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**Abstract** Given a triangulation of a planar region, the reduced Hsieh-Clough-Tocher (rHCT) triangular element enables the construction of a smooth piecewise-cubic surface. In preparation for the use of energy minimization to select interpolants from that family of surfaces, a formula for the bending energy of the generic rHCT element is determined, treating the element as a thin and almost flat plate. The aim is to find an approach to interpolation which displays low sensitivity to the choice of triangulation. The problem arose in terrain modeling.

**Keywords:** Delaunay triangulation, finite elements, Hsieh-Clough-Tocher element, interpolation, spline, surface, terrain modeling, triangulation

## 1. Introduction

Lawson [9],[10] pioneered the use of  $C^1$ -compatible finite elements for the task of interpolating a continuously differentiable (“ $C^1$ ”) function  $z = f(x, y)$  from a finite set of spatial points

$$(x_i, y_i, z_i), \quad i = 1, \dots, n,$$

so that  $z_i = z(x_i, y_i)$ . An important application is to terrain modeling from large sets of elevation data, where the function values  $z_i$  are elevations at specified data locations  $(x_i, y_i)$ .

For his work, Lawson chose an element generally ascribed to Clough and Tocher [4], but frequently referred to in the literature (e.g. Ciarlet [2]) as the *reduced Hsieh-Clough-Tocher (rHCT) element*. For a description of that and related elements, we recommend the text by Bernadou and Boisserie [1]. Farin [7] formulated Clough-Tocher interpolation in terms of Bernstein-Bezier polynomials and also provided a modification of the rHCT element which trades  $C^2$ -continuity at the barycenter – where subtriangles with different cubics join (see Sections 2 and 4 below) – for improved approximation to  $C^2$ -continuity at the edges of the triangular element. For general information, the reader may want to consult Ciarlet [3] and Zienkiewicz [18], to name just two representatives of a large body of literature on the Finite Element Method.

The rHCT element is a triangular surface patch, that is, it is defined over a footprint triangle in the  $x, y$ -plane. Its use in the context of interpolation thus presupposes a “*triangulation*” of the data locations  $(x_i, y_i)$ ,  $i = 1, \dots, n$ , that is, a set of triangles whose interiors do not meet, whose vertices are the data locations, and whose union covers the convex hull of the latter. Two different triangles of the triangulation thus have either a single edge or a single vertex in common, or do not meet at all. In the context of terrain modeling, a set of elevation data locations triangulated in this fashion is now frequently called a “*triangulated irregular network (TIN)*”. Any set of planar data locations  $(x_i, y_i)$  can be triangulated in many different ways and this affects the surface to be constructed. A frequently used generic method is the *Delaunay triangulation* [5].



The rHCT elements – by their construction – join smoothly at triangle boundaries, thus ensuring a continuously differentiable fit. The specification of an rHCT element over a particular triangle requires that the function value  $z_i$  and the gradient  $(z_{ix}, z_{iy})$  be given at each triangle vertex, that is, at each data location  $(x_i, y_i)$ . The resulting function is to agree with those prescribed values and slopes.

Unless such gradient information is also provided, it must be estimated from given function values  $z_i$  in order to complete the specification of rHCT elements for each triangle of the TIN. Thus one distinction between alternate methods for surface interpolation based on the rHCT element is what method for estimating gradients at data locations is chosen.

Lawson's approach [10] is to select at least six neighbors of a data point, assign them weights which decrease with distance from the data point, and then consider 6-parameter quadratic bivariate functions which pass through the data point. From among those functions select the one which minimizes the weighted least squares error. The tangent to that quadratic function at the data point provides the gradient estimate. Franke [8] and Stead [15] compare various procedures for triangulation based interpolation, in particular, aspects of gradient estimation.

In the context of terrain modeling, with elevation data given along digitized contour lines, Mandel, Bernal, and Witzgall [11] arrived at gradient estimates by minimizing the elastic energy of a mechanical surrogate structure for the surface consisting of thin beams along the edges of the triangular patches and joined tangentially to thin plates, one at each vertex. The orientation of the plates can be adjusted to minimize the elastic energy of the beams, thus defining gradients at triangulation vertices, that is, at data locations. That procedure was chosen because of the distribution of data points along lines, which rendered local fitting procedures less attractive. It also eliminated the somewhat arbitrary choice of neighboring data points and their weights.

The two rHCT methods mentioned above are less sensitive to changes in the underlying triangulation than the still most frequently employed *linear* TIN methods. In those linear methods, each footprint triangle in the TIN gives rise to a planar triangular facet spanned by the elevations at the triangle vertices. The resulting piecewise linear surface is, indeed, extremely sensitive to the choice of triangulation.

