

THE INTEGRAL OVER AN ELLIPSOID AND THE SECOND BORN APPROXIMATION

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Abstract

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MATHEMATICS

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THE INTEGRAL OVER AN ELLIPSOID AND THE SECOND BORN APPROXIMATION

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Let us write the equation

$$\Delta\psi + k^2\psi - q\psi = 0, \quad (1)$$

where $\psi - e^{ikx} \rightarrow 0$ as $r \rightarrow \infty$. 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 $k \rightarrow \infty$, using the properties of the integral over a paraboloid.

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

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

where

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

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 $k \rightarrow \infty$.

Relation (3) can be represented in the form

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

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

$$I(q, P, P', \rho) = \frac{1}{4\pi\rho} \int_{-\rho}^\rho \int_0^{2\pi} q \left(\frac{x+x'}{2} + a_{11}s + a_{12}t + a_{13}u, \frac{y+y'}{2} + a_{21}s + a_{22}t + a_{23}u, \frac{z+z'}{2} + a_{31}s + a_{32}t + a_{33}u \right) d\psi ds, \quad (5)$$

$$I(q, P, P', \rho) = \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi q \left(\frac{x+x'}{2} + a_{31}s + a_{12}t + a_{33}u, \frac{y+y'}{2} + a_{21}s + a_{22}t + a_{23}u, \frac{z+z'}{2} + a_{31}s + a_{32}t + a_{33}u \right) D(\rho, \theta, \varphi) d\theta d\psi, \quad (6)$$

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)

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

and in formula (6)

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

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

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

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

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

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

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

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

where

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

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

$$I(q, \rho, c) = 0, \quad (10)$$

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

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

$$I(q, \rho, c) = \frac{(n-1)!!(m-1)!!}{2^{(m+n)/2} \left(\frac{m+n}{2}\right)!} \frac{1}{2\rho} \int_{-\rho}^{\rho} a \left(\rho - \frac{c}{\rho}s, \rho + \frac{c}{\rho}s \right) \times \\ \times \left[\frac{\sqrt{(\rho^2 - c^2)(\rho^2 - s^2)}}{\rho} \right]^{m+n} ds. \quad (11)$$

3. Suppose the relation

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

holds, where the functions

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

are bounded and $\lim_{n \rightarrow \infty} I(q_n, \rho, c) = 0$. 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

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

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

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

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

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

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

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 $\rho \rightarrow c$.

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

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

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

$$I(q, \rho, c) = \frac{1}{2c} \int_{-c}^c q(s, 0, 0) ds + \frac{\rho - c}{c} \frac{q(c, 0, 0) + q(-c, 0, 0)}{2} - \\ - \frac{\rho - c}{2c^2} \int_{-c}^c q(s, 0, 0) ds + \frac{\rho - c}{4c^2} \int_{-c}^c \left(\frac{\partial^2 q}{\partial t^2} + \frac{\partial^2 q}{\partial u^2} \right)_{\substack{t=0 \\ u=0}} (c^2 - s^2) ds + o(\rho - c) \quad \text{as } \rho \rightarrow c.$$

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

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

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

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

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

$$R(P, P') = -\frac{e^{2ikc}}{4ikc} \int_l q(P'') dl - \frac{1}{2ik} \int_c^\infty e^{2ik\rho} \frac{d}{d\rho} I(q, P, P', \rho) d\rho, \\ c = \frac{PP'}{2}, \quad (14)$$

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

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

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

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

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

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

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

where l coincides with the segment PP' .

Let us note that condition (3) ensures the absolute convergence of the integral (15) as $\rho \rightarrow \infty$, while condition 4 ensures it as $\rho \rightarrow c$. 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 $k \rightarrow \infty$.

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

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

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

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