microwave absorption spectrum. We have made an analysis of the infra-red band[17] of H_2Se at 4.3μ and find the effective moments of inertia are in the neighborhood of $I_A=3.14$, $I_B=3.89$, $I_C=7.18\times10^{-40}$ g cm^2.

These values were substituted in the formulae for the rigid rotor and the positions of the transitions in the microwave region (0.2 cm and longer) calculated as shown in Table II*E*. These positions are only approximate, but indicate that one line might be detectable in the one-centimeter region.

[17] D. M. Cameron, W. C. Sears, and H. H. Nielsen, J. Chem. Phys. **7**, 994 (1939).

The dipole moment of H_2Se is not known. A guess of 0.7×10^{-18} esu-cm was used in estimating the order of magnitude of the absorption coefficient. If the $7_{1,6}-6_{4,3}$ line can be detected, its intensity will serve to determine the dipole moment.

The spectrum of HDSe will be of considerable interest in relation to those of HDO and HDS.

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Note on the Spherical Harmonic Method As Applied to the Milne Problem for a Sphere*

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The spherical analog of the Milne problem for the half-plane is treated by an approximate method based on expanding the neutron distribution function in a finite number of spherical harmonics. The results are improved markedly in going from the first to the second approximation and more slowly in higher approximations. The neutron distribution is calculated in the first two approximations. Values of the "extrapolated endpoint"—as predicted by the first three approximations—are tabulated in Table I as a function of the radius of the sphere.

1.

We consider the following problem: a black sphere of radius a, i.e., a sphere which absorbs completely all neutrons which fall upon it, is surrounded by an infinite non-capturing medium which scatters neutrons isotropically without changing their velocity. No sources are present in the outer medium except that a current density of amount $(F/4\pi r^2)$ (F is a constant) is assumed to exist in the direction $(-r)$. We wish to determine the neutron density in the (outer) medium.[1]

This problem is the complete analog of the Milne problem for the semi-infinite plane since the albedo of the black core is zero just as the albedo of vacuum is zero in the plane case. If the black core is replaced by vacuum, the albedo is no longer zero, and the physical conditions are altered in an essential way. The modified problem is not treated in this note.

* The contents of this note were published in a Montreal Report (MT-49) dated April 15, 1944. The Central Records File Reference giving authority for declassification is 11-5-3, serial No. 47. The spherical harmonic method has been generalized and applied to a great variety of neutron diffusion problems by C. Mark (declassified Montreal report MT-97), B. Carlson (declassified Los Alamos report LADC No. 108), R. Glauber, and W. Rarita. Another approximation method based on the Gauss formula for numerical integration, which is equivalent in certain ways to the spherical harmonic method (cf. footnotes below), was developed independently by G. C. Wick, Zeits. f. Physik **121**, 702 (1943), and applied to problems of the stellar atmosphere by S. Chandrasekhar, Astrophys. J. **100**, 76 (1944) and succeeding papers. Because of the war, Wick's paper did not come to the attention of the author until the present work was completed.

[1] S. Chandrasekhar, Astrophys. J. **101**, 95 (1945) has worked out the converse of this problem, namely the determination of the distribution function due to a point source in a spherical scattering medium surrounded by vacuum, by Wick's method.

An exact solution of the present problem, in contrast to the Milne problem for the plane, seems impossible. Recourse must therefore be had to approximate methods. The simplest approximation is the diffusion approximation which consists in expanding the neutron distribution function up to and including the first spherical harmonic. A natural extension of the diffusion approximation is the inclusion of a larger number of spherical harmonics in the expansion of the neutron distribution function. In the limit, of course, the approximate solutions go over into the exact solution. The great virtue of the spherical harmonic method (as we shall call it) is its rapid convergence in the early approximations.

2.