With the goal of further reducing the sensitivity of the interpolating surface to the choice of triangulation, we propose to examine an alternate method for estimating the gradients at data locations. The idea is to replace the surrogate mechanical structure consisting of thin beams used in [11] by a surrogate mechanical structure consisting of the actual rHCT elements, joined together smoothly, and to minimize the total elastic energy of the resulting interpolating surface considered as consisting of almost flat thin plates. More precisely, we determine that

interpolating surface  $z = z(x, y)$  which consists of rHCT elements and minimizes

$$(1.1) \quad \int \int \left[ \left( \frac{\partial^2 z}{\partial x^2} \right)^2 + 2 \left( \frac{\partial^2 z}{\partial x \partial y} \right)^2 + \left( \frac{\partial^2 z}{\partial y^2} \right)^2 \right] dx dy$$

with respect to the choice of gradients at triangulation vertices.

A critical first step in this direction is to develop closed formulas for that energy operator as applied to the generic rHCT element, and that is the purpose of this report. Those formulas are unwieldy, and the availability of symbolic computation packages was instrumental in their derivation. This work relied on Mathematica (see for instance [16]).

Powell-Sabin splines [14] also provide a unique piecewise polynomial  $C_1$ -function which meets prescribed values and gradients at the vertices of a triangulation. The concept of thin plate energy minimization has also been considered for various other approaches to bivariate interpolation (e.g. Powell [13]). Mansfield [12] minimizes the full strain energy functional. The reader may want to consult Dierckx [6].

We also revisit the definition of the rHCT element and verify its main properties. This exposition as well as the derivation of the energy formulas is conducted in terms of *barycentric coordinates*. In this fashion, the inherent symmetries of the element are preserved.

In particular, the roles of the vertices of the element and their associated quantities are interchangeable. More precisely, many formulas involving indexed quantities follow from each other by

$$(1.2) \quad \text{cyclic substitution : } 1 \rightarrow 2 \rightarrow 3 \rightarrow 1,$$

where each index value is replaced by its cyclic successor.

We will not always write all three instances of formulas that arise from each other by cyclic substitution of indices. Instead, we will write one instance of the formula, and indicate that the remaining instances can be generated by cyclic substitution.

## 2. Definition of the rHCT Element

In this section we define various quantities which are used to calculate the generic element. Suppose we are given three triangle vertices,

$$(x_1, y_1), (x_2, y_2), (x_3, y_3),$$

with associated function values, i.e., elevations,

$$z_1, z_2, z_3,$$

and partial derivatives with respect to  $x$  and  $y$ , i.e. coordinate slopes,

$$z_{1x}, z_{1y}, z_{2x}, z_{2y}, z_{3x}, z_{3y}.$$

We wish to define the elevation  $z = z(x, y)$  at any location  $(x, y)$  in the footprint triangle of the rHCT element, so that

$$z_i = z(x_i, y_i), \quad z_{ix} = \frac{\partial z}{\partial x}(x_i, y_i), \quad z_{iy} = \frac{\partial z}{\partial y}(x_i, y_i), \quad i = 1, 2, 3.$$

For that purpose, it is convenient to express functions over triangles using “*barycentric coordinates*”. For any point  $(x, y)$  in the plane, its barycentric coordinates

$$\lambda_1, \lambda_2, \lambda_3$$

are defined by the relations

$$(2.1) \quad \begin{aligned} \lambda_1 + \lambda_2 + \lambda_3 &= 1 \\ \lambda_1 x_1 + \lambda_2 x_2 + \lambda_3 x_3 &= x \\ \lambda_1 y_1 + \lambda_2 y_2 + \lambda_3 y_3 &= y. \end{aligned}$$

Following Zienkiewicz [17], we use the abbreviations

$$x_{ij} := x_i - x_j, \quad y_{ij} := y_i - y_j, \quad z_{ij} := z_i - z_j, \quad i, j = 1, 2, 3, \quad i \neq j.$$

The following determinants will play a role:

$$(2.2) \quad \begin{aligned} D_{xy} = -D_{yx} &:= \det \begin{vmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{vmatrix} = x_1 y_{23} + x_2 y_{31} + x_3 y_{12}, \\ D_{zy} = -D_{yz} &:= \det \begin{vmatrix} 1 & 1 & 1 \\ z_1 & z_2 & z_3 \\ y_1 & y_2 & y_3 \end{vmatrix} = z_1 y_{23} + z_2 y_{31} + z_3 y_{12}, \\ D_{zx} = -D_{xz} &:= \det \begin{vmatrix} 1 & 1 & 1 \\ z_1 & z_2 & z_3 \\ x_1 & x_2 & x_3 \end{vmatrix} = z_1 x_{23} + z_2 x_{31} + z_3 x_{12}. \end{aligned}$$

