')$ belonging to D_1^* is the generalized function defined as a continuous linear functional on D_2 by

[1]J. J. McINERNEY, *Nucl. Sci. Eng.*, 22, 215-234 (1965).

[2]A. M. JACOBS, J. J. McINERNEY, *Nucl. Sci. Eng.*, 22, 119-120 (1965).

[3]I. KUŠČER, N. J. McCORMICK, *Nucl. Sci. Eng.*, letter to the Editor (preprint).

[4]I. M. GELFAND, G. E. SCHILOW, *Verallgemeinerte Funktionen (Distributionen)*, Vol. 1 VEB - Deutscher Verlag der Wissenschaften, Berlin (1960).

$$\langle T(\nu)\times T(\nu'),\ \phi(\nu,\nu')\rangle_2 \equiv \langle T(\nu),\ \langle T(\nu'),\ \phi(\nu,\nu')\rangle_1\rangle_1$$

for every $\phi\in D_2$.

As is proved in Ref. 4, p. 106, the direct product defined above satisfies the commutative law, i.e. $T(\nu)\times T(\nu') = T(\nu')\times T(\nu)$.

Note that the square of a generalized function is not defined.

It follows from these definitions that the generalized function $(\nu-\mu)^{-1}\times(\nu'-\mu)^{-1}$ for fixed μ is defined as a continuous linear functional on D_2 by

$$\left\langle \frac{1}{\nu-\mu}\times\frac{1}{\nu'-\mu},\ \phi(\nu,\nu')\right\rangle_2 = ⨍_{-1}^{+1}\frac{1}{\nu-\mu}\times\left\{⨍_{-1}^{+1}\frac{\phi(\nu,\nu')}{\nu'-\mu}\,d\nu'\right\}d\nu.$$

However, if one deals with $(\nu-\mu)^{-1}(\nu'-\mu)^{-1}$ as a function of μ for fixed ν and ν' (the $\times$-sign is omitted deliberately), then this (ordinary) product should be considered as a generalized function belonging to D_1^*, corresponding to the functional

$$\left\langle \frac{1}{(\nu-\mu)(\nu'-\mu)},\ \phi(\mu)\right\rangle_1 = ⨍_{-1}^{+1}\frac{\phi(\mu)\,d\mu}{(\nu-\mu)(\nu'-\mu)},$$

i.e. the limit ($\epsilon\to 0$) of the integral over all the values of μ in $[-1,+1]$ with the exception of those values of μ for which $|\nu-\mu|\leqslant\epsilon$ or $|\nu'-\mu|\leqslant\epsilon$. Here ν and ν' stand for *different* variables that may have the *same* value.

We now come to the crucial theorem concerning the orthonormality of the generalized eigenfunctions. A proof will be given in detail.

Theorem 2 - The generalized functions $T_\mu(\nu)$ defined in (3) obey an orthonormality relation of the form

$$\int_{-1}^{+1}\mu\left(\frac{T(\nu)}{N^{\frac12}(\nu)}\times\frac{T(\nu')}{N^{\frac12}(\nu')}\right)_\mu d\mu = 1(\nu)\times\delta(\nu'-\nu),$$

with

$$N(\nu) = \nu[\lambda^2(\nu) + (\tfrac12\pi c\nu)^2],$$

where the generalized function $1(\nu)$ is defined as a continuous linear functional on D_1 by

$$\langle 1(\nu),\phi(\nu)\rangle_1 \equiv \int_{-1}^{+1}\phi(\nu)\,d\nu$$

for every $\phi\in D_1$.

Proof. The proof requires the verification of the identity

$$\left\langle\int_{-1}^{+1}\mu\left(\frac{T(\nu)}{N^{\frac12}(\nu)}\times\frac{T(\nu')}{N^{\frac12}(\nu')}\right)_\mu d\mu,\ \tilde\phi(\nu,\nu')\right\rangle_2 = \langle 1(\nu)\times\delta(\nu'-\nu),\ \tilde\phi(\nu,\nu')\rangle_2$$

for every $\tilde\phi\in D_2$, or equivalently

$$\left\langle\int_{-1}^{+1}\mu\,(T(\nu)\times T(\nu'))_\mu\,d\mu,\ \phi(\nu,\nu')\right\rangle_2 = \langle 1(\nu)\times\delta(\nu'-\nu),\ N^{\frac12}(\nu)N^{\frac12}(\nu')\phi(\nu,\nu')\rangle_2 \qquad (5)$$

for every $\phi\in D_2$; $\phi(\nu,\nu')\equiv N^{-\frac12}(\nu)N^{-\frac12}(\nu')\tilde\phi(\nu,\nu')$.