The transport equation governing the distribution of neutrons in the medium surrounding the black core is:

$$\mu\frac{\partial\psi(r,\mu)}{\partial r}+\frac{(1-\mu^2)}{r}\frac{\partial\psi(r,\mu)}{\partial\mu}+\psi(r,\mu)=\frac{\psi_0(r)}{2}, \quad (1)$$

where the origin of coordinates is taken at the center of the black core, μ is the cosine of the angle between the direction of motion of the neutron and the radius r (pointing away from the origin), and $\psi(r, \mu)d\mu$ is the number of neutrons per unit volume at distance r with direction cosine between μ and $\mu+d\mu$. The quantity $\psi_0(r)$ is the neutron density, defined as $\int_{-1}^{1}\psi(r, \mu)d\mu$. Finally, the mean free path is taken as unit of length, and the neutron velocity is set equal to unity.

It is easy to show, by integrating Eq. (1) over $d\mu$, that the total flux $[4\pi r^2 j(r)](j(r) = -\int_{-1}^{1}\mu\psi(r, \mu)d\mu)$ is a constant independent of r. We choose the constant as 4π so that $j(r)=1/r^2$. Equation (1) is to be solved, subject to the boundary condition

$$\psi(a, \mu)=0 \quad \text{for} \quad \mu>0, \quad (A)$$

where a is the radius of the black core.

The spherical harmonic method we propose consists in expanding $\psi(r, \mu)$ in a series of Legendre polynomials and breaking off the series after a finite number of terms. Thus we write:

$$\psi(r,\mu)=\sum_{l=0}^{l_0}\tfrac{1}{2}(2l+1)\psi_l(r)P_l(\mu), \quad (2)$$

where $\psi_l(r)=\int_{-1}^{1}P_l(\mu)\psi(r, \mu)d\mu$, and l_0 is an integer which determines the order of the approximation. For example, if l_0 is taken as 1, we say we are dealing with the P_1-approximation, if $l_0=3$, the P_3-approximation, and so on. It is natural to choose l_0 as an odd integer for successive approximations since the even approximations contain singular parts which have no clear physical significance.

The representation of $\psi(r, \mu)$ by a finite number of Legendre polynomials, as defined by Eq. (2), is inconsistant with the boundary condition (A). Instead, this boundary condition must be relaxed and replaced by a series of boundary conditions appropriate to the order of the approximation which is being considered. Thus, if we are working with the P_1-approximation (the diffusion approximation), one boundary condition is sufficient to determine all the arbitrary constants, and it is reasonable to require that the total current entering the (outer) medium from the black core is zero, namely that:

$$\int_0^1 \mu\psi(a, \mu)d\mu=0. \quad (3)$$

The next approximation, the P_3-approximation, requires one additional boundary condition besides Eq. (3). There is some arbitrariness involved in the choice of this added boundary condition since we could require that $\int_0^1 P_2(\mu)\psi(a, \mu)d\mu=0$ or $\int_0^1 P_3(\mu)\psi(a, \mu)d\mu=0$, etc. It turns out that the solution for $\psi_0(r)$ is negligibly affected by the particular choice made and always gives a distinct improvement over the P_1-approximation. In an odd approximation, it seems most sensible to choose a boundary condition on an odd moment.[2]

[2] Dr. Mark has pointed out that the apparent ambiguity in the choice of the boundary conditions is removed if one recalls that in the Milne problem for the half-plane the exact even "half-moments" have an infinite derivative at the boundary, whereas the exact odd "half-moments" have a finite derivative, just as they do in any odd P-approximation. Furthermore, it is possible to obtain unique boundary conditions at $r=a$ by regarding the black sphere as *black* not as *vacuum*, i.e., by regarding the black sphere as a second medium which is completely absorbing, solving the equations, and equating (at $r=a$) the ψ_l's to the ψ_l's of the outside medium. The latter procedure turns out to be equivalent to Wick's choice of boundary conditions. The procedure we adopt gives more accurate results for the "extrapolated end point." For example, in the limit $a\rightarrow\infty$ (cf. Table I), we obtain 0.667, 0.705, 0.709 for the extrapolated end point in the P_1-, P_3-, P_5-approximations respectively as compared to 0.577, 0.694, 0.704 with the "black" or Wick boundary conditions; the correct value is

