Generalized second-order partial derivatives of $1/r$

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Abstract
The generalized second-order partial derivatives of $1/r$, where $r$ is the radial distance in three dimensions (3D), are obtained using a result of the potential theory of classical analysis. Some non-spherical-regularization alternatives to the standard spherical-regularization expression for the derivatives are derived. The utility of a spheroidal-regularization expression is illustrated on an example from classical electrodynamics.

1. Introduction

The expression for the Laplacian of $1/r$,

$$\nabla^2 \frac{1}{r} = -4\pi \delta(r),$$  

(1)

where $r = |\mathbf{r}| = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ is the magnitude of a vector $\mathbf{r} = (x_1, x_2, x_3)$, the Laplacian $\nabla^2$ is the differential operator $\partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2$ and $\delta(r) = \delta(x_1)\delta(x_2)\delta(x_3)$ is the three-dimensional (3D) delta function, is well known and its correct use involves only the elementary rules of the delta-function formalism. The Laplacian (1) is useful in innumerable calculations of electrodynamics, but sometimes the second-order partial derivatives $(\partial^2/\partial x_i \partial x_j)(1/r)$ themselves are needed. Examples are the calculation of the electromagnetic fields of point dipoles [1] and solving the Poisson equation for the difference between the Coulomb- and Lorenz-gauge vector potentials of a uniformly moving point charge [2].

While the expression for $(\partial^2/\partial x_i \partial x_j)(1/r)$ has been known for some time, its correct use is rather more intricate than that of $\nabla^2(1/r)$. This expression is usually written as [3]

$$\frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r} = \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} - \frac{4\pi}{3} \delta(r) \delta_{ij},$$  

(2)

which hides an important fact that an integration of the product of the first term on the right-hand side and a ‘well-behaved’ test function over a 3D domain that includes the origin...
$r = 0$ still has to be regularized because of the term’s $1/r^3$ behaviour at the origin\. The regularization assumed in (2) is of a specific, ‘spherical’ kind, which can be effected in many equivalent forms, e.g.

$$\frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \to w\lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{(r^2 + \epsilon^2)^{5/2}}$$

(3)

$$\to w\lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \Theta(r - \epsilon).$$

(4)

Here, the symbol w\lim indicates the weak limit\(^2\) and $\Theta(\cdot)$ is the Heaviside step function. The form (4) is implemented automatically when spherical coordinates are used in integration and the angular integration is done first.

Relation (2) was derived as a delta-function identity by Frahm [3]. In the present paper, we obtain it easily as a generalized (distributional) derivative using a result of the potential theory of classical analysis. We also derive some ‘non-spherical’ alternatives to (2); while integration in spherical coordinates provides a straightforward implementation of the spherical regularization implied in (2), the use of a non-spherical regularization may be more advantageous computationally in some applications. An example from classical electrodynamics where a spheroidal regularization is useful is given in the appendix. Apart from the utility, awareness of non-spherical alternatives is important for the correct use of the standard, ‘spherical’ expression.

Our treatment assumes no knowledge of the theory of generalized functions and generalized (distributional) derivatives beyond the elementary delta-function formalism, but it should help elucidate the operational meaning of some essentially non-classical mathematical objects\(^3\). Presenting the second-order partial derivatives of $1/r$ from the very beginning as generalized (distributional) derivatives should help avoid the pitfalls that would await anyone attempting to use expression (2), or its very recent ‘generalization’ [6] (remarked on in the last section), in an integration in non-spherical coordinates. This topic and its treatment are suitable for graduate and advanced undergraduate courses of electrodynamics.

A generalized-function treatment of the singularities that may arise at the origin $r = 0$ of a spherical (polar) coordinate system has recently been presented in this journal by Gsponer [7]. In contrast to Gsponer, our approach does not rely on any specific choice of coordinates.

2. Derivation using derivatives of the potential of an extended density

Let

$$\phi(r) = \int d^3r', \frac{\rho(r')}{R}, \quad R = |r - r'|,$$

(5)

be the ‘potential’ created by a density $\rho(r)$ that is assumed to be a ‘well-behaved’ localized function of $r$. While the second-order partial derivatives $\partial^2 \phi(r)/\partial x_i \partial x_j$ perfectly exist at any point $r$ if the density $\rho(r)$ is sufficiently ‘smooth’\(^4\), they cannot be calculated by

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\(^1\) An expression for the (generalized) second-order derivative of $1/r$ that takes this circumstance into account explicitly seems to have been given first in [4], p 28.

\(^2\) $w\lim_{a \to a_0} g_a(r) = g(r)$ iff $\lim_{a \to a_0} \int d^3r f(r) g_a(r) = \int d^3r f(r) g(r)$, where $g(r)$ is in general a generalized function (distribution) and $f(r)$ is any well-behaved test function.

