

THE INTEGRAL OVER A PARABOLOID AND THE FIRST BORN APPROXIMATION

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Abstract

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MATHEMATICS

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THE INTEGRAL OVER A PARABOLOID AND THE FIRST BORN APPROXIMATION

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Consider the equation

$$\Delta\psi + k^2\psi = qe^{ikx}. \quad (1)$$

As is known, a particular solution of this equation has the form

$$\psi_1(x, y, z) = -\frac{1}{4\pi} \int e^{ik(x'-r')} q(x', y', z') \frac{dv'}{r'}, \quad (2)$$

where the integral is taken over all space, $dv' = dx' dy' dz'$, $r'^2 = (x - x')^2 + (y - y')^2 + (z - z')^2$. In quantum mechanics, ψ_1 gives the correction of the first Born approximation to the wave function (1). In the present paper we study in detail the dependence of ψ_1 on q and k as $k \rightarrow \infty$.

Equality (2) can be written in the form

$$\psi_1(x, y, z) = -\frac{1}{4\pi} e^{ikx} \int e^{ik(s+r)} q(x+s, y+t, z+u) \frac{dv}{r}, \quad (3)$$

where $r^2 = s^2 + t^2 + u^2$, $dv = ds dt du$.

In addition to the Cartesian coordinates of the point $Q(s, t, u)$, introduce two more new coordinate systems $Q(\rho, \varphi, \theta)$ and $Q(\rho, s, \psi)$. Here φ and θ are defined as in the spherical system, $\rho = s+r$, $\text{tg } \psi = u/t$. Relation (3) can be represented as follows:

$$\psi_1(x, y, z) = -\frac{1}{2} e^{ikx} \int_0^\infty e^{ik\rho} I(q, P, \rho) d\rho. \quad (4)$$

Here, to define $I(q, P, \rho)$ at the point $P(x, y, z)$, we use either of two formulas:

$$I(q, P, \rho) = \frac{1}{2\pi} \int_0^{2\pi} \int_0^\pi \frac{\rho \sin \theta}{(1 + \cos \varphi \sin \theta)^2} q \left(x + \frac{\rho \sin \theta \cos \varphi}{1 + \cos \varphi \sin \theta}, y + \frac{\rho \sin \theta \sin \varphi}{1 + \cos \varphi \sin \theta}, z + \frac{\rho \cos \theta}{1 + \cos \varphi \sin \theta} \right) d\theta d\varphi, \quad (5)$$

$$I(q, P, \rho) = \frac{1}{2\pi} \int_{-\infty}^{\rho/2} \int_0^{2\pi} q \left(x + s, y + \sqrt{\rho^2 - 2\rho s} \cos \psi, z + \sqrt{\rho^2 - 2\rho s} \sin \psi \right) d\psi ds. \quad (6)$$

The expression $I(q, P, \rho)$ is the integral of the function q over the paraboloid of revolution $s + r = \rho$ with focus at the point P .

1. Basic properties of the integral over a paraboloid.

Introduce the notation $I(q, \rho) = I(q, P, \rho)$ if $x = y = z = 0$.

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

$$\frac{d}{d\rho} I(q, \rho) = \frac{1}{\rho} I(f, \rho).$$

The stated property is obtained as a result of differentiating both sides of (5).

2. Let $q(s, t, u) = a(s, r) t^m u^n$, where $a(s, \rho - s) s^k \in L(-\infty, \rho/2)$ ($0 \leq k \leq (m+n)/2$), and m and n are nonnegative integers. Then

the equality holds

$$I(q, \rho) = 0, \quad (7)$$

if at least one of the numbers m or n is odd. If, however, m and n are even numbers, then

$$I(q, \rho) = \frac{(n-1)!(m-1)!!}{2^{(m+n)/2}((m+n)/2)!} \int_{-\infty}^{\rho/2} a(s, \rho - s) (\rho^2 - 2\rho s)^{(m+n)/2} ds. \quad (8)$$

Putting $n = 0$, $m = 0$ in (8), we obtain

$$I(q, \rho) = \int_{-\infty}^{\rho/2} a(s, \rho - s) ds, \quad \text{where } q(s, t, u) = q(s, r). \quad (9)$$

3. Suppose that 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

$$a_{kl}(s) = \left. \frac{\partial^{k+l}}{\partial t^k \partial u^l} q \right|_{t=0, u=0}, \quad a_{k,l}(s) s^m \in L(-\infty, \rho/2), \quad 0 \leq m \leq (k+l)/2,$$

and

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

Then the equality

$$I(q, \rho) = \sum_{k,l=0}^{\infty} \frac{1}{2^{2(k+l)} (k+l)! k! l!} \int_{-\infty}^{\rho/2} a_{2k,2l}(s) (\rho^2 - 2\rho s)^{k+l} ds \quad (10)$$

is valid.