We therefore choose as the second boundary condition in the P_3-approximation:

$$\int_0^1 P_3(\mu)\psi(a,\mu)d\mu=0. \qquad (4)$$

Since $P_3(\mu)$ is a linear combination of μ and μ^3, Eqs. (3) and (4) are equivalent to (3) and the condition $\int_0^1 \mu^3\psi(a,\mu)d\mu=0$. (This is an added attraction for the "odd moment" boundary conditions.) In this manner it is possible, except for increasing algebraic complications, to arrive at closer and closer approximations to the neutron density $\psi_0(r)$.

3.

We now carry through the P_1 and P_3-approximations in accordance with the procedure outlined above. Let us multiply both sides of Eq. (1) by $P_l(\mu)$. Integrating over $d\mu$ and using well-known relations between Legendre polynomials, we get a series of equations:[3]

$$\frac{1}{(2l+1)}\{l\psi_{l-1}'(r)+(l+1)\psi_{l+1}'(r)\} + \frac{1}{r(2l+1)}\{(l+1)(l+2)\psi_{l+1}(r) - l(l-1)\psi_{l-1}(r)\}+\psi_l(r)=\psi_0(r)\delta_{0l}. \qquad (5)$$

In Eq. (5) the primes denote differentiation with respect to r and δ_{0l} is the Kronecker delta-function. If we choose $l_0=1$ (P_1-approximation), then Eq. (5) becomes equivalent to the two equations:

$$\psi_1'(r)+2\psi_1(r)/r=0, \qquad (6a)$$

$$\tfrac{1}{3}\psi_0'(r)+\psi_1(r)=0, \qquad (6b)$$

of which the solutions are:

$$\psi_1(r)=-1/r^2, \qquad (7a)$$

$$\psi_0(r)=-3/r+B \text{ (B is a constant).} \qquad (7b)$$

The total flux has been taken as 4π. Equation (7b) is, of course, the usual diffusion result and on the crude assumption, $\psi_0(a)=0$, would lead to the value $B=3/a$. However, one should use the improved boundary condition (3) which becomes in the present case:

$$\tfrac{1}{2}\psi_0(a)+\psi_1(a)=0, \qquad (8)$$

from which

$$B=3(1+2/3a)/a. \qquad (9)$$

It is convenient to rewrite Eq. (7b) in the form:

$$r\psi_0(r)=B[r-a+r_0] \quad \text{where} \quad r_0=a-3/B.$$

The quantity r_0 is called the extrapolated end point and has the value (in the P_1-approximation):

$$r_0=2/3(1+2/3a). \qquad (9a)$$

We consider next the P_3-approximation; setting $l_0=3$ in Eq. (2), we get from Eq. (5) the following set of equations:

$$r\psi_1'(r)+2\psi_1(r)=0; \qquad (10a)$$

$$r\psi_0'(r)+2r\psi_2'(r)+6\psi_2(r)+3r\psi_1=0; \qquad (10b)$$

$$2r\psi_1'(r)+3r\psi_3'(r)-2\psi_1(r)+12\psi_3(r)+5r\psi_2(r)=0; \qquad (10c)$$

$$3r\psi_2'(r)-6\psi_2(r)+7r\psi_3(r)=0. \qquad (10d)$$

These equations are to be solved subject to the boundary conditions (3) and (4) which may be rewritten as:

$$4\psi_0(a)+8\psi_1(a)+5\psi_2(a)=0; \qquad (11a)$$

$$8\psi_1(a)+25\psi_2(a)+32\psi_3(a)=0. \qquad (11b)$$

The solutions are:[4]

$$\psi_0(r)=-3/r+B-2Ge^{-kr}/r; \qquad (12a)$$

$$\psi_1(r)=-1/r^2; \qquad (12b)$$

$$\psi_2(r)=-6/5r^3+G(1+3/kr+3/k^2r^2)e^{-kr}/r; \qquad (12c)$$

$$\psi_3(r)=-18/7r^4+5G(1+6/kr+15/k^2r^2+15/k^3r^3)e^{-kr}/3kr \qquad (12d)$$

0.7104. However, the neutron density at the boundary (for the limiting case $a\rightarrow\infty$) is given exactly by the Wick method. One would then suppose that for finite a, the present method would give more rapidly converging values of the extrapolated endpoint whereas the Wick method would give more rapidly converging values of the neutron density, at least at the boundary.