\(^3\) For a general-function theoretic underpinning of our approach, the interested reader is directed to the canonical regularization method of Gelfand and Shilov and the completeness theorem of generalized functions [5].

\(^4\) If the density $\rho_a(r)$ has a sharp surface, the second-order derivatives of the potential are discontinuous at that surface.
a straightforward differentiating inside the integral that defines the potential because the resulting integrand is not integrable at the point \( r' = r \). A correct way of performing here the differentation under the integral sign is given by the following formula,

\[
\frac{\partial^2 \phi(r)}{\partial x_i \partial x_j} = \lim_{\epsilon \to 0} \int_{R>\epsilon} d^3r' \rho(r') \frac{\partial^2}{\partial x_i \partial x_j} \left( \frac{1}{R} - \frac{4\pi}{3} \rho(r) \delta_{ij} \right) = \lim_{\epsilon \to 0} \int_{R>\epsilon} d^3r' \rho(r') \frac{3(x_i - x_i')(x_j - x_j') - R^2 \delta_{ij}}{R^5} \Theta(R - \epsilon) - \frac{4\pi}{3} \rho(r) \delta_{ij}.
\]

Here, the integration domain excludes a ball of radius \( \epsilon \) and centre at \( r' = r \); the second line is a more explicit transcription of the first line, with the integration domain \( R = |r' - r| > \epsilon \) expressed by the Heaviside step-function factor \( \Theta(R - \epsilon) \) in the integrand. An instructive derivation of formula (6) is given in the well-known text of Tikhonov and Samarskii [8] (they consider the most involved case \( i = j \), but the generalization to any \( i, j = 1, 2, 3 \) is straightforward). This derivation uses the divergence theorem with a function that has only a 1/\( r \) singularity at the point \( R = 0 \) and thus, unlike the informal proof in [3], is fully legitimate in classical analysis.\(^5\)

Note that the regularization of the integral on the right-hand side of (6) is explicitly of the spherical kind. If the excluded integration domain was assumed to have a non-spherical shape, the ensuing regularization would in general yield a different value for the integral, resulting in an incorrect value for the derivative in question. The reason why different regularizations yield in general different values of the regularized integral is that, because of the factor \( \Theta(1/R) \), the integrand goes through large positive and negative variations near the point \( R = 0 \). The integral thus can be made convergent only conditionally [8].

Defining a generalized (distributional) derivative

\[
\frac{\partial^2}{\partial x_i \partial x_j} \equiv \lim_{\epsilon \to 0} \frac{3(x_i - x_i')(x_j - x_j') - R^2 \delta_{ij}}{R^5} \Theta(1/R) - \frac{4\pi}{3} \delta(r - r')(R - \epsilon) \delta_{ij}
\]

(7)

(denoted by a bar to distinguish it from a classical derivative [4, 10, 11]), formula (6) can be written simply as

\[
\frac{\partial^2 \phi(r)}{\partial x_i \partial x_j} = \int d^3r' \rho(r') \frac{\partial^2}{\partial x_i \partial x_j} \left( \frac{1}{R} \right).
\]

The generalized derivative (7) can thus be seen as the mathematical operation using which the second-order differentiation with respect to components of \( r \) of a function defined as the integral with respect to \( r' \) of an integrand involving the factor \( 1/R = 1/|r - r'| \) may be performed under the integral sign.

\[
\frac{\partial^2}{\partial x_i \partial x_j} \int d^3r' \rho(r') \frac{\partial^2}{\partial x_i \partial x_j} \left( \frac{1}{R} \right) = \int d^3r' \rho(r') \frac{\partial^2}{\partial x_i \partial x_j} \left( \frac{1}{R} \right),
\]

(9)

where the ‘density’ \( \rho(r) \) now plays the role of a well-behaved test function.

Expression (2) is a special case \( r' = 0 \) (so that \( R \equiv r - r' = r \)) of the generalized derivative (7),

\[
\frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r} = \lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \Theta(r - \epsilon) - \frac{4\pi}{3} \delta(r) \delta_{ij}.
\]

(10)

Adding expressions (10) with \( i = j = 1, 2, 3 \), the non-delta-function terms cancel out, and we obtain the full Laplacian (1) as

\[
\nabla^2 \frac{1}{r} = -4\pi \delta(r).
\]

(11)

\(^5\) As the informal proof in [3], informal derivations of the full Laplacian relation (1) typically use the divergence theorem with a function that has a 1/\( r^2 \) singularity at \( r = 0 \); for a more rigorous alternative, see [9].
where
\[ \tilde{\nabla}^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \]  
(12)
is now the generalized Laplacian operator.