According to definition 5 and the definition of the generalized functions $T_\mu(\nu)$ the left hand side of the relation (5) can be written as

In the first term in (6) the integral between braces must be evaluated for all values of ν and ν', $(\nu,\nu')\in S$, including those values for which $\nu'=\nu$.

If ν' and ν have different values it is easy to verify that

$$\frac12 c\,⨍_{-1}^{+1}\frac{\mu\,d\mu}{(\nu-\mu)(\nu'-\mu)} = \frac{\frac12 c}{\nu-\nu'}\left\{\nu'\,⨍_{-1}^{+1}\frac{d\mu}{\nu'-\mu} - \nu\,⨍_{-1}^{+1}\frac{d\mu}{\nu-\mu}\right\}$$
$$= -1(\nu)\times\frac{\lambda(\nu')}{\nu-\nu'} + 1(\nu')\times\frac{\lambda(\nu)}{\nu-\nu'} \qquad (\nu'\neq\nu). \qquad (7\text{-}1)$$

In order to evaluate the integral on the diagonal $\nu'=\nu$ we recall the Poincaré-Bertrand formula[5], p. 57:

$$\int_L\frac{dt}{t-t_0}\int_L\frac{F(t,t_1)}{t_1-t}\,dt_1 = -\pi^2F(t_0,t_0) + \int_L dt_1\int_L\frac{F(t,t_1)}{(t-t_0)(t_1-t)}\,dt, \qquad (8)$$

valid for every function F that satisfies the Hölder condition with respect to both variables t and t_1. In (8) the integrals in the second term of the right-hand side must be interpreted as

$$\lim_{\epsilon\to0}\int_{|t_1-t_0|>\epsilon}\left\{\lim_{\eta\to0}\int_{|t-t_0|>\eta,\,|t_1-t|>\eta}\frac{F(t,t_1)}{(t-t_0)(t_1-t)}\,dt\right\}dt_1;$$

the integrals in the left-hand side are principal values in the usual sense. We note that in the integrals of the left-hand side of (8) the domain of integration extends over the whole square $L\times L$. In the integrals of the right-hand side of (8) the domain of integration also extends over the whole square $L\times L$, from which, however, the point $t=t_1=t_0$ has been excluded; the contribution from this point is given explicitly by the term $-\pi^2F(t_0,t_0)$. Since this term can also be written as

$$-\pi^2\lim_{\epsilon\to0}\int_{|t_1-t_0|\leqslant\epsilon}F(t_0,t_1)\delta(t_1-t_0)\,dt_1,$$

one may concluded that for $t_1=t_0$

$$\int_L\frac{F(t,t_1)dt}{(t-t_0)(t_1-t)}\text{ is equal to }-\pi^2F(t_0,t_0)\delta(t_1-t_0).$$

This means that for $\nu=\nu'$

$$⨍_{-1}^{+1}\frac{\mu\,d\mu}{(\nu-\mu)(\nu'-\mu)}\text{ is equal to }\pi^2\nu\times\delta(\nu'-\nu). \qquad (7\text{-}2)$$

The results (7-1) and (7-2) give the following identity in D_2^*:

$$\frac12 c\,⨍_{-1}^{+1}\frac{\mu\,d\mu}{(\nu-\mu)(\nu'-\mu)} = -1(\nu)\times\frac{\lambda(\nu')}{\nu-\nu'} + 1(\nu')\times\frac{\lambda(\nu)}{\nu-\nu'} + \frac12\pi^2c\nu\times\delta(\nu'-\nu). \qquad (7\text{-}3)$$

[5] N. I. MUSKHELISHVILI, *Singular Integral Equations*, Noordhoff, Groningen (1953).

