

Analysis of Atkinson's variable transformation for numerical integration over smooth surfaces in \mathbb{R}^3

Avram Sidi

Computer Science Department, Technion - Israel Institute of Technology, Haifa 32000,
Israel; e-mail: asidi@cs.technion.ac.il

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Summary. Recently, a variable transformation for integrals over smooth surfaces in \mathbb{R}^3 was introduced in a paper by Atkinson. This interesting transformation, which includes a “grading” parameter that can be fixed by the user, makes it possible to compute these integrals numerically via the product trapezoidal rule in an efficient manner. Some analysis of the approximations thus produced was provided by Atkinson, who also stated some conjectures concerning the unusually fast convergence of his quadrature formulas observed for certain values of the grading parameter. In a recent report by Atkinson and Sommariva, this analysis is continued for the case in which the integral is over the surface of a sphere and the integrand is smooth over this surface, and optimal results are given for special values of the grading parameter. In the present work, we give a complete analysis of Atkinson's method over arbitrary smooth surfaces that are homeomorphic to the surface of the unit sphere. We obtain optimal results that explain the actual rates of convergence, and we achieve this for all values of the grading parameter.

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1 Introduction

Recently, Atkinson [2] considered the problem of numerically computing the integral

$$(1.1) \quad I[f] = \iint_S f(\xi, \eta, \zeta) dA_S,$$

where S is the surface of an arbitrary bounded and simply connected body in \mathbb{R}^3 and dA_S is the associated area element. We assume that S is infinitely smooth and homeomorphic to the surface U of the unit sphere; namely, to the set

$$(1.2) \quad U = \{(x, y, z) : x^2 + y^2 + z^2 = 1\}.$$

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 [2], Atkinson considers both smooth integrands $f(\xi, \eta, \zeta)$ and ones with point singularities of the single and double layer types. In the present work, we restrict our attention to smooth integrands; thus, $f \in C^\infty(S)$ throughout our treatment.

In his method, Atkinson first makes the following change of variables on U :

$$(1.3) \quad (x, y, z) = (\psi(\theta) \cos \phi, \psi(\theta) \sin \phi, v(\theta));$$

$$\psi(\theta) = \frac{\sin^q \theta}{(\cos^2 \theta + \sin^{2q} \theta)^{1/2}}, \quad v(\theta) = \frac{\cos \theta}{(\cos^2 \theta + \sin^{2q} \theta)^{1/2}},$$

$$0 \leq \theta \leq \pi, \quad 0 \leq \phi \leq 2\pi.$$

Obviously, when $q = 1$, (θ, ϕ) are simply the standard spherical coordinates on U . For $q > 1$, the variable θ is being “graded” in such a way that the north and south poles of U remain fixed, but the areas around them are distorted. Following this transformation of variables, Atkinson proposes to approximate the resulting (transformed) integral by the product trapezoidal rule with the same stepsize in both θ and ϕ . The complete mathematical description of this procedure is given in the next paragraph.

Denote the mapping from U to S via

$$(1.4) \quad \boldsymbol{\rho} = [\xi, \eta, \zeta]^T = [\xi(x, y, z), \eta(x, y, z), \zeta(x, y, z)]^T,$$

so that the Jacobian matrix of this mapping is

$$(1.5) \quad J(x, y, z) = \begin{bmatrix} \partial\xi/\partial x & \partial\xi/\partial y & \partial\xi/\partial z \\ \partial\eta/\partial x & \partial\eta/\partial y & \partial\eta/\partial z \\ \partial\zeta/\partial x & \partial\zeta/\partial y & \partial\zeta/\partial z \end{bmatrix}.$$

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

$$(1.6) \quad \mathbf{r} = [x, y, z]^T.$$

Now, by expressing $I[f]$ as an integral over U via (1.4), and by introducing the variables θ and ϕ on U as in (1.3), 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 dA_S on S becomes

$$(1.7) \quad dA_S = \left\| \frac{\partial \boldsymbol{\rho}}{\partial \theta} \times \frac{\partial \boldsymbol{\rho}}{\partial \phi} \right\| d\theta d\phi,$$

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

$$(1.8) \quad I[f] = \int_0^\pi \left[\int_0^{2\pi} F(\theta, \phi) d\phi \right] d\theta; \quad F(\theta, \phi) \equiv f(\xi, \eta, \zeta) \left\| \frac{\partial \boldsymbol{\rho}}{\partial \theta} \times \frac{\partial \boldsymbol{\rho}}{\partial \phi} \right\|.$$

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

$$(1.9) \quad \frac{\partial \boldsymbol{\rho}}{\partial \theta} = J \frac{\partial \mathbf{r}}{\partial \theta}, \quad \frac{\partial \boldsymbol{\rho}}{\partial \phi} = J \frac{\partial \mathbf{r}}{\partial \phi}.$$

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

$$(1.10) \quad \frac{\partial \mathbf{r}}{\partial \theta} = \begin{bmatrix} \psi'(\theta) \cos \phi \\ \psi'(\theta) \sin \phi \\ \nu'(\theta) \end{bmatrix}, \quad \frac{\partial \mathbf{r}}{\partial \phi} = \psi(\theta) \begin{bmatrix} -\sin \phi \\ \cos \phi \\ 0 \end{bmatrix}.$$

As mentioned above, Atkinson approximates the transformed integral $\int_0^\pi [\int_0^{2\pi} F(\theta, \phi) d\phi] d\theta$ via the product trapezoidal rule with stepsize $h = \pi/n$ both in θ and ϕ , where n is some positive integer. In the present work, we take the product trapezoidal rule with *different* stepsizes in θ and ϕ via

$$(1.11) \quad T_{n,n'}[F] = hh' \sum_{j=1}^{n-1} \sum_{k=1}^{n'} F(jh, kh'); \quad h = \frac{\pi}{n}, \quad h' = \frac{2\pi}{n'},$$

where n and n' are positive integers. In the sequel, we let $n' \sim \alpha n^\beta$ as $n \rightarrow \infty$ for some fixed positive constants α and β . (Thus, in [2], $n' = 2n$, in which case $h' = h$.)