The generalized derivative (10) is the weak limit \( a \to 0 \) of the corresponding classical derivative of the potential
\[ \phi_a(r) = \int d^3 r' \frac{\rho_a(r')}{R}, \quad R = |r - r'|, \]
(13)
that is due to a localized density \( \rho_a(r) \) the spatial extension of which depends on a parameter \( a \) so that
\[ \lim_{a \to 0} \int d^3 r \ f(r) \rho_a(r) = f(0), \]
(14)
where \( f(r) \) is any well-behaved test function; this condition is transcribed formally as
\[ \lim_{a \to 0} \rho_a(r) = \delta(r). \]
(15)
This can be shown by calculating the limit \( a \to 0 \) of the integral of the product of (6) with \( \phi(r) = \phi_a(r) \) and a well-behaved function \( f(r) \). It suffices to consider the case \( i = j = 1 \).

\[ \lim_{a \to 0} \int d^3 r \ f(r) \frac{\partial^2 \phi_a(r)}{\partial x_1^2} \]
\[ = \lim_{a \to 0} \int d^3 r \ f(r) \lim_{\epsilon \to 0} \int d^3 r' \rho_a(r') \frac{3(x_1 - x_1')^2 - R^2}{R^5} \Theta(R - \epsilon) - \frac{4\pi}{3} \lim_{a \to 0} \int d^3 r f(r) \rho_a(r) \]
\[ = \lim_{a \to 0} \int d^3 r' \rho_a(r') \int d^3 r \ f(r) \frac{3(x_1 - x_1')^2 - R^2}{R^5} \Theta(R - \epsilon) - \frac{4\pi}{3} \int d^3 r f(r) \delta(r) \]
\[ = \lim_{a \to 0} \int d^3 r' \rho_a(r') \int d^3 r \ f(r) \frac{3(x_1 - x_1')^2 - R^2}{R^5} \Theta(R - \epsilon) - \frac{4\pi}{3} f(0) \]
(16)
where
\[ F(r') = \lim_{\epsilon \to 0} \int d^3 r f(r) \frac{3(x_1 - x_1')^2 - R^2}{R^5} \Theta(R - \epsilon). \]
(17)
The function \( F(r') \) is well behaved, and thus
\[ \lim_{a \to 0} \int d^3 r' \rho_a(r') F(r') = \int d^3 r' \delta(r') F(r') \]
\[ = F(0) \]
\[ = \lim_{\epsilon \to 0} \int d^3 r f(r) \frac{3x_1^2 - r^2}{r^5} \Theta(r - \epsilon). \]
(18)
The algebraic manipulations in (16) are legitimate operations of moving limits without changing their sequential order and of interchanging the orders of integration.

Equations similar to (16) and (18) obviously hold for all the derivatives \( \partial^2 \phi_a(r) / \partial x_i \partial x_j \), \( i, j = 1, 2, 3 \). We thus have that, for any well-behaved test function \( f(r) \),
\[ \lim_{a \to 0} \int d^3 r f(r) \frac{\partial^2 \phi_a(r)}{\partial x_i \partial x_j} = \lim_{\epsilon \to 0} \int d^3 r f(r) \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \Theta(r - \epsilon) - \frac{4\pi}{3} f(0) \delta_{ij}, \]
(19)
which is expressed formally as
\[
\lim_{a \to 0} \frac{\partial^2 \phi_a(r)}{\partial x_i \partial x_j} = \lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \Theta(r - \epsilon) - \frac{4\pi}{3} \delta(r) \delta_{ij}
\]
\[
\Rightarrow \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r}.
\]

(20)

Since the limit \( a \to 0 \) of the potential \( \phi_a(r) \) itself is the potential \( 1/r \) of a point density \( \delta(r) \), this result is the formal underpinning of a natural interpretation of the generalized derivative \( \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r} \) as the second-order derivative of the potential of a point source. Note that while the regularization used in (20) is of the spherical kind, the extended density \( \rho_a(r) \) that generates the potential \( \phi_a(r) \) does not have to have any particular symmetry as a function of \( r \).

Using the powerful methods and results of the theory of generalized functions and derivatives, result (20) can be obtained almost immediately (see [12], appendix), but the approach adopted here required only a little more effort.

