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New Variational Principle for Transport Theory

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A general variational principle of Kahan, Rideau, and Roussopoulos is shown to be applicable to problems of transport theory and in particular to the solution of the Milne problem. The variational principle yields directly the flux at every point, not only at infinity, unlike the classical methods for asymptotic densities.

MATHEMATICAL DEVELOPMENT

TRANSPORT theory has made a great use of variational principles, whose inception began with the work of LeCaine,[1] Marshak,[2] Davison,[3] and Kourganoff.[4] Later on, Pryce,[5] Fuchs,[6] and Wilson[7] used variational principles for the determination of the critical radius of a neutron reacting sphere, and Corngold[8] has done likewise for slowing-down problems. In all those problems but the last, a given functional was shown to be a maximum. The utility of variational principles is, however, not restricted to the cases of extrema, and for the purpose of practical computation it is sometimes quite sufficient to use functionals leading to saddle points.

Many problems of neutron transport theory are given in the form of an integral equation of the Fredholm type:

$$\phi(x)=\lambda\int K(x,x')\phi(x')dx'+S(x), \tag{1}$$

where the limits are given, and the kernel $K(x,x')$ is real, symmetrical or symmetrizable. The exact solution of (1) is often unknown but it is quite easy to find approximate solutions $u(x)$. Given

$$\phi(x)=u(x)+q(x), \tag{2}$$

the problem is to find reasonably accurate values of $q(x)$. Introducing (2) into (1), we have

$$q(x)=\lambda\int K(x,x')q(x')dx'+f(x), \tag{3}$$

where

$$f(x)=\lambda\int K(x,x')u(x')dx'-u(x)+S(x).$$

If, on the other hand, $G(x_0\rightarrow x)$ is the Green's function of (1), one has

$$G(x_0\rightarrow x)=\lambda\int K(x,x')G(x_0\rightarrow x')dx'+\lambda K(x,x_0). \tag{4}$$

Given the integral operator

$$L\equiv\int[\delta(x-x')-\lambda K(x,x')]\cdots dx',$$

Eqs. (3) and (4) take the form

$$Lq(x_0)=f(x_0), \tag{3'}$$

$$LG(x_0\rightarrow x)=\lambda K(x,x_0). \tag{4'}$$

A theorem of Kahan and Rideau[9] (generalized by Roussopoulos[10] for the case of unsymmetric L operators) shows that the two quantities

$$\lambda\int q(x_0)K(x,x_0)dx_0 \quad\text{and}\quad \int f(x_0)G(x_0\rightarrow x)dx_0$$

[1] J. LeCaine, Phys. Rev. **72**, 564 (1947).
[2] R. E. Marshak, Phys. Rev. **71**, 688 (1947).
[3] B. Davison, Phys. Rev. **71**, 694 (1947).
[4] V. Kourganoff, Compt. rend **227**, 895 (1948).
[5] H. L. Pryce, Birmingham Report MSP 2A (unpublished).
[6] K. Fuchs, Birmingham Report MS 85 (unpublished).
[7] A. H. Wilson, Birmingham Report MS 115 (unpublished).
[8] N. Corngold, Proc. Phys. Soc. (London) **A70**, 793 (1957).
[9] T. Kahan and G. Rideau, Compt. rend. **233**, 1446 (1951).
[10] P. Roussopoulos, Compt. rend. **236**, 1858 (1953).

are equal to the same stationary value (SV),

$$\left.\begin{array}{l}\lambda\displaystyle\int q(x_0)K(x,x_0)dx_0\\ \displaystyle\int f(x_0)G(x,x_0)dx_0\end{array}\right\}=\mathrm{SV}\frac{\displaystyle\int \tilde{G}(x\rightarrow x_0)f(x_0)dx_0\int \tilde{q}(x_0)K(x,x_0)dx_0}{\displaystyle\int \tilde{G}(x\rightarrow x_0)L\tilde{q}(x_0)dx_0}, \quad (5)$$

where $\tilde{G}(x\rightarrow x_0)$ and $\tilde{q}(x_0)$ are approximate values of $G(x\rightarrow x_0)$ and $q(x_0)$. The functional (5) retains its stationary property independently of the particular significance of $q(x_0)$, $f(x_0)$, $G(x\rightarrow x_0)$, and $K(x\rightarrow x_0)$.

