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Abstract

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ON BOUNDARY CONDITIONS IN THE METHOD OF SPHERICAL HARMONICS

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As is known ([1–6]), the method of spherical harmonics for the approximate solution of the kinetic equation

$$\left(s, \frac{1}{\alpha}\operatorname{grad}\varphi\right) + \varphi = \frac{\lambda}{4\pi}\int_{\Omega}\theta(P,\mu_0)\varphi(s',P)\,ds' + F(s,P), \qquad \mu_0 = (s,s'), \quad (1)$$

consists in seeking an approximate solution in the form of a sum of a finite number of spherical functions

$$\sum_{0\le k\le n}(2k+1)\sum_{-k\le i\le k}\frac{1}{1+\delta_{0i}}\frac{(k-|i|)!}{(k+|i|)!}\varphi_{ki}(P)P_{ki}(s) \equiv \sum_{0\le k\le n}(2k+1)\varphi_k(s,P) \quad (2)$$

(P_n-approximation) with unknown coefficients $\varphi_{ki}(P) = \varphi_{ki}(x_1,x_2,x_3)$. In expression (2), $P_{ki}(s) = P_{ki}(\theta,\psi)$ are linearly independent spherical functions (harmonics) of order k,

$$P_{ki}(s) = P_k^{(|i|)}(\cos\theta)\begin{cases}\sin|i|\psi, & i=-k,\dots,-1,\\ \cos i\psi, & i = 0,1,\dots,k,\end{cases}$$

where $P_k^{(i)}$ are the associated Legendre functions of the first kind; δ_{0i} is the Kronecker symbol.

The usual procedure for determining the unknown functions φ_{ki} is as follows: substitute the sum (2) into equation (1), multiply by $P_{ki}(s)$ ($k = 0,1,\dots,n$; $i = 0,\pm1,\dots,\pm k$), and integrate the resulting expressions with respect to the angular variables s. In this way, for the functions $\varphi_{ki}(P)$ one obtains a system of linear partial differential equations which is an approximation to equation (1). To this system it is still necessary to adjoin approximate boundary conditions, which, for a given n, would approximate in the best possible way (in some sense) the exact boundary conditions both at the interfaces of two media and at the boundary with vacuum. The approximate boundary conditions at the interfaces of two media are determined uniquely and reduce to the requirement that the functions φ_{ki} be continuous in a neighborhood of these boundaries ($^{3-7}$). The situation is more complicated with the approximate boundary conditions at the boundary with vacuum. The clarification of this question is the purpose of the present work.

We shall assume that the region G, where the process of particle transport takes place, is convex and bounded by a piecewise-smooth surface Γ. Then the exact boundary condition expressing the absence of particles incident from outside on the boundary Γ of the region G has the form

$$\varphi(s, P) = 0, \quad \text{if } P \in \Gamma \text{ and } (s, n) < 0, \tag{3}$$

where n is the vector of the outward normal at the point P of the boundary Γ.

It would seem natural that, in order to obtain approximate boundary conditions on Γ, one should multiply the sum (2) by a sufficient number of the first harmonics P_{ki}, integrate over those s for which $(s, n) < 0$, and set the resulting expressions equal to zero.

However, such boundary conditions will not be the best ones. This circumstance was apparently first noted by Marshak (^{2}) (see also ($^{3-5}$)) in numerical examples in the solution of spherically symmetric problems. It turned out that for such problems the error of the approximate solution becomes considerably smaller if the approximate boundary conditions on the outer boundary of the sphere are taken as follows (we assume n odd, $n = 2m - 1$): multiply the sum (2) by the odd Legendre polynomials P_{2k-1} $(k = 1, 2, \dots, m)$ and then, as usual, integrate over the interval $(-1, 0)$. Thus, equating to zero the first m moments of the sum (2) with respect to an obviously incomplete system of functions on $(-1, 0)$ leads to a smaller error than, for example, the same procedure for the complete system $P_0, P_1, \dots$.

This empirical fact had no theoretical justification, and therefore it was unclear how to write analogous approximate boundary conditions for problems with more complicated geometries (for example, cylindrical). The circumstances described served as the reason for discussing the question of the choice of (best) boundary conditions on the boundary with vacuum in the method of spherical harmonics ($^{3-5}$).

In papers ($^{6-7}$), on the basis of a new variational principle for the problem (1) + (3), established in (^{8}), the best boundary conditions in the method of spherical harmonics for arbitrary geometry were derived. At the same time, a new derivation is given of the spherical-harmonic equations themselves. The boundary conditions obtained are "best" in the sense that, together with their system of spherical-harmonic equations, they provide the least value of the corresponding functional within the framework of the P_n-approximation.