3. Non-spherical regularizations

3.1. Spheroidal regularization

Let us replace the spherical excluded integration domain used in (6), (7) and (10) by a spheroid of semiaxes \( \epsilon/\gamma \), \( \epsilon \) and \( \epsilon \) along the \( x_1 \), \( x_2 \) and \( x_3 \) axes, respectively, with the parameter \( \gamma \) given by
\[
\gamma = \frac{1}{\sqrt{1 - v^2}}, \quad 0 < |v| < 1.
\]

(21)

Regularization using such a domain may be suitable in applications involving effects of special relativity, according to which a spherical charge of radius \( \epsilon \) contracts to an oblate spheroid of this geometry when it is set in motion with a speed \( v \) along the \( x_1 \) axis. To find the modification of expression (10) for the generalized derivative \( \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r} \) that such spheroidal regularization entails, we only need to evaluate the difference,
\[
\lim_{\epsilon \to 0} \int_{\gamma^2 x_1^2 + x_2^2 + x_3^2 > \epsilon^2} d^3r f(r) \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} - \lim_{\epsilon \to 0} \int_{r > \epsilon} d^3r f(r) \frac{3x_i x_j - r^2 \delta_{ij}}{r^5}.
\]

(22)

where \( f(r) \) is again a well-behaved test function and the integration domain \( \mathcal{U}_\epsilon \) is the region delimited by the oblate surface \( \gamma^2 x_1^2 + x_2^2 + x_3^2 = \epsilon^2 \) and the spherical surface \( r^2 = x_1^2 + x_2^2 + x_3^2 = \epsilon^2 \).

(23)

As \( \epsilon \) tends to zero, the integration domain \( \mathcal{U}_\epsilon \) gets progressively smaller and closer to the origin \( r = 0 \) so that, for any \( r \in \mathcal{U}_\epsilon \), \( f(r) \to f(0) \) as \( \epsilon \to 0 \). The right-hand side of (22) can therefore be written as
\[
\lim_{\epsilon \to 0} \int_{\mathcal{U}_\epsilon} d^3r f(r) \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} = f(0) \lim_{\epsilon \to 0} \int_{\mathcal{U}_\epsilon} d^3r \frac{3x_i x_j - r^2 \delta_{ij}}{r^5}.
\]

(24)
Here, the integral on the right-hand side can be evaluated easily in spherical coordinates. With \( x_1 \) axis as the polar axis and \( \cos \theta = \xi \), we obtain for \( i = j = 1 \)

\[
\int_{\Omega} d^3r \frac{3x_i^2 - r^2}{r^5} = 2\pi \int_{-1}^{1} d\xi \frac{(3\xi^2 - 1)}{\sqrt{1 - \xi^2}} \int_{\epsilon/\sqrt{1 - \xi^2 - \xi^2}}^{1} \frac{dr}{r} = \pi \int_{-1}^{1} d\xi \frac{(3\xi^2 - 1)}{\cos^2 \phi} \ln[1 + (\gamma^2 - 1)\xi^2] = 2\pi \left( \frac{2}{\gamma^2} - 2 \arcsin \frac{v}{\gamma v^3} - \frac{2}{3} \right).
\]

(25)

The case \( i = j = 2 \) gives

\[
\int_{\Omega} d^3r \frac{3x_i^2 - r^2}{r^5} = \frac{1}{2} \int_{-1}^{1} d\xi \int_{0}^{2\pi} d\phi \left[ 3(1 - \xi^2) \cos^2 \phi - 1 \right] \ln[1 + (\gamma^2 - 1)\xi^2] = \frac{\pi}{2} \int_{-1}^{1} d\xi \left( 1 - 3\xi^2 \right) \ln[1 + (\gamma^2 - 1)\xi^2] = 2\pi \left( \frac{1}{\xi^2} - 1 \arcsin \frac{v}{\gamma v^3} \right).
\]

(26)

and the same result obviously will be obtained for \( i = j = 3 \). The mixed cases \( i \neq j \) will all yield zero on account of the integration with respect to the azimuthal angle \( \phi \). A notable feature of results (25) and (26) is that they are independent of \( \epsilon \). Collecting all these results, equation (24) can be written as

\[
\lim_{\epsilon \to 0} \int_{\Omega} d^3r \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} = 2\pi \left[ g_{ij}(v) - \frac{2}{3} \delta_{ij} \right] f(0).
\]

(27)

where

\[
g_{ij}(v) = \begin{cases} 2/\gamma^2 - (2/\gamma v^3) \arcsin v, & i = j = 1 \\ 1 - 1/\xi^2 + (1/\gamma v^3) \arcsin v, & i = j = 2, 3 \\ 0, & i \neq j. \end{cases}
\]

(28)

This result establishes a generalized-function identity,

\[
\lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \Theta(\gamma^2 x_i^2 + x_j^2 + x_3^2 - \epsilon^2) - \Theta(r - \epsilon) = 2\pi \left[ g_{ij}(v) - \frac{2}{3} \delta_{ij} \right] \delta(r),
\]