Note that the product trapezoidal rule for an arbitrary integral $\int_0^\pi [\int_0^{2\pi} F(\theta, \phi) d\phi] d\theta$, where $F(\theta, \phi)$ is continuous for $(\theta, \phi) \in [0, \pi] \times [0, 2\pi]$, is actually $hh' \sum''_{j=0}^n \sum''_{k=0}^{n'} F(jh, kh')$, where the double prime on a summation means that the first and the last terms in the summation are to be multiplied by $1/2$. $T_{n,n'}[F]$ in (1.11) is indeed the product trapezoidal rule because (i) $F(\theta, \phi)$ is 2π -periodic in ϕ , and (ii) $F(0, \phi) = 0 = F(\pi, \phi)$, which is the case we have here, as we will see shortly.

The variable transformation above turns out to be very effective in that the accuracy of $T_{n,n'}[F]$ increases with increasing q . Some analysis of the error has been carried out by Atkinson [2] for integration over U . In this paper, Atkinson reports that very high accuracies are achieved for certain values of q ; for example, he reports that when $f(\xi, \eta, \zeta)$ is smooth over S , especially high accuracies are obtained with $2q$ equal to an odd integer. Actual rates of convergence are not given in [2], however. Further analysis, again for the case of integration of smooth $f(\xi, \eta, \zeta)$ over U , the surface of the unit sphere, is given in a recent work of Atkinson and Sommariva [3], where results are

given for special values of q . We mention these results in the last section of this paper.

In the present work, we tackle the general problem in which integration is carried out on S , the surface of an arbitrary bounded and simply connected body in \mathbb{R}^3 , precisely as explained in the first paragraph of this section, and with different stepsizes for the variables θ and ϕ , and prove optimal results concerning $T_{n,n}[F]$ for *all* values of q . The proof techniques we use here are those introduced in the paper Sidi [7] for the same integrals, but with a different variable transformation of the author. The variable transformation of [7] belongs to the extension of the class \mathcal{S}_m , which was previously introduced in the paper Sidi [6]. Surprisingly, the approximations introduced in [2] and [7] seem to have very similar mathematical and numerical properties. The extended class \mathcal{S}_m transformations and their analysis appear also in a separate paper [10] by the author. The application of the variable transformations in the extended class \mathcal{S}_m to the same problem is also treated in greater detail in the paper Sidi [11].

In Section 2, we give some important theoretical preliminaries. Following these, in Sections 3 and 4 we give the optimal convergence results concerning the cases, respectively, (i) $2q \neq$ odd integer, for which the error is $O(h^{2q})$, and (ii) $2q =$ odd integer, for which the error is $O(h^{4q})$. Theorems 3.1 and 4.2 are the main results of this work.

Note that Euler–Maclaurin expansions concerning the trapezoidal rule approximations of finite-range integrals $\int_a^b u(x) dx$ are the main analytical tool we use in our study. For the sake of easy reference, we reproduce here the relevant Euler–Maclaurin expansions as Theorems 1.1 and 1.2. Of these, Theorem 1.1, concerns the integrals $\int_a^b u(x) dx$ in the case the integrands $u(x)$ are in $C^{2m}[a, b]$; this theorem can be found in most books on numerical analysis. See, for example, Davis and Rabinowitz [4], Ralston and Rabinowitz [5], and Atkinson [1]. See also the brief review in Sidi [8, Appendix D]. Theorem 1.2 is a special case of a very general theorem from Sidi [9] that concerns integrands that are smooth in the open interval (a, b) but may have arbitrary algebraic–logarithmic singularities at $x = a$ and $x = b$, and is expressed in terms of the asymptotic expansions of $u(x)$ as $x \rightarrow a+$ and $x \rightarrow b-$ and is very easy to write down and use. Below, B_k is the k th Bernoulli number and $\zeta(z)$ is the Riemann Zeta function. The following relations are well known:

$$\zeta(0) = -\frac{1}{2}; \quad \zeta(-2j) = 0, \quad \zeta(1-2j) = -\frac{B_{2j}}{2j}, \quad j = 1, 2, \dots$$

Theorem 1.1 *Let $u \in C^{2m}[a, b]$, and let $h = (b - a)/n$ for $n = 1, 2, \dots$. Then, for some $\xi_{m,n} \in (a, b)$,*

$$\begin{aligned}
 h \sum_{i=0}^n u(a + ih) &= \int_a^b u(x) dx + \sum_{k=1}^{m-1} \frac{B_{2k}}{(2k)!} [u^{(2k-1)}(b) - u^{(2k-1)}(a)] h^{2k} \\
 &\quad + (b - a) \frac{B_{2m}}{(2m)!} u^{(2m)}(\xi_{m,n}) h^{2m}.
 \end{aligned}$$

Theorem 1.2 Let $u \in C^\infty(a, b)$, and assume that $u(x)$ has the following asymptotic expansions as $x \rightarrow a+$ and $x \rightarrow b-$:

$$\begin{aligned}
 u(x) &\sim \sum_{s=0}^{\infty} c_s (x - a)^{\gamma_s} \quad \text{as } x \rightarrow a+, \\
 u(x) &\sim \sum_{s=0}^{\infty} d_s (b - x)^{\delta_s} \quad \text{as } x \rightarrow b-,
 \end{aligned}$$

where the γ_s and δ_s are complex in general, and satisfy

$$\gamma_s \neq -1, -2, \dots; \Re\gamma_0 \leq \Re\gamma_1 \leq \Re\gamma_2 \leq \dots; \lim_{s \rightarrow \infty} \Re\gamma_s = +\infty,$$

$$\delta_s \neq -1, -2, \dots; \Re\delta_0 \leq \Re\delta_1 \leq \Re\delta_2 \leq \dots; \lim_{s \rightarrow \infty} \Re\delta_s = +\infty.$$

Assume also that, for each k , the derivative $u^{(k)}(x)$ also has asymptotic expansions as $x \rightarrow a+$ and $x \rightarrow b-$ that are obtained by differentiating those of $u(x)$ term by term k times. Let $h = (b - a)/n$ for $n = 1, 2, \dots$. Then

$$\begin{aligned}
 (1.12) \quad h \sum_{i=1}^{n-1} u(a + ih) &\sim \int_a^b u(x) dx + \sum_{\substack{s=0 \\ \gamma_s \notin \{2, 4, \dots\}}}^{\infty} c_s \zeta(-\gamma_s) h^{\gamma_s+1} \\
 &\quad + \sum_{\substack{s=0 \\ \delta_s \notin \{2, 4, \dots\}}}^{\infty} d_s \zeta(-\delta_s) h^{\delta_s+1} \quad \text{as } h \rightarrow 0,
 \end{aligned}$$

where $\zeta(z)$ is the Riemann Zeta function. [Note that in case $\Re\gamma_0 \leq -1$ and $\Re\delta_0 \leq -1$, $\int_a^b u(x) dx$ does not exist in the ordinary sense, but is defined in the sense of Hadamard finite part.]