$$\frac14 c^2\int_{-1}^{+1}\nu\left[\int_{-1}^{+1}\nu'\phi(\nu,\nu')\left\{⨍_{-1}^{+1}\frac{\mu\,d\mu}{(\nu-\mu)(\nu'-\mu)}\right\}d\nu'\right]d\nu + \frac12 c\int_{-1}^{+1}\nu\left[\int_{-1}^{+1}\lambda(\nu')\phi(\nu,\nu')\left\{⨍_{-1}^{+1}\frac{\mu}{\nu-\mu}\times\delta(\nu'-\mu)\,d\mu\right\}d\nu'\right]d\nu$$
$$+\frac12 c\int_{-1}^{+1}\lambda(\nu)\left[\int_{-1}^{+1}\nu'\phi(\nu,\nu')\left\{⨍_{-1}^{+1}\frac{\mu}{\nu'-\mu}\times\delta(\nu-\mu)\,d\mu\right\}d\nu'\right]d\nu + \int_{-1}^{+1}\lambda(\nu)\left[\int_{-1}^{+1}\lambda(\nu')\phi(\nu,\nu')\left\{\int_{-1}^{+1}\mu\,\delta(\nu-\mu)\times\delta(\nu'-\mu)\,d\mu\right\}d\nu'\right]d\nu. \qquad (6)$$

With (7-3) it follows that

$$\frac{1}{4}c^2 \int_{-1}^{+1} \nu \left[\int_{-1}^{+1} \nu'\phi(\nu,\nu') \left\{ ⨍_{-1}^{+1} \frac{\mu d\mu}{(\nu-\mu)(\nu'-\mu)} \right\} d\nu' \right] d\nu$$

$$= -\frac{1}{2}c \int_{-1}^{+1} \nu \left[⨍_{-1}^{+1} \frac{\nu'\lambda(\nu')}{\nu-\nu'} \phi(\nu,\nu')d\nu' \right] d\nu$$

$$+\frac{1}{2}c \int_{-1}^{+1} \nu\lambda(\nu) \left[⨍_{-1}^{+1} \frac{\nu'}{\nu-\nu'} \phi(\nu,\nu')d\nu' \right] d\nu$$

$$+\frac{1}{4}\pi^2 c^2 \int_{-1}^{+1} \nu^3 \left[\int_{-1}^{+1} \phi(\nu,\nu')\delta(\nu'-\nu)d\nu' \right] d\nu \; . \tag{9}$$

In the second term in (6) one may interchange the order of the integrations with respect to μ and ν'. The integral over ν' can be evaluated. After the substitution of ν' for μ under the integral sign one finds:

$$\frac{1}{2}c \int_{-1}^{+1} \nu \left[\int_{-1}^{+1} \lambda(\nu')\phi(\nu,\nu') \left\{ \int_{-1}^{+1} \frac{\mu}{\nu-\mu} \times \delta(\nu'-\mu)d\mu \right\} d\nu' \right] d\nu$$

$$= \frac{1}{2}c \int_{-1}^{+1} \nu \left[⨍_{-1}^{+1} \frac{\nu'\lambda(\nu')}{\nu-\nu'} \phi(\nu,\nu')d\nu' \right] d\nu. \tag{10}$$

For the third term in (6) one finds in an analogous way:

$$\frac{1}{2}c \int_{-1}^{+1} \lambda(\nu) \left[\int_{-1}^{+1} \nu'\phi(\nu,\nu') \left\{ ⨍_{-1}^{+1} \frac{\mu}{\nu'-\mu} \times \delta(\nu-\mu)d\mu \right\} d\nu' \right] d\nu$$

$$= \frac{1}{2}c \int_{-1}^{+1} \nu\lambda(\nu) \left[⨍_{-1}^{+1} \frac{\nu'}{\nu'-\nu} \phi(\nu,\nu')d\nu' \right] d\nu. \tag{11}$$

The fourth term in (6) gives according to definition 5:

$$\int_{-1}^{+1} \lambda(\nu) \left[\int_{-1}^{+1} \lambda(\nu')\phi(\nu,\nu') \left\{ \int_{-1}^{+1} \mu\delta(\nu-\mu) \times \delta(\nu'-\mu)d\mu \right\} d\nu' \right] d\nu$$

$$= \int_{-1}^{+1} \nu\lambda^2(\nu) \left[\int_{-1}^{+1} \delta(\nu'-\nu)\phi(\nu,\nu')d\nu' \right] d\nu. \tag{12}$$

With the results (9) - (12) one derives the following expression for the left-hand side of the relation (5):

$$\left\langle \int_{-1}^{+1} \mu(T(\nu) \times T(\nu'))_\mu \, d\mu, \; \phi(\nu,\nu') \right\rangle_2$$

$$= \int_{-1}^{+1} N(\nu) \left[\int_{-1}^{+1} \delta(\nu'-\nu)\phi(\nu,\nu')d\nu' \right] d\nu \tag{13}$$

with $N(\nu) = \nu[\lambda^2(\nu) + (\frac{1}{2}\pi c\nu)^2]$.