The determinant  $D_{xy}$  is double the area of the footprint triangle. It is assumed that the area of that triangle does not vanish. The footprint triangle is required, moreover, to have positive orientation, that is,

$$D_{xy} > 0.$$



Solving the linear system of equations (2.1) yields

$$(2.3) \quad \begin{aligned} \lambda_1 &= (y_{23}x + x_{32}y + x_2y_3 - y_2x_3)/D_{xy} \\ \lambda_2 &= (y_{31}x + x_{13}y + x_3y_1 - y_3x_1)/D_{xy} \\ \lambda_3 &= (y_{12}x + x_{21}y + x_1y_2 - y_1x_2)/D_{xy}. \end{aligned}$$

Note that the above formulas arise from each other by cyclic substitution (1.2). Indeed, barycentric coordinates treat all vertices of a triangle symmetrically. Their signs indicate whether a location lies inside or outside the footprint triangle: a negative barycentric coordinate means the location is outside the triangle; if all three coordinates are positive, the location lies in the interior of the triangle.

Edges of the footprint triangle are characterized by the vanishing of one of the barycentric coordinates. At vertex  $i$ ,  $\lambda_i = 1$  and  $\lambda_j = 0$  for  $j \neq i$ . The *barycenter* or *centroid*

$$(x_0, y_0) := \left( \frac{x_1 + x_2 + x_3}{3}, \frac{y_1 + y_2 + y_3}{3} \right)$$

of the triangle is characterized by  $\lambda_1 = \lambda_2 = \lambda_3 = 1/3$ .

The barycenter plays a key role in the definition of the rHCT element. It is used to define a “*barycentric partition*” of the triangle into four subsets, the barycenter itself and three subtriangles (see Figure 1):

$$\begin{aligned} B_0 &:= \{(\lambda_1, \lambda_2, \lambda_3) : \lambda_1 = \lambda_2 = \lambda_3 = 1/3\} \\ B_1 &:= \{(\lambda_1, \lambda_2, \lambda_3) : 0 \leq \lambda_1 < \lambda_2, \lambda_1 \leq \lambda_3\} \\ B_2 &:= \{(\lambda_1, \lambda_2, \lambda_3) : 0 \leq \lambda_2 < \lambda_3, \lambda_2 \leq \lambda_1\} \\ B_3 &:= \{(\lambda_1, \lambda_2, \lambda_3) : 0 \leq \lambda_3 < \lambda_1, \lambda_3 \leq \lambda_2\}. \end{aligned}$$

Note that in each of the subtriangles  $B_i, i = 1, 2, 3$ , the corresponding barycentric coordinate is dominated by the remaining ones; e.g.,

$$(2.4) \quad \lambda_1 \leq \min\{\lambda_2, \lambda_3\} \quad \text{in } B_1.$$

The rHCT function is defined in terms of three *correction functions* [10]

$$\rho_1, \rho_2, \rho_3,$$

which are piecewise cubic polynomials in the barycentric coordinates, each defined in a piecewise manner with respect to the subtriangles of the barycentric partition.

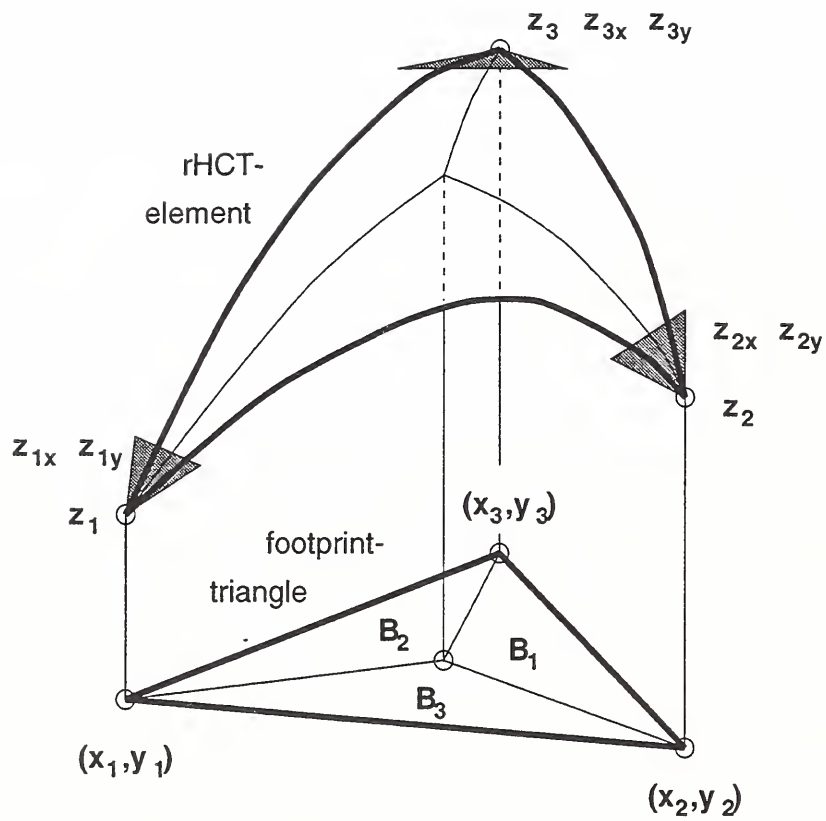


Figure 2.1: Reduced Hsieh-Clough-Tocher Element (rHCT).