(29)

using which difference (22) with any well-behaved function \( f(r) \) can be evaluated immediately. According to this identity,

\[
\lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \Theta(r - \epsilon)
\]

\[
= \lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \Theta(\gamma^2 x_i^2 + x_j^2 + x_3^2 - \epsilon^2) - 2\pi \left[ g_{ij}(v) - \frac{2}{3} \delta_{ij} \right] \delta(r),
\]

(30)

and thus the generalized derivative (10) can be rewritten as

\[
\frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r} = \lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \Theta(\gamma^2 x_i^2 + x_j^2 + x_3^2 - \epsilon^2) - 2\pi g_{ij}(v) \delta(r),
\]

(31)

which is a spheroidal-regularization alternative to the standard, spherical-regularization expression (10) for the generalized derivative \((\partial^2/\partial x_i \partial x_j)(1/r)\); equation (31) reduces to (10) in the limit \( v \to 0 \) since \( \lim_{v \to 0} \gamma = 1 \) and \( \lim_{v \to 0} g_{ij}(v) = \frac{2}{\xi^2} \delta_{ij} \). An electrodynamic example in which expression (31) is useful is given in the appendix.
3.2. Cylindrical regularization

In some applications, cylindrical coordinates are natural to the problem and the requisite integrations are performed most easily in these coordinates. We can find the expression for \((\partial^2/\partial x_i \partial x_j)(1/r)\) that employs a cylindrical regularization by evaluating the difference

\[
\lim_{\epsilon \to 0} \int_{r>\epsilon} d^3r f(r) \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} = \lim_{\epsilon \to 0} \int_{T_{\epsilon,\kappa}} d^3r f(r) \frac{3x_i x_j - r^2 \delta_{ij}}{r^5}
\]

\[
= \lim_{\epsilon \to 0} \left( \int_{V_{\epsilon,\kappa}^{(1)}} d^3r f(r) \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} - \int_{V_{\epsilon,\kappa}^{(2)}} d^3r f(r) \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \right). \tag{32}
\]

Here, the integration domain \(T_{\epsilon,\kappa}\) is defined as

\[
T_{\epsilon,\kappa} = \{(x_1, x_2, x_3); |x_1| > \kappa \epsilon \cup x_2^2 + x_3^2 > \epsilon^2\}, \tag{33}
\]

which is the complement of a cylinder of base radius \(\epsilon\) and half-height \(\kappa \epsilon\), parallel to the \(x_1\) axis and centred at the origin \(r = 0\), and the integration domains \(V_{\epsilon,\kappa}^{(1)}\) and \(V_{\epsilon,\kappa}^{(2)}\) are defined as

\[
V_{\epsilon,\kappa}^{(1)} = \{(x_1, x_2, x_3); x_1^2 + x_2^2 + x_3^2 > \epsilon^2 \cap x_2^2 + x_3^2 < \epsilon^2 \cap |x_1| < \kappa \epsilon\}, \tag{34}
\]

\[
V_{\epsilon,\kappa}^{(2)} = \{(x_1, x_2, x_3); x_1^2 + x_2^2 + x_3^2 < \epsilon^2 \cap x_2^2 + x_3^2 < \epsilon^2 \cap |x_1| > \kappa \epsilon\}, \tag{35}
\]

which are regions delimited by the surface of the cylinder and the spherical surface \(r^2 = x_1^2 + x_2^2 + x_3^2 = \epsilon^2\). The region \(V_{\epsilon,\kappa}^{(2)}\) is nonempty only when \(\kappa < 1\), in which case the integral over \(V_{\epsilon,\kappa}^{(2)}\) has to be subtracted from that over the region \(V_{\epsilon,\kappa}^{(1)}\).

As \(\epsilon\) tends to zero, the regions \(V_{\epsilon,\kappa}^{(1,2)}\) progressively shrink and collapse onto the origin \(r = 0\) so that, for any \(r \in V_{\epsilon,\kappa}^{(1,2)}\), \(f(r) \to f(0)\) as \(\epsilon \to 0\), and thus

\[
\lim_{\epsilon \to 0} \left[ \int_{V_{\epsilon,\kappa}^{(1)}} d^3r - \int_{V_{\epsilon,\kappa}^{(2)}} d^3r \right] f(r) \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} = f(0) \lim_{\epsilon \to 0} \left[ \int_{V_{\epsilon,\kappa}^{(1)}} d^3r - \int_{V_{\epsilon,\kappa}^{(2)}} d^3r \right] \frac{3x_i x_j - r^2 \delta_{ij}}{r^5}, \tag{36}
\]

where the large brackets are used to denote the difference in the indicated integrals. The integrals on the right-hand side are evaluated easily in cylindrical coordinates \(s, \phi, x_1\). The case \(i = j = 1\) gives

\[
\left[ \int_{V_{\epsilon,\kappa}^{(1)}} d^3r - \int_{V_{\epsilon,\kappa}^{(2)}} d^3r \right] \frac{3x_1^2 - r^2}{r^5} = 4\pi \int_0^\epsilon s \, ds \int_{\sqrt{s^2 - r^2}}^{\epsilon} \, dx_1 \frac{2x_1^2 - s^2}{(x_1^2 + s^2)^{5/2}} = 4\pi \left( \frac{\kappa}{\sqrt{1 + \kappa^2}} - \frac{2}{3} \right). \tag{37}
\]

