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# The Variational Method for Asymptotic Neutron Densities*

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Inhomogeneous integral equations connected with a certain class of neutron diffusion problems are treated by means of a variational method. It is shown how to obtain quite accurate values of the asymptotic neutron density in the following three cases: (a) Milne's problem for the plane, (b) infinite scattering medium surrounding black spherical core, (c) infinite scattering medium surrounding black spherical core with air gap.

THE variational method for solving eigenvalue problems associated with integral equations is well known. One starts with the integral equation:

$$\rho_0(\mathbf{r}) = c\int d\mathbf{r}'\rho_0(\mathbf{r}')K(\mathbf{r}, \mathbf{r}'), \tag{1}$$

where $c$ is the (lowest) eigenvalue to be determined, $\rho_0(\mathbf{r})$ is, say, the neutron density as a function of the coordinates, and $K(\mathbf{r}, \mathbf{r}')$ is the kernel (assumed to be symmetric in $\mathbf{r}$ and $\mathbf{r}'$); the integration is over the medium in question. It can then be shown that the functional:

$$\int d\mathbf{r}\rho(\mathbf{r})\left\{\rho(\mathbf{r}) - c\int d\mathbf{r}'\rho(\mathbf{r}')K(\mathbf{r}, \mathbf{r}')\right\} \tag{2}$$

is an extremum[1] for the actual solution $\rho_0$ of Eq. (1); furthermore, it is evident that:

$$c = \frac{\int d\mathbf{r}\rho_0^2(\mathbf{r})}{\int d\mathbf{r}\rho_0(\mathbf{r})\int d\mathbf{r}'\rho_0(\mathbf{r}')K(\mathbf{r}, \mathbf{r}')} \tag{3}$$

Since the first variation of (2) vanishes, we may expect that the value predicted for the eigenvalue $c$ by the insertion of some trial function for the unknown $\rho_0$ will be closer to the correct value of $c$ than the trial function is to $\rho_0$. It can be proved that the approximate eigenvalue is always larger than the correct eigenvalue.

The extension of the variational method to inhomogeneous integral equations is possible and leads to a simple procedure for obtaining fairly accurate solutions for a certain class of neutron diffusion problems. We shall first present briefly the method in general terms and then discuss specific applications. Suppose the inhomogeneous integral equation is:[2]

$$q_0(x) = \int dx'K(x, x')q_0(x') + f(x), \tag{4}$$

where $q_0(x)$ is the unknown function, $K(x, x')$ is a positive symmetric kernel, and $f(x)$ is bounded so that $\int |f(x)|dx$ exists. Suppose, further, that we can express $[\int dxq_0(x)]$ in terms of $q_0(\infty)$, say

$$q_0(\infty) = k_1\int dxq_0(x)f(x) + k_2$$

* This work was done in the Montreal Laboratory of the National Research Council of Canada during the Spring of 1944 and is now declassified.

1 This can be seen easily by writing the trial function $\rho(\mathbf{r})$ as $[\rho_0(\mathbf{r})+\epsilon(\mathbf{r})]$ ($\epsilon(\mathbf{r})$ is the correction function), and showing that the term of first order in $\epsilon$ vanishes identically.

2 The method is presented for a function of one variable; the generalization to more than one variable, as in the case of the homogeneous integral equations, is also possible.

with $k_1$, $k_2$ known constants. Let us define the functional:

$$\frac{\int dxq(x)\left\{q(x)-\int dx'K(x,x')q(x')\right\}}{\left[\int dxq(x)f(x)\right]^2}. \tag{5}$$

The reasoning then proceeds along the same lines as in the homogeneous case: (5) is an extremum[3] for the actual solution, $q_0(x)$, of Eq. (4), and can be equated to $[k_1/(q_0(\infty)-k_2)]$. For an arbitrary trial function, $q(x)$, the equation determining $q_0(\infty)$ is:

$$\frac{\int dxq(x)\left\{q(x)-\int dx'K(x,x')q(x')\right\}}{\left[\int dxq(x)f(x)\right]^2}=\frac{k_1}{q_0(\infty)-k_2}. \tag{6}$$

We shall now show how several neutron diffusion problems requiring a knowledge of the asymptotic neutron density can be written in the form (4). The application of (6) will follow immediately.

