Available online at www.sciencedirect.com
ScienceDirect
Applied Mathematics and Computation 181 (2006) 291–309
APPLIED MATHEMATICS AND COMPUTATION
www.elsevier.com/locate/amc

Numerical integration over smooth surfaces in $\mathbb{R}^3$ via class $\mathscr{S}_m$ variable transformations. Part II: Singular integrands

Avram Sidi

Computer Science Department, Technion – Israel Institute of Technology, Technian city, Haifa 32000, Israel

Abstract

Class $\mathscr{S}_m$ variable transformations with integer m for finite-range integrals were introduced by the author about a decade ago. These transformations "periodize" the integrand functions in a way that enables the trapezoidal rule to achieve very high accuracy, especially with even m. In a recent work by the author, these transformations were extended to *arbitrary* real m, and their role in improving the convergence of the trapezoidal rule for different classes of integrands was studied in detail. It was shown that, with m chosen appropriately, exceptionally high accuracy can be achieved by the trapezoidal rule. The present work is Part II of a series of two papers dealing with the use of these transformations in the computation of integrals on surfaces of simply connected bounded domains in $\mathbb{R}^3$, in conjunction with the product trapezoidal rule. We assume these surfaces are smooth and homeomorphic to the surface of the unit sphere. In Part I, we treat the cases in which the integrands are smooth. In the present work, we treat integrands that have point singularities of the single-layer and double-layer types on these surfaces. We propose two methods, one in which the product trapezoidal rule is applied with a standard variable transformation from $\mathscr{S}_m$, and another in which the trapezoidal rule is applied with a rather unconventional transformation derived from $\mathscr{S}_m$ and achieves higher accuracy than the former. We give thorough analyses of the errors incurred by both methods, which show that surprisingly high accuracies can be achieved with suitable values of m. We also illustrate the theoretical results with numerical examples.

Keywords: Numerical integration; Integration over smooth surfaces in $\mathbb{R}^3$; Singular integrands; Product trapezoidal rule; Variable transformations; Sin^m-transformation; Euler–Maclaurin expansions; Asymptotic expansions

1. Introduction

This is Part II of a series of two papers dealing with a new approach to the numerical evaluation of integrals over smooth surfaces in three dimensions. In these papers, we treat integrals of the form

$$I[f] = \int\int_{\mathrm{S}} f(Q)\mathrm{d}A_{\mathrm{S}}, \tag{1.1}$$

E-mail address: asidi@cs.technion.ac.il
URL: http://www.cs.technion.ac.il/~asidi/

0096-3003/$ - see front matter © 2006 Elsevier Inc. All rights reserved.
doi:10.1016/j.amc.2006.01.035

where S is the surface of an arbitrary bounded and simply connected domain in $\mathbb{R}^3$ and $\mathrm{d}A_S$ is the associated area element. We assume that S is infinitely smooth and homeomorphic to the surface of the unit sphere, which we shall denote by U throughout. We also assume that the transformation from U to S is one-to-one and infinitely differentiable and that it has a nonsingular Jacobian matrix.

In Part I [11], we consider integrand functions $f(Q)$ that are smooth over S. In the present work, we treat the cases in which the integrand functions have point singularities of the single-layer and double-layer types over S. That is, $f(Q)$ is either of the form

$$f(Q) = \frac{g(Q)}{|Q-P|}, \quad P \in S \quad \text{(single-layer)}, \tag{1.2}$$

or of the form

$$f(Q) = \frac{g(Q)[(Q-P)\cdot \mathbf{n}_Q]}{|Q-P|^3}, \quad P \in S \quad \text{(double-layer)}, \tag{1.3}$$

where $g(Q)$ is smooth over S, $|Q-P|$ denotes the Euclidean distance between P and Q, $\mathbf{n}_Q$ is the outward normal to S at Q, and $(Q-P)\cdot\mathbf{n}_Q$ is the dot product of the vectors $(Q-P)$ and $\mathbf{n}_Q$.

Such singular integrals arise in boundary integral equation formulations of partial differential equations in continuum problems. For a review of this subject, see Atkinson [1] and [2, Chapter 5].

The fact that S is a general surface in $\mathbb{R}^3$, as well as the fact that the integrand $f(Q)$ has a point singularity on S, makes the treatment of this problem considerably more involved than the case of smooth $f(Q)$ studied in [11]. The analysis of the case of singular $f(Q)$ turns out to be simpler when $S = U$, however, and this case is treated in a recent paper by the author [9]. The study of [9] may facilitate the study of the present work somewhat.

Here are the steps of the method of integration we present in this work:

(i) Using the mapping of U, the surface of the unit sphere, to S, express $I[f]$ as an integral over U.
(ii) Rotate the coordinate system on U such that either the north pole or the south pole is mapped to P, the point of singularity of $f(Q)$ on S.
(iii) Express the (twice-transformed) integral over U in terms of the standard spherical coordinates θ and ϕ, $0 \leqslant \theta \leqslant \pi$ and $0 \leqslant \phi \leqslant 2\pi$. The resulting integral can be written in the form $I[f] = \int_0^{\pi}[\int_0^{2\pi} F(\theta,\phi)d\phi]\mathrm{d}\theta$.
(iv) Transform θ by an appropriate variable transformation $\theta = \Psi(t)$, $0 \leqslant t \leqslant 1$, where $\Psi(t)$ is derived from standard variable transformations in the extended classes $\mathscr{S}_m$ of Sidi [10]. The resulting integral is $I[f] = \int_0^1[\int_0^{2\pi}\widehat{F}(t,\phi)\mathrm{d}\phi]\mathrm{d}t$, where $\widehat{F}(t,\phi) = F(\Psi(t),\phi)\Psi'(t)$.
(v) Approximate the final integral in the variables t and ϕ by the product trapezoidal rule.

Before proceeding further, we advise the reader to study Part I [11] concerning the smooth $f(Q)$, which presents the essentials of this approach in detail. It presents a discussion on the merits of employing variable transformations in general. In addition, Part I provides the definition and a summary of the properties of transformations in the extended classes $\mathscr{S}_m$, and also the $\sin^m$-transformation in $\mathscr{S}_m$ that we have used in our computations. Finally, it also provides the relevant Euler–Maclaurin expansions, including an extension of them due to Sidi [7]. All these comprise the analytical tools necessary for the study of the methods of the present work. In the sequel, we will refer freely to [11] for these tools.

We now turn to the complete mathematical description of the methods we have sketched above.

Let $Q = (\xi,\eta,\zeta)$ and $P = (\xi_0,\eta_0,\zeta_0)$ in (1.1)–(1.3), and let U, the surface of the unit sphere, be given as in

$$U := \{(x,y,z):\ x^2+y^2+z^2 = 1\}. \tag{1.4}$$

Denote the mapping from U to S via

$$\boldsymbol{\rho} = [\xi,\eta,\zeta]^{\mathrm{T}} = [\xi(x,y,z),\eta(x,y,z),\zeta(x,y,z)]^{\mathrm{T}}, \tag{1.5}$$

so that the Jacobian matrix of this mapping is

$$J(x,y,z) = \begin{bmatrix} \partial\xi/\partial x & \partial\xi/\partial y & \partial\xi/\partial z \\ \partial\eta/\partial x & \partial\eta/\partial y & \partial\eta/\partial z \\ \partial\zeta/\partial x & \partial\zeta/\partial y & \partial\zeta/\partial z \end{bmatrix}. \tag{1.6}$$

Thus, $J(x,y,z)$ is known as a function of x, y and z.

Let $P = (\xi_0, \eta_0, \zeta_0) \in S$ be the mapping of the point $(x_0, y_0, z_0) \in U$. That is,

$$P = (\xi_0, \eta_0, \zeta_0) = (\xi(x_0,y_0,z_0), \eta(x_0,y_0,z_0), \zeta(x_0,y_0,z_0)). \tag{1.7}$$

Now rotate the (x,y,z) coordinate system such that the point (x_0,y_0,z_0) is mapped to the north pole or the south pole of U. In other words, map U onto itself (orthogonally) via a fixed 3×3 real orthogonal matrix H (that is, $H^{-1} = H^{\mathrm{T}}$) such that

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}, \quad \begin{bmatrix} x_0 \\ y_0 \\ z_0 \end{bmatrix} = \mu H e_3; \quad \mu = \pm 1, \quad e_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{1.8}$$

Here μ should be chosen in a way that does not cause loss of accuracy numerically.

Let now

$$\tilde{\mathbf{r}} = [\tilde{x}, \tilde{y}, \tilde{z}]^{\mathrm{T}}, \tag{1.9}$$

and switch to the standard spherical coordinates θ and ϕ:

$$(\tilde{x}, \tilde{y}, \tilde{z}) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta); \quad 0 \leqslant \theta \leqslant \pi, \; 0 \leqslant \phi \leqslant 2\pi. \tag{1.10}$$

Now, by expressing $I[f]$ (expressed originally in terms of the coordinates ξ, η, ζ) as an integral over U (expressed in terms of the coordinates $\tilde{x}, \tilde{y}, \tilde{z}$) via (1.5) and (1.8), and by introducing the variables θ and ϕ on U as in (1.10), we are actually generating a two-parameter representation of S, these parameters being θ and ϕ. Thus, in terms of θ and ϕ, the area element $\mathrm{d}A_S$ on S becomes

$$\mathrm{d}A_S = \left\| \frac{\partial\boldsymbol{\rho}}{\partial\theta} \times \frac{\partial\boldsymbol{\rho}}{\partial\phi} \right\| \mathrm{d}\theta\,\mathrm{d}\phi, \tag{1.11}$$

where $\|\mathbf{p}\| = \sqrt{\mathbf{p}^{\mathrm{T}}\mathbf{p}}$ for $\mathbf{p} \in \mathbb{R}^3$. We, therefore, have

$$I[f] = \int_0^{\pi} \left[\int_0^{2\pi} F(\theta,\phi)\,\mathrm{d}\phi \right] \mathrm{d}\theta; \qquad F(\theta,\phi) \equiv f(\xi,\eta,\zeta) \left\| \frac{\partial\boldsymbol{\rho}}{\partial\theta} \times \frac{\partial\boldsymbol{\rho}}{\partial\phi} \right\|. \tag{1.12}$$

The vectors $\partial\boldsymbol{\rho}/\partial\theta$ and $\partial\boldsymbol{\rho}/\partial\phi$ can be computed by the chain rule, as in

$$\frac{\partial\boldsymbol{\rho}}{\partial\theta} = JH\frac{\partial\tilde{\mathbf{r}}}{\partial\theta}, \qquad \frac{\partial\boldsymbol{\rho}}{\partial\phi} = JH\frac{\partial\tilde{\mathbf{r}}}{\partial\phi}. \tag{1.13}$$

Here, J stands for $J(x,y,z)$ for short, and

$$\frac{\partial\tilde{\mathbf{r}}}{\partial\theta} = \begin{bmatrix} \cos\theta\cos\phi \\ \cos\theta\sin\phi \\ -\sin\theta \end{bmatrix}, \qquad \frac{\partial\tilde{\mathbf{r}}}{\partial\phi} = \sin\theta \begin{bmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{bmatrix}. \tag{1.14}$$

Next, we make the further variable transformation $\theta = \Psi(t)$, $0 \leqslant t \leqslant 1$, as explained above; this results in the transformed integral

$$I[f] = \int_0^1 \left[\int_0^{2\pi} \widehat{F}(t,\phi)\,\mathrm{d}\phi \right] \mathrm{d}t; \qquad \widehat{F}(t,\phi) \equiv F(\Psi(t),\phi)\Psi'(t). \tag{1.15}$$

Finally, we approximate the transformed integral via the product trapezoidal rule (with the boundary points taken out)

$$\widehat{T}_{n,n'}[f] = hh' \sum_{j=1}^{n-1} \sum_{k=1}^{n'} \widehat{F}(jh, kh'); \quad h = \frac{1}{n}, \; h' = \frac{2\pi}{n'}, \tag{1.16}$$

where n and n' are positive integers. We let $n' \sim \alpha n^{\beta}$ as $n \to \infty$ for some fixed positive α and β in the sequel.