$$(2.5) \quad \rho_1 := \begin{cases} \frac{1}{81} & \text{for } (\lambda_1, \lambda_2, \lambda_3) \in B_0 \\ \lambda_1 \lambda_2 \lambda_3 + \frac{5}{6} \lambda_1^3 - \frac{1}{2} \lambda_1^2 & \text{for } (\lambda_1, \lambda_2, \lambda_3) \in B_1 \\ -\frac{1}{6} \lambda_2^3 + \frac{1}{2} \lambda_2^2 \lambda_3 & \text{for } (\lambda_1, \lambda_2, \lambda_3) \in B_2 \\ -\frac{1}{6} \lambda_3^3 + \frac{1}{2} \lambda_3^2 \lambda_2 & \text{for } (\lambda_1, \lambda_2, \lambda_3) \in B_3. \end{cases}$$

Expressions for the remaining correction functions  $\rho_2$  and  $\rho_3$  follow directly from the above expression by cyclic substitution (1.2).

The edge of the footprint triangle spanned by vertices 1 and 2 is characterized by  $\lambda_3 = 0$ , and essentially lies in subtriangle  $B_3$ . Since the  $B_3$ -expression for each correction function contains  $\lambda_3$  as a common factor, those functions vanish along that edge. In general,

$$(2.6) \quad \rho_1 = \rho_2 = \rho_3 = 0 \quad \text{on the triangle boundary.}$$

Each function  $\rho_i$ ,  $i = 1, 2, 3$ , is continuous across the subtriangle boundaries. This is readily verified for the correction function  $\rho_1$  as follows. At the boundary between subtriangles  $B_2$  and  $B_3$ , we have  $\lambda_2 = \lambda_3$ . If we substitute the single quantity  $\lambda$  for these values, the expressions for  $\rho_1$  in  $B_2$  and  $B_3$  become identical. At the boundary between subtriangles  $B_1$  and  $B_2$ , we have similarly  $\lambda_1 = \lambda_2 := \lambda$ . Substituting  $\lambda$  into the expressions keyed to  $B_1$  and  $B_2$  yields

$$\frac{1}{2} \lambda^2 - \frac{7}{6} \lambda^3$$

in both cases. The argument is analogous for the remaining two correction functions. It will be seen in the next section that the correction functions are also smooth at subtriangle boundaries, and thus belong to the class  $C^1$ .

The following quantities can be calculated easily from the initial triangle data.

$$(2.7) \quad \begin{aligned} M_{ji} &= z_{ix} x_{ji} + z_{iy} y_{ji}, \quad i, j = 1, 2, 3, \quad i \neq j, \\ Q_{ij} &= \frac{M_{ji} + M_{ij}}{2}, \quad C_{ij} = \frac{M_{ji} - M_{ij}}{2} - z_{ji} \\ L_i &= \sqrt{x_{jk}^2 + y_{jk}^2}, \quad i \neq j, \quad j \neq k, \quad k \neq i, \\ K_1 &= \frac{3(L_2^2 - L_3^2)}{L_1^2}, \quad K_2 = \frac{3(L_3^2 - L_1^2)}{L_2^2}, \quad K_3 = \frac{3(L_1^2 - L_2^2)}{L_3^2}. \end{aligned}$$

The six quantities  $M_{ji}$  represent the directional derivatives at vertex  $i$  with respect to the direction vector  $(x_{ij}, y_{ij})$ , which represents an entire directed edge of the triangle. Note

that for a linear function  $z = z(x, y)$ ,  $M_{ji} = -M_{ij} = z_{ij}$ , and for a quadratic function,  $M_{ji} - M_{ij} = 2z_{ji}$ . As a consequence, the quantities  $Q_{ij}$  and  $C_{ij}$  both vanish for linear functions, and the quantities  $C_{ij}$  for quadratic functions. Also note

$$Q_{ji} = Q_{ij}, \quad \text{and} \quad C_{ji} = -C_{ij}.$$

We also define three functions

$$V_1, V_2, V_3$$

in terms of the previously (2.5) introduced correction functions  $\rho_1, \rho_2, \rho_3$ :

$$(2.8) \quad V_1 := \lambda_2 \lambda_3 (\lambda_2 - \lambda_3) + K_1 \rho_1 - \rho_2 + \rho_3$$