We consider first the well-known Milne problem, i.e., the case of a semi-infinite, isotropically scattering (but non-capturing) medium bounded by vacuum which sustains a constant current from infinity. A rigorous expression for the asymptotic neutron density is known for this problem;[4] this is not the case for the other two problems discussed below where at present only approximate solutions are available. The application of the variational method to the Milne problem will disclose the manner in which values of the asymptotic neutron density are arrived at and give an indication of the power of the method.

The integral equation for the neutron density, $\rho_0(x)$ (the boundary is taken at $x=0$ and the scattering mean free path is taken as the unit of length), in the Milne problem is:

$$\rho_0(x)=\tfrac{1}{2}\int_0^\infty dx'E_1(|x-x'|)\rho_0(x'), \tag{7}$$

where $E_1(x)$ is the exponential integral function of order one.[5] Since the asymptotic neutron density is linear, we write $\rho_0(x)=x+q_0(x)$; for large $x$, $q_0(x)$ approaches a constant which we denote by $q_0(\infty)$. Substitution for $\rho_0(x)$ into (7) yields:

$$q_0(x)=\tfrac{1}{2}\int_0^\infty dx'E_1(|x-x'|)q_0(x')+\frac{E_3(x)}{2}, \tag{8}$$

where $E_3(x)$ is the exponential integral function of order three. Equation (8) is of the form (4) but we still require an expression for $\int_0^\infty dxq_0(x)E_3(x)$ in terms of $q_0(\infty)$ before applying (6).

To obtain such a relation,[6] we make use of a theorem proved by Davison,[7] namely that if we have

[3] Dr. B. Davison, in the following article, discusses the conditions under which (5) is a minimum, not only an extremum, for the actual solution.
[4] E. Hopf, *Mathematical Problems of Radiative Equilibrium*, Cambridge Tracts No. 31 (1934).
[5] The exponential integral function of order $n$ is: $E_n(x)=\int_1^\infty[e^{-xt}]dt/t^n$.
[6] In the original report, the relation between $q_0(\infty)$ and $\int_0^\infty dxq_0(x)f(x)$ in all three problems considered, was derived by another method. It is more elegant to make use of Davison's theorem.
[7] The proof of this theorem is simply as follows: $Q(r)$ in (9) can be regarded as $r$ times the neutron density in an infinite (isotropically) scattering medium due to a spherically symmetrical system of continuously distributed sources, the source density at distance $r$ from the origin being $F(r)/r$. The total output of these sources will be $\int d\mathbf{r}(F(r)/r)=4\pi\int_0^\infty rdrF(r)$ and $Q(\infty)$ is equal to $3/4\pi$ times the output of all sources; this leads to (10).

an integral equation of the form:

$$Q(r)=\tfrac{1}{2}\int_0^\infty dr'Q(r')[E_1(|r-r'|)-E_1(r+r')]+F(r) \tag{9}$$

and $Q(r)$ is its solution bounded at infinity, then

$$Q(\infty)=3\int_0^\infty rdrF(r). \tag{10}$$

A comparison of Eqs. (8) and (9) yields:

$$q_0(\infty)=\tfrac{3}{2}\int_0^\infty xdxE_3(x)+\tfrac{3}{2}\int_0^\infty xdx\int_0^\infty dx'q_0(x')E_1(x+x'). \tag{11}$$

Interchanging the order of integration in the second term on the right-hand-side (r.h.s.) of (11) and evaluating the resulting integral and the first term on the r.h.s., we get:

$$q_0(\infty)=\tfrac{3}{2}\int_0^\infty dxq_0(x)E_3(x)+\tfrac{3}{8}. \tag{12}$$

Equation (12) is of the desired form and Eq. (6) becomes:

$$\frac{\displaystyle\int_0^\infty dxq(x)\left\{q(x)-\tfrac{1}{2}\int_0^\infty dx'q(x')E_1(|x-x'|)\right\}}{\displaystyle\tfrac{1}{2}\left[\int_0^\infty dxq(x)E_3(x)\right]^2}=\frac{1}{\tfrac{2}{3}q_0(\infty)-\tfrac{1}{4}}. \tag{13}$$

Equation (13) is the final result, and from it we may calculate $q_0(\infty)$ for different choices of the trial function $q(x)$. The procedure now is to assume a function for $q(x)$, and choose the parameters in this function so that the left-hand side (l.h.s.) of (10) is an extremum; the resulting function is then used to calculate $q_0(\infty)$. In this process the trial function $q(x)$ is determined except for a constant factor; this factor may be taken so that $q(x)$ is asymptotic to the value obtained for $q_0(\infty)$.