It is clear from (1.12) that the powers $(x - a)^{2s}$ and $(b - x)^{2s}$, if present in the asymptotic expansions of $u(x)$ as $x \rightarrow a+$ and $x \rightarrow b-$, do not contribute to the asymptotic expansion of $h \sum_{i=1}^{n-1} u(a + ih)$ as $h \rightarrow 0$.

In addition, if γ_p is the first of the γ_s that is different from 2, 4, 6, . . . , and if δ_q is the first of the δ_s that is different from 2, 4, 6, . . . , then $h \sum_{i=1}^{n-1} u(a + ih) = O(h^\sigma)$ as $h \rightarrow 0$, where $\sigma = \min\{\Re\gamma_p, \Re\delta_q\}$. This is a useful observation we make use of later.

Before we end this section, we sketch the ideas that yield the proofs of the main results of Sections 3 and 4. Because these proofs involve many

technical details, we believe such a sketch may help the reader not to get lost in the details. We first observe that the asymptotic expansion of the error $T_{n,n'}[F] - I[f]$ as $h \rightarrow 0$ is the same as that of $\bar{T}_n[F] - I[f]$, where $\bar{T}_n[F]$ is the trapezoidal rule approximation to the one-dimensional integral $I[f] = \int_0^\pi v(\theta) d\theta$ with $v(\theta) = \int_0^{2\pi} F(\theta, \phi) d\phi$. As a result, it is enough to study $\bar{T}_n[F] - I[f]$ only. In view of Theorem 1.2, this study can be carried out by a careful analysis of $v(\theta)$ as $\theta \rightarrow 0$ and $\theta \rightarrow \pi$, which, in turn, is done by studying the expansions of $F(\theta, \phi)$ as $\theta \rightarrow 0$ and $\theta \rightarrow \pi$ and integrating them carefully with respect to ϕ . [As a result of this integration, many of the terms in the expansions of $F(\theta, \phi)$ disappear; this is a crucial fact that we use in the treatment of the cases in which $2q$ is an odd integer.] Now, for all values of the grading parameter q , the function $v(\theta)$ is infinitely smooth for $0 < \theta < \pi$; it is not regular at $\theta = 0$ and $\theta = \pi$ for all values of q , however. Nevertheless, in all cases, $v(\theta)$ has asymptotic expansions as $\theta \rightarrow 0$ and $\theta \rightarrow \pi$ in (not necessarily integral) powers of θ and $(\pi - \theta)$, respectively. At this point, Theorem 1.2 is invoked to obtain the main results.

2 Preliminaries

Let us assume that $f(\xi, \eta, \zeta)$ is infinitely differentiable over S . This and the fact that the transformation in (1.4) is infinitely differentiable over U imply that $f(\xi, \eta, \zeta)$ is an infinitely differentiable function of x, y, z over U . Let us observe that x, y, z , as functions of ϕ , are analytic and 2π -periodic as well. Therefore, as a function of ϕ , $f(\xi, \eta, \zeta)$ is infinitely differentiable on $(-\infty, \infty)$ and also 2π -periodic. There is an analogous statement that can be made concerning $\|\partial \rho / \partial \theta \times \partial \rho / \partial \phi\|$, and we turn to it next.

In the sequel, we use the notation

$$(\xi_1, \xi_2, \xi_3) = (\xi, \eta, \zeta) \quad \text{and} \quad (x_1, x_2, x_3) = (x, y, z)$$

whenever convenient.

2.1 Analysis of $\|\partial \rho / \partial \theta \times \partial \rho / \partial \phi\|$

Theorem 2.1 *With S as in the first paragraph of Section 1, there holds*

$$(2.1) \quad \left\| \frac{\partial \rho}{\partial \theta} \times \frac{\partial \rho}{\partial \phi} \right\| = L(\theta) R(x, y, z),$$

where

$$(2.2) \quad L(\theta) = |v'(\theta)| = \frac{\sin^{2q-1} \theta (q \cos^2 \theta + \sin^2 \theta)}{(\cos^2 \theta + \sin^{2q} \theta)^{3/2}},$$

and

$$(2.3) \quad R(x, y, z) = \sqrt{\beta_{12}^2 + \beta_{23}^2 + \beta_{31}^2}; \quad \beta_{ij} = (\nabla \xi_i \times \nabla \xi_j) \cdot \mathbf{r},$$

∇u being the gradient of the function $u(x, y, z)$, that is, $\nabla u = (\partial u/\partial x, \partial u/\partial y, \partial u/\partial z)$. $R(x, y, z)$ is strictly positive on U and is in $C^\infty(U)$. Consequently, $R(x, y, z)$, as a function of ϕ , is infinitely differentiable on $(-\infty, \infty)$ and 2π -periodic as well.