The cases \(i = j = 2, 3\) give

\[
\left[ \int_{V_{\epsilon,\kappa}^{(1)}} d^3r - \int_{V_{\epsilon,\kappa}^{(2)}} d^3r \right] \frac{3x_i^2 - r^2}{r^5} = 2\pi \int_0^\epsilon s \, ds \int_{\sqrt{s^2 - r^2}}^{\epsilon} \, dx_1 \int_0^{2\pi} \, d\phi \frac{(3 \cos^2 \phi - 1)s^2 - x_i^2}{(x_1^2 + s^2)^{5/2}} = 2\pi \int_0^\epsilon s \, ds \int_{\sqrt{s^2 - r^2}}^{\epsilon} \, dx_1 \frac{s^2 - 2x_1^2}{(x_1^2 + s^2)^{5/2}} = 2\pi \left( \frac{2}{3} - \frac{\kappa}{\sqrt{1 + \kappa^2}} \right), \tag{38}
\]

and the mixed cases \(i \neq j\) yield zero because of the integration with respect to \(\phi\).
Similar to the establishing of identity (30), these results now establish a generalized-function identity,

\[
\lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \Theta(r - \epsilon) = \lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \left[ \Theta(|x_1| - \kappa \epsilon) + \Theta(x_2^2 + x_3^2 - \epsilon^2) \Theta(\kappa \epsilon - |x_1|) \right] \\
- 2\pi \left[ h_{ij}(\kappa) - \frac{2}{3} \delta_{ij} \right] \delta(r),
\]

(39)

where

\[
h_{ij}(\kappa) = \begin{cases} 
2 - 2\kappa/\sqrt{1 + \kappa^2}, & i = j = 1 \\
\kappa/\sqrt{1 + \kappa^2}, & i = j = 2, 3 \\
0, & i \neq j.
\end{cases}
\]

(40)

Using identity (39), the generalized derivative (10) can be written as

\[
\frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r} = \lim_{\epsilon \to 0} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \left[ \Theta(|x_1| - \kappa \epsilon) + \Theta(x_2^2 + x_3^2 - \epsilon^2) \Theta(\kappa \epsilon - |x_1|) \right] \\
- 2\pi h_{ij}(\kappa) \delta(r).
\]

(41)

This is a cylindrical-regularization alternative to (10). In the limit \( \kappa \to 0 \), the delta-function term in (41) simplifies to \(-4\pi \delta(r)\) for \( i = j = 1 \) ([4], p 29) and to 0 otherwise; such regularization is implemented automatically by using the cylindrical coordinates \( s, \phi, x_1 \) and performing the requisite integration over the whole space \( \mathbb{R}^3 \), so that the integration with respect to the variable \( x_1 \) is done last,

\[
\int d^3 r \quad f(r) \quad \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r} = \int_{-\infty}^{\infty} dx_1 \left( \int_{-\infty}^{\infty} s \ ds \int_{0}^{2\pi} d\phi \ f(s, \phi, x_1) \frac{d_{ij}(s, \phi, x_1)}{(x_1^2 + s^2)^{3/2}} \right) \\
- 4\pi f(0) \delta_{ij},
\]

(42)

where \( d_{ij}(s, \phi, x_1) \) is the function obtained by the transformation of \( 3x_i x_j - r^2 \delta_{ij} \) from the Cartesian to the cylindrical coordinates (e.g. \( d_{11}(s, \phi, x_1) = 2x_1^2 - s^2 \)).

4. Concluding remarks

In [12], the equivalence of the spherical- and spheroidal-regularization expressions for the generalized second-order partial derivatives of \( 1/r \) was illustrated by a relatively laborious explicit calculation of the weak limit \( a \to 0 \) of the derivatives of the Coulomb potential of a charged conducting spheroid of finite extension \( a \). The derivation of the generalized derivatives given here, together with the presented results on non-spherical regularization, ensures that any similar explicit calculation must yield the same result.

A point worth making is that while the standard, spherical-regularization expression (10) and the non-spherical-regularization expressions (31) and (41) for the generalized derivatives \( (\partial^2/\partial x_i \partial x_j)(1/r) \) are guaranteed to yield the same results in an integral with a well-behaved function, care should be taken in numerical work to use an integration grid that is compatible with the kind of regularization employed [4].