We next discuss in more detail the choice of the matrix H in (1.8) and the choice of the variable transformation $\theta = \Psi(t)$ in (1.15).

As mentioned already, when determining H, we should choose μ in a way that does not cause loss of accuracy numerically. For example, following Atkinson [3], we can take H to be a real Householder matrix, with μ fixed such that H is computed in the most stable way possible: When $z_0 \neq 0$,

$$\mu = -\mathrm{sgn}(z_0); \qquad H = I - 2pp^{\mathrm{T}}, \qquad p = \frac{1}{\sqrt{2+2|z_0|}} \begin{bmatrix} x_0 \\ y_0 \\ \mathrm{sign}(z_0)(|z_0|+1) \end{bmatrix}, \tag{1.17}$$

and when $z_0 = 0$, we have

$$\mu = +1 \text{ or } \mu = -1; \qquad H = I - 2pp^{\mathrm{T}}, \qquad p = \frac{1}{\sqrt{2}} \begin{bmatrix} x_0 \\ y_0 \\ -\mu \end{bmatrix}. \tag{1.18}$$

(Recall that, if H is a real Householder matrix, then it is symmetric, and hence satisfies $H^{-1} = H$, in addition to $H^{-1} = H^{\mathrm{T}}$.)

We now describe a procedure proposed in [9] that enables us to use only (1.17) for determining $H = I - 2pp^{\mathrm{T}}$, $p^{\mathrm{T}}p = 1$. Letting $\rho = \max\{|x_0|, |y_0|, |z_0|\}$, so that $\rho \geqslant 1/\sqrt{3} > 0$, we consider three separate cases:

(i) If $|x_0| = \rho$, then

$$\begin{bmatrix} y \\ z \\ x \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}, \quad \begin{bmatrix} y_0 \\ z_0 \\ x_0 \end{bmatrix} = -\mathrm{sign}(x_0) H e_3; \qquad p = \frac{1}{\sqrt{2+2|x_0|}} \begin{bmatrix} y_0 \\ z_0 \\ \mathrm{sign}(x_0)(|x_0|+1) \end{bmatrix}. \tag{1.19}$$

(ii) If $|y_0| = \rho$, then

$$\begin{bmatrix} z \\ x \\ y \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}, \quad \begin{bmatrix} z_0 \\ x_0 \\ y_0 \end{bmatrix} = -\mathrm{sign}(y_0) H e_3; \qquad p = \frac{1}{\sqrt{2+2|y_0|}} \begin{bmatrix} z_0 \\ x_0 \\ \mathrm{sign}(y_0)(|y_0|+1) \end{bmatrix}. \tag{1.20}$$

(iii) If $|z_0| = \rho$, then

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}, \quad \begin{bmatrix} x_0 \\ y_0 \\ z_0 \end{bmatrix} = -\mathrm{sign}(z_0) H e_3; \qquad p = \frac{1}{\sqrt{2+2|z_0|}} \begin{bmatrix} x_0 \\ y_0 \\ \mathrm{sign}(z_0)(|z_0|+1) \end{bmatrix}. \tag{1.21}$$

Note that, in these transformations, x, y, and z are permuted cyclically to preserve the orientation of the coordinate system.

As for the choice of the variable transformation $\theta = \Psi(t)$, we propose two different ways. Below, we recall that transformations in the classes $\mathscr{S}_m$ are monotonically increasing functions that map the interval $[0, 1]$ onto itself.

1. Choose $\psi \in \mathscr{S}_m$ for arbitrary $m > 0$, and let

$$\Psi(t) = \Psi_1(t) = \pi\psi(t). \tag{1.22}$$

2. Choose $\varpi \in \mathscr{S}_q$ for some *fixed* even integer $q > 0$ and $\psi \in \mathscr{S}_m$ for arbitrary $m > -q/(q+1)$, and define the transformation $\Psi(t) = \Psi_2(t)$ as follows:
   - When P is the mapping of the south pole, let

$$\Psi(t) = \Psi_{2,\mathrm{S}}(t) = 2\pi\psi\left(\frac{1}{2}\varpi(t)\right). \tag{1.23}$$

   - When P is the mapping of the north pole, let

$$\Psi(t) = \Psi_{2,\mathrm{N}}(t) = \pi - \Psi_{2,\mathrm{S}}(1-t) = \pi\left[1 - 2\psi\left(\frac{1}{2}\varpi(1-t)\right)\right]. \tag{1.24}$$

Notes

1. The product trapezoidal rule for the transformed integral $\int_0^1 \left[\int_0^{2\pi} \widehat{F}(t,\phi)\mathrm{d}\phi\right]\mathrm{d}t$ in (1.12) is actually

$$hh'{\sum_{j=0}^{n}}''{\sum_{k=0}^{n'}}''\widehat{F}(jh,kh'), \tag{1.25}$$

to begin with. (Here, the double prime on a summation means that the first and the last terms in the summation are to be multiplied by 1/2.) First, our transformed integrand $\widehat{F}(t,\phi)$ is 2π-periodic in ϕ, hence $\widehat{F}(t,0) = \widehat{F}(t,2\pi)$. This implies that the summation ${\sum''}_{k=0}^{n'}$ in (1.25) can be written as $\sum_{k=1}^{n'}$. In addition, as we will see later in this work, the integrand $F(\theta,\phi)$ is continuous for all $\theta \in [0,\pi]$ and $\phi \in [0,2\pi]$, despite the fact that $\lim_{Q\to P}|f(Q)| = \infty$. [In fact, $F(\theta,\phi)$ is infinitely differentiable for $\theta \in [0,\pi]$ and $\phi \in (-\infty,\infty)$, and 2π-periodic in ϕ as well.] Because $m > 1$, there holds $\Psi_1'(0) = \Psi_1'(1) = 0$. Similarly, because $q > 0$ and $m > -q/(q+1)$, there holds $\Psi_2'(0) = \Psi_2'(1) = 0$. [These indeed follow from the facts that $\Psi_{2,\mathrm{S}}(t) = \mathrm{O}(t^{(m+1)(q+1)})$ as $t \to 0+$, and $\pi - \Psi_{2,\mathrm{S}}(t) = \mathrm{O}((1-t)^{q+1})$ as $t \to 1-$.] These facts and $\widehat{F}(t,\phi) = F(\Psi(t),\phi)\Psi'(t)$ imply that $\widehat{F}(0,\phi) = \widehat{F}(1,\phi) = 0$. This means that the summation ${\sum''}_{j=0}^{n}$ in (1.25) can be written as $\sum_{j=1}^{n-1}$. As a result, the rule in (1.25) becomes $\widehat{T}_{n,n'}[f]$ given in (1.16).
2. The variable transformation $\Psi_1(t)$ in the present work is the same as that given in [9]. The transformation $\Psi_2(t)$ given here is different from that of [9], however. With $\Psi_2(t)$ of [9], we have $\Psi_2'(0) \neq 0$ when $\mu = +1$ and $\Psi_2'(1) \neq 0$ when $\mu = -1$. This implies that, to form $\widehat{T}_{n,n'}[f]$, we need to compute $F(0,\phi)$ when $\mu = +1$ and $F(\pi,\phi)$ when $\mu = -1$. This computation must be done separately, because these values of $F(\theta,\phi)$ can be computed only as limits as $Q \to P$ when S is arbitrary. (As shown in [9], when $S = U$, they are available immediately.) Because we want to obviate the need to do extra computation (or programming), we have chosen to modify $\Psi_2(t)$ as in (1.23) and (1.24) so that $\Psi_2'(0) = \Psi_2'(1) = 0$, which forces $\widehat{F}(0,\phi) = \widehat{F}(1,\phi) = 0$, whether P is the mapping of the north pole or of the south pole, as mentioned above.
3. With $\Psi_{2,\mathrm{S}}(t)$ available, we can obtain $\Psi_{2,\mathrm{N}}(t)$ as follows:

$$\begin{aligned}\int_0^{\pi} v(\theta)\mathrm{d}\theta &= \int_0^{\pi} v(\pi-\theta)\mathrm{d}\theta = \int_0^1 v(\pi - \Psi_{2,\mathrm{S}}(t))\Psi_{2,\mathrm{S}}'(t)\mathrm{d}t = \int_0^1 v(\pi - \Psi_{2,\mathrm{S}}(1-t))\Psi_{2,\mathrm{S}}'(1-t)\mathrm{d}t \\ &= \int_0^1 v(\Psi_{2,\mathrm{N}}(t))\Psi_{2,\mathrm{N}}'(t)\mathrm{d}t.\end{aligned}$$

The variable transformations $\theta = \Psi(t)$ above turn out to be very effective in that the accuracy of $\widehat{T}_{n,n'}[f]$ increases with increasing m, and in a subtle way. For some special values of m, unusually high accuracies are achieved, as we will see later. Also, the approximations produced with $\Psi_2(t)$ have better accuracies than those produced with $\Psi_1(t)$.

The plan of this paper is as follows: In the next section, we give a preliminary analysis of $\widehat{T}_{n,n'}[f]$, in which we show that it is sufficient to analyze the trapezoidal rule for the one-dimensional integral $\int_0^1 \hat{v}(t)\mathrm{d}t$, where $\hat{v}(t) = v(\Psi(t))\Psi'(t)$ with $v(\theta) = \int_0^{2\pi} F(\theta,\phi)\mathrm{d}\phi$. In Section 3, which is a most important (and, theoretically, the most involved) part of this work, we give a detailed analysis of the transformed integrand $F(\theta,\phi)$. The main result of this section is Theorem 3.9. In Section 4, we analyze the asymptotic behavior of the integral

$v(\theta)$ as $\theta \to 0$ and as $\theta \to \pi$, Theorem 4.2 being the main result of this section. In Sections 5 and 6, we provide the complete analysis of the rule $\widehat{T}_{n,n'}[f]$, Theorem 5.1 [for $\Psi_1(t)$] and Theorem 6.2 [for $\Psi_2(t)$] being the main results. In Section 7, we provide a numerical example with both $\Psi_1(t)$ and $\Psi_2(t)$, and verify the validity of our theoretical results.

Before closing, we mention that the basic method described above is related to a recent method of Atkinson [3]. As it turns out, the numerical performance of our basic method with $\Psi(t) = \Psi_1(t)$ is very similar to that of [3], and some of the theoretical results of Section 5 concerning our basic method are analogous to those of [3]. There is no analogue of our method with $\Psi(t) = \Psi_2(t)$ and its corresponding theory in [3], however. One of the major differences between the methods of the present paper and that of [3] is that in the present paper, the variable θ on the unit sphere is transformed (by a variable transformation in the extended class $\mathscr{S}_m$), whereas in [3], θ is "graded" in a special and interesting way by the introduction of a grading parameter q, instead of being transformed. The convergence analysis of the numerical integration formula for the case in which $f(Q)$ is smooth has been given recently by Atkinson and Sommariva [4] (for $S = U$ and for certain values of q) and by Sidi [8] (for arbitrary S and for all values of q).