Proof Denoting

$$\begin{bmatrix} \psi'(\theta) \cos \phi \\ \psi'(\theta) \sin \phi \\ \nu'(\theta) \end{bmatrix} = \boldsymbol{\kappa}, \quad \begin{bmatrix} -\sin \phi \\ \cos \phi \\ 0 \end{bmatrix} = \boldsymbol{\lambda}$$

in (1.10), letting also

$$\mathbf{K} = J\boldsymbol{\kappa}, \quad \mathbf{L} = J\boldsymbol{\lambda},$$

and using the fact that for any two vectors \mathbf{a}, \mathbf{b} in \mathbb{R}^3 , there holds

$$\|\mathbf{a} \times \mathbf{b}\|^2 = \|\mathbf{a}\|^2 \|\mathbf{b}\|^2 - (\mathbf{a} \cdot \mathbf{b})^2,$$

we have

$$(2.4) \quad \left\| \frac{\partial \boldsymbol{\rho}}{\partial \theta} \times \frac{\partial \boldsymbol{\rho}}{\partial \phi} \right\|^2 = [\psi(\theta)]^2 [\|\mathbf{K}\|^2 \|\mathbf{L}\|^2 - (\mathbf{K}^T \mathbf{L})^2].$$

Next, by Lemmas 7.1 and 7.2 in Sidi [7], letting $\boldsymbol{\kappa} = [\kappa_1, \kappa_2, \kappa_3]^T$ and $\boldsymbol{\lambda} = [\lambda_1, \lambda_2, \lambda_3]^T$, it follows that

$$(2.5) \quad \|\mathbf{K}\|^2 \|\mathbf{L}\|^2 - (\mathbf{K}^T \mathbf{L})^2 = \sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2,$$

where

$$(2.6) \quad \sigma_{ij} = \sum_{r=1}^3 \sum_{s=1}^3 J_{ir} J_{js} \tau_{rs}; \quad \tau_{rs} = \kappa_r \lambda_s - \kappa_s \lambda_r.$$

Here, J_{ij} is the (i, j) element of the matrix J . Now, $\tau_{ji} = -\tau_{ij}$; this implies that $\tau_{ii} = 0$ and hence the only relevant τ_{ij} are $\tau_{12}, \tau_{23}, \tau_{31}$. From the definitions of $\boldsymbol{\kappa}$ and $\boldsymbol{\lambda}$, it follows that

$$\tau_{12} = \psi'(\theta), \quad \tau_{23} = -\nu'(\theta) \cos \phi, \quad \tau_{31} = -\nu'(\theta) \sin \phi.$$

By (1.3), we have that $[\psi(\theta)]^2 + [\nu(\theta)]^2 = 1$ for all θ , and by differentiation it follows that $\psi(\theta)\psi'(\theta) + \nu(\theta)\nu'(\theta) = 0$, from which we have $\nu'(\theta) = -\psi(\theta)\psi'(\theta)/\nu(\theta)$. Using this, and invoking (1.3), we obtain

$$\tau_{12} = \frac{\psi'(\theta)}{\nu(\theta)} z, \quad \tau_{23} = \frac{\psi'(\theta)}{\nu(\theta)} x, \quad \tau_{31} = \frac{\psi'(\theta)}{\nu(\theta)} y.$$

With x, y, z replaced by x_1, x_2, x_3 , these can be rewritten in the form

$$\tau_{ij} = \frac{\psi'(\theta)}{\nu(\theta)} \sum_{k=1}^3 \epsilon_{ijk} x_k,$$

where $\epsilon_{123} = 1$, and $\epsilon_{ijk}, 1 \leq i, j, k \leq 3$, is odd under an interchange of any two of the indices i, j, k , which means that $\epsilon_{ijk} = 0$ when any two of these indices have the same value. Substituting these in (2.6), and observing that $J_{ij} = \partial \xi_i / \partial x_j$, we obtain

$$\sigma_{ij} = \frac{\psi'(\theta)}{\nu(\theta)} \sum_{r=1}^3 \sum_{s=1}^3 \sum_{k=1}^3 \epsilon_{rsk} \frac{\partial \xi_i}{\partial x_r} \frac{\partial \xi_j}{\partial x_s} x_k = \frac{\psi'(\theta)}{\nu(\theta)} \beta_{ij},$$

with β_{ij} as defined in (2.3). Combining all the above in (2.5) and (2.4), and invoking again $\nu'(\theta) = -\psi(\theta)\psi'(\theta)/\nu(\theta)$, the results in (2.1)–(2.3) follow.

Since all elements of $J(x, y, z)$ are in $C^\infty(U)$, so are β_{ij} ; consequently, $M(x, y, z) \equiv \beta_{12}^2 + \beta_{23}^2 + \beta_{31}^2$ is in $C^\infty(U)$ as well. We now show that $M(x, y, z)$ is strictly positive on U , which will guarantee that $R(x, y, z) = \sqrt{M(x, y, z)}$ is in $C^\infty(U)$. [Note that if $M(x, y, z)$ vanishes at some point on U , then $\sqrt{M(x, y, z)}$ is not necessarily in $C^\infty(U)$.] Assume, to the contrary, that $M(a, b, c) = 0$ at some point $(a, b, c) \in U$. This means that $\beta_{12} = \beta_{23} = \beta_{31} = 0$ at this point, which, in turn, means that all three vectors $\nabla \xi_i(a, b, c), i = 1, 2, 3$, lie in a plane orthogonal to the vector $[a, b, c]^T$, hence lie in the same plane, thus becoming linearly dependent. This is equivalent to $\det J(a, b, c) = 0$, which contradicts our assumption that the matrix $J(x, y, z)$ is nonsingular on U . This completes the proof of the theorem. \square

Note that the result of Theorem 2.1 is true whether S has symmetry properties or not.

As an example, let us consider the case in which S is the surface of an ellipsoid, which we take to be

$$S = \{(\xi, \eta, \zeta) : (\xi/a)^2 + (\eta/b)^2 + (\zeta/c)^2 = 1\}.$$

Here, a, b, c are the lengths of the semi-axes of this ellipsoid. The mapping from U to S can be taken to be $(\xi, \eta, \zeta) = (ax, by, cz)$. In this case, $J = \text{diag}(a, b, c)$ hence is nonsingular on U . This example was treated in [2], where the result

$$R(x, y, z) = [(bcx)^2 + (cay)^2 + (abz)^2]^{1/2},$$

is also given. This result can also be obtained from Theorem 2.1. It is easy to see that $R(x, y, z)$ in this case is in $C^\infty(U)$, and this is in accordance with Theorem 2.1.

