THE INTEGRAL OVER AN ELLIPSOID AND THE SECOND BORN APPROXIMATION

MATHEMATICS

1966

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Abstract

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UDC 517.37

MATHEMATICS

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THE INTEGRAL OVER AN ELLIPSOID AND THE SECOND BORN APPROXIMATION

(Presented by Academician I. M. Vinogradov, 11 IX 1965)

Let us write the equation

$$\Delta\psi + k^2\psi - q\psi = 0, \tag{1}$$

where $\psi - e^{ikx} \to 0$ as $r \to \infty$. The correction ψ_1 of the first Born approximation to the wave function ψ can, as is known, be written in the form

$$\psi_1(x, y, z) = -\frac{1}{4\pi}\int e^{ik(x'+r')} q(x', y', z')\frac{dv'}{r'},$$

$$r'^2 = (x - x')^2 + (y - y')^2 + (z - z')^2,$$

and the integral is taken over all space. In article (1) we studied the behavior of ψ_1 as $k \to \infty$, using the properties of the integral over a paraboloid.

Let us now write the second correction ψ_2 to the wave function:

$$\psi_2(P) = \frac{1}{4\pi}\int e^{ikx'} q(P')R(P, P')\,dv', \tag{2}$$

where

$$R(P, P') = \frac{1}{4\pi}\int e^{ik(r'+r'')} q(P'')\frac{dv''}{r'r''}. \tag{3}$$

Here the points P, P', P'' have, respectively, the coordinates (x, y, z), (x', y', z'), (x'', y'', z''); $r' = PP'$, $r'' = P'P''$. The purpose of this article is to study the behavior of $R(P, P')$ as $k \to \infty$.

Relation (3) can be represented in the form

$$R(P,P')=\int_c^\infty e^{2ik\rho}I(q,P,P',\rho)\,d\rho,\qquad c=\frac{PP'}{2}. \tag{4}$$

The integral $I(q,P,P',\rho)$ is determined by either of two formulas:

$$I(q,P,P',\rho)=\frac{1}{4\pi\rho}\int_{-\rho}^{\rho}\int_0^{2\pi} q\left(\frac{x+x'}{2}+a_{11}s+a_{12}t+a_{13}u,\ \frac{y+y'}{2}+a_{21}s+\right.$$

$$\left.+a_{22}t+a_{23}u,\ \frac{z+z'}{2}+a_{11}s+a_{32}t+a_{13}u\right)d\psi\,ds, \tag{5}$$

$$I(q,P,P',\rho)=\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} q\left(\frac{x+x'}{2}+a_{31}s+a_{12}t+a_{33}u,\ \frac{y+y'}{2}+\right.$$

$$\left.+a_{21}s+a_{22}t+a_{23}u,\ \frac{z+z'}{2}+a_{31}s+a_{32}t+a_{33}u\right)D(\rho,\theta,\varphi)\,d\theta\,d\psi, \tag{6}$$

where the matrix $A=\|a_{ij}\|$ is orthogonal and the vector $\bar{h}[a_{11}a_{21}a_{31}]$ is parallel to the vector PP'. In addition, in formula (5)

$$t=\frac{\sqrt{(\rho^2-c^2)(\rho^2-s^2)}}{\rho}\cos\psi,\qquad u=\frac{\sqrt{(\rho^2-c^2)(\rho^2-s^2)}}{\rho}\sin\psi,$$

and in formula (6)

$$s=r\cos\varphi\sin\theta,\qquad t=r\sin\varphi\sin\theta,\qquad u=r\cos\theta,\qquad r=\rho\sqrt{\frac{\rho^2-c^2}{\rho^2-c^2\cos^2\varphi\sin^2\theta}},$$

$$D(\rho,\theta,\varphi)=\frac{\rho^2\sqrt{\rho^2-c^2}\,\sin\theta}{(\rho^2-c^2\cos^2\varphi\sin^2\theta)^{1/2}}.$$

Let, in particular, $q(P'')=q(r'r'')$. Then formula (5) gives

$$I(q,\ P,\ P',\ \rho)=\frac{1}{2c}\int_{\rho^2-c^2}^{\rho^2} q(t)\frac{1}{\sqrt{\rho^2-t}}\,dt, \tag{7}$$

If $q(P'')=q(r',r'')$, then

$$I(q,\ P,\ P',\ \rho) = \frac{1}{2\rho}\int_{-\rho}^{\rho} q\left(\rho - \frac{c}{\rho}t,\ \rho + \frac{c}{\rho}t\right)\,dt. \tag{8}$$

The expression $I(q, P, P', \rho)$ is the integral of the function q over an ellipsoid of revolution with foci at the points P and P'.

1. Basic properties of the integral over an ellipsoid

Introduce the notation $I(q, \rho, c) = I(q, P, P', \rho)$, $\rho > c$, if $y' = y = 0$, $z' = z = 0$, $x' + x = 0$ $(c = |x|)$. The properties of the integral over an ellipsoid formulated below are in many respects similar to the properties of the integral over a paraboloid (1).