Note that the extended class $\mathscr{S}_m$ of [10] for arbitrary m is indeed an extension of that first introduced in Sidi [5] with integer m. It is described briefly also in [9,11].

Finally, this paper is partly based on the report [6] by the author.

2. Preliminary results on $\widehat{T}_{n,n'}[f]$

Let us define

$$v(\theta) = \int_0^{2\pi} F(\theta, \phi)\mathrm{d}\phi, \qquad \hat{v}(t) = \int_0^{2\pi} \widehat{F}(t, \phi)\mathrm{d}\phi. \tag{2.1}$$

Thus,

$$\hat{v}(t) = v(\Psi(t))\Psi'(t), \qquad I[f] = \int_0^{\pi} v(\theta)\mathrm{d}\theta = \int_0^1 \hat{v}(t)\mathrm{d}t. \tag{2.2}$$

As we show in Theorem 3.9 in the next section, despite the singularity of $f(Q)$ at the point $P \in S$, the function $F(\theta, \phi)$ is infinitely differentiable as a function of both $\theta \in [0, \pi]$ and $\phi \in (-\infty, \infty)$, and also 2π-periodic as a function of ϕ. [Recall that the point $P = (\xi_0, \eta_0, \zeta_0)$ is the mapping of the north pole ($\theta = 0$) or of the south pole ($\theta = \pi$) of the transformed U.] This being the case, the developments of [11, Section 3] apply, and we have that

$$\widehat{T}_{n,n'}[f] = \widetilde{T}_n[f] + \mathrm{O}(h'^{\nu}) \text{ as } h' \to 0, \quad \text{for every } \nu > 0, \tag{2.3}$$

where

$$\widetilde{T}_n[f] = h{\sum_{j=0}^{n}}'' \int_0^{2\pi} \widehat{F}(jh, \phi)\mathrm{d}\phi = h{\sum_{j=0}^{n}}'' \hat{v}(jh). \tag{2.4}$$

(Recall that the double prime on the summation $\sum_{j=0}^{\prime\prime n}$ means that the $j = 0$ and $j = n$ terms are to be multiplied by 1/2.) Thus, if we let $n' \sim \alpha n^{\beta}$ as $n \to \infty$ for some fixed positive α and β, then (2.3) becomes

$$\widehat{T}_{n,n'}[f] = \widetilde{T}_n[f] + \mathrm{O}(h^{\nu}) \text{ as } h \to 0 \quad \text{for every } \nu > 0. \tag{2.5}$$

In the sequel, we let $n' \sim \alpha n^{\beta}$ as $n \to \infty$.

As is clear from (2.5), the error in $\widehat{T}_{n,n'}[f]$ as $h \to 0$ has the same asymptotic expansion as that of $\widetilde{T}_n[f]$. Thus, we need to concern ourselves only with the asymptotic expansion as $h \to 0$ of $\widetilde{T}_n[f]$, the trapezoidal rule approximation to the one-dimensional integral $\int_0^1 \hat{v}(t)\mathrm{d}t$. For this, we need to study $\hat{v}(t)$ as $t \to 0+$ and $t \to 1-$, by [11, Theorem A.2]. For this, in turn, we need to expand $\widehat{F}(t, \phi)$ about $t = 0$ and $t = 1$. This we do by expanding $v(\theta)$ about $\theta = 0$ and $\theta = \pi$, for which we need to expand $F(\theta, \phi)$ about $\theta = 0$ and $\theta = \pi$.

Throughout, we make use of the fact that the sequence $\{(\sin\theta)^i\}_{i=1}^{\infty}$ is a bona fide asymptotic scale both as $\theta\to 0$ and as $\theta\to\pi$.

3. The transformed integrand

In this section, we do an asymptotic analysis as $\theta\to 0$ and as $\theta\to\pi$ of the integrand $F(\theta,\phi)$ in (1.12). This analysis will help us in determining the precise nature of the asymptotic expansions of $v(\theta)$ as $\theta\to 0$ and as $\theta\to\pi$, respectively. We achieve this by studying the different factors that make up $F(\theta,\phi)$. Definition 3.1 and Lemmas 3.2 and 3.3 that follow serve to simplify the analysis.

Definition 3.1. We say that a function $A(\theta,\phi)$ belongs to the set $\mathscr{K}$ if it is infinitely differentiable for $0\leqslant\theta\leqslant\pi$ and $-\infty\leqslant\phi\leqslant\infty$ and 2π-periodic in ϕ, and is of the form

$$A(\theta,\phi)=M_1(\theta,\phi)+M_2(\theta,\phi)\cos\phi\sin\phi+N_1(\theta,\phi)\cos\phi+N_2(\theta,\phi)\sin\phi,$$

where the functions $M_s(\theta,\phi)$ and $N_s(\theta,\phi)$ have asymptotic expansions of the form

$$M_s(\theta,\phi)\sim\sum_{i=0}^{\infty}c_{si}(\phi)\theta^{2i}\quad\text{as }\theta\to 0,\quad s=1,2,$$

$$N_s(\theta,\phi)\sim\sum_{i=0}^{\infty}d_{si}(\phi)\theta^{2i+1}\quad\text{as }\theta\to 0,\quad s=1,2,$$

$c_{si}(\phi)$ and $d_{si}(\phi)$ being π-periodic and even functions of ϕ, and infinitely differentiable for $\phi\in(-\infty,\infty)$.

Lemma 3.2 that follows is easy to prove; we leave its verification to the reader. The observation that $(\cos\phi)^i(\sin\phi)^j$ is even and π-periodic in ϕ only when both i and j are even integers is helpful in this verification.

Lemma 3.2. *If $A_1(\theta,\phi)$ and $A_2(\theta,\phi)$ are in the set $\mathscr{K}$, then so are their sum and their product.*

Lemma 3.3. *Let $W(\tilde{x},\tilde{y},\tilde{z})$ be infinitely differentiable about the point $(\tilde{x},\tilde{y},\tilde{z})=(0,0,1)$ on (the transformed) U. Then, with $(\tilde{x},\tilde{y},\tilde{z})=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$ [recall (1.10)], the function $A(\theta,\phi)\equiv W(\tilde{x},\tilde{y},\tilde{z})$ is in the set $\mathscr{K}$.*

Proof. We start by noting that, $\tilde{z}=\sqrt{1-\tilde{x}^2-\tilde{y}^2}$ is an infinitely differentiable function of $\tilde{x}$ and $\tilde{y}$ in any neighborhood of the point $(\tilde{x},\tilde{y})=(0,0)$. This implies that $W(\tilde{x},\tilde{y},\tilde{z})$ is also an infinitely differentiable function of the variables $\tilde{x}$ and $\tilde{y}$ in any neighborhood of $(\tilde{x},\tilde{y},\tilde{z})=(0,0,1)$ on (the transformed) U. As such, we denote it by $\widetilde{W}(\tilde{x},\tilde{y})$. Let us now expand $\widetilde{W}(\tilde{x},\tilde{y})$ in a Taylor series about $(0,0)$ (equivalently, at $\theta=0$). We obtain

$$\widetilde{W}(\tilde{x},\tilde{y})\sim\sum_{i,j\geqslant 0}^{\infty}\widetilde{W}_{i,j}\tilde{x}^i\tilde{y}^j\quad\text{as }(\tilde{x},\tilde{y})\to(0,0);\qquad\widetilde{W}_{i,j}=\frac{1}{i!j!}\left.\frac{\partial^{i+j}\widetilde{W}}{\partial\tilde{x}^i\partial\tilde{y}^j}\right|_{(\tilde{x},\tilde{y})=(0,0)}.\tag{3.1}$$

In terms of θ and ϕ, this can be expressed as in

$$\widetilde{W}(\tilde{x},\tilde{y})=A(\theta,\phi)\sim\sum_{i,j\geqslant 0}^{\infty}\widetilde{W}_{i,j}(\sin\theta)^{i+j}(\cos\phi)^i(\sin\phi)^j\quad\text{as }\theta\to 0.\tag{3.2}$$

We observe that the summation on i and j in (3.2) can be divided into four summations: The first, second, third, and fourth summations contain the terms with, respectively, i and j both even, i and j both odd, i odd and j even, and i even and j odd. Thus, they can immediately be identified with, respectively, $M_1(\theta,\phi)$, $M_2(\theta,\phi)\cos\phi\sin\phi$, $N_1(\theta,\phi)\cos\phi$, and $N_2(\theta,\phi)\sin\phi$ in Definition 3.1. For example,

$$N_1(\theta,\phi)\sim\sum_{s=0}^{\infty}\left[\sum_{\substack{i,j\geqslant 0\\ i+j=s}}\widetilde{W}_{2i+1,2j}(\cos\phi)^{2i}(\sin\phi)^{2j}\right](\sin\theta)^{2s+1}\quad\text{as }\theta\to 0.$$

[Note that $(\cos\phi)^{2i}(\sin\phi)^{2j}$, $i,j = 0,1,2,\ldots$, are even π-periodic functions of ϕ and are infinitely differentiable for $\phi \in (-\infty,\infty)$. Similarly, $(\sin\theta)^r$, as $\theta \to 0$, has an asymptotic expansion in even (odd) powers of θ when r is an even (odd) integer.] We leave the details to the reader. □

3.1. The function g(Q)

We start with $g(Q) = g(\xi,\eta,\zeta)$, as this is the simplest part. We have already assumed that $g(Q)$ is infinitely differentiable on S. Because the transformations from the coordinates $(\tilde{x},\tilde{y},\tilde{z})$ to (x,y,z) and from (x,y,z) to (ξ,η,ζ) are one-to-one and infinitely differentiable, $g(Q)$ is an infinitely differentiable function of $\tilde{x},\tilde{y},\tilde{z}$ over U. Therefore, Lemma 3.3 applies to $g(Q)$, and $g(Q) = A_1(\theta,\phi)$ for some $A_1(\theta,\phi) \in \mathscr{K}$.