2.2 Preliminary analysis of $T_{n,n'}[F]$

Substituting (2.1) in the function $F(\theta, \phi)$ defined in (1.8), we have that

$$(2.7) \quad F(\theta, \phi) = L(\theta) w(x, y, z); \quad w(x, y, z) = f(\xi, \eta, \zeta)R(x, y, z),$$

with $L(\theta)$ and $R(x, y, z)$ as in (2.2) and (2.3), respectively. By our discussion in the first paragraph of this section and by Theorem 2.1, it is clear that $w(x, y, z)$ is in $C^\infty(U)$. Therefore, as a function of ϕ , it is also infinitely differentiable on $(-\infty, \infty)$ and 2π -periodic as well. As a result, $F(\theta, \phi)$, as a function of ϕ , is also infinitely differentiable on $(-\infty, \infty)$ and is also 2π -periodic. Furthermore, since $w(x, y, z)$ is continuous on U , and $L(0) = L(\pi) = 0$ because $q \geq 1$, it follows that $F(0, \phi) = F(\pi, \phi) = 0$.

With this information on the function $F(\theta, \phi)$ available, we next give a preliminary analysis of $T_{n,n'}[F]$ that is defined in (1.11).

Now, $h' \sum_{k=1}^{n'} F(\theta, kh')$ is the trapezoidal rule approximation to the integral $\int_0^{2\pi} F(\theta, \phi) d\phi$. Therefore, by the Euler–Maclaurin summation formula in Theorem 1.1, we have

$$(2.8) \quad h' \sum_{k=1}^{n'} F(\theta, kh') = \int_0^{2\pi} F(\theta, \phi) d\phi + r_m(\theta; h'),$$

where

$$(2.9) \quad |r_m(\theta; h')| \leq 2\pi \frac{B_{2m}}{(2m)!} \left(\max_{\substack{0 \leq \theta \leq \pi \\ 0 \leq \phi \leq 2\pi}} \left| \frac{\partial^{2m}}{\partial \phi^{2m}} F(\theta, \phi) \right| \right) h'^{2m} \\ \equiv C_m h'^{2m} \quad \text{for every } m,$$

C_m being constants independent of h' and θ . Consequently, we easily have the following important intermediate result:

Theorem 2.2 *With $f \in C^\infty(S)$, and for n fixed, there holds*

$$(2.10) \quad T_{n,n'}[F] = \bar{T}_n[F] + O(h'^\mu) \quad \text{as } h' \rightarrow 0, \quad \text{for every } \mu > 0,$$

uniformly in n , hence in h , where

$$(2.11) \quad \bar{T}_n[F] = h \sum_{j=1}^{n-1} \int_0^{2\pi} F(jh, \phi) d\phi.$$

Thus, when n' is chosen such that $n' \sim \alpha n^\beta$ as $n \rightarrow \infty$ for some fixed positive constants α and β , there holds

$$(2.12) \quad T_{n,n'}[F] = \bar{T}_n[F] + O(h^\mu) \quad \text{as } h \rightarrow 0, \quad \text{for every } \mu > 0,$$

and, therefore,

$$(2.13) \quad T_{n,n'}[F] - I[f] = (\overline{T}_n[F] - I[f]) + O(h^\mu) \quad \text{as } h \rightarrow 0, \quad \text{for every } \mu > 0.$$

Thus, we need to concern ourselves only with the asymptotic expansion as $h \rightarrow 0$ of $\overline{T}_n[F] - I[f]$. Note that $\overline{T}_n[F]$ is nothing but the (one-dimensional) trapezoidal rule approximation to the integral

$$(2.14) \quad I[f] = \int_0^\pi v(\theta) d\theta; \quad v(\theta) = \int_0^{2\pi} F(\theta, \phi) d\phi.$$

This means that, by Theorem 1.2, we need to study $v(\theta)$ as $\theta \rightarrow 0$ and $\theta \rightarrow \pi$.

2.3 Asymptotic analysis of $\int_0^{2\pi} w(x, y, z) d\phi$

By (2.7),

$$(2.15) \quad v(\theta) = \int_0^{2\pi} F(\theta, \phi) d\phi = \int_0^{2\pi} L(\theta)w(x, y, z) d\phi = L(\theta)G(\theta),$$

where

$$(2.16) \quad G(\theta) = \int_0^{2\pi} w(x, y, z) d\phi.$$

Therefore, we need to study the asymptotic behavior of the functions $L(\theta)$ and $G(\theta)$ as $\theta \rightarrow 0$ and $\theta \rightarrow \pi$. Here, we give some preliminary analysis of $G(\theta)$, which we make use of in the next sections. The analysis of $L(\theta)$ is left to the next sections.

Now, when $\theta = 0$, there holds $(x, y, z) = (0, 0, 1)$, while when $\theta = \pi$, there holds $(x, y, z) = (0, 0, -1)$. Let also

$$\xi(0, 0, \pm 1) = \xi_\pm, \quad \eta(0, 0, \pm 1) = \eta_\pm, \quad \zeta(0, 0, \pm 1) = \zeta_\pm.$$

Because $w(x, y, z) = f(\xi, \eta, \zeta)R(x, y, z)$ is in $C^\infty(U)$, it has the asymptotic expansions

$$w(x, y, z) \sim \sum_{i=0}^\infty \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{w^{(i,j,k)}(0, 0, 1)}{i! j! k!} x^i y^j (z - 1)^k \quad \text{as } \theta \rightarrow 0,$$

$$w(x, y, z) \sim \sum_{i=0}^\infty \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{w^{(i,j,k)}(0, 0, -1)}{i! j! k!} x^i y^j (z + 1)^k \quad \text{as } \theta \rightarrow \pi,$$

where

$$w^{(i,j,k)}(x_0, y_0, z_0) = \frac{\partial^{i+j+k} w}{\partial x^i \partial y^j \partial z^k} \Big|_{(x,y,z)=(x_0,y_0,z_0)}.$$

Obviously, these are the Taylor series expansions of $w(x, y, z)$ about $(0, 0, 1)$ and $(0, 0, -1)$, respectively.