Expressions for  $V_2, V_3$  follow by cyclic substitution (1.2). The functions  $V_i$  are continuous and, by (2.6),

$$(2.9) \quad V_1 = V_2 = V_3 = 0 \quad \text{at each triangle vertex.}$$

With the preceding definitions, we are now ready to present a formula for the rHCT function, expressing the elevation  $z = z(x, y)$  at any location  $(x, y)$  in the footprint triangle:

$$(2.10) \quad \begin{aligned} z = & z_1 \lambda_1 + z_2 \lambda_2 + z_3 \lambda_3 + \\ & Q_{23} \lambda_2 \lambda_3 + Q_{31} \lambda_3 \lambda_1 + Q_{12} \lambda_1 \lambda_2 + \\ & C_{23} V_1 + C_{31} V_2 + C_{12} V_3 . \end{aligned}$$

This indeed defines a function  $z = z(x, y)$ , since the quantities  $\lambda_i$  are functions of  $x$  and  $y$  by (2.3). To see that  $z = z(x, y)$  assumes the prescribed elevations  $z_i$  at the vertices of the footprint triangle, recall (2.9) and that, at vertices, one  $\lambda_i$  equals 1 while the others are zero.

Recall also that for a quadratic function the coefficients  $C_{ij}$  vanish, so that the first two lines of the above expression for  $z = z(x, y)$  describe an interpolation that is quadratic. Similarly, if both sets of coefficients  $Q_{ij}, C_{ij}$  vanish, then the first three terms of (2.10) describe a linear interpolation. This observation is significant because the energy integral (1.1) vanishes for linear functions, and will thus be a homogeneous quadratic form in the six coefficients  $Q_{ij}, C_{ij}$ .

### 3. First Derivatives of the rHCT element

In this section, the partial derivatives of  $z = z(x, y)$  will be determined, enabling us to establish continuous differentiability. The derivatives of the rHCT function  $z = z(x, y)$  are in the final

instance based on the derivatives of the barycentric coordinates  $\lambda_i$ .

$$(3.1) \quad \begin{aligned} \frac{\partial \lambda_1}{\partial x} &= \frac{y_{23}}{D_{xy}} \quad , \quad \frac{\partial \lambda_1}{\partial y} = \frac{x_{23}}{D_{yx}} \quad , \\ \frac{\partial \lambda_2}{\partial x} &= \frac{y_{31}}{D_{xy}} \quad , \quad \frac{\partial \lambda_2}{\partial y} = \frac{x_{31}}{D_{yx}} \quad , \\ \frac{\partial \lambda_3}{\partial x} &= \frac{y_{21}}{D_{xy}} \quad , \quad \frac{\partial \lambda_3}{\partial y} = \frac{x_{21}}{D_{yx}} \quad . \end{aligned}$$

Notice the use of both determinants  $D_{xy}$  and  $D_{yx} = -D_{xy}$  as defined in (2.2). This convention permits us to write the above formulas symmetrically in  $x$  and  $y$ .

For the correction functions  $\rho_i$  defined in (2.5), the Chain Rule yields

$$\frac{\partial \rho_1}{\partial x} = \frac{\partial \rho_1}{\partial \lambda_1} \frac{\partial \lambda_1}{\partial x} + \frac{\partial \rho_1}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial x} + \frac{\partial \rho_1}{\partial \lambda_3} \frac{\partial \lambda_3}{\partial x} \quad ,$$

and

$$(3.2) \quad \frac{\partial \rho_1}{\partial x} = \frac{1}{D_{xy}} \left\{ \begin{array}{ll} \left[ -\frac{1}{18} y_{23} \right] & \text{in } B_0 \\ \left[ \left( \lambda_2 \lambda_3 + \frac{5}{2} \lambda_1^2 - \lambda_1 \right) y_{23} + \lambda_1 \lambda_3 y_{31} + \lambda_1 \lambda_2 y_{12} \right] & \text{in } B_1 \\ \left[ \left( -\frac{1}{2} \lambda_2^2 + \lambda_2 \lambda_3 \right) y_{31} + \frac{1}{2} \lambda_2^2 y_{12} \right] & \text{in } B_2 \\ \left[ \frac{1}{2} \lambda_3^2 y_{31} + \left( -\frac{1}{2} \lambda_3^2 + \lambda_3 \lambda_2 \right) y_{12} \right] & \text{in } B_3 . \end{array} \right.$$