4. If the function $q(s, t, u)$ is continuous and satisfies the inequality

$$|q(s, \sqrt{\rho^2 - 2\rho s} \cos \psi, \sqrt{\rho^2 - 2\rho s} \sin \psi)| \leq \varphi(s), \quad s \leq 0, \quad \varphi(s) \in L(-\infty, 0),$$

then

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

5. Suppose that the function $q(s, t, u)$ is bounded and that the relation

$$|q(s, t, u) - \varphi_1(s)| \leq \varphi_2(s) (t^2 + u^2)^\alpha, \quad s \leq 0,$$

holds, where

$$\varphi_1(s) \in L(-\infty, 0), \quad \varphi_2(s) s^\beta \in L(-\infty, 0), \quad 0 \leq \beta \leq \alpha, \quad \alpha \leq \frac{1}{2}.$$

Then

$$I(q, \rho) = \int_{-\infty}^0 \varphi_1(s) ds + O(\rho^\alpha) \quad \text{as } \rho \rightarrow 0.$$

6. Suppose that $q(s, t, u)$ is continuous at the point $O(0, 0, 0)$ and the equality

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

holds, where

$$a_{k,l}(s) = \frac{\partial^{k+l}}{\partial t^k \partial u^l} q \Big|_{t=0, u=0}, \quad a_{kl}(s) s^m \in L(-\infty, \rho/2), \quad 0 \leq m \leq$$

$$\leq (k+l)/2, \quad |q_2(s, t, u)| \leq \varphi(s)(t^2 + u^2)^\alpha, \quad s^m \varphi(s) \in L(-\infty, \rho/2),$$

$$0 \leq m \leq \alpha, \quad \alpha > 1.$$

Then

$$I(q, \rho) = \int_{-\infty}^0 q(s, 0, 0) ds + \frac{\rho}{2} \left[q(0, 0, 0) - \int_{-\infty}^0 \left(\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial u^2} \right) q \Big|_{t=0, u=0} s ds + o(1) \right]. \quad (11)$$

7. From the inequality $|q(s, t, u)| \leq \varphi(r)$ it follows that

$$|I(q, \rho)| \leq \int_{\rho/2}^{\infty} \varphi(r) dr. \quad (12)$$

§ 2. Integral over a paraboloid of a function equal to zero outside a convex body

According to Property 1, for smooth functions $q(s, t, u)$ there exists the derivative $\frac{d}{d\rho} I(q, \rho)$ ($\rho > 0$). We shall now clarify the conditions for existence and the method of computing $\frac{d}{d\rho} I(q, \rho)$ in the case when $q(s, t, u)$ has a discontinuity on some convex surface.

Let $\Phi(s, t, u) = 0$ be the equation of a convex surface S , dividing all space into two nonintersecting parts R_1 and R_2 (R_1 is the convex part). In what follows we shall assume that $\Phi(s, t, u)$ has continuous first partial derivatives.

Denote by $\chi(s, t, u)$ the characteristic function of the closure of the set R_1 , and by γ_ρ the line of intersection of the surface S with the paraboloid $\rho = s + r$. Define on γ_ρ the function

$$\Delta(s, t, u) = \frac{\partial \Phi}{\partial s} \left(\sqrt{s^2 + t^2 + u^2} - s \right) - t \frac{\partial \Phi}{\partial t} - u \frac{\partial \Phi}{\partial u}. \quad (13)$$

If at some point $M(s, t, u)$ of the line γ_ρ the equality $\Delta(s, t, u) = 0$ holds, this means that the tangent to the meridian of the paraboloid at the point M belongs to the plane tangent to the surface S at the point M .

Theorem 1. Let on γ_ρ the inequality

$$|\Delta(s, t, u)| \geq \delta > 0 \quad (14)$$

hold.