Invoking (1.3), these expansions can be rewritten in the form

$$w(x, y, z) \sim \sum_{i,j,k \geq 0} e_{i,j,k}^{(+)} \cos^i \phi \sin^j \phi [\psi(\theta)]^{i+j} [\nu(\theta) - 1]^k \quad \text{as } \theta \rightarrow 0,$$

$$w(x, y, z) \sim \sum_{i,j,k \geq 0} e_{i,j,k}^{(-)} \cos^i \phi \sin^j \phi [\psi(\theta)]^{i+j} [\nu(\theta) + 1]^k \quad \text{as } \theta \rightarrow \pi,$$

where

$$e_{i,j,k}^{(\pm)} = \frac{w^{(i,j,k)}(0, 0, \pm 1)}{i! j! k!}.$$

Substituting these in the integral $\int_0^{2\pi} w(x, y, z) d\phi$, and interchanging the order of integration and summation (which is legitimate, as can be verified easily), we obtain

$$(2.17) \quad G(\theta) \sim \sum_{i,j,k \geq 0} e_{i,j,k}^{(+)} \mu_{i,j} [\psi(\theta)]^{i+j} [\nu(\theta) - 1]^k \quad \text{as } \theta \rightarrow 0,$$

$$G(\theta) \sim \sum_{i,j,k \geq 0} e_{i,j,k}^{(-)} \mu_{i,j} [\psi(\theta)]^{i+j} [\nu(\theta) + 1]^k \quad \text{as } \theta \rightarrow \pi,$$

where $\mu_{i,j}$ is defined by

$$(2.18) \quad \mu_{i,j} = \int_0^{2\pi} \cos^i \phi \sin^j \phi d\phi.$$

By Lemma 3.1 in [11] (originally, Lemma 4.1 in [7]), we have

$$(2.19) \quad \mu_{i,j} = 0 \quad \text{when } i \text{ or } j \text{ or both odd.}$$

Consequently,

$$(2.20) \quad G(\theta) \sim \sum_{i,j,k \geq 0} A_{i,j,k}^{(+)} [\psi(\theta)]^{2i+2j} [\nu(\theta) - 1]^k \quad \text{as } \theta \rightarrow 0,$$

$$G(\theta) \sim \sum_{i,j,k \geq 0} A_{i,j,k}^{(-)} [\psi(\theta)]^{2i+2j} [\nu(\theta) + 1]^k \quad \text{as } \theta \rightarrow \pi,$$

where

$$(2.21) \quad A_{i,j,k}^{(\pm)} = e_{2i,2j,k}^{(\pm)} \mu_{2i,2j}.$$

Note that, by the fact that $w(x, y, z) = f(\xi, \eta, \zeta)R(x, y, z)$ and $\mu_{0,0} = 2\pi$, we have

$$(2.22) \quad A_{0,0,0}^{(\pm)} = 2\pi w(0, 0, \pm 1) = 2\pi f(\xi_{\pm}, \eta_{\pm}, \zeta_{\pm}) R(0, 0, \pm 1).$$

The result in (2.19) and its consequences in (2.20) and (2.21) are of importance in that they lead to the optimal result for the case in which $2q$ is an odd integer, as we will see in Section 4.

3 Convergence analysis for $T_{n,n'}[F]$ when $2q \neq$ odd integer

Theorem 3.1 *Let $f \in C^\infty(S)$ and let $q \geq 1$ such that $2q \neq$ an odd integer. Then, with $n' \sim \alpha n^\beta$ as $n \rightarrow \infty$ for some fixed positive constants α and β , there holds*

$$(3.1) \quad T_{n,n'}[F] - I[f] = O(h^{2q}) \quad \text{as } h \rightarrow 0.$$

In case $w(0, 0, 1) + w(0, 0, -1) \neq 0$, there holds

$$(3.2) \quad T_{n,n'}[F] - I[f] \sim 2\pi q \zeta(-2q + 1) [w(0, 0, 1) + w(0, 0, -1)] h^{2q} \quad \text{as } h \rightarrow 0.$$

Proof Since $\psi(\theta)$ and $v(\theta)$ in (1.3) are both in $C^\infty(0, \pi)$ with possible (end-point) singularities at $\theta = 0$ and $\theta = \pi$, the functions $L(\theta)$ and $G(\theta)$ are also in $C^\infty(0, \pi)$ with possible singularities at $\theta = 0$ and $\theta = \pi$, and so is their product.

In the sequel, we analyze their behavior only as $\theta \rightarrow 0$, the analysis as $\theta \rightarrow \pi$ being identical.

Analysis of $L(\theta)$: We start by analyzing the behavior of $L(\theta)$ as $\theta \rightarrow 0$. First,

$$\sin^{2q-1} \theta \sim \sum_{i=0}^{\infty} a_i \theta^{2q+2i-1} \quad \text{as } \theta \rightarrow 0, \quad a_0 = 1.$$

Next,

$$q \cos^2 \theta + \sin^2 \theta \sim \sum_{i=0}^{\infty} b_i \theta^{2i} \quad \text{as } \theta \rightarrow 0, \quad b_0 = q.$$

Next,

$$\cos^2 \theta + \sin^{2q} \theta \sim 1 + \sum_{i=1}^{\infty} c_i \theta^{\delta_i} \quad \text{as } \theta \rightarrow 0; \quad 2 = \delta_1 < \delta_2 < \dots,$$

so that

$$(\cos^2 \theta + \sin^{2q} \theta)^{-3/2} \sim 1 + \sum_{i=1}^{\infty} d_i \theta^{\sigma_i} \quad \text{as } \theta \rightarrow 0; \quad 2 = \sigma_1 < \sigma_2 < \dots .$$

Combining all these in (2.2), we obtain

$$L(\theta) \sim \sum_{i=0}^{\infty} e_i \theta^{\tau_i} \quad \text{as } \theta \rightarrow 0; \quad 2q - 1 = \tau_0 < \tau_1 < \tau_2 < \dots, \quad e_0 = q.$$

This completes the analysis of $L(\theta)$ for $\theta \rightarrow 0$. As for $\theta \rightarrow \pi$, we have

$$L(\theta) \sim \sum_{i=0}^{\infty} e_i (\pi - \theta)^{\tau_i} \quad \text{as } \theta \rightarrow \pi,$$

which follows immediately from the fact that $L(\pi - \theta) = L(\theta)$.