As has already been remarked, the whole point of the variational method is that the choice of $q(x)$ may be quite rough and yet give a fairly accurate value for $q_0(\infty)$. Thus, in the present instance, even if we assume $q(x)=$constant (for which no variation is necessary in the left-hand side of (13)), we get:

$$q_0(\infty)=\tfrac{3}{8}\left\{1+\frac{\left[\int_0^\infty dxE_3(x)\right]^2}{\displaystyle\int_0^\infty dx\left[1-\tfrac{1}{2}\int_0^\infty dx'E_1(|x-x'|)\right]}\right\} \tag{14}$$

$$=17/24=0.7083,$$

which is only 0.3 percent less than the correct value 0.7104.[8] The result can be considerably improved by starting from a more elaborate trial function and actually using the extremum property of the functional. In fact, LeCaine has shown that by choosing a trial function which simulates more closely the the actual $q(x)$, namely:

$$q(x)=\text{const.}[1-AE_2(x)+BE_3(x)]$$

[8] Cf. E. Hopf, reference 4; the value 0.7083 should be less than the true value (which it is!) since the l.h.s. of (13) should give a minimum for the correct solution of the integral equation (8) (cf. reference 3).

and extremizing the left-hand side of (13) with respect to $A$ and $B$, one arrives at a value of $q_0(\infty)$ which agrees with the correct value to six decimal places (0.7104457 as compared to the correct value 0.7104461).

The second application of the variational method considered here is an estimate of the asymptotic neutron density in an infinite, isotropically scattering (but non-capturing) medium supporting a constant flux from infinity and surrounding a perfectly absorbing spherical core. This problem was treated by the spherical harmonic method,[9] and we shall compare the results of the variational method with those results. The integral equation for the neutron density in the medium surrounding the black core can easily be derived; we find:

$$\rho_0(r)=\tfrac{1}{2}\int_a^\infty dr'\rho_0(r')\{E_1(|r-r'|)-E_1((r^2-a^2)^{\frac{1}{2}}+(r'^2-a^2)^{\frac{1}{2}})\}, \tag{15}$$

where $\rho_0(r)$ is $r$ times the neutron density and $a$ is the radius of the black core.

We are interested in a solution of (15) which is asymptotically linear, and we write this solution as

$$\rho_0(r)=r-Q(r). \tag{16}$$

The existence of this solution can be established in the same way as the existence of the solution of Eq. (7). On substituting (16) into (15), we find the integral equation for $Q(r)$, namely:

$$Q(r)=\int_a^\infty dr'Q(r')K(r,r')+\epsilon_3(r) \tag{17}$$

where

$$K(r,r')=\tfrac{1}{2}\{E_1(|r-r'|)-E_1((r^2-a^2)^{\frac{1}{2}}+(r'^2-a^2)^{\frac{1}{2}})\}, \tag{17a}$$

$$\epsilon_3(r)=\tfrac{1}{2}[aE_2(r-a)+E_3((r^2-a^2)^{\frac{1}{2}})-E_3(r-a)]. \tag{17b}$$

The kernel $K(r, r')$ is obviously symmetric; it is also positive, as can be seen by noting that $|r-r'|<[(r^2-a^2)^{\frac{1}{2}}+(r'^2-a^2)^{\frac{1}{2}}]$ and that $E_1(x)$ is a monotonically decreasing function of $x$. Moreover, the function $\epsilon_3(r)$ is bounded and the integral $\int_a^\infty|\epsilon_3(r)|dr$ exists. Hence, the variational method can be employed to estimate $Q(\infty)$ provided $Q(\infty)$ can be expressed in terms of $\int_a^\infty drQ(r)\epsilon_3(r)$.