1. If the functions $q(s, t, u)$ and $f = s\,\partial q/\partial s + t\,\partial q/\partial t + u\,\partial q/\partial u$ are bounded, then

$$\frac{d}{d\rho}I(q,\rho,c) = \frac{1}{\rho(\rho^2-c^2)}I(fr'r'',\rho,c) + \frac{3\rho^2-c^2}{\rho(\rho^2-c^2)}I(q,\rho,c) - \frac{3}{\rho(\rho^2-c^2)}I(qr^2,\rho,c), \tag{9}$$

where

$$r^2 = s^2+t^2+u^2, \qquad r' = \rho - \frac{c}{\rho}s, \qquad r'' = \rho + \frac{c}{\rho}s.$$

2. Let $q(s,t,u) = a(r', r'')t^n u^m$, where $a(r', r'')$ is a bounded function and m and n are nonnegative integers. Then the equality

$$I(q,\rho,c) = 0, \tag{10}$$

holds if at least one of the numbers m or n is odd.

If, however, m and n are even numbers, then

$$I(q,\rho,c) = \frac{(n-1)!!(m-1)!!}{2^{(m+n)/2}\left(\frac{m+n}{2}\right)!}\,\frac{1}{2\rho}\int_{-\rho}^{\rho} a\left(\rho - \frac{c}{\rho}s,\ \rho + \frac{c}{\rho}s\right)\times$$

$$\times\left[\frac{\sqrt{(\rho^2-c^2)(\rho^2-s^2)}}{\rho}\right]^{m+n} ds. \tag{11}$$

3. Suppose the relation

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$$q(s,t,u) = \sum_{\substack{k,l \geq 0 \\ k+l \leq n}} a_{k,l}(s) t^k u^l \frac{1}{k!\, l!} + q_n(s,t,u)$$

holds, where the functions

$$a_{k,l}(s) = \frac{\partial^{k+l}}{\partial t^k \partial u^l} q \bigg|_{\substack{t=0 \\ u=0}}$$

are bounded and $\lim_{n\to\infty} I(q_n, \rho, c) = 0$. Then the equality is true:

$$I(q,\rho,c) = \sum_{k,l=0}^{\infty} \frac{1}{2^{2(k+l)}(k+l)!\, k!\, l!} \frac{1}{2\rho} \int_{-\rho}^{\rho} a_{2k,2l}(s) \left[\frac{(\rho^2 - c^2)(\rho^2 - s^2)}{\rho^2} \right]^{k+l} ds.$$

4. Let the function $q(s,t,u)$ be bounded and have the form $q(s,t,u) = a(r', r'') e^{\beta t + \gamma u}$. Then

$$I(q,\rho,c) = \frac{1}{2\rho} \int_{-\rho}^{\rho} a\left(\rho - \frac{c}{\rho} s,\ \rho + \frac{c}{\rho} s\right) J_0 \left[\frac{\sqrt{(\beta^2+\gamma^2)(\rho^2 - c^2)(\rho^2 - s^2)}}{\rho} \right] ds, \tag{12}$$

where $J_0(z)$ is the Bessel function.

5. If $q(s,t,u)$ is a continuous function, then

$$\lim_{\rho\to c} I(q,\rho,c) = \frac{1}{2c} \int_{-c}^{c} q(s,0,0)\, ds.$$

6. Let the function $q(s,t,u)$ be bounded and let the relation

$$|q(s,t,u) - \varphi_1(s)| \leq \varphi_2(s)(t^2 + u^2)^{\alpha}, \quad |s| \leq c, \quad 0 < \alpha \leq \frac{1}{2},$$

hold, where the functions $\varphi_1(s)$ and $\varphi_2(s)$ are also bounded. Then

$$I(q,\rho,c) = \frac{1}{2c} \int_{-c}^{c} q(s,0,0)\, ds + O\left[\left(\frac{\rho - c}{\rho} \right)^{\alpha} \right] \quad \text{as } \rho \to c. \tag{13}$$

By imposing additional smoothness requirements on $q(s,t,u)$, one can find the subsequent terms of the expansion of $I(q,\rho,c)$ in powers of $\rho - c$ as $\rho \to c$.