This derivation is valid under the following assumptions on the scattering indicatrix $\theta(P, \mu_0)$: 1) the function $\theta(P, \mu_0)$ is the sum of a finite number of terms of the form $b_i(P)\theta_i(\mu_0)$, where $b_i(P)$ are piecewise continuous on $\overline{G}$, and $\theta_i(\mu_0)$ are summable functions on $(-1, 1)$; 2) the function $\theta(P, \mu_0) \neq 0$ and is even in μ_0; and 3) the inequalities

$$h_k(P) = \frac{1}{2}\int_{-1}^{1} \theta(P, \mu_0) P_k(\mu_0)\, d\mu_0 \geq 0, \qquad k = 0, 1, \ldots$$

are satisfied.

The function $\alpha(P)$ is assumed to be piecewise continuous and positive on $\overline{G}$. The surfaces of discontinuity of the functions α and θ correspond to the boundaries of separation of the media constituting the region G.

Under the assumptions formulated, for the homogeneous problem (1) + (3) the following variational principle holds: the first eigenvalue λ_1 is equal to the least value of the functional

$$\frac{\int_\Omega \int_\Gamma |(s, n)| u^2\, d\Gamma\, ds + \int_\Omega \int_G \alpha(P) \left[\left(s, \frac{1}{\alpha} \operatorname{grad} u \right)^2 + u^2 \right] dP\, ds}{\frac{1}{4\pi} \int_G \int_\Omega \int_\Omega \alpha(P)\theta(P, \mu_0) u(s, P) u(s', P)\, ds'\, ds\, dP} \tag{4}$$

on the set of such functions u for which the numerator in (4) exists and is finite. (From this, in particular, it follows that the boundary condition (3) is natural.) The minimum of the functional (4) is realized on the function $\varphi_1(s, P) + \varphi_1(-s, P)$, where φ_1 is the eigenfunction corresponding to λ_1. An analogous variational principle also holds for higher

eigenvalues, and also for the inhomogeneous problem (1) + (3) for $\lambda < \lambda_1$ (for details see ([7],[8])).

We shall seek an approximate solution of the homogeneous problem (1) + (3) in the form of the sum (2), assuming n odd, $n = 2m - 1$ ($m = 1, 2, \ldots$).

From the assumption that the function $\hat{\theta}(P, \mu_0)$ is even in μ_0, the relation immediately follows

$$\sum_{0 \leq k \leq m-1} \left[(4k+3)\varphi_{2k+1} + (4k+1) \left(s, \frac{1}{\alpha} \operatorname{grad} \varphi_{2k} \right) \right] = 0,$$

or, by virtue of the properties of spherical functions ($k = 0, 1, \ldots, m-1$),

$$(4k+1)(s, \operatorname{grad} \varphi_{2k}) - \operatorname{div}_s \operatorname{grad} \varphi_{2k} + \operatorname{div}_s \operatorname{grad} \varphi_{2k+2} + (4k+3)\alpha\varphi_{2k+1} = 0. \tag{5}$$

The expressions on the left in (5) are spherical functions of orders $1, 3, \dots, 2m-1$. Therefore, equating to zero the coefficients of all linearly independent spherical functions entering the equalities (5), we obtain $2m^2 + m$ partial differential equations with respect to φ_{ki}. We shall not write out this system.

The remaining $2m^2 - m$ equations and the conditions on the boundary Γ will be derived from the requirement that functions of the form

$$u(s,P) = \varphi(s,P) + \varphi(-s,P) = 2 \sum_{0 \le k \le m-1} (4k+1)\varphi_{2k}(s,P)$$

give the least value to the functional (4). Carrying out the corresponding calculations, we obtain the equations

$$\frac{1}{4\pi}\int_\Omega \left[(4k-1)(s, \operatorname{grad}\varphi_{2k-1}) - \operatorname{div}_s \operatorname{grad}\varphi_{2k-1} + \operatorname{div}_s \operatorname{grad}\varphi_{2k+1}\right] P_{2k,j}(s)\, ds + \alpha(1-\lambda h_{2k})\varphi_{2k,j} = 0 \tag{6}$$

and the same number of boundary conditions

$$\sum_{0 \le i \le m-1} \int_\Omega \left[(4i+1)|(s,n)|\varphi_{2i} - (4i+3)(s,n)\varphi_{2i+1}\right] P_{2k,j}(s)\, ds = 0, \qquad P \in \Gamma \tag{7}$$

$$(k = 0, 1, \dots, m-1; \quad j = -2k, \dots, 0, 1, \dots, 2k).$$

From the system (5) + (6) and from the boundary conditions (7), all odd harmonics can be eliminated. As a result we obtain

$$-\frac{1}{4\pi}\sum_{0 \le i \le m-1} (4i+1) \int_\Omega \left(s, \frac{1}{\alpha}\operatorname{grad}\right)^2 \varphi_{2i} P_{2k,j}(s)\, ds + (1-\lambda h_{2k})\varphi_{2k,j} = 0, \tag{8}$$

$$\sum_{0 \le i \le m-1} (4i+1) \int_\Omega \left[|(s,n)|\varphi_{2i} + (s,n)^2 \frac{1}{\alpha}\frac{\partial \varphi_{2i}}{\partial n}\right] P_{2k,j}(s)\, ds = 0, \qquad P \in \Gamma, \tag{9}$$

or

$$\int_{(s,n)<0} (s,n)\varphi(s,P)\, P_{2k,j}(s)\, ds = 0, \qquad P \in \Gamma. \tag{9'}$$

In the system (8) one can get rid of the summation sign and obtain equations relating only φ_{2k-2}, φ_{2k}, and φ_{2k+2} ($\varphi_{-2} = \varphi_{2m} = 0$).