A relation between $Q(\infty)$ and $\int_a^\infty drQ(r)\epsilon_3(r)$ can be found by again making use of Davison's theorem (cf. Eqs. (9) and (10)). For this purpose, we must define $Q(r)$ and $\epsilon_3(r)$ in the interval $0\leqslant r<a$; we choose:[10]

$$Q(r)=\tfrac{1}{2}\int_a^\infty dr'Q(r')\{E_1(|r-r'|)-E_1(r+r')\}, \quad (0\leqslant r<a), \tag{18a}$$

$$\epsilon_3(r)=0, \qquad (0\leqslant r<a). \tag{18b}$$

Further, we write:

$$\Lambda Q(r)=\tfrac{1}{2}\int_0^\infty dr'Q(r')\{E_1(|r-r'|)-E_1(r+r')\}, \tag{19a}$$

$$\Delta_1 Q(r)=\tfrac{1}{2}\int_0^a dr'Q(r')\{E_1(|r-r'|)-E_1(r+r')\}, \tag{19b}$$

$$\Delta_2 Q(r)=\tfrac{1}{2}\int_a^\infty dr'Q(r')\{E_1((r^2-a^2)^{\frac{1}{2}}+(r'^2-a^2)^{\frac{1}{2}})-E_1(r+r')\}, \quad (r\geqslant a), \tag{19c}$$

$$=0, \quad (0\leqslant r<a). \tag{19d}$$

[9] R. E. Marshak, Phys. Rev. **71**, 688 (1947).
[10] Cf. Davison's declassified Montreal report MT-232, "Influence of an Air Gap Surrounding a Small Black Sphere Upon the Linear Extrapolation Length of the Neutron Density in the Surrounding Medium."

In view of the above definitions, Eq. (17) becomes:

$$Q(r) = \Lambda Q(r) - \Delta_1 Q(r) - \Delta_2 Q(r) + \epsilon_3(r). \tag{20}$$

Equation (20) is also satisfied for $0 \leqslant r < a$. If we now use Eq. (9), we get:

$$Q(\infty) = 3\left\{\int_a^\infty r dr \epsilon_3(r) - \int_0^\infty r dr [\Delta_1 Q(r)] - \int_a^\infty r dr \Delta_2 Q(r)\right\}. \tag{21}$$

The evaluation of the first term on the r.h.s. of (21) is straightforward; the result is $3a^2/4$. The second term on the r.h.s. can be evaluated by interchanging the order of integration to give $-3\int_0^a r dr Q(r)$. However, $Q(r)$ for $0 \leqslant r < a$ is defined by (18a); inserting (18a) and interchanging the order of integration a second time yields:

$$-\tfrac{3}{2}\int_a^\infty dr' Q(r') \int_0^a r dr \{E_1(|r-r'|) - E_1(r+r')\}.$$

The third term on the r.h.s. becomes, on interchanging the order of integration:

$$-\tfrac{3}{2}\int_a^\infty dr' Q(r') \int_a^\infty r dr \{E_1((r^2-a^2)^{\frac{1}{2}} + (r'^2-a^2)^{\frac{1}{2}}) - E_1(r+r')\}.$$

It is easy to show that:

$$\tfrac{1}{2}\left\{\int_0^a r dr E_1(|r-r'|) + \int_a^\infty r dr E_1((r^2-a^2)^{\frac{1}{2}} + (r'^2-a^2)^{\frac{1}{2}}) - \int_0^\infty r dr E_1(r+r')\right\} = \epsilon_3(r'). \tag{22}$$

Hence, Eq. (21) leads to the desired relation:

$$Q(\infty) = \frac{3a^2}{4} - 3\int_a^\infty dr Q(r) \epsilon_3(r). \tag{23}$$

Substituting (23) into (6) yields an equation corresponding to (13), namely:

$$\frac{\int_a^\infty dr Q(r)\left\{Q(r) - \frac{1}{2}\int_a^\infty dr' Q(r') K(r, r')\right\}}{\left[\int_a^\infty dr Q(r) \epsilon_3(r)\right]^2} = \frac{1}{\frac{a^2}{4} - \frac{Q(\infty)}{3}}. \tag{24}$$