3.2. The vector $\frac{\partial\boldsymbol{\rho}}{\partial\theta} \times \frac{\partial\boldsymbol{\rho}}{\partial\phi}$ and the function $\|\frac{\partial\boldsymbol{\rho}}{\partial\theta} \times \frac{\partial\boldsymbol{\rho}}{\partial\phi}\|$

For simplicity of notation, let us denote (ξ,η,ζ) by (ξ_1,ξ_2,ξ_3), (x,y,z) by (x_1,x_2,x_3), and $(\tilde{x},\tilde{y},\tilde{z})$ by $(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3)$. Thus,

$$\tilde{\mathbf{r}} = [\tilde{x},\tilde{y},\tilde{z}]^{\mathrm{T}} = [\tilde{x}_1,\tilde{x}_2,\tilde{x}_3]^{\mathrm{T}}, \qquad (\tilde{x}_1,\tilde{x}_2,\tilde{x}_3) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta),$$
$$\boldsymbol{\rho} = [\xi,\eta,\zeta]^{\mathrm{T}} = [\xi_1(x_1,x_2,x_3), \xi_2(x_1,x_2,x_3), \xi_3(x_1,x_2,x_3)]^{\mathrm{T}}.$$

Thus, $\partial\xi_i/\partial x_j$ is the (i,j) element of the Jacobian matrix $J(x_1,x_2,x_3)$ in (1.6). It is now easy to see that the Jacobian matrix of the mapping from the transformed U to S is

$$\widetilde{J}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3) = J(x_1,x_2,x_3)H,$$

its (i,j) element being $\partial\xi_i/\partial\tilde{x}_j = \sum_{k=1}^{3}(\partial\xi_i/\partial x_k)[H]_{kj}$. By Theorem 2.1 in [11] and Lemma 3.3, we can now state the following result:

Theorem 3.4. *Let* $\widetilde{\mathbf{\nabla}}u$ *denote the gradient of the function* $u(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3)$, *that is*, $\widetilde{\mathbf{\nabla}}u = (\partial u/\partial\tilde{x}_1, \partial u/\partial\tilde{x}_2, \partial u/\partial\tilde{x}_3)$. *Define*

$$\tilde{\sigma}_{ij} = \left(\widetilde{\mathbf{\nabla}}\xi_i \times \widetilde{\mathbf{\nabla}}\xi_j\right)\cdot\tilde{\mathbf{r}}, \qquad \widetilde{R}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3) = \sqrt{\tilde{\sigma}_{23}^2 + \tilde{\sigma}_{31}^2 + \tilde{\sigma}_{12}^2}. \tag{3.3}$$

Then

$$\frac{\partial\boldsymbol{\rho}}{\partial\theta} \times \frac{\partial\boldsymbol{\rho}}{\partial\phi} = [\tilde{\sigma}_{23},\tilde{\sigma}_{31},\tilde{\sigma}_{12}]^{\mathrm{T}}\sin\theta, \qquad \left\|\frac{\partial\boldsymbol{\rho}}{\partial\theta} \times \frac{\partial\boldsymbol{\rho}}{\partial\phi}\right\| = \widetilde{R}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3)\sin\theta. \tag{3.4}$$

With S as in the first paragraph of Section 1, $\widetilde{R}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3)$ *is strictly positive on the transformed U and is in* $C^\infty(U)$. *Consequently,* $\widetilde{R}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3)$, *as a function of* ϕ, *is infinitely differentiable and* 2π*-periodic as well. As a result, we also have that* $\widetilde{R}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3) = A_2(\theta,\phi)$ *for some* $A_2(\theta,\phi) \in \mathscr{K}$.

Now, the computation of $\partial\boldsymbol{\rho}/\partial\theta \times \partial\boldsymbol{\rho}/\partial\phi$ and $\widetilde{R}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3)$ can be simplified as in Theorem 3.5 that follows:

Theorem 3.5. *Let* $\mathbf{r} = [x_1,x_2,x_3]^{\mathrm{T}}$ *and let* $\mathbf{\nabla}u$ *denote the gradient of the function* $u(x_1,x_2,x_3)$, *that is*, $\mathbf{\nabla}u = (\partial u/\partial x_1, \partial u/\partial x_2, \partial u/\partial x_3)$. *Define*

$$\sigma_{ij} = (\mathbf{\nabla}\xi_i \times \mathbf{\nabla}\xi_j)\cdot\mathbf{r} \quad \textit{and} \quad R(x_1,x_2,x_3) = \sqrt{\sigma_{23}^2 + \sigma_{31}^2 + \sigma_{12}^2}. \tag{3.5}$$

Then

$$\tilde{\sigma}_{ij} = (\det H)\sigma_{ij}, \quad \textit{hence}\ \widetilde{R}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3) = R(x_1,x_2,x_3). \tag{3.6}$$

Consequently,

$$\frac{\partial\boldsymbol{\rho}}{\partial\theta} \times \frac{\partial\boldsymbol{\rho}}{\partial\phi} = (\det H)[\sigma_{23},\sigma_{31},\sigma_{12}]^{\mathrm{T}}\sin\theta, \qquad \left\|\frac{\partial\boldsymbol{\rho}}{\partial\theta} \times \frac{\partial\boldsymbol{\rho}}{\partial\phi}\right\| = R(x_1,x_2,x_3)\sin\theta. \tag{3.7}$$

We give the proof of this result in Appendix to this work.

3.3. The singular factors

We now come to the analysis of the singular factors $V(Q) \equiv f(Q)/g(Q)$,

$$V(Q) = \frac{1}{|Q-P|} \quad \text{(single-layer)}, \qquad V(Q) = \frac{(Q-P)\cdot \mathbf{n}_Q}{|Q-P|^3} \quad \text{(double-layer)}. \tag{3.8}$$

It is these factors that make the study of $v(\theta)$ and hence of $\widehat{T}_{n,n'}[f]$ difficult.

We will give the full treatment with $\mu = +1$ in (1.8), that is, with the point of singularity $P \in S$ being the mapping of $(\tilde{x},\tilde{y},\tilde{z}) = (0,0,1)$ hence of $\theta = 0$ in the transformed U; the treatment of the case $\mu = -1$ is analogous.

3.3.1. Study of $Q-P$ and $|Q-P|^\beta$

First, it is obvious from our assumptions that $Q-P$ is infinitely differentiable as a function of $\tilde{x},\tilde{y},\tilde{z}$, hence also as a function of θ and ϕ, and is 2π-periodic in ϕ, and vanishes only when $\theta = 0$.

We would now like to investigate the nature of the dependence of $Q-P$ on θ and ϕ as $\theta \to 0$ in case $\mu = +1$. Recalling that $\tilde{z} = \sqrt{1-\tilde{x}^2-\tilde{y}^2}$, in every small neighborhood of $(\tilde{x},\tilde{y},\tilde{z}) = (0,0,1)$, we can view $Q = (\xi,\eta,\zeta)$ as an infinitely differentiable function of $\tilde{x}$ and $\tilde{y}$. Thus,

$$Q = \boldsymbol{\rho} = \tilde{\boldsymbol{\rho}}(\tilde{x},\tilde{y}), \quad P = \boldsymbol{\rho}_0 = \tilde{\boldsymbol{\rho}}(0,0).$$

Expanding $\tilde{\boldsymbol{\rho}}(\tilde{x},\tilde{y})$ a in a Taylor series about $(\tilde{x},\tilde{y}) = (0,0)$, we have

$$Q-P = \tilde{\boldsymbol{\rho}}(\tilde{x},\tilde{y}) - \tilde{\boldsymbol{\rho}}(0,0) \sim \sum_{\substack{i,j\geqslant 0\\ i+j\geqslant 1}} \tilde{\boldsymbol{\rho}}_{i,j}\tilde{x}^i\tilde{y}^j \quad \text{as } \theta\to 0; \qquad \tilde{\boldsymbol{\rho}}_{i,j} = \frac{1}{i!j!}\frac{\partial^{i+j}\tilde{\boldsymbol{\rho}}}{\partial\tilde{x}^i\partial\tilde{y}^j}\bigg|_{(\tilde{x},\tilde{y})=(0,0)}. \tag{3.9}$$

Using the chain rule for partial derivatives, and using the fact that $\partial\tilde{z}/\partial\tilde{x}$ and $\partial\tilde{z}/\partial\tilde{y}$ both vanish at $(\tilde{x},\tilde{y}) = (0,0)$, it can be shown that the linear terms in this series satisfy

$$\tilde{\boldsymbol{\rho}}_{1,0}\tilde{x} + \tilde{\boldsymbol{\rho}}_{0,1}\tilde{y} = \widetilde{J}_0\begin{bmatrix}\tilde{x}\\ \tilde{y}\\ 0\end{bmatrix}; \qquad \widetilde{J}_0 = J(x_0,y_0,z_0)H. \tag{3.10}$$

Thus,

$$Q-P = \sin\theta\left[\widetilde{J}_0\boldsymbol{\sigma}(\phi) + \mathrm{O}(\theta)\right] \quad \text{as } \theta\to 0; \qquad \boldsymbol{\sigma}(\phi) = \begin{bmatrix}\cos\phi\\ \sin\phi\\ 0\end{bmatrix}. \tag{3.11}$$

Note that $\boldsymbol{\sigma}(\phi) \neq 0$ and the matrix $\widetilde{J}_0$ is nonsingular. As a result, $Q-P$ has a *simple* zero at $\theta = 0$, and so does $|Q-P|$.

Lemma 3.6. *Let $\mu = +1$ in (1.8). Then for every β, there holds*

$$|Q-P|^\beta = (\sin\theta)^\beta A_3(\theta,\phi) \quad \textit{for some } A_3(\theta,\phi)\in\mathscr{K}.$$

Proof. Let $B = \widetilde{J}_0^{\mathrm{T}}\widetilde{J}_0 = [b_{ij}]_{i,j=1}^3$. Because $\widetilde{J}_0$ is a nonsingular matrix, B is a real symmetric positive definite matrix. Then, by (3.9),

$$|Q-P|^2 = (Q-P)^{\mathrm{T}}(Q-P) \sim \sum_{\substack{i,j\geqslant 0\\ i+j\geqslant 2}} \omega_{i,j}\tilde{x}^i\tilde{y}^j \quad \text{as } \theta\to 0, \tag{3.12}$$

where $\omega_{2,0} = b_{11}$, $\omega_{0,2} = b_{22}$, and $\omega_{1,1} = b_{12} = b_{21}$ by (3.10). Using the fact that

$$\tilde{x}^i\tilde{y}^j = (\sin\theta)^{i+j}(\cos\phi)^i(\sin\phi)^j = \mathrm{O}(\theta^{i+j}) \quad \text{as } \theta\to 0,$$

we rearrange the expansion of $|Q-P|^2$ in (3.12) according to the size of its terms as $\theta \to 0$. We obtain,

$$|Q-P|^2 \sim \sum_{s=2}^{\infty} \gamma_s(\theta,\phi) \quad \text{as } \theta \to 0, \tag{3.13}$$

where

$$\begin{aligned}\gamma_2(\theta,\phi) &= \omega_{2,0}\tilde{x}^2 + \omega_{0,2}\tilde{y}^2 + 2\omega_{1,1}\tilde{x}\tilde{y} = b_{11}\tilde{x}^2 + b_{22}\tilde{y}^2 + 2b_{12}\tilde{x}\tilde{y},\\ \gamma_s(\theta,\phi) &= \sum_{\substack{i,j\geqslant 0\\ i+j=s}} \omega_{i,j}\tilde{x}^i\tilde{y}^j, \quad s=3,4,\ldots\end{aligned} \tag{3.14}$$

In terms of θ and ϕ, we have

$$\begin{aligned}\gamma_2(\theta,\phi) &= (\sin\theta)^2[b_{11}\cos^2\phi + b_{22}\sin^2\phi + 2b_{12}\cos\phi\sin\phi],\\ \gamma_s(\theta,\phi) &= (\sin\theta)^s \sum_{\substack{i,j\geqslant 0\\ i+j=s}} \omega_{i,j}(\cos\phi)^i(\sin\phi)^j, \quad s=3,4,\ldots\end{aligned} \tag{3.15}$$

Clearly, $\gamma_s(\theta,\phi)$ is a sum of products $(\cos\phi)^i(\sin\phi)^j$ with $i+j$ even (odd) when s is even (odd), and its expansion about $\theta=0$ contains only even (odd) powers of θ when s is even (odd). In addition, $\gamma_s(\theta,\phi)=\mathrm{O}(\theta^s)$ as $\theta \to 0$. Also note that, with i and j even integers, the product $(\cos\phi)^i(\sin\phi)^j$ is an even and π-periodic function of ϕ.