Analysis of $G(\theta)$: We again start with the analysis of the case $\theta \rightarrow 0$. We begin with the results in (2.20)–(2.22). From (1.3) and the preceding developments used in the analysis of $L(\theta)$,

$$[\psi(\theta)]^m \sim \sum_{i=0}^{\infty} c'_{mi} \theta^{\delta'_i} \quad \text{as } \theta \rightarrow 0; \quad mq = \delta'_0 < \delta'_1 < \dots,$$

$$[v(\theta) - 1]^k \sim \sum_{i=0}^{\infty} d'_{ki} \theta^{\sigma'_i} \quad \text{as } \theta \rightarrow 0; \quad 2k = \sigma'_0 < \sigma'_1 < \dots .$$

As a result,

$$G(\theta) \sim 2\pi w(0, 0, 1) + \sum_{i=1}^{\infty} e'_i \theta^{\tau'_i} \quad \text{as } \theta \rightarrow 0; \quad 0 < \tau'_1 < \tau'_2 < \dots .$$

This completes the analysis of the case $\theta \rightarrow 0$. As for the case $\theta \rightarrow \pi$, we have similarly

$$G(\theta) \sim 2\pi w(0, 0, -1) + \sum_{i=1}^{\infty} e'_i (\pi - \theta)^{\tau'_i} \quad \text{as } \theta \rightarrow \pi.$$

This follows immediately from the fact that

$$\psi(\pi - \theta) = \psi(\theta) \quad \text{and} \quad v(\theta) + 1 = -[v(\pi - \theta) - 1].$$

Combining the results we have obtained for $L(\theta)$ and $G(\theta)$, we conclude [recall (2.15)] that $v(\theta) = L(\theta)G(\theta)$ has the asymptotic expansions

$$v(\theta) \sim \sum_{i=0}^{\infty} E_i^{(+)} \theta^{\alpha_i} \quad \text{as } \theta \rightarrow 0; \quad E_0^{(+)} = 2\pi q w(0, 0, 1),$$

$$v(\theta) \sim \sum_{i=0}^{\infty} E_i^{(-)} (\pi - \theta)^{\alpha_i} \quad \text{as } \theta \rightarrow \pi; \quad E_0^{(-)} = 2\pi q w(0, 0, -1),$$

with

$$2q - 1 = \alpha_0 < \alpha_1 < \alpha_2 < \dots .$$

Applying now Theorem 1.2, we obtain

$$\bar{T}_n[F] - \int_0^\pi v(\theta) d\theta \sim \sum_{i=0}^\infty (E_i^{(+)} + E_i^{(-)}) \zeta(-\alpha_i) h^{\alpha_i+1} \quad \text{as } h \rightarrow 0,$$

from which the results in (3.1) and (3.2) follow. □

4 Convergence analysis for $T_{n,n'}[F]$ when $2q = \text{odd integer}$

When $2q$ is an odd integer, the approximation $T_{n,n'}[F]$ turns out to have very high accuracy. The optimal theoretical result for this case can be obtained by a more refined study of the asymptotic expansions of $v(\theta)$ as $\theta \rightarrow 0$ and $\theta \rightarrow \pi$. To achieve this goal, we start with the following definition:

Definition 4.1 $R_\mu(\theta)$ stands generically for any function of θ that has an asymptotic expansion of the form

$$R_\mu(\theta) \sim \sum_{i=0}^\infty r_i \theta^{\mu+2i} \quad \text{as } \theta \rightarrow 0.$$

Remark Note that, in Definition 4.1, we do not require $r_0 \neq 0$, because such a requirement is not needed in the sequel.

By Definition 4.1, we have

$$(4.1) \quad R_\mu(\theta) + R_{\mu+2k}(\theta) = R_\mu(\theta), \quad k = 1, 2, \dots ,$$

$$\text{hence} \quad \sum_{k=0}^\infty R_{\mu+2k}(\theta) = R_\mu(\theta).$$

We also have

$$(4.2) \quad R_\mu(\theta)R_\nu(\theta) = R_{\mu+\nu}(\theta), \quad [R_\mu(\theta)]^\alpha = R_{\alpha\mu}(\theta).$$

Theorem 4.2 Let $f \in C^\infty(S)$ and let $2q$ be an odd integer greater than 2; that is, $q = 3/2, 5/2, \dots$. Then, with $n' \sim \alpha n^\beta$ as $n \rightarrow \infty$ for some fixed positive constants α and β , there holds

$$(4.3) \quad T_{n,n'}[F] - I[f] = O(h^{4q}) \quad \text{as } h \rightarrow 0.$$

Proof We give a detailed analysis for $\theta \rightarrow 0$; that for $\theta \rightarrow \pi$ is analogous. First, as we have also seen in the preceding section,

$$(4.4) \quad \begin{aligned} \cos^\alpha \theta &= 1 + R_2(\theta) = R_0(\theta), & \sin^\alpha \theta &= R_\alpha(\theta), \\ \cos^2 \theta + q \sin^2 \theta &= R_0(\theta), \end{aligned}$$

and, because $2q$ is an odd integer,

$$(4.5) \quad \begin{aligned} \cos^2 \theta + \sin^{2q} \theta &= 1 - \sin^2 \theta + \sin^{2q} \theta \\ &= 1 + R_2(\theta) + R_{2q}(\theta) = R_0(\theta) + R_{2q}(\theta). \end{aligned}$$

[It is important to realize that, by the fact that $2q$ is not an even integer, (4.1) does not apply to $R_0(\theta) + R_{2q}(\theta)$; that is, $R_0(\theta) + R_{2q}(\theta) \neq R_0(\theta)$.]

Note that, for $k = 0, 1, 2, \dots$, $R_{2k}(\theta)$ has only even powers in its expansion, while $R_{2qk}(\theta)$ has only even (odd) powers in its expansion when k is an even (odd) integer. Consequently, by (4.1) and (4.2), and by the fact that $2q > 2$,

$$(4.6) \quad (R_2 + R_{2q})^k = \sum_{i=0}^k (R_2)^{k-i} (R_{2q})^i = \sum_{i=0}^k R_{2k-2i} R_{2qi} = R_{2k} + R_{2q+2k-2}.$$

Therefore, by (4.5) and (4.6), by the fact that

$$R_2(\theta) + R_{2q}(\theta) = O(\theta^2) = o(1) \quad \text{as } \theta \rightarrow 0,$$

and by the binomial theorem, there holds for every $\alpha \neq 0$

$$(4.7) \quad \begin{aligned} (\cos^2 \theta + \sin^{2q} \theta)^\alpha &= [1 + (R_2 + R_{2q})]^\alpha \\ &= 1 + \sum_{k=1}^\infty (R_2 + R_{2q})^k = 1 + R_2 + R_{2q} = R_0 + R_{2q}. \end{aligned}$$

[Note that here we have suppressed θ in $R_\mu(\theta)$. We shall continue to do so in the sequel for convenience.] In view of the above, we now analyze the behavior of $L(\theta)$ and $G(\theta)$ as $\theta \rightarrow 0$. In this analysis, we make free use of (4.1) and (4.2).