7. Let the function $q(s,t,u)$ be continuous and let the equality

$$q(s,t,u) = \sum_{\substack{k,l\geq 0\\ k+l\leq 2}} a_{k,l}(s)\, t^k u^l\, \frac{1}{k!\, l!} + q_2(s,t,u),$$

hold, where the functions

$$a_{k,l}(s) = \left.\frac{\partial^{k+l}}{\partial t^k \partial u^l} q\right|_{\substack{t=0\\ u=0}}$$

are bounded and $|q_2(s,t,u)| \leq C(t^2+u^2)^\alpha$, $\alpha > 1$. Then

$$I(q,\rho,c) = \frac{1}{2c}\int_{-c}^{c} q(s,0,0)\, ds + \frac{\rho - c}{c}\, \frac{q(c,0,0)+q(-c,0,0)}{2} -$$

$$-\frac{\rho-c}{2c^2}\int_{-c}^{c} q(s,0,0)\, ds + \frac{\rho-c}{4c^2}\int_{-c}^{c}\left(\frac{\partial^2 q}{\partial t^2} + \frac{\partial^2 q}{\partial u^2}\right)_{\substack{t=0\\ u=0}} (c^2 - s^2)\, ds + o(\rho - c) \quad \text{as } \rho \to c.$$

8. Let $|q(s,t,u)| \leq \varphi(r)$, where the function $\varphi(r)$ decreases monotonically. Then

$$|I(q,\rho,c)| \leq \varphi\left(\sqrt{\rho^2 - c^2}\right).$$

The last inequality characterizes the behavior of $I(q,\rho,c)$ as $\rho \to \infty$.

2. Asymptotics of $R(P,P')$ as $k \to \infty$.

Theorem 1. Let the following conditions be satisfied:

1. The function $q(x,y,z)$ has bounded first-order derivatives.
2. There exists a monotonically decreasing function $\varphi(r)$ such that

$$\left| q\left(\frac{x+x'}{2} + s,\ \frac{y+y'}{2} + t,\ \frac{z-z'}{2} + u\right)\right| \leq \varphi(r), \quad \varphi(r) \in L(-\infty, 0),$$

$$r^2 = s^2 + t^2 + u^2.$$

Then the equality

$$R(P,P') = -\frac{e^{2ikc}}{4ikc}\int_l q(P'')\, dl - \frac{1}{2ik}\int_c^\infty e^{2ik\rho}\, \frac{d}{d\rho} I(q,P,P',\rho)\, d\rho,$$

$$c = \frac{PP'}{2}, \tag{14}$$

holds, where the integration contour l coincides with the segment PP'.

The expression $\frac{d}{d\rho} I(q, P, P', \rho)$ in the right-hand side of (14) can be found by means of formula (9).

Suppose, additionally, that the following conditions are satisfied:

3. There exists a monotonically decreasing function $\psi(r)$ such that, for

$$q_1(s,t,u) = q\left(\frac{x+x'}{2} + s, \frac{y+y'}{2} + t, \frac{z+z'}{2} + u\right),$$

 the inequality

$$|\partial q_1/\partial s| + |\partial q_1/\partial t| + |\partial q_1/\partial u| \le \psi(r), \quad \psi(r) \in L(0,\infty).$$

4. The function $q_1(s,t,u)$ satisfies, for some K and $\alpha > 0$, the Hölder condition. Then the integral

$$\int_c^\infty e^{2ik\rho} \frac{d}{d\rho} I(q, P, P', \rho)\, d\rho \tag{15}$$

converges absolutely and, consequently, tends to zero as $k \to \infty$.

Thus, if conditions (1)–(4) are satisfied, then

$$R(P, P') = \frac{e^{2ikc}}{4ikc}\left[\int_l q(P'')\, dl + o(1)\right], \qquad k \to \infty, \tag{16}$$

where l coincides with the segment PP'.

Let us note that condition (3) ensures the absolute convergence of the integral (15) as $\rho \to \infty$, while condition 4 ensures it as $\rho \to c$. Condition 4 admits a substantial weakening.

Let us also note that, imposing additional requirements on $q(x, y, z)$ and using the properties of $I(q, P, P', \rho)$ (item 1), one can find the subsequent terms of the expansion of $R(P, P')$ in powers of $1/k$ as $k \to \infty$.

Consider the case, frequently encountered in applications, when $q(x, y, z)$ has a discontinuity at the points of some bounded convex closed surface S. The surface S divides all space into two nonintersecting parts R_1 and R_2, where R_1 denotes the convex part of space. We shall say that the points P and P' form a focal pair of the surface S if the common points P'' of the surface S and of some ellipsoid $P''P + P''P' = 2\rho$ form a set of positive planar measure. Denote by $\chi(x, y, z)$ the characteristic function of R_1.

Theorem 2. Let $\Phi(x, y, z) = 0$ be the equation of the surface S, and let the function $\Phi(x, y, z)$ have continuous first partial derivatives. Suppose, moreover, that $q(P'') = q_1(P'')\chi(P'')$, where $q_1(P'')$ has continuous first partial derivatives satisfying, for some α, the Hölder condition. If the points P and P' $(P, P' \in R_1)$ do not form a focal pair of the surface S, then equality (16) holds.

In some cases the smoothness restrictions on $q_1(P'')$ may be weakened. If the function $q_1(P'')$ has the form $q_1(P'') = q_1(r', r'')$, then for Theorem 2 to hold it is sufficient to require continuity of the partial derivatives

$$\frac{\partial}{\partial r'} q_1(r', r'') \quad \text{and} \quad \frac{\partial}{\partial r''} q(r', r'').$$

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Received
9 IX 1965

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