We now rewrite $\gamma_2(\theta,\phi)$ in the form

$$\begin{aligned}&\gamma_2(\theta,\phi) = \gamma_2^{(1)}(\theta,\phi) + \gamma_2^{(2)}(\theta,\phi);\\ &\gamma_2^{(1)}(\theta,\phi) = (\sin\theta)^2[b_{11}\cos^2\phi + b_{22}\sin^2\phi], \quad \gamma_2^{(2)}(\theta,\phi) = (\sin\theta)^2[2b_{12}\cos\phi\sin\phi],\end{aligned} \tag{3.16}$$

and let

$$\begin{aligned}H_0(\theta,\phi) &= \frac{\gamma_2^{(2)}(\theta,\phi)}{\gamma_2^{(1)}(\theta,\phi)} = \frac{2b_{12}\cos\phi\sin\phi}{b_{11}\cos^2\phi + b_{22}\sin^2\phi};\\ H_s(\theta,\phi) &= \frac{\gamma_{s+2}(\theta,\phi)}{\gamma_2^{(1)}(\theta,\phi)} = (\sin\theta)^s \frac{\sum_{\substack{i,j\geqslant 0\\ i+j=s+2}} \omega_{i,j}(\cos\phi)^i(\sin\phi)^j}{b_{11}\cos^2\phi + b_{22}\sin^2\phi}, \quad s=1,2,\ldots\end{aligned} \tag{3.17}$$

(Note that, $b_{11}\cos^2\phi + b_{22}\sin^2\phi \neq 0$ for all ϕ because $b_{11}>0$ and $b_{22}>0$ by the positive definiteness of B.) In addition,

$$|H_0(\theta,\phi)| \leqslant \frac{|b_{12}|}{\sqrt{b_{11}b_{22}}} \equiv v < 1; \qquad H_s(\theta,\phi) = \mathrm{O}(\theta^s) = \mathrm{o}(1) \quad \text{as } \theta \to 0, \quad s=1,2,\ldots \tag{3.18}$$

The assertion that $v<1$ follows from (i) the fact that the maximum of $|H_0(\theta,\phi)|$ is v and (ii) the fact that the matrix B is positive definite, hence $b_{11}b_{22}-b_{12}^2>0$. In terms of the $\widehat{H}(\theta,\phi)$, we now re-express the expansion of $|Q-P|^2$ in (3.13) as in

$$|Q-P|^2 = \gamma_2^{(1)}(\theta,\phi)[1+\widehat{H}(\theta,\phi)]; \qquad \widehat{H}(\theta,\phi) \sim \sum_{s=0}^{\infty} H_s(\theta,\phi) \quad \text{as } \theta \to 0. \tag{3.19}$$

First, from the structure of the $H_s(\theta,\phi)$, we conclude that $\widehat{H}(\theta,\phi)$ is in $\mathscr{K}$ and so is $1+\widehat{H}(\theta,\phi)$. Next, clearly, $\widehat{H}(\theta,\phi) = H_0(\theta,\phi) + \mathrm{o}(1)$ as $\theta \to 0$. By this and by the fact that $|H_0(\theta,\phi)| \leqslant v < 1$, we have that $|\widehat{H}(\theta,\phi)| \leqslant v' < 1$ for some $v' > v$ and all small θ. Thus, we can apply the binomial theorem to (3.19), to obtain the following convergent series representation that is valid for all small θ:

$$|Q-P|^{\beta} = (\sin\theta)^{\beta}(b_{11}\cos^2\phi + b_{22}\sin^2\phi)^{\beta/2} \sum_{k=0}^{\infty} \binom{\beta/2}{k} [\widehat{H}(\theta,\phi)]^k. \tag{3.20}$$

By repeated application of Lemma 3.2 to the terms $[\widehat{H}(\theta,\phi)]^k$, $k=0,1,\ldots$, we conclude that this summation represents a function in $\mathscr{K}$. Observing that the factor $(b_{11}\cos^2\phi+b_{22}\sin^2\phi)^{\beta/2}$ in (3.20) is an even and π-periodic function of ϕ and is independent of θ, we complete the proof. We leave the details to the reader. □

3.3.2. Study of $(Q-P)\cdot\mathbf{n}_Q$

Let us treat the variables $\tilde{x}$ and $\tilde{y}$ as the parameters that describe S. Thus, the outward normal $\mathbf{n}_Q$ to S at the point $Q=\tilde{\boldsymbol{\rho}}(\tilde{x},\tilde{y})$ is given by

$$\mathbf{n}_Q=\frac{\mathbf{L}(\tilde{x},\tilde{y})}{\|\mathbf{L}(\tilde{x},\tilde{y})\|};\qquad \mathbf{L}(\tilde{x},\tilde{y})=\frac{\partial\tilde{\boldsymbol{\rho}}(\tilde{x},\tilde{y})}{\partial\tilde{x}}\times\frac{\partial\tilde{\boldsymbol{\rho}}(\tilde{x},\tilde{y})}{\partial\tilde{y}}. \tag{3.21}$$

Then, remembering that $P\in S$, and that it is the image in (transformed) U (with $\mu=+1$) of the point with coordinates $(\tilde{x},\tilde{y},\tilde{z})=(0,0,1)$, we have

$$\frac{\partial\tilde{\boldsymbol{\rho}}(\tilde{x},\tilde{y})}{\partial\tilde{x}}\sim\sum_{i,j\geqslant 0}^{\infty}(i+1)\tilde{\boldsymbol{\rho}}_{i+1,j}\tilde{x}^i\tilde{y}^j\quad\text{as }\theta\to 0,$$

$$\frac{\partial\tilde{\boldsymbol{\rho}}(\tilde{x},\tilde{y})}{\partial\tilde{y}}\sim\sum_{i,j\geqslant 0}^{\infty}(j+1)\tilde{\boldsymbol{\rho}}_{i,j+1}\tilde{x}^i\tilde{y}^j\quad\text{as }\theta\to 0,$$

with $\tilde{\boldsymbol{\rho}}_{i,j}$ as defined in (3.9). Consequently,

$$\mathbf{L}(\tilde{x},\tilde{y})\sim\boldsymbol{\alpha}_{0,0}+\sum_{\substack{i,j\geqslant 0\\ i+j\geqslant 1}}^{\infty}\boldsymbol{\alpha}_{i,j}\tilde{x}^i\tilde{y}^j\quad\text{as }\theta\to 0;\qquad \boldsymbol{\alpha}_{0,0}=\tilde{\boldsymbol{\rho}}_{1,0}\times\tilde{\boldsymbol{\rho}}_{0,1}, \tag{3.22}$$

where $\boldsymbol{\alpha}_{i,j}$ are constant vectors and $\boldsymbol{\alpha}_{0,0}$ is a *nonzero* vector in the direction of $\mathbf{n}_P$. Hence $\|\mathbf{L}(\tilde{x},\tilde{y})\|^\beta=\|\boldsymbol{\alpha}_{0,0}+\mathrm{o}(1)\|^\beta$ as $\theta\to 0$, and, therefore,

$$\|\mathbf{L}(\tilde{x},\tilde{y})\|^\beta=D_1(\theta,\phi)\quad\text{for some }D_1(\theta,\phi)\in\mathscr{K},\ \text{for every }\beta. \tag{3.23}$$

From (3.9), we have

$$Q-P=(\tilde{\boldsymbol{\rho}}_{1,0}\tilde{x}+\tilde{\boldsymbol{\rho}}_{0,1}\tilde{y})+\left(\tilde{\boldsymbol{\rho}}_{2,0}\tilde{x}^2+\tilde{\boldsymbol{\rho}}_{1,1}\tilde{x}\tilde{y}+\tilde{\boldsymbol{\rho}}_{0,2}\tilde{y}^2\right)+M(\tilde{x},\tilde{y}), \tag{3.24}$$

where $M(\tilde{x},\tilde{y})$ has a Taylor series expansion about $(0,0)$ that contains the powers $\tilde{x}^i\tilde{y}^j$, $i+j\geqslant 3$. Because $\boldsymbol{\alpha}_{0,0}=\tilde{\boldsymbol{\rho}}_{1,0}\times\tilde{\boldsymbol{\rho}}_{0,1}$ is orthogonal to $\tilde{\boldsymbol{\rho}}_{1,0}$ and $\tilde{\boldsymbol{\rho}}_{0,1}$, and because $\tilde{x}^i\tilde{y}^j=(\sin\theta)^{i+j}(\cos\phi)^i(\sin\phi)^j=\mathrm{O}(\theta^{i+j})$ as $\theta\to 0$, by (3.22) and (3.24), we obtain in terms of the variables θ and ϕ

$$(Q-P)\cdot\mathbf{L}(\tilde{x},\tilde{y})=D_2(\theta,\phi)\sin^2\theta\quad\text{for some }D_2(\theta,\phi)\in\mathscr{K}. \tag{3.25}$$

Combining (3.21), (3.23), and (3.25), and proceeding as before, we obtain the following result:

Lemma 3.7. *Let $\mu=+1$ in (1.8). Then*

$$(Q-P)\cdot\mathbf{n}_Q=(\sin\theta)^2D(\theta,\phi)\quad\textit{for some }D(\theta,\phi)\in\mathscr{K}.$$

3.3.3. Asymptotic expansions of the singular factors V(Q)

Using Lemmas 3.2, 3.6, and 3.7, we obtain the following result concerning the singular factors in (3.8):

Lemma 3.8. *Let $\mu=+1$ in (1.8). Then*

$$V(Q)=V(\xi,\eta,\zeta)=(\sin\theta)^{-1}A_4(\theta,\phi)\quad\textit{for some }A_4(\theta,\phi)\in\mathscr{K}.$$

3.4. Asymptotic expansions of $F(\theta,\phi)$

We now combine the results that we obtained above in $F(\theta,\phi)$. Let us recall that

$$F(\theta,\phi)=g(\xi,\eta,\zeta)\widetilde{R}(\tilde{x},\tilde{y},\tilde{z})V(\xi,\eta,\zeta)\sin\theta. \tag{3.26}$$

By the fact that $g(\xi,\eta,\zeta) = A_1(\theta,\phi) \in \mathscr{K}$, $\widetilde{R}(\tilde{x},\tilde{y},\tilde{z}) = A_2(\theta,\phi) \in \mathscr{K}$, by Lemma 3.8, and by Lemma 3.2, we have that $F(\theta,\phi) = A(\theta,\phi) \in \mathscr{K}$ when $\mu = +1$ in (1.8). This result, of course, concerns the behavior of $F(\theta,\phi)$ as $\theta \to 0$ only. As for the behavior of $F(\theta,\phi)$ as $\theta \to \pi$, by the fact that $g(\xi,\eta,\zeta)$, $\widetilde{R}(\tilde{x},\tilde{y},\tilde{z})$, and $V(\xi,\eta,\zeta)$ are all infinitely differentiable in every small neighborhood of $(\tilde{x},\tilde{y},\tilde{z}) = (0,0,-1)$, it follows from the developments in [11, Section 3] that $F(\theta,\phi) = (\sin\theta)A'(\pi-\theta,\phi)$ for some $A'(\theta,\phi) \in \mathscr{K}$. The complete details are given in Theorem 3.9 below, whose proof is left to the reader.