We start with $L(\theta)$. From (2.2), (4.4), and (4.7),

$$(4.8) \quad L(\theta) = R_{2q-1} R_0 (R_0 + R_{2q}) = R_{2q-1} + R_{4q-1}.$$

The analysis of $G(\theta)$ as $\theta \rightarrow 0$ is done by studying the first of the asymptotic expansions in (2.20). First, by (1.3), (4.4), and (4.7),

$$(4.9) \quad \begin{aligned} [\psi(\theta)]^{2r} &= \frac{\sin^{2qr} \theta}{(\cos^2 \theta + \sin^{2q} \theta)^r} = R_{2qr} (R_0 + R_{2q}) \\ &= R_{2qr} + R_{2q(r+1)}, \quad r = 1, 2, \dots \end{aligned}$$

Next, again by (1.3), (4.4), and (4.7), there holds

$$v(\theta) = (1 + R_2)(1 + R_2 + R_{2q}) = 1 + R_2 + R_{2q},$$

so that

$$v(\theta) - 1 = R_2 + R_{2q},$$

hence, by (4.6),

$$(4.10) \quad [v(\theta) - 1]^k = R_{2k} + R_{2q+2k-2}, \quad k = 1, 2, \dots .$$

Combining (4.9) and (4.10), we have

$$(4.11) \quad [\psi(\theta)]^{2r} [v(\theta) - 1]^k = R_{2qr+2k} + R_{2q(r+1)+2k-2}, \quad r, k = 1, 2, \dots .$$

Substituting (4.11) in the asymptotic expansion of $G(\theta)$ as $\theta \rightarrow 0$ that is given in (2.20), after analyzing the first few terms, we observe that

$$\begin{aligned} G(\theta) \sim & A_{0,0,0}^{(+)} + \left(A_{1,0,0}^{(+)} + A_{0,1,0}^{(+)} \right) (R_{2q} + R_{4q}) + A_{0,0,1}^{(+)} (R_2 + R_{2q}) \\ & + \left(A_{2,0,0}^{(+)} + A_{1,1,0}^{(+)} + A_{0,2,0}^{(+)} \right) (R_{4q} + R_{6q}) \\ & + \left(A_{1,0,1}^{(+)} + A_{0,1,1}^{(+)} \right) (R_{2q+2} + R_{4q}) \\ & + A_{0,0,2}^{(+)} (R_4 + R_{2q+2}) + \dots, \quad \text{as } \theta \rightarrow 0, \end{aligned}$$

from which we conclude that

$$(4.12) \quad G(\theta) = R_0 + R_{2q}.$$

Combining (4.8) and (4.12) in [recall (2.15)] $v(\theta) = L(\theta)G(\theta)$, we obtain

$$v(\theta) = (R_{2q-1} + R_{4q-1})(R_0 + R_{2q}) = R_{2q-1} + R_{4q-1},$$

which can be written in the form

$$(4.13) \quad v(\theta) \sim \sum_{i=0}^{\infty} D_i^{(+)} \theta^{2q-1+2i} + \sum_{i=0}^{\infty} C_i^{(+)} \theta^{4q-1+2i} \quad \text{as } \theta \rightarrow 0.$$

In an analogous manner,

$$(4.14) \quad v(\theta) \sim \sum_{i=0}^{\infty} D_i^{(-)} (\pi - \theta)^{2q-1+2i} + \sum_{i=0}^{\infty} C_i^{(-)} (\pi - \theta)^{4q-1+2i} \quad \text{as } \theta \rightarrow \pi.$$

Now, the series $\sum_{i=0}^{\infty} D_i^{(+)} \theta^{2q-1+2i}$ and $\sum_{i=0}^{\infty} D_i^{(-)} (\pi - \theta)^{2q-1+2i}$ contain only even powers; therefore, they do not contribute to the Euler–Maclaurin

expansion of $\int_0^\pi v(\theta) d\theta$. By (4.13) and (4.14), by Theorem 1.2, and by the fact that $\zeta(1 - 4q - 2i) = -B_{4q+2i}/(4q + 2i) \neq 0$, there holds

$$\bar{T}_n[F] - \int_0^\pi v(\theta) d\theta \sim - \sum_{i=0}^{\infty} \frac{B_{4q+2i}}{4q + 2i} (C_i^{(+)} + C_i^{(-)}) h^{4q+2i} \quad \text{as } h \rightarrow 0,$$

from which the result in (4.3) follows. \square

5 Concluding Remarks

In this paper, we have given a complete analysis of the quadrature method introduced by Atkinson [2] for smooth integrands over an arbitrary smooth surface S in \mathbb{R}^3 . Our main results, namely, Theorems 3.1 and 4.2, cover *all* values of the grading parameter q . These results are valid when the relevant surface S is homeomorphic to U , the surface of the unit sphere, and when the mapping from U to S is one-to-one, infinitely differentiable, and has a nonsingular Jacobian matrix.

After this work was completed, the author was provided by Professor Kendall Atkinson with a copy of the recent paper Atkinson and Sommariva [3], which deals with the same problem and uses techniques similar to those developed in [7]. The paper [3] differs from the present work in the following ways: The results of [3] concern integration of smooth functions over the surface of the unit sphere. Theorem 2.2 of [3] (analogue of our Theorem 3.1) is about the case in which $2q$ is not an odd integer with $1 < q < 2$. Similarly, Theorem 2.3 of [3] (analogue of our Theorem 4.2), which is about the case in which $2q$ is an odd integer, treats the cases $q = 1.5, 2.5, 3.5$ only.

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