Similarly,

$$(3.3) \quad \frac{\partial \rho_1}{\partial y} = \frac{1}{D_{yx}} \left\{ \begin{array}{ll} \left[ -\frac{1}{18} x_{23} \right] & \text{in } B_0 \\ \left[ \left( \lambda_2 \lambda_3 + \frac{5}{2} \lambda_1^2 - \lambda_1 \right) x_{23} + \lambda_1 \lambda_3 x_{31} + \lambda_1 \lambda_2 x_{12} \right] & \text{in } B_1 \\ \left[ \left( -\frac{1}{2} \lambda_2^2 + \lambda_2 \lambda_3 \right) x_{31} + \frac{1}{2} \lambda_2^2 x_{12} \right] & \text{in } B_2 \\ \left[ \frac{1}{2} \lambda_3^2 x_{31} + \left( -\frac{1}{2} \lambda_3^2 + \lambda_3 \lambda_2 \right) x_{12} \right] & \text{in } B_3 . \end{array} \right.$$

The above two formulas are symmetric in  $x$  and  $y$ . The corresponding formulas for the derivatives of the other correction functions  $\rho_2$  and  $\rho_3$  follow by cyclic substitution (1.2).



It is also readily seen that the gradient of  $\rho_1$  vanishes along the  $B_2$ -edge – characterized by  $\lambda_2 = 0$  – and the  $B_3$ -edge – characterized by  $\lambda_3 = 0$  – of the footprint triangle (compare 2.6):

$$(3.4) \quad \frac{\partial \rho_i}{\partial x} = \frac{\partial \rho_i}{\partial y} = 0 \quad \text{for } \lambda_i = 0, \quad i = 1, 2, 3.$$

We are now able to ascertain that the correction functions  $\rho_i$  are indeed continuously differentiable, that is, that they join smoothly at subtriangle boundaries. We consider only  $\rho_1$ . The other cases follow by cyclic substitution (1.2). The boundary between subtriangles  $B_2$  and  $B_3$  is characterized by  $\lambda_2 = \lambda_3$ . The expressions specified in both (3.2) and (3.3) for those subtriangles are identical in this case. At the boundary between  $B_1$  and  $B_2$  we have  $\lambda_1 = \lambda_2 := \lambda$  and  $\lambda_3 = 1 - 2\lambda$ . Applying these substitutions for subtriangle  $B_1$  yields

$$(\lambda(1 - 2\lambda) + \frac{5}{2}\lambda^2 - \lambda)y_{23} + \lambda(1 - 2\lambda)y_{31} + \lambda^2y_{12}$$

or, taking into account that  $y_{23} = -y_{12} - y_{31}$ ,

$$(-\frac{5}{2}\lambda^2 + \lambda)y_{31} + \frac{1}{2}\lambda^2y_{12}.$$

The same expression clearly results in subtriangle  $B_2$ . The argument for the derivative with respect to  $y$  is analogous, and so is the consideration of the boundary between  $B_1$  and  $B_3$ .

Since the correction functions  $\rho_i$  are continuously differentiable, the same holds for the functions  $V_i$  in formula (2.10) for the function  $z = z(x, y)$ . As a consequence, the rHCT element belongs to the class  $C^1$ .

Using the Chain Rule and formulas (3.1), we find

$$\begin{aligned} \frac{\partial z}{\partial x} &= \frac{\partial z}{\partial \lambda_1} \frac{\partial \lambda_1}{\partial x} + \frac{\partial z}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial x} + \frac{\partial z}{\partial \lambda_3} \frac{\partial \lambda_3}{\partial x} \\ &= \frac{1}{D_{xy}} [(z_1 + Q_{31}\lambda_3 + Q_{12}\lambda_2)y_{23} + \dots + (z_3 + Q_{23}\lambda_2 + Q_{31}\lambda_1)y_{12}] + \\ &\quad C_{23} \frac{\partial V_1}{\partial x} + C_{31} \frac{\partial V_2}{\partial x} + C_{12} \frac{\partial V_3}{\partial x}. \end{aligned}$$

Thus,

$$(3.5) \quad \frac{\partial z}{\partial x} = \frac{1}{D_{xy}} [z_1y_{23} + z_2y_{31} + z_3y_{12} + \lambda_1(Q_{12}y_{31} + Q_{31}y_{12}) + \lambda_2(Q_{23}y_{12} + Q_{12}y_{23}) + \lambda_3(Q_{31}y_{23} + Q_{23}y_{31})] + C_{23} \frac{\partial V_1}{\partial x} + C_{31} \frac{\partial V_2}{\partial x} + C_{12} \frac{\partial V_3}{\partial x}.$$

Exchanging  $x$  and  $y$  then yields

$$(3.6) \quad \frac{\partial z}{\partial y} = \frac{1}{D_{yx}} [z_1 x_{23} + z_2 x_{31} + z_3 x_{12} + \lambda_1(Q_{12}x_{13} + Q_{31}x_{21}) + \lambda_2(Q_{23}x_{21} + Q_{12}x_{32}) + \lambda_3(Q_{31}x_{31} + Q_{23}y_{13})] + C_{23} \frac{\partial V_1}{\partial y} + C_{31} \frac{\partial V_2}{\partial y} + C_{12} \frac{\partial V_3}{\partial y}.$$

Note that the constants in both expressions equal the determinants  $D_{zy}$  and  $D_{zx}$ , respectively, as defined in (2.2).