Theorem 3.9. *The transformed integrand $F(\theta,\phi)$ is infinitely differentiable for all θ and ϕ. Furthermore,*

(i) *When $\mu = +1$ in (1.8), the integrand $F(\theta,\phi)$ satisfies*

$$\begin{aligned} &F(\theta,\phi) = D_0^+(\theta,\phi) \quad \text{for some } D_0^+(\theta,\phi) \text{ in } \mathscr{K}, \\ &F(\theta,\phi) = (\pi-\theta)D_\pi^+(\pi-\theta,\phi) \quad \text{for some } D_\pi^+(\theta,\phi) \text{ in } \mathscr{K}. \end{aligned} \tag{3.27}$$

(ii) *When $\mu = -1$ in (1.8), the integrand $F(\theta,\phi)$ satisfies*

$$\begin{aligned} &F(\theta,\phi) = \theta D_0^-(\theta,\phi) \quad \text{for some } D_0^-(\theta,\phi) \text{ in } \mathscr{K}, \\ &F(\theta,\phi) = D_\pi^-(\pi-\theta,\phi) \quad \text{for some } D_\pi^+(\theta,\phi) \text{ in } \mathscr{K}. \end{aligned} \tag{3.28}$$

Note that the first of the relations in (3.27) and (3.28) concern the asymptotic expansions of $F(\theta,\phi)$ as $\theta \to 0$ and the second ones concern the asymptotic expansions of $F(\theta,\phi)$ as $\theta \to \pi$.

4. Asymptotic expansions of $v(\theta)$

We next consider the asymptotic behavior of $v(\theta)$, which, we recall, is given by

$$v(\theta) = \int_0^{2\pi} F(\theta,\phi)\,\mathrm{d}\phi,$$

as $\theta \to 0$ and $\theta \to \pi$. This we achieve by using Lemma 3.1 in [11] (originally, Lemma 3.1 in [6]), which we reproduce here for convenience as Lemma 4.1.

Lemma 4.1. *Let $M(\phi)$ be an even and π-periodic function of ϕ. Define $u(\phi) = M(\phi)(\cos\phi)^i(\sin\phi)^j$ and $q_{i,j} = \int_0^{2\pi} u(\phi)\mathrm{d}\phi$. If i or j or both are odd integers, then $q_{i,j} = 0$. Thus, $q_{i,j}$ is possibly nonzero if and only if i and j are both even integers.*

An important implication of Lemma 4.1 that concerns functions $A(\theta,\phi) \in \mathscr{K}$ (precisely as in Definition 3.1) is the following:

$$\int_0^{2\pi} A(\theta,\phi)\mathrm{d}\phi \sim \sum_{i=0}^{\infty}\left[\int_0^{2\pi} c_{1i}(\phi)\mathrm{d}\phi\right]\theta^{2i} \quad \text{as } \theta \to 0. \tag{4.1}$$

Note that the only contribution to the asymptotic expansion of $\int_0^{2\pi} A(\theta,\phi)\mathrm{d}\phi$ comes from $M_1(\theta,\phi)$; $M_2(\theta,\phi)$, $N_1(\theta,\phi)$, and $N_2(\theta,\phi)$ contribute nothing by Lemma 4.1.

Theorem 4.2 below, whose proof we leave to the reader, follows from Theorem 3.9 and (4.1). It also covers Theorems 3.1 and 3.2 in [9] as a special case.

Theorem 4.2

(i) *When $\mu = +1$ in (1.8), the integral $v(\theta)$ satisfies*

$$v(\theta) \sim \sum_{i=0}^{\infty} \mu_i^{(+,0)}\theta^{2i} \quad \text{as } \theta \to 0, \qquad v(\theta) \sim \sum_{i=0}^{\infty} \mu_i^{(+,\pi)}(\pi-\theta)^{2i+1} \quad \text{as } \theta \to \pi. \tag{4.2}$$

(ii) *When $\mu = -1$ in (1.8), the integral $v(\theta)$ satisfies*

$$v(\theta) \sim \sum_{i=0}^{\infty} \mu_i^{(-,0)}\theta^{2i+1} \quad \text{as } \theta \to 0, \qquad v(\theta) \sim \sum_{i=0}^{\infty} \mu_i^{(-,\pi)}(\pi-\theta)^{2i} \quad \text{as } \theta \to \pi. \tag{4.3}$$

5. Study of $\widehat{T}_{n,n'}[f]$ under $\Psi_1(t)$

We now analyze the behavior of $\widehat{T}_{n,n'}[f]$ as $h \to 0$ for $\Psi(t) = \Psi_1(t)$ defined in (1.23). Theorem 5.1 that follows and that is the main result of this section is essentially Theorem 4.1 in [9].

For the details of the proof, we refer the reader to [9].

Theorem 5.1. *Let $\psi(t) \in \mathscr{S}_m$. With $\Psi(t) = \Psi_1(t) = \pi\psi(t)$ and with $n' \sim \alpha n^\beta$ as $n \to \infty$ for some fixed positive α and β, there holds*

$$\widehat{T}_{n,n'}[f] - I[f] = \begin{cases} O(h^{2m+2}) & \text{as } h \to 0, \quad \text{if } m \text{ even integer}, \\ O(h^{m+1}) & \text{as } h \to 0, \quad \text{otherwise}. \end{cases}$$

For m an even integer, we also have the complete Euler–Maclaurin expansion

$$\widehat{T}_{n,n'}[f] \sim I[f] + \sum_{i=0}^{\infty} \rho_i h^{2m+2+2i} \quad \text{as } h \to 0.$$

Note the better accuracy that $\widehat{T}_{n,n'}[f]$ can achieve when m is an even integer.

6. Study of $\widehat{T}_{n,n'}[f]$ under $\Psi_2(t)$

We next analyze the behavior of $\widehat{T}_{n,n'}[f]$ as $h \to 0$ for $\Psi(t) = \Psi_2(t)$ defined (1.24). This analysis requires a good understanding of the properties of $\Psi_2(t)$. Therefore, we study $\Psi_2(t)$ first. As can be verified, it is enough to study the case that suits the mapping of the south pole of the transformed U to the point of singularity P on S, that is, the case $\mu = -1$ in (1.8). We recall that, in this case, $\Psi_2(t) = \Psi_{2,S}(t) = 2\pi\psi(\frac{1}{2}\varpi(t))$, where $\varpi \in \mathscr{S}_q$ and $\psi \in \mathscr{S}_m$, with $q > 0$ an even integer and $m > -q/(q+1)$ but arbitrary otherwise.

Below, we will make use of the following facts concerning $\psi \in \mathscr{S}_m$:

$$\psi(0) = 0, \quad \psi(1) = 1; \qquad \psi'(t) > 0 \quad \text{for } t \in (0,1), \tag{6.1}$$

$$\psi'(1-t) = \psi'(t), \qquad \psi(1-t) = 1 - \psi(t), \tag{6.2}$$

$$\psi(t) \sim \sum_{i=0}^{\infty} a_i t^{m+2i+1} \quad \text{as } t \to 0+, \tag{6.3}$$

$$\psi(t) \sim 1 - \sum_{i=0}^{\infty} a_i (1-t)^{m+2i+1} \quad \text{as } t \to 1-. \tag{6.4}$$

From (6.2), it follows that

$$\psi\left(\frac{1}{2}\right) = \frac{1}{2}; \qquad \psi^{(2k)}\left(\frac{1}{2}\right) = 0, \quad k = 1, 2, \ldots, \tag{6.5}$$

so that

$$\psi(t) \sim \frac{1}{2} + \sum_{k=0}^{\infty} b_k \left(\frac{1}{2} - t\right)^{2k+1} \quad \text{as } t \to \frac{1}{2}. \tag{6.6}$$

Lemma 6.1. *The function $\Psi_{2,S}(t)$ has the asymptotic expansions*

$$\Psi_{2,S}(t) \sim \sum_{i=0}^{\infty} c_i t^{M+2i+1} \quad \text{as } t \to 0+; \qquad M = (q+1)(m+1) - 1, \tag{6.7}$$

and

$$\Psi_{2,S}(t) \sim \pi - \sum_{i=0}^{\infty} d_i (1-t)^{q+2i+1} \quad \text{as } t \to 1-. \tag{6.8}$$

Therefore, there also hold

$$\Psi'_{2,S}(t) \sim \sum_{i=0}^{\infty} c'_i t^{M+2i} \quad as\ t \to 0+, \tag{6.9}$$

and

$$\Psi'_{2,S}(t) \sim \sum_{i=0}^{\infty} d'_i (1-t)^{q+2i} \quad as\ t \to 1-. \tag{6.10}$$

Proof. We start by observing that, by (6.3),

$$\varpi(t) \sim \sum_{i=0}^{\infty} \tilde{a}_i t^{q+2i+1} \quad \text{as } t \to 0+, \tag{6.11}$$

so that $\varpi(t) = O(t^{q+1}) = o(1)$ as $t \to 0+$ since $q > 0$. Thus, again by (6.3),

$$\Psi_{2,S}(t) \sim 2\pi \sum_{i=0}^{\infty} a_i \left[\frac{1}{2}\varpi(t)\right]^{m+2i+1} \quad \text{as } t \to 0+. \tag{6.12}$$

Substituting (6.11) in (6.12), and re-expanding in powers of t, and realizing that

$$u(t) \sim \sum_{i=0}^{\infty} d_i t^{s+2i} \quad \text{as } t \to 0+ \Rightarrow [u(t)]^{\alpha} \sim \sum_{i=0}^{\infty} e_i t^{\alpha s+2i} \quad \text{as } t \to 0+, \tag{6.13}$$

we obtain the result in (6.7).

For the proof of (6.8), we proceed as follows: By (6.4), we have

$$\varpi(t) \sim 1 - \sum_{i=0}^{\infty} \tilde{a}_i (1-t)^{q+2i+1} \quad \text{as } t \to 1-, \tag{6.14}$$

hence $\lim_{t\to 1-}[\frac{1}{2}\varpi(t)] = \frac{1}{2}$. By this and by (6.6), there holds

$$\Psi_{2,S}(t) \sim \pi - 2\pi \sum_{k=0}^{\infty} b_k \left[\frac{1}{2} - \frac{1}{2}\varpi(t)\right]^{2k+1} \quad \text{as } t \to 1-. \tag{6.15}$$

Substituting (6.14) in (6.15), and re-expanding in powers of t with (6.13) in mind, we obtain the result in (6.8). □

Theorem 6.2 that follows and that is the main result of this section is the analogue of Theorem 4.2 in [9].

Theorem 6.2. *With $\Psi(t) = \Psi_{2,S}(t)$ when $\mu = -1$ in (1.8), or $\Psi(t) = \Psi_{2,N}(t)$ when $\mu = +1$ in (1.8), and with $n' \sim \alpha n^{\beta}$ as $n \to \infty$ for some fixed positive α and β, there holds*

$$\widehat{T}_{n,n'}[f] - I[f] = \begin{cases} O(h^{4M+4}) & as\ h \to 0, \quad \text{if } 2M \text{ odd integer}, \\ O(h^{2M+2}) & as\ h \to 0, \quad otherwise, \end{cases} \tag{6.16}$$

where $M = (m+1)(q+1) - 1$, as in (6.7). For $2M$ an odd integer, we also have the complete Euler–Maclaurin expansion

$$\widehat{T}_{n,n'}[f] \sim I[f] + \sum_{i=0}^{\infty} \rho_i h^{4M+4+2i} \quad as\ h \to 0. \tag{6.17}$$

Remark. Note that, because q is an (even) integer, $2M$ can be an odd integer if and only if $2(q+1)m$ is an odd integer. Thus, when $q = 2$, which is the value we have chosen for q in our numerical examples, $2M$ is an odd integer if and only if $6m$ is an odd integer.