An important particular case is the evaluation of

$$\lim_{x\rightarrow\infty}\int K(x,x_0)q(x_0)dx_0.$$

If

$$\lim_{x\rightarrow\infty}K(x,x_0)=0 \quad \text{and} \quad \lim_{x\rightarrow\infty}S(x)=0,$$

we have

$$\lim_{x\rightarrow\infty}G(x_0\rightarrow x)=\mu\phi(x_0),$$

where μ is a constant factor to be determined in each particular case by physical considerations. Under such conditions,

$$\lim_{x\rightarrow\infty}\int q(x_0)K(x,x_0)dx_0=\mu\int f(x_0)\phi(x_0)dx_0$$
$$=\mu\int f(x_0)u(x_0)dx_0+\mu\int f(x_0)q(x_0)dx_0. \quad (6)$$

It is quite evident from inspection of (3) that the last term can be evaluated by means of the Schwinger variational principle

$$\int f(x_0)q(x_0)dx_0=\mathrm{SV}\frac{[\int \tilde{q}(x_0)f(x_0)dx_0]^2}{\int \tilde{q}(x_0)L\tilde{q}(x_0)dx_0}. \quad (7)$$

It has not been possible to determine the direction of the error in (5). However, in the case of (7) it can be shown[3] that under specific conditions imposed on L and $f(x_0)$, the functional (7) is a maximum.

We remark also that the functional (5) give us an estimate of $q(x)$ for every point in the interval of integration, in contrast to the methods expounded in (1), (2), and (3).

THE MILNE PROBLEM

We shall apply the functional (5) to the determination of the neutron (or photon) flux in a semi-infinite isotropically scattering and noncapturing medium, which is bounded by vacuum and which sustains a constant current from infinity, i.e., the Milne problem.

We have $\lambda=1$; $S(x)=0$; $K(x,x')=\frac{1}{2}E_1(|x-x'|)$, and the diffusion approximation gives us $u(x)=x$, that is $f(x)=\frac{1}{2}E_3(|x|)$, with

$$E_n(|x|)=\int_1^\infty \frac{e^{-t|x|}}{t^n}dt.$$

Since $\lim_{x\rightarrow\infty}K(x,x')=0$, we could as well apply (7) with

$$q(\infty)=\lim_{x\rightarrow\infty}\int K(x,x')q(x')dx', \quad (8)$$

since $\lim_{x\rightarrow\infty}f(x)=0$ and obtain

$$q(\infty)=\frac{\mu}{2}\int_0^\infty E_3(x)xdx+\mu\,\mathrm{SV}\left\{\left[\int_0^\infty \tfrac{1}{2}E_3(x)\tilde{q}(x)dx\right]^2\Big/\int_0^\infty \tilde{q}(x)dx\left[\tilde{q}(x)-\tfrac{1}{2}\int_0^\infty E_1(|x-x'|)\tilde{q}(x')dx'\right]\right\}. \quad (9)$$

Physical considerations[2,11] show that $\mu=3$. Solution (9) is nothing but the well-known variational estimate of the extrapolation length.