The derivatives of the functions  $V_i$ ,  $i = 1, 2, 3$ , (2.8) are next. Again, we display only the derivatives of  $V_1$ , since the expressions for the derivatives of the remaining functions follow by cyclic substitution (1.2). The first term of the function  $V_1$  is the polynomial  $\lambda_2 \lambda_3 (\lambda_2 - \lambda_3)$ . By (3.1), the partial derivative of this expression with respect to  $x$  is given by

$$\frac{1}{D_{xy}} [(2\lambda_2 \lambda_3 - \lambda_3^2) y_{31} + (\lambda_2^2 - 2\lambda_2 \lambda_3) y_{12}].$$

Thus, – and symmetrically for the derivative with respect to  $y$  –,

$$(3.7) \quad \begin{aligned} \frac{\partial V_1}{\partial x} &= \frac{1}{D_{xy}} [(2\lambda_2 \lambda_3 - \lambda_3^2) y_{31} + (\lambda_2^2 - 2\lambda_2 \lambda_3) y_{12}] + K_1 \frac{\partial \rho_1}{\partial x} - \frac{\partial \rho_2}{\partial x} + \frac{\partial \rho_3}{\partial x} \\ \frac{\partial V_1}{\partial y} &= \frac{1}{D_{yx}} [(2\lambda_2 \lambda_3 - \lambda_3^2) x_{31} + (\lambda_2^2 - 2\lambda_2 \lambda_3) x_{12}] + K_1 \frac{\partial \rho_1}{\partial y} - \frac{\partial \rho_2}{\partial y} + \frac{\partial \rho_3}{\partial y}. \end{aligned}$$

It now follows from (3.5,3.6) that, at vertex 1,

$$\begin{aligned} D_{xy} \frac{\partial z}{\partial x}(x_1, y_1) &= D_{zy} + (Q_{12} + C_{12}) y_{31} + (Q_{31} - C_{31}) y_{12} \\ D_{yx} \frac{\partial z}{\partial y}(x_1, y_1) &= D_{zx} + (Q_{12} + C_{12}) x_{13} + (Q_{31} - C_{31}) x_{21}. \end{aligned}$$

In view of  $Q_{12} + C_{12} = M_{21} - z_{21}$ ,  $Q_{31} - C_{31} = M_{31} + z_{31}$  – by the definition (2.7) of those quantities, – a short calculation yields

$$\begin{aligned} D_{xy} \frac{\partial z}{\partial x}(x_1, y_1) &= M_{21} y_{31} + M_{31} y_{12} = D_{xy} z_{1x}, \\ D_{yx} \frac{\partial z}{\partial y}(x_1, y_1) &= M_{21} x_{31} + M_{31} x_{12} = D_{yx} z_{1y}. \end{aligned}$$

This – and cyclic substitution (1.2) – show that the rHCT function  $z = z(x, y)$  indeed assumes the prescribed derivative values at the vertices of the footprint triangle.

## 4. The Linear Derivative Condition

The salient property of the rHCT element – as opposed to the nonreduced HCT element – is that it satisfies (see for example [10]) the following

- (4.1) *Linear Derivative Condition:* Along each edge of the footprint triangle, the derivative taken in the direction perpendicular to the edge varies linearly between the values it assumes at the ends of the edge.

The purpose of the Linear Derivative Condition is to ensure that adjacent triangles in a triangulation fit together smoothly. Indeed, all directional derivatives at a vertex can be determined from the – given – gradient at that vertex. At the endpoints of the common edge, both elevations and derivatives in the direction of the edge are therefore predetermined. Since the rHCT function  $z = z(x, y)$  induces a cubic function on the edge, that function is fully specified – say, by Hermite’s formula – and the specification is the same in both the adjacent triangles, because that specification is solely based on quantities given at the two vertices of the boundary edge. Continuity across the edge therefore holds, as does commonality of the derivative in the direction of the edge. In order to ensure smoothness, that is, a common gradient in both triangles along the edge, it therefore suffices that the derivatives perpendicular to the edge are also fully specified by their values at the vertices of the edge.

Now if the perpendicular derivative along an edge is a linear function, that is, if the Linear Derivative Condition is satisfied, then that derivative is fully specified by its values at the vertices of the edge. This is all that is needed to ensure smoothness across triangle boundaries.