Let us consider three examples.

1. **The diffusion approximation** ([6]), $m = 1$.

$$-\sum_{1\le i\le 3} \frac{\partial}{\partial x_i}\frac{1}{\alpha}\frac{\partial \varphi_0}{\partial x_i} + 3\alpha(1-\lambda h_0)\varphi_0 = 0, \qquad \varphi_0 + \frac{2}{3\alpha}\frac{\partial \varphi_0}{\partial n}\bigg|_{P\in\Gamma} = 0.$$

The boundary condition obtained—to set equal to zero the flux of particles incident on the boundary Γ—was known from physical considerations.

2. Problems with plane and spherical symmetry. The boundary conditions (9) turn into the Marshak conditions formulated above. The equations of spherical harmonics for these cases are well known ([2–7]).

3. Infinite cylinder. Equation (1) and boundary condition (3) have the form

$$\left[\cos\psi\sqrt{1-\mu^2}\frac{\partial}{\partial r} - \frac{\sin\psi}{r}\sqrt{1-\mu^2}\frac{\partial}{\partial \psi} + \alpha(r)\right] =$$

$$= \frac{\lambda\alpha(r)}{4\pi}\int_0^{2\pi}\int_{-1}^{1}\theta(r,\mu_0)\,\varphi(r,\mu',\psi')\,d\mu'\,d\psi', \tag{10}$$

$$\varphi(R,\mu,\psi) = 0, \qquad \frac{\pi}{2} < \psi < \frac{3\pi}{2}. \tag{11}$$

Taking into account the symmetry properties of the solution of the problem (10) + (11), $\varphi(r,\mu,\psi) = \varphi(r,-\mu,\psi) = \varphi(r,\mu,2\pi-\psi)$, within the P_3-approximation it is evidently necessary to set in (2) $\varphi_{ki}(r) = 0$, except for $\varphi_{00}, \varphi_{11}, \varphi_{20}, \varphi_{22}, \varphi_{31}$, and φ_{33}. For these 6 unknown functions we have the following system of (ordinary) differential equations (5) + (6):

$$\varphi_{11}' + \frac{1}{r}\varphi_{11} + \alpha(1-\lambda h_0)\varphi_{00} = 0, \qquad \varphi_{00}' - \varphi_{20}' + \frac{1}{2}\varphi_{22}' + \frac{1}{r}\varphi_{22} + 3\alpha\varphi_{11} = 0,$$

$$-\varphi_{11}' + \varphi_{31}' - \frac{1}{r}\varphi_{11} + \frac{1}{r}\varphi_{31} + 5\alpha(1-\lambda h_2)\varphi_{20} = 0,$$

$$6\varphi_{11}' - \varphi_{31}' + \frac{1}{2}\varphi_{33}' - \frac{6}{r}\varphi_{11} + \frac{1}{r}\varphi_{31} + \frac{3}{2r}\varphi_{33} + 5\alpha(1-\lambda h_2)\varphi_{22} = 0,$$

$$6\varphi_{20}' - \frac{1}{2}\varphi_{22}' - \frac{1}{r}\varphi_{22} + 7\alpha\varphi_{31} = 0, \qquad 15\varphi_{22}' - \frac{30}{r}\varphi_{22} + 7\alpha\varphi_{33} = 0$$

and 3 boundary conditions (7) (for $r = R$):

$$16\varphi_{00} - 32\varphi_{11} - 10\varphi_{20} + 5\varphi_{22} = 0, \quad -40\varphi_{00} + 128\varphi_{11} + 250\varphi_{20}$$

$$-25\varphi_{22} - 128\varphi_{31} = 0,$$

$$120\varphi_{00} - 384\varphi_{11} - 150\varphi_{20} + 175\varphi_{22} + 64\varphi_{31} - 32\varphi_{33} = 0.$$

The remaining 3 boundary conditions are determined by the symmetry properties of the solution at $r = 0$: $\varphi'_{00} = 0,\ \varphi_{11} = 0,\ \varphi'_{20} = 0$ (if $\alpha,\ h_0$, and h_2 are sufficiently regular at zero).

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Note: Figure translations are in progress. See original paper for figures.