If, on the other hand, we want to determine $q(\infty)$ by (5), we take $\tilde{q}(x)=z_0$ and replacing $G(x\rightarrow x_0)$ by $\phi(x_0)=x_0+z_0$, obtain

$$q(\infty)=\mathrm{SV}\lim_{x\rightarrow\infty}\left\{\int_0^\infty (x_0+z_0)\tfrac{1}{2}E_3(x_0)dx_0\int_0^\infty \tfrac{1}{2}z_0E_1(|x-x_0|)dx_0\Big/\int_0^\infty (x_0+z_0)\left[z_0-\tfrac{1}{2}\int_0^\infty E_1(|x_0-x_0'|)z_0dx_0'\right]dx_0\right\}, \quad (10)$$

which gives us by straightforward integration

$$q(\infty)=\frac{3+4z_0}{4+6z_0}.$$

This result is dependent on the normalization chosen for $q(x)$ [through $\phi(x)$] but if we take a value consistent with an iteration scheme, we must take $z_0=q(\infty)$ which gives us immediately

$$q(\infty)=\frac{1}{\sqrt{2}}=0.7071;$$

this differs by less than 0.5% from the exact value 0.7104. LeCaine[1] found, with a constant trial function

[11] B. Davison, *Neutron Transport Theory* (Oxford University Press, New York, 1957), p. 210.

$\tilde{q}(x)$ in (9), the value $q(\infty)=0.7083$ which is slightly more precise.

Let us determine $q(x)$ for every point of the medium by means of the functional (5). Since the Green's function for the diffusion approximation in a noncapturing half-space is

$$2\pi|x+x_0|-2\pi|x-x_0|,$$

we choose the following approximate Green's function:

$$\tilde{G}(x\rightarrow x_0)=2\pi|x+x_0|-2\pi|x-x_0|+4\pi q(\infty), \quad (11)$$

which has the property that

$$\lim_{x\rightarrow\infty}\tilde{G}(x\rightarrow x_0)=4\pi[x_0+q(\infty)],$$

i.e., $\mu=4\pi$. The conjunction of (5) with (3) leads to

$$q(x)\simeq\tfrac{1}{2}E_3(x)+\frac{\int_0^\infty[|x+x_0|-|x-x_0|+2q(\infty)]\tfrac{1}{2}E_3(z_0)dx_0\int_0^\infty\tfrac{1}{2}E_1(|x-x_0|)dx_0}{\int_0^\infty[|x+x_0|-|x-x_0|+2q(\infty)]\tfrac{1}{2}E_2(x_0)dx_0}. \quad (12)$$

We shall omit the resulting integrations which are long but straightforward, giving the final result

$$q(x)=\tfrac{1}{2}E_3(x)+q(\infty)[1-\tfrac{1}{2}E_2(x)]\times\left[1-\frac{12E_5(x)}{4q(\infty)+3}\right]\left[1-\frac{6E_4(x)}{3q(\infty)+2}\right]^{-1}, \quad (13)$$

which has the correct asymptotic form

$$q(x)=q(\infty)[1-\tfrac{1}{2}E_2(x)]+\tfrac{1}{2}E_3(x).$$

The value at the boundary $q(0)=7/12=0.584$ differs by 1% from the exact value 0.577. The error never exceeds 1.5% at other points. It is expected that the greater error near the boundary is caused by the rather incorrect form of the Green's function at the boundary.

CONCLUSION

The use of the new variational principle—whose precision is satisfactory for most purposes—has two interesting properties:

1. We make no use whatsoever of any hypothesis on the development of $\tilde{q}(x)$ in a series of functions, and moreover we reach satisfactory accuracy with the rough trial function $\tilde{q}(x)=z_0$. Much greater precision could have been obtained if we had taken a development of $\tilde{q}(x)$ in a series of functions $E_n(x)$ with unknown coefficients.

2. We have no extremum to compute and we avoid the rather cumbersome work of computation of the coefficients of $E_n(x)$.

In general the method expounded above could equally well be applied to problems of transport theory whose exact solution is unknown (e.g., the slab or sphere problem), in contrast to the classical methods[1–3] valid for asymptotic densities. We have found a direct determination of $q(x)$ through (5) and not through $q(\infty)$, which would moreover be impossible in the case where all the points of the reacting medium are at finite distances. The approximate Green's functions $\tilde{G}(x_0\rightarrow x)$ could always be taken as the Green's functions pertaining to the diffusion approximation, which are quite easy to construct for a great number of problems.

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