Again, as in the plane Milne case, we choose the simplest trial function, i.e. $Q(r) \equiv$ const.; we get

$$Q(\infty) = \frac{3a^2}{4} - \frac{3\left[\frac{a}{2} - \frac{1}{3} + \int_a^\infty dr E_3((r^2-a^2)^{\frac{1}{2}})\right]^2}{\left[1 + 2\int_a^\infty dr \int_a^\infty dr' E_1((r^2-a^2)^{\frac{1}{2}} + (r'^2-a^2)^{\frac{1}{2}})\right]}. \tag{25}$$

Values of $[a - Q(\infty)]$—i.e., the "extrapolated endpoint"—as a function of $a$ computed on the basis of (25) are given in column 2 of Table I, while the values of the extrapolated endpoint predicted by the $P_5$-approximation of spherical harmonic method[9] are given in column 3. It is seen how powerful the variational method is for the determination of the asymptotic neutron density. Of course, a slightly more accurate choice of trial function, which takes into account the exponential-type approach of $Q(r)$ to $Q(\infty)$, would lead to considerably more accurate values of the extrapolated endpoint. Table I further indicates that the actual solution of (17) maximizes the extrapolated endpoint as is to be expected from Davison's paper.[3]

TABLE I. Extrapolation endpoint as function of $a$.

| $a$ | Variational method | $P_5$-approximation |
|---|---|---|
| 0.5 | 0.347 | 0.334 |
| 1.0 | .506 | .494 |
| 2.0 | .626 | .620 |
| 5.0 | .688 | .690 |
| $\infty$ | .708 | .709 |

Finally, we have applied the variational method developed above to the case of a black sphere (of radius $a$) surrounded by an "air gap" (of outer radius $b$) which in turn is surrounded by an isotropically scattering (but non-capturing) medium supporting a constant flux from infinity. The integral equation for $r$ times the neutron density turns out to be:

$$\rho_0(r)=\tfrac{1}{2}\int_b^\infty dr'\rho_0(r')\bar{K}(r,r') \tag{26}$$

where:

$$\bar{K}(r,r')=\Big\{E_1(|r-r'|)-E_1((r^2-b^2)^{\frac{1}{2}}+(r'^2-b^2)^{\frac{1}{2}}) \\ +\int_\alpha^\beta \frac{dR}{R}\exp\Big[-R+\frac{1}{R}((R^2+r^2-r'^2)^2-4R^2(r^2-b^2))^{\frac{1}{2}}\Big]\Big\}.$$

with

$$\alpha=(r^2-b^2)^{\frac{1}{2}}+(r'^2-b^2)^{\frac{1}{2}},\quad \beta=(r^2-a^2)^{\frac{1}{2}}+(r'^2-a^2)^{\frac{1}{2}}.$$

As in the two preceding cases, since capture is absent in the outside medium, the asymptotic solution is linear. Following the procedure for the black sphere without gap, we obtain the integral equation for $Q(r)$, ($\rho_0(r)=r-Q(r)$), namely:

$$Q(r)=\tfrac{1}{2}\int_b^\infty dr'Q(r')\bar{K}(r,r')+\bar{\epsilon}_3(r), \tag{27}$$

where:

$$\bar{\epsilon}_3(r)=\tfrac{1}{2}[bE_2(r-b)-E_3(r-b)+E_3((r^2-a^2)^{\frac{1}{2}}-(b^2-a^2)^{\frac{1}{2}})-(b^2-a^2)^{\frac{1}{2}}E_2((r^2-a^2)^{\frac{1}{2}}-(b^2-a^2)^{\frac{1}{2}})]. \tag{27a}$$

We find for $Q(\infty)$ (cf. Eq. (23)):

$$Q(\infty)=\frac{3a^2}{4}-3\int_b^\infty drQ(r)\bar{\epsilon}_3(r). \tag{28}$$

Substitution of (28) into Eq. (6) then permits an immediate application of the variational method to estimate $Q(\infty)$. No numerical results have been obtained for this case.

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