[3] The set of Eqs. (5) is a straightforward consequence of the expansion of Eq. (2); compare, however, the roundabout treatment of the spherical problem (see ref. in footnote 1) necessitated by the use of Wick's method. In the end, the final equations are identical. In general, the spherical harmonic method has an advantage over Wick's method in its easy adaptability to problems of several media and different geometries.

[4] The terms having G as coefficient are essentially Hankel functions (of the first kind) of half-integral order having ($i\,kr$) as argument.

where

$$k=(35)^{\frac{1}{2}}/3;$$

$$B=\frac{3}{a}\left[1+\frac{2}{3a}+\frac{1}{2a^2}\right]+\frac{7k\delta}{2a}\left[1-\frac{5}{ka}-\frac{5}{k^2a^2}\right];$$

$$G=14k\delta e^{ka}/3;$$

$$\delta=\frac{[1/8k^2a][1+15/4a+72/7a^2]}{\left\{\left(1+\frac{175}{96k}\right)+\frac{6}{ka}\left(1+\frac{175}{192k}\right)+\frac{15}{k^2a^2}\left(1+\frac{35}{96k}\right)+\frac{15}{k^3a^3}\right\}}.$$

We rewrite Eq. (12a) to exhibit the extrapolated endpoint and the novel feature of the P_3-approximation:

$$r\psi_0(r)=B[(r-a+r_0)-\gamma e^{-k(r-a)}], \quad (13)$$

where

$$B=3/(a-r_0), \quad \gamma=2G/kB.$$

It is seen from Eq. (13) that the P_3-approximation gives a different (and necessarily improved) value for r_0. Moreover, a correction of exponential order is added to the asymptotic expression $(r-a+r_0)$.

Each higher P-approximation improves the extrapolated end point and adds one more term of exponential order. Thus, we would obtain the following form for $\psi_0(r)$ in the $P_{(2l_0+1)}$-approximation:

$$r\psi_0(r)=B\left\{(r-a+r_0)-\sum_{j=1}^{l_0}\gamma_j e^{-k_j(r-a)}\right\}. \quad (14)$$

Substitution of Eq. (14) into the series of Eq. (6) would lead to an algebraic equation of order l_0 in k^2 which would yield l_0 distinct roots[5] k_j and permit the determination of $\psi_1, \psi_2, \cdots\psi_{(2l_0+1)}$. Knowledge of the ψ_l's together with the application of the (l_0+1) boundary conditions:

$$\int_0^1 \mu^{(2j+1)}\psi(a,\mu)d\mu=0 \quad (j=0,1,\cdots l_0) \quad (15)$$

would then yield the (l_0+1) constants $r_0, \gamma_1, \gamma_2, \cdots\gamma_{l_0}$.

4.

Since knowledge of the "extrapolated end point," r_0, is of special interest for pile design (e.g., control rods, upper limit on thermal utilization of strongly capturing sphere, etc.) we present some numerical results in Table I. Values of r_0 are given for several values of a in the P_1, P_3, and P_5-approximations. Table I exhibits a fairly general property of the spherical harmonic method: the great improvement of the P_3-approximation over the P_1-approximation and the less rapid improvement registered by still higher approximations.

TABLE I. Extrapolated end point r_0.

a	P_1	P_3	P_5
0.5	0.286	0.323	0.334
1.0	0.400	0.480	0.494
2.0	0.500	0.608	0.620
5.0	0.588	0.682	0.690
∞	0.667	0.705	0.709

[5] The roots k_j are identical with the ones obtained by an application of Wick's method; they are independent of the geometry.