Very recently, Frahm’s formula (2) has been criticized as being valid only when averaged over smooth functions, and, to remedy that, an expression,

\[
\frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{r} = \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} - 4\pi \frac{x_i x_j}{r^2} \delta(r),
\]

(43)
Generalized second-order partial derivatives of $1/r$

has been proposed [6]. However, our analysis shows that the only ‘flaw’ in Frahm’s formula is that it does not indicate explicitly the spherical regularization that it assumes. We note that expression (43) still suffers from the lack of an appropriate regularization of the non-delta function term. Moreover, the delta-function term as it stands there is ill-defined; it would become meaningful in an integration in spherical coordinates and the replacement of the 3D delta function $\delta(r)$ by the radial equivalent $\delta(r)/(4\pi r^2)$. Clearly, the ‘general’ expression (43) will yield correct results only in an integration in spherical coordinates, with the angular integration of the term involving the non-delta-function part being done first.

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Appendix

We shall employ here a spheroidal-regularization generalized derivative in a calculation of the difference $A^{(C)}_{x_1} - A^{(L)}_{x_1}$ between the $x_1$-components of the Coulomb- and Lorenz-gauge vector potentials of a unit point charge moving uniformly with a velocity $v$ along the $x_1$ axis.

The difference $A^{(C)}_{x_1} - A^{(L)}_{x_1}$ satisfies an inhomogeneous wave equation [2],

$$\Box[A^{(C)}_{x_1}(r, t) - A^{(L)}_{x_1}(r, t)] = -v \frac{\partial^2}{\partial x_1^2} \phi^{(C)}(r, t),$$

(A.1)

where $\Box = \nabla^2 - \partial^2/\partial t^2$ is the d’Alembertian operator (we use Gaussian units with the speed of light $c = 1$) and

$$\phi^{(C)}(r, t) = \frac{1}{\sqrt{(x_1 - vt)^2 + x_2^2 + x_3^2}},$$

(A.2)

is the Coulomb-gauge scalar potential of the charge. But an inhomogeneous wave equation,

$$\Box f = s(x_1 - vt, x_2, x_3),$$

(A.3)

whose source term is ‘moving’ with a constant velocity $v$ along the $x_1$ axis, can be simplified by a simple transformation of the variables to a Poisson equation, the vanishing-at-infinity solution of which is given in terms of the original variables by

$$f(r, t) = -\frac{\gamma}{4\pi} \int d^3 r' \frac{s(x_1' - vt, x_2, x_3)}{\sqrt{\gamma^2 (x_1 - x_1')^2 + (x_2 - x_2')^2 + (x_3 - x_3')^2}},$$

(A.4)

where $\gamma = (1 - v^2)^{-1/2}$ [13] (see also [2, 14]). The wave equation (A.1) is therefore solved by

$$A^{(C)}_{x_1}(r, t) - A^{(L)}_{x_1}(r, t) = \frac{\gamma \gamma}{4\pi} \int d^3 r' \frac{(\partial^2/\partial x_1'^2) \phi^{(C)}(r', t)}{\sqrt{\gamma^2 (x_1 - x_1')^2 + (x_2 - x_2')^2 + (x_3 - x_3')^2}}.$$

(A.5)

Note that, in order that the integral is defined properly, the second-order derivative of the point-charge potential $\phi^{(C)}$ must here be a generalized one. However, instead of using the standard spherical-regularization expression for the derivative, it will be seen that the evaluation of the
expression is used. Following (31), this is given by
\[
\frac{\partial^2 \phi^{(C)}(r, t)}{\partial x_1^2} = \lim_{\epsilon \to 0} \frac{3(x_1 - vt)^2 - R^2}{R^5} \Theta(R^* - \epsilon)
\]
\[-4\pi \left( \frac{1}{v^2} - \frac{\arcsin v}{v^3} \right) \delta(x_1 - vt) \delta(x_2) \delta(x_3),
\]
where
\[
R = \sqrt{x_1^2 + x_2^2 + x_3^2} \quad \text{and} \quad R^* = \sqrt{\gamma^2(x_1 - vt)^2 + x_2^2 + x_3^2}.
\]

The integration in (A.5) is now done in two steps. First, the term involving the delta-function term of (A.6) is integrated readily and a transformation \( \gamma(x_1 - vt) \to x_1 \) is performed in the remaining integrand. This gives
\[
A^{(C)}(r, t) - A^{(D)}(r, t) = G(r, t) - \left( \frac{\gamma}{v} - \frac{\arcsin v}{v^2} \right) \frac{1}{R^*},
\]
where
\[
G(r, t) = \lim_{\epsilon \to 0} \frac{v}{4\pi} \int \frac{d^3 r'}{|R^* - r'|} \left( \frac{2x_1^2/\gamma^2 - x_2^2 - x_3^2}{(x_1^2/\gamma^2 + x_2^2 + x_3^2)^{5/2}} \right) \Theta(r' - \epsilon).
\]