Proof. As we have seen earlier, we have to analyze the asymptotic behavior of $\widetilde{T}_n[f]$, the trapezoidal rule approximation of the one-dimensional integral, $\int_0^1 \hat{v}(t)\mathrm{d}t$, where $\hat{v}(t) = v(\Psi(t))\Psi'(t)$. Here, we give the proof for the case $\mu = -1$, hence $\Psi(t) = \Psi_{2,\mathrm{S}}(t)$. In this case, $v(\theta)$ has the asymptotic expansions given in (4.3) in Theorem 4.2. Thus,

$$\hat{v}(t) \sim \Psi'(t)\sum_{i=0}^{\infty}\mu_i^{(-,0)}[\Psi(t)]^{2i+1} \quad \text{as } t \to 0+, \tag{6.18}$$

$$\hat{v}(t) \sim \Psi'(t)\sum_{i=0}^{\infty}\mu_i^{(-,\pi)}[\pi - \Psi(t)]^{2i} \quad \text{as } t \to 1-. \tag{6.19}$$

Substituting the asymptotic expansions of $\Psi_{2,\mathrm{S}}(t)$ given in (6.7) and (6.8) and those of $\Psi'_{2,\mathrm{S}}(t)$ given in (6.9) and (6.10), and re-expanding in powers of t, we obtain

$$\hat{v}(t) \sim \sum_{i=0}^{\infty} t^{M+(M+1)(2i+1)}\left(\sum_{j=0}^{\infty}\alpha_{i,j}t^{2j}\right) \quad \text{as } t \to 0+, \tag{6.20}$$

$$\hat{v}(t) \sim \sum_{i=0}^{\infty}\beta_i(1-t)^{q+2i} \text{ as } t \to 1-, \tag{6.21}$$

Recalling that q is an even integer, and applying Corollary 2.2 of [7] (see, also Theorem 4.4 of [10]), we obtain the results in (6.16). □

As mentioned in [10], a fair comparison of the effects of two variable transformations demands that their abscissas should have similar amounts of clustering at the endpoints of the integration interval. As mentioned in the same paper, the clustering of the abscissas at the endpoints $t = 0$ and $t = 1$ is determined directly by the asymptotic behavior (as $t \to 0+$ and/or $t \to 1-$) of the variable transformation used. Now, $\Psi_1(t) = \mathrm{O}(t^{m+1})$ as $t \to 0+$ and $\Psi_1(t) = \mathrm{O}((1-t)^{m+1})$ as $t \to 1-$. Similarly, when $\mu = -1$ (and it is enough to look only at this case) $\Psi_{2,\mathrm{S}}(t) = \mathrm{O}(t^{M+1})$ as $t \to 0+$ and $\Psi_{2,\mathrm{S}}(t) = \mathrm{O}((1-t)^{q+1})$ as $t \to 1-$, and because $M \geqslant q$ when $m \geqslant 1$, the amount of clustering is largest at $t = 0$. The conclusion from this is that a fair comparison of the effects of $\Psi_1(t)$ and $\Psi_2(t)$ can be made when $M = (m+1)(q+1) - 1$ for $\Psi_2(t)$ is the same as m in $\Psi_1(t)$. Thus, by Theorems 5.1 and 6.2, the rule $\widehat{T}_{n,n'}[f]$ with $\Psi_2(t)$ is always superior to that with $\Psi_1(t)$.

7. Numerical example

Let S be the surface of the ellipsoid whose equation is $(\xi/a)^2 + (\eta/b)^2 + (\zeta/c)^2 = 1$, and let $f(Q) = g(Q)/|Q - P|$, with $g(Q) = g(\xi, \eta, \zeta) = \exp[0.1(\xi + 2\eta + 3\zeta)]$. We take $(a, b, c) = (1, 2, 3)$ and $P = (\xi_0, \eta_0, \zeta_0) = (1/2, 1, 3/\sqrt{2}) \in S$, and consider the computation of the integral

$$I[f] = \int\int_{\mathrm{S}} f(Q)\mathrm{d}A_{\mathrm{S}} = 38.2549189698039\ldots.$$

This is one of the numerical examples treated in [3].

We take the mapping of U to S to be

$$(\xi, \eta, \zeta) = (ax, by, cz),$$

by which, P is the mapping of

$$(x_0, y_0, z_0) = (\xi_0/a, \eta_0/b, \zeta_0/c) = (1/2, 1/2, 1/\sqrt{2}) \in U.$$

This point is mapped to the south pole via the (orthogonal) Householder matrix H,

$$H = I - 2pp^{\mathrm{T}}, \qquad p = \frac{1}{\sqrt{2+\sqrt{2}}}\begin{bmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2}+1 \end{bmatrix},$$

precisely as in (1.17), that is,

$$\begin{bmatrix} x_0 \\ y_0 \\ z_0 \end{bmatrix} = \mu H \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \mu = -1.$$

The function $R(x, y, z)$ is given as in

$$R(x,y,z) = [(bcx)^2 + (cay)^2 + (abz)^2]^{1/2}; \qquad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}.$$

Clearly, because S is infinitely smooth and $g(Q)$ is infinitely differentiable over S, Theorems 5.1 and 6.2 apply.

The function $\psi(t)$ we use in constructing the variable transformation $\Psi(t)$—whether $\Psi_1(t)$ or $\Psi_2(t)$—for the variable θ is the extended $\sin^m$-transformation for various values of m. This transformation has been used in the numerical examples of [11,9]. The function $\varpi(t)$ used in constructing the variable transformation $\Psi_2(t)$ is the $\sin^q$-transformation. We have chosen the simplest case of $q = 2$ for which $\varpi(t) = t - (\sin 2\pi t)/(2\pi)$.

The numerical results in Tables 1 and 2, which were computed via $\Psi_1(t) = \pi\psi(t)$, and the results in Tables 3 and 4, which were computed via $\Psi_{2,S}(t) = 2\pi\psi(\frac{1}{2}\varpi(t))$, in quadruple-precision arithmetic, illustrate the conclusions of, respectively, Theorems 5.1 and 6.2 very clearly. Tables 1 and 3 give the relative errors in the $\widehat{T}_n[f] \equiv \widehat{T}_{n,n}[f]$, $n = 2^k$, $k = 1, 2, \ldots, 9$, for various values of m. Tables 2 and 4 present the numbers

$$\mu_{m,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\widehat{T}_{2^k}[f] - I[f]|}{|\widehat{T}_{2^{k+1}}[f] - I[f]|} \right)$$

Table 1
Relative errors in the rules $\widehat{T}_n[f] = \widehat{T}_{n,n}[f]$ for the integral of Section 7, obtained via the transformation $\Psi_1(t)$ with $n = 2^k$, $k = 1(1)9$, and $m = 1(1)10$

n	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$	$m = 8$	$m = 9$	$m = 10$
2	6.22D + 00	1.84D + 01	2.85D + 01	3.73D + 01	4.51D + 01	5.24D + 01	5.90D + 01	6.53D + 01	7.12D + 01	7.68D + 01
4	1.40D + 00	1.62D + 00	1.90D + 00	1.34D + 00	7.76D − 01	5.09D − 01	5.95D − 01	1.01D + 00	1.68D + 00	2.57D + 00
8	5.99D − 01	8.98D − 02	1.77D − 01	1.94D − 01	9.45D − 02	6.35D − 02	2.26D − 01	3.60D − 01	4.53D − 01	4.99D − 01
16	1.45D − 01	5.01D − 04	7.05D − 05	9.26D − 04	1.61D − 04	9.12D − 04	6.51D − 03	1.85D − 02	3.64D − 02	5.83D − 02
32	3.61D − 02	2.09D − 08	5.24D − 05	6.39D − 08	3.77D − 07	1.30D − 06	4.22D − 06	4.81D − 06	2.91D − 05	5.20D − 05
64	9.03D − 03	1.46D − 10	3.26D − 06	2.80D − 14	4.69D − 09	4.11D − 12	7.00D − 12	3.90D − 11	1.92D − 10	6.96D − 10
128	2.26D − 03	2.27D − 12	2.04D − 07	1.68D − 18	7.32D − 11	2.04D − 24	5.40D − 14	1.92D − 20	6.68D − 17	1.17D − 18
256	5.64D − 04	3.55D − 14	1.27D − 08	1.64D − 21	1.14D − 12	4.38D − 28	2.11D − 16	1.65D − 29	6.50D − 20	1.65D − 29
512	1.41D − 04	5.55D − 16	7.97D − 10	1.60D − 24	1.79D − 14	1.66D − 29	8.23D − 19	1.65D − 29	6.34D − 23	1.65D − 29

The transformation $\Psi_1(t)$ is as in (1.22), $\psi(t)$ there being the $\sin^m$-transformation.

Table 2
The numbers $\mu_{m,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\widehat{T}_{2^k}[f] - I[f]|}{|\widehat{T}_{2^{k+1}}[f] - I[f]|} \right)$, for $k = 1(1)8$ and $m = 1(1)10$, for the integral of Section 7, where $\widehat{T}_n[f]$ are those of Table 1

k	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$	$m = 8$	$m = 9$	$m = 10$
1	2.154	3.500	3.906	4.802	5.863	6.684	6.632	6.021	5.403	4.903
2	1.223	4.176	3.427	2.780	3.036	3.004	1.399	1.480	1.894	2.362
3	2.046	7.487	11.289	7.714	9.195	6.122	5.115	4.283	3.636	3.098
4	2.006	14.550	0.429	13.822	8.742	9.455	10.593	11.910	10.290	10.131
5	2.000	7.162	4.004	21.122	6.328	18.271	19.200	16.913	17.205	16.190
6	2.000	6.001	4.001	14.022	6.002	40.871	7.017	30.921	21.457	29.150
7	2.000	6.000	4.000	10.002	6.001	12.187	8.001	30.116	10.007	36.044
8	2.000	6.000	4.000	10.001	6.000	4.724	8.000	−0.002	10.001	−0.003

Table 3
Relative errors in the rules $\widehat{T}_n[f] = \widehat{T}_{n,n}[f]$ for the integral of Section 7, obtained via the transformation $\Psi_2(t)$ with $n = 2^k$, $k = 1(1)9$, and $m = -3/6(1/6)6/6$

n	$m=-3/6$ $M=0.5$	$m=-2/6$ $M=1$	$m=-1/6$ $M=1.5$	$m=0$ $M=2$	$m=1/6$ $M=2.5$	$m=2/6$ $M=3$	$m=3/6$ $M=3.5$	$m=4/6$ $M=4$	$m=5/6$ $M=4.5$	$m=6/6$ $M=5$
2	2.34D + 01	3.02D + 01	2.69D + 01	1.84D + 01	8.76D + 00	3.68D − 02	7.42D + 00	1.34D + 01	1.81D + 01	2.19D + 01
4	1.39D + 00	2.90D + 00	2.77D + 00	1.62D + 00	2.97D − 01	8.12D − 01	1.60D + 00	2.07D + 00	2.29D + 00	2.30D + 00
8	2.33D − 02	8.61D − 03	4.38D − 02	8.98D − 02	8.43D − 02	2.04D − 02	7.57D − 02	1.73D − 01	2.49D − 01	2.92D − 01
16	5.72D − 04	5.24D − 04	5.78D − 04	5.01D − 04	5.38D − 04	7.24D − 04	8.37D − 04	7.29D − 04	4.65D − 04	2.15D − 04
32	3.02D − 09	3.57D − 06	3.13D − 08	2.09D − 08	3.50D − 08	2.20D − 08	2.52D − 08	6.06D − 08	6.63D − 08	2.03D − 09
64	5.30D − 10	2.21D − 07	1.45D − 15	1.46D − 10	5.53D − 17	1.96D − 13	3.72D − 16	1.91D − 15	3.51D − 15	3.38D − 15
128	8.27D − 12	1.38D − 08	1.33D − 18	2.27D − 12	1.14D − 24	7.65D − 16	1.65D − 30	4.30D − 19	5.13D − 29	3.63D − 22
256	1.29D − 13	8.62D − 10	1.30D − 21	3.55D − 14	6.94D − 29	2.99D − 18	2.47D − 32	4.19D − 22	9.86D − 32	8.84D − 26
512	2.02D − 15	5.39D − 11	1.27D − 24	5.55D − 16	3.70D − 32	1.17D − 20	1.23D − 32	4.10D − 25	9.24D − 32	2.16D − 29

The transformation $\Psi_2(t)$ is as in (1.23), $\psi(t)$ and $\varpi(t)$ there being the $\sin^m$-transformation and the $\sin^2$-transformation, respectively.