According to definition 2 the right-hand side of the identity (13) is equivalent to

$$\left\langle 1(\nu), \; \left\langle \delta(\nu'-\nu), \; N^{\frac{1}{2}}(\nu)\, N^{\frac{1}{2}}(\nu')\, \phi(\nu,\nu') \right\rangle_1 \right\rangle_1 \; ,$$

which, according to definition 5, is in turn equivalent to

$$\left\langle 1(\nu) \times \delta(\nu'-\nu), \; N^{\frac{1}{2}}(\nu)\, N^{\frac{1}{2}}(\nu')\, \phi(\nu,\nu') \right\rangle_2 .$$

This proves the relation (5) for every $\phi \epsilon D_2$.

We remark that the relation (5) can also be proved starting from the fact that the generalized function $[T(\nu) \times T(\nu')]_\mu$ is a continuous function of the parameter μ in the sense of Ref. 4, Kap. 1 Anhang 2. This enables one to write the left-hand side of (5) as

$$\int_{-1}^{+1} \mu \left\langle (T(\nu) \times T(\nu'))_\mu, \; \phi(\nu,\nu') \right\rangle_2 d\mu \; ,$$

which is equivalent to

$$\int_{-1}^{+1} \mu \left\langle T_\mu(\nu), \; \left\langle T_\mu(\nu'), \; \phi(\nu,\nu') \right\rangle_1 \right\rangle_1 d\mu \; .$$

If one uses theorem 1 and the Poincaré-Bertrand formula (8) it is not difficult to show that this is equal to the expression in the right-hand side of (5) for every $\phi \epsilon D_2$.

Having established the results above one deduces all other formulae that have appeared in the literature, e.g. the full-range closure relation and the angular Green's function, using exactly analogous methods.

DISCUSSION

From the proof of theorem 2 above one concludes that McInerney's relation (Eq. (35)) is valid only if $\nu' \neq \nu$; in essence it corresponds to our relation (7-1). Therefore its use in the identity (Eq. (32)) is not justified, since (32) holds and is used also if $\nu' = \nu$. The correct form of (35) should contain a supplementary factor in the right-hand side to account for the contribution from the diagonal $\nu' = \nu$; this factor is essentially expressed in our result (7-2).

The statement of Kuščer and McCormick concerning the ambiguity in the Poincaré-Bertrand formula is due to a misinterpretation of the integrals occurring in this formula. In the notation of Ref. 3 the meaning of the integral over ν in the right-hand side of Eq. (2B) when $\mu' = \mu$ is uniquely defined by the factor $\pi^2 F(\mu,\mu)$ representing the contribution to the integral over μ' at the point $\mu' = \mu$. As we demonstrated above this contribution is equal to $\pi^2 F(\mu,\mu)\delta(\mu-\mu')$.

In conclusion we should like to make the following remarks.

The introduction of generalized functions in neutron transport theory requires proper definitions and their proper handling as functionals. Though the theorems may be stated in the usual shorthand notation, proofs should always be given with reference to the space of test-functions.

The symbol T for a generalized function is preferred to ϕ since in mathematical literature the symbol ϕ is commonly used to denote a test-function.

The symbol P only denotes a meaningful operator if placed before an integral sign. Therefore formulae like (2A) and (2B) in Ref. 3 are mathematically senseless.

The same warning is appropriate to formulae (4) and (7) in Ref. 2, where one silently passes from generalized functions ϵD_1^* in the left-hand side to generalized functions ϵD_2^* in the right-hand side. Such ambiguities cause confusion and should therefore be avoided.

To summarize we have given a rigorous proof that there is only one consistent system of formulae in neutron transport theory. It is the system that is currently used in this field, following the work of Case et al.

H. G. Kaper

Mathematical Institute
Groningen University
Groningen, The Netherlands.

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Comment to the Preceding Letter by Kaper

We appreciate the effort of Kaper to mathematically justify what we hoped to convey in a heuristic manner. It is indeed reassuring to see that his Eq. (7-3) follows from our Eq. (3A), and that his derivation is closely related to ours (so that it seems to the same extent arbitrary).

We admit not having explained one symbol which has created doubt about the mathematical sense of the equations. Our $\int P$ stands for $P\int$ or $⨍$ of other authors, whereas