Here, \( R^* \) is a vector with components \( \gamma(x_1 - vt), x_2, x_3 \). The expansion of the factor \( 1/|R^* - r'| \) in Legendre polynomials can now be used to separate angular and radial integrations; moreover, the use of spherical coordinates \( r', \theta', \phi' \) with the angular integration done first implements the regularization limit \( \epsilon \to 0 \) automatically. Thus,
\[
G(r, t) = \frac{v}{2R^*} \sum_{l=0}^{\infty} \frac{(4l + 1) P_2(\xi^*)}{2l(2l + 1)} \int_{-1}^{1} d\xi' \frac{(3 - 2v^2)\xi'^2 - 1}{(1 - v^2\xi'^2)^{5/2}} P_2(\xi'),
\]
where \( \xi^* = \gamma(x_1 - vt)/R^* \), \( \xi' = x_1^*/r' = \cos \theta' \), and the result,
\[
\int_{0}^{\infty} \frac{dr'}{r'} \frac{r'^2}{r^2} = \frac{4l + 1}{2l(2l + 1)} \frac{1}{R^*}, \quad l \geq 1,
\]
where \( r_0 (r_\infty) \) is the lesser (greater) of \( r' \) and \( R^* \), is used. The summation in (A.10) runs only over Legendre polynomials of even non-zero order since the integration with respect to \( \xi^* \) yields zero when the Legendre-polynomial order is zero or odd.

Second, the \( v \)-dependent part of the integrand is expanded in powers of \( v^2 \) to facilitate the integration with respect to \( \xi^* \),
\[
\frac{(3 - 2v^2)\xi'^2 - 1}{(1 - v^2\xi'^2)^{5/2}} = \sum_{n=0}^{\infty} \frac{(2n + 1)!!}{(2n)!!} [(2n + 3)\xi'^2 - 2n - 1] \xi'^{2n} v^{2n}.
\]

Using this expansion in (A.10), we obtain after interchanging the orders of summation and integrating term by term with respect to \( \xi^* \):
\[
G(r, t) = \frac{v}{2\sqrt{\pi} R^*} \sum_{n=0}^{\infty} \left[ \Gamma \left( n + \frac{3}{2} \right) \right]^2 v^{2n} \sum_{l=1}^{n+1} \frac{(4l + 1) P_{2l}(\xi^*)}{\Gamma(n - l + 2) \Gamma(n + l + \frac{3}{2})}
\]
\[= \frac{1}{v R^*} \sum_{n=1}^{\infty} \frac{[(2n - 1)!!]^2}{(2n + 1)!} \frac{[2n + 1]((v \xi^*)^{2n} - v^{2n})}{[(2n + 3)v^{2n} - 2n - 1] \xi'^{2n}} \]
\[= \left( \frac{1}{\sqrt{1 - v^2\xi'^2}} - \frac{\arcsin v}{v} \right) \frac{1}{v R^*}.
\]
Here, in the first line, the series over \( l \) terminates at \( l = n + 1 \) since all its \( l > n + 1 \) terms vanish; in the second line, the terminated series is summed and the resulting series over \( n \) rearranged so that it has an overall multiplier \( 1/v \); and, in the third line, the series over \( n \) is summed using the well-known expansions of the functions \((1 + x)^{-1/2}\) and \(\arcsin x\) in powers of \( x \). Using (A.13) in (A.8) and then the definition \( \xi^* = \gamma (x_1 - vt)/R^* \) with definition (A.7) of \( R^* \), we obtain finally

\[
A_{x_1}^{(C)}(r, t) - A_{x_1}^{(L)}(r, t) = \left( \frac{1}{\sqrt{1 - v^2 \xi^*}} - \gamma \right) \frac{1}{v R^*} \\
= \frac{1}{v} \left( \frac{1}{\sqrt{(x_1 - vt)^2 + x_2^2 + x_3^2}} - \frac{1}{\sqrt{(x_1 - vt)^2 + (x_2^2 + x_3^2)/\gamma^2}} \right).
\]  
(A.14)

The same closed-form expression for the difference between the \( x_1 \) components of the Coulomb- and Lorenz-gauge vector potentials of a point charge moving uniformly along the \( x_3 \) axis was obtained in [2] by calculating the requisite gauge function for the transformation between the Lorenz and Coulomb gauges using a formula derived by Jackson [15].

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