Table 4
The numbers $\mu_{m,k} = \frac{1}{\log 2} \cdot \log\left(\frac{|\widehat{T}_{2^k}[f]-I[f]|}{|\widehat{T}_{2^{k+1}}[f]-I[f]|}\right)$, for $k = 1(1)8$ and $m = -3/6(1/6)6/6$, for the integral of Section 7, where $\widehat{T}_n[f]$ are those of Table 3

k	$m=-3/6$ $M=0.5$	$m=-2/6$ $M=1$	$m=-1/6$ $M=1.5$	$m=0$ $M=2$	$m=1/6$ $M=2.5$	$m=2/6$ $M=3$	$m=3/6$ $M=3.5$	$m=4/6$ $M=4$	$m=5/6$ $M=4.5$	$m=6/6$ $M=5$
1	4.072	3.382	3.281	3.500	4.883	−4.465	2.217	2.694	2.988	3.249
2	5.902	8.395	5.981	4.176	1.815	5.316	4.398	3.579	3.196	2.979
3	5.346	4.039	6.243	7.487	7.291	4.815	6.500	7.893	9.066	10.409
4	17.530	7.197	14.173	14.550	13.910	15.007	15.021	13.554	12.778	16.691
5	2.512	4.015	24.362	7.162	29.236	16.775	26.010	24.916	24.172	19.196
6	6.001	4.001	10.093	6.001	25.531	8.001	47.680	12.120	45.957	23.152
7	6.000	4.000	10.001	6.000	14.005	8.001	6.066	10.001	9.024	12.002
8	6.000	4.000	10.000	6.000	10.874	8.000	1.000	10.000	0.093	12.003

for the same values of m and for $k = 1, 2, \ldots, 8$. It is seen that, with increasing k, the $\mu_{m,k}$ in Table 2 are tending to $2m + 2$ for even integer values of m, while for other values of m, the $\mu_{m,k}$ are tending to $m + 1$, completely in accordance with Theorem 5.1. It is also seen that, with increasing k, the $\mu_{m,k}$ in Table 4 are tending to $4M + 4$ for odd integer values of $2M = 2[3(m + 1) - 1] = 6m + 4$, while for other values of M, the $\mu_{m,k}$ are tending to $2M + 2$, completely in accordance with Theorem 6.2. Note that, with $q = 2$, $2M$ is an odd integer $\geqslant 1$ when $m = (2j - 5)/6$, $j = 1, 2, \ldots$

8. Concluding remarks

In this work, we have described numerical quadrature formulas based on the trapezoidal rule for computing integrals of functions with point singularities over smooth surfaces in $\mathbb{R}^3$ that are homeomorphic to the unit sphere. These formulas are obtained as follows: We first transform the integrals to the unit sphere mapping the point of singularity to one of the poles of the unit sphere, and express the transformed integrals in terms of the standard spherical coordinates θ and ϕ, $0 \leqslant \theta \leqslant \pi$ and $0 \leqslant \phi \leqslant 2\pi$. We then transform the variable θ via $\theta = \Psi(t)$, $0 \leqslant t \leqslant 1$, where $\Psi(t)$ is a variable transformation related to a transformation in the class $\mathscr{S}_m$; this is done in two different ways. Finally, we apply the product trapezoidal rule to the integral in t and ϕ. We have shown that, with one of the variable transformations, the error in the approximations obtained can be as high as $O(h^{2m+2})$ when m is an even integer, while with the other transformation, the error can be as high as $O(h^{4M+4})$ with $M = (m + 1)(q + 1) - 1$, when $2M$ is an odd integer or, equivalently, when $2(q + 1)m$ is an odd integer, where, we recall, q is an even integer.

Acknowledgement

The author wishes to thank Professor Kendall E. Atkinson for making available his lecture notes that preceded [3] and for a very interesting discussion that inspired this work.

Appendix. Proof of Theorem 3.5

By (3.3), we first have (see also [11, Eq. (2.10)])

$$\tilde{\sigma}_{ij} = \begin{vmatrix} \partial\xi_i/\partial\tilde{x}_1 & \partial\xi_i/\partial\tilde{x}_2 & \partial\xi_i/\partial\tilde{x}_3 \\ \partial\xi_j/\partial\tilde{x}_1 & \partial\xi_j/\partial\tilde{x}_2 & \partial\xi_j/\partial\tilde{x}_3 \\ \tilde{x}_1 & \tilde{x}_2 & \tilde{x}_3 \end{vmatrix}. \tag{A.1}$$

Next,

$$\frac{\partial\xi_i}{\partial\tilde{x}_s} = \sum_{p=1}^{3} \frac{\partial\xi_i}{\partial x_p}[H]_{ps}. \tag{A.2}$$

Next, $\mathbf{r} = H\tilde{\mathbf{r}}$ by (1.8), so that $\tilde{\mathbf{r}} = H^{-1}\mathbf{r}$, which, by the fact that $H^{-1} = H^{\mathrm{T}}$, becomes $\tilde{\mathbf{r}} = H^{\mathrm{T}}\mathbf{r}$. Consequently,

$$\tilde{x}_k = \sum_{r=1}^{3}[H^{\mathrm{T}}]_{kr}x_r = \sum_{r=1}^{3}[H]_{rk}x_r. \tag{A.3}$$

Substituting (A.2) and (A.3) in (A.1), the determinant expression for $\tilde{\sigma}_{ij}$ becomes

$$\tilde{\sigma}_{ij} = \begin{vmatrix} \sum_{p=1}^{3}\partial\xi_i/\partial x_p[H]_{p1} & \sum_{p=1}^{3}\partial\xi_i/\partial x_p[H]_{p2} & \sum_{p=1}^{3}\partial\xi_i/\partial x_p[H]_{p3} \\ \sum_{q=1}^{3}\partial\xi_j/\partial x_q[H]_{q1} & \sum_{q=1}^{3}\partial\xi_j/\partial x_q[H]_{q2} & \sum_{q=1}^{3}\partial\xi_j/\partial x_q[H]_{q3} \\ \sum_{r=1}^{3}[H]_{r1}x_r & \sum_{r=1}^{3}[H]_{r2}x_r & \sum_{r=1}^{3}[H]_{r3}x_r \end{vmatrix},$$

which, by the multilinearity property of determinants, in turn, becomes

$$\tilde{\sigma}_{ij} = \sum_{p=1}^{3}\sum_{q=1}^{3}\sum_{r=1}^{3} \frac{\partial\xi_i}{\partial x_p}\frac{\partial\xi_j}{\partial x_q}x_r V_{pqr}, \tag{A.4}$$

where

$$V_{pqr} = \begin{vmatrix} [H]_{p1} & [H]_{p2} & [H]_{p3} \\ [H]_{q1} & [H]_{q2} & [H]_{q3} \\ [H]_{r1} & [H]_{r2} & [H]_{r3} \end{vmatrix}.$$

Clearly,

$$V_{pqr} = \epsilon_{pqr}(\det H), \tag{A.5}$$

where $\epsilon_{123} = 1$ and ϵ_{pqr} is odd under an interchange of any two of the indices p, q, and r, which means that $\epsilon_{pqr} = 0$ when any two of these indices have the same value. Substituting (A.5) in (A.4), we thus obtain

$$\tilde{\sigma}_{ij} = (\det H)\sum_{p=1}^{3}\sum_{q=1}^{3}\sum_{r=1}^{3} \epsilon_{pqr}\frac{\partial\xi_i}{\partial x_p}\frac{\partial\xi_j}{\partial x_q}x_r,$$

which can be rewritten in the form

$$\tilde{\sigma}_{ij} = (\det H)\begin{vmatrix} \partial\xi_i/\partial x_1 & \partial\xi_i/\partial x_2 & \partial\xi_i/\partial x_3 \\ \partial\xi_j/\partial x_1 & \partial\xi_j/\partial x_2 & \partial xi_j/\partial x_3 \\ x_1 & x_2 & x_3 \end{vmatrix} = (\det H)[(\nabla\xi_i \times \nabla\xi_j)\cdot \boldsymbol{r}] = (\det H)\sigma_{ij}. \tag{A.6}$$

By (A.6), the fact that H is orthogonal and hence $|\det H| = 1$, and (3.3) and (3.5), we obtain $\widetilde{R}(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3) = R(x_1, x_2, x_3)$. This completes the proof of (3.6). The result in (3.7) is an immediate consequence of (3.6) and (3.4).

References

[1] K.E. Atkinson, The numerical solution of boundary integral equations, in: I.S. Duff, G.A. Watson (Eds.), State of the Art in Numerical Analysis, Oxford University Press, Oxford, 1997, pp. 223–259.

[2] K.E. Atkinson, The Numerical Solution of Integral Equations of the Second Kind, Cambridge Monographs on Applied and Computational Mathematics, vol. 4, Cambridge University Press, Cambridge, 1997.

[3] K.E. Atkinson, Quadrature of singular integrands over surfaces, Electr. Trans. Numer. Anal. 17 (2004) 133–150.

[4] K.E. Atkinson, A. Sommariva, Quadrature over the sphere, Electr. Trans. Numer. Anal. 20 (2005) 104–118.

[5] A. Sidi, A new variable transformation for numerical integration, in: H. Brass, G. Hämmerlin (Eds.), Numerical Integration IV, ISNM, vol. 112, Birkhäuser, Basel, 1993, pp. 359–373.

[6] A. Sidi, Class $\mathscr{S}_m$ variable transformations and application to numerical integration over smooth surfaces in $\mathbb{R}^3$, Computer Science Department, Technion – Israel Institute of Technology, 2003, preprint.

[7] A. Sidi, Euler–Maclaurin expansions for integrals with endpoint singularities: a new perspective, Numer. Math. 98 (2004) 371–387.

[8] A. Sidi, Analysis of Atkinson's variable transformation for numerical integration over smooth surfaces in $\mathbb{R}^3$, Numer. Math. 100 (2005) 519–536.

[9] A. Sidi, Application of class $\mathscr{S}_m$ variable transformations to numerical integration over surfaces of spheres, J. Comput. Appl. Math. 184 (2005) 475–492.

[10] A. Sidi, Extension of a class of periodizing variable transformations for numerical integration, Math. Comput. 75 (2006) 327–343.

[11] A. Sidi, Numerical integration over smooth surfaces in $\mathbb{R}^3$ via class $\mathscr{S}_m$ variable transformations. Part I: Smooth integrands, Appl. Math. Comput. 171 (2005) 646–674.