If the functions $q\chi$, $f\chi = (s \partial q / \partial s + t \partial q / \partial t + u \partial q / \partial u + q)\chi$ are integrable over the paraboloid and q is bounded on γ_ρ , then the relation

$$\begin{aligned} & \frac{d}{d\rho} I(q\chi, \rho) = \\ & = \frac{1}{\rho} I(f\chi, \rho) + \frac{1}{2\pi\rho} \int_{\gamma_\rho} \left(s \frac{\partial \Phi}{\partial s} + t \frac{\partial \Phi}{\partial t} + u \frac{\partial \Phi}{\partial u} \right) q(s, t, u) \varepsilon(s, t, u) \frac{\rho - 2s}{\Delta(s, t, u)} d\psi, \end{aligned} \quad (15)$$

where $\varepsilon(P) = -1$, if $P(s, t, u)$ is a point of entry into the body R_1 of the meridian of the paraboloid $\rho = str$, and $\varepsilon(P) = 1$, if P is a point of exit.

§ 3. Asymptotics of ψ_1 as $k \rightarrow \infty$

Theorem 2. Let the inequalities

$$|q(x + s, y + t, z + u)| \leq \varphi_1(r, P), \quad |f(x, y, z; s, t, u)| \leq \varphi_2(r, P)$$

hold,

$$(r^2 = s^2 + t^2 + u^2),$$

where

$$\begin{aligned} f(x, y, z; s, t, u) &= q(x + s, y + t, z + u) + \\ &+ (s \partial / \partial s + t \partial / \partial t + u \partial / \partial u) q(x + s, y + t, z + u), \end{aligned}$$

$$\int_0^\infty r^n \varphi_k(r, P) dr < \infty \quad (k = 1, n = 0, 1; k = 2, n = 0).$$

Then the formula holds

$$\psi_1(x, y, z) = \frac{1}{2ik} e^{ikx} \left[\int_{-\infty}^x q(s, y, z) ds + \int_0^\infty e^{ik\rho} \frac{1}{\rho} I(f, P, \rho) d\rho \right].$$

Assume in addition that the following conditions are satisfied.

1. The integral exists

$$\int_0^\infty \varphi_2(r, P) |\ln r| dr < \infty.$$

2. For some a ($a > 0$) the inequality

$$|f(x, y, z; s, t, u) - f(x, y, z, s, 0, 0)| \leq a(s)(t^2 + u^2)^\alpha, \quad s \leq 0,$$

holds, where $a(s)s^\beta \in L(-\infty, 0)$, $0 \leq \beta \leq \alpha$.

Then the integral

$$\int_0^\infty e^{ik\rho} \frac{1}{\rho} I(f, P, \rho) d\rho$$

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

Thus (see (1)),

$$\psi_1(x, y, z) = \frac{1}{2ik} e^{ikx} \left[\int_{-\infty}^x q(s, y, z) ds + o(1) \right], \quad k \rightarrow \infty.$$

Consider a bounded closed convex surface S , whose equation is $\Phi(x, y, z) = 0$, where $\Phi(x, y, z)$ has continuous partial derivatives of first order. We shall say that $P(x, y, z)$ is a point of focus type of the surface S if the common points $Q(x', y', z')$ of the surface S and of some paraboloid

$$(y' - y)^2 + (z' - z)^2 = \rho^2 - 2\rho(x' - x)$$

form a set of positive planar measure. Let the function $q_1(x, y, z)$ have continuous partial derivatives of first order and, for some K and α , satisfy the inequality

$$|s| \left| \frac{\partial}{\partial s} q_1(x + s, y + t, z + u) - \frac{\partial}{\partial s} q_1(x + s, y, z) \right| \leq K(t^2 + u^2)^\alpha, \quad s \leq 0, \alpha > 0.$$

Finally, put $q(x, y, z) = q_1(x, y, z)\chi(x, y, z)$, where $\chi(x, y, z)$ is the characteristic function of R_1 (see item 2).

If $P(x, y, z) \in R_1$ and P is not a point of focus type of the surface S , then as $k \rightarrow \infty$

$$\psi_1(x, y, z) = \frac{1}{2ik} e^{ikx} \left[\int_{x_0}^x q(s, y, z) ds + o(1) \right],$$

where $\Phi(x_0, y, z) = 0$ and $x_0 < x$.

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REFERENCES

1. L. D. Landau, E. M. Lifshitz, *Quantum Mechanics*, Moscow, 1963.

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

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