A directional derivative of  $z = z(x, y)$  perpendicular to the edge, say, from vertex  $i$  to vertex  $j$  is given by

$$(4.2) \quad y_{ji} \frac{\partial z}{\partial x} - x_{ji} \frac{\partial z}{\partial y},$$

because the vector  $(y_{jk}, -x_{jk})$  is perpendicular to the direction  $(x_{jk}, y_{jk})$  of the edge. Any other definition of the perpendicular derivative differs by a constant factor; so it does not matter which definition we choose.

In order to verify that the rHCT indeed satisfies the Linear Derivative Condition that (4.2) is a linear function, we need to consider only the three functions  $V_i$  (2.8), since they contain all the cubic terms of the function  $z = z(x, y)$ . In particular, we need to consider only  $V_1$ , because the argument extends by cyclic substitution (1.2) to the two remaining functions  $V_i$ .

We first evaluate

$$(4.3) \quad D_{xy} \left( y_{23} \frac{\partial V_1}{\partial x} - x_{23} \frac{\partial V_1}{\partial y} \right),$$

in subtriangle  $B_1$ , for the edge connecting vertices 2 and 3. Here  $\lambda_1 = 0$ , whence  $\lambda_2 + \lambda_3 = 1$ .

Since the gradients of  $\rho_2$  and  $\rho_3$  vanish along that edge (see 3.4), and since the gradient of  $\rho_1$  becomes

$$\lambda_2 \lambda_3 \left( \frac{y_{23}}{D_{xy}}, \frac{x_{23}}{D_{yx}} \right),$$

we find for (4.3), taking into account  $D_{yx} = -D_{xy}$ ,

(4.4)

$$\lambda_3(2\lambda_2 - \lambda_3)(x_{23}x_{31} + y_{23}y_{31}) - \lambda_2(2\lambda_3 - \lambda_2)(x_{23}x_{12} + y_{23}y_{12}) + \lambda_2\lambda_3 K_1(x_{23}^2 + y_{23}^2).$$

From definitions (2.7),  $K_1(x_{23}^2 + y_{23}^2) = 3(L_2^2 - L_3^2)$ . Moreover, the scalar products,

$$S_2 := x_{23}x_{12} + y_{23}y_{12}, \quad S_3 := x_{31}x_{23} + y_{31}y_{23},$$

can be used to express squares of edge lengths  $L_i^2$ :

$$L_2^2 - L_3^2 = S_3 - S_2.$$

Expression (4.4) thus reduces to

$$(\lambda_2 + \lambda_3)(\lambda_2 S_2 - \lambda_3 S_3) = \lambda_2 S_2 - \lambda_3 S_3,$$

and is therefore linear in  $x$  and  $y$ .

Along the edge in subtriangle  $B_2$ , we have  $\lambda_2 = 0$ ,  $\lambda_3 + \lambda_1 = 1$ . Only the gradient of  $\rho_2$  does not vanish. Similarly to (4.3) we find

$$(\lambda_3 + \lambda_1)(-\lambda_3 L_2^2) = -\lambda_3 L_2^2,$$

which again establishes linearity. In subtriangle  $B_3$ ,  $\lambda_3 = 0$ ,  $\lambda_1 + \lambda_2 = 1$ . Thus

$$(\lambda_1 + \lambda_2)(-\lambda_2 L_3^2) = -\lambda_2 L_3^2.$$

The rHCT is therefore seen to satisfy the Linear Derivative Condition.

## 5. Second Derivatives of the rHCT Element

We now aim to express the second partial derivatives

$$\frac{\partial^2 z}{\partial x^2}, \quad \frac{\partial^2 z}{\partial x \partial y}, \quad \frac{\partial^2 z}{\partial y^2}$$

as linear functions of the barycentric coordinates  $\lambda_1, \lambda_2, \lambda_3$ . We start with the correction functions  $\rho_i$ , based on the following applications of the Chain Rule.

$$\begin{aligned}\frac{\partial^2 \rho_1}{\partial x^2} &= \frac{\partial}{\partial \lambda_1} \left( \frac{\partial \rho_1}{\partial x} \right) \cdot \frac{\partial \lambda_1}{\partial x} + \frac{\partial}{\partial \lambda_2} \left( \frac{\partial \rho_1}{\partial x} \right) \cdot \frac{\partial \lambda_2}{\partial x} + \frac{\partial}{\partial \lambda_3} \left( \frac{\partial \rho_1}{\partial x} \right) \cdot \frac{\partial \lambda_3}{\partial x}, \\ \frac{\partial^2 \rho_1}{\partial x \partial y} &= \frac{\partial}{\partial \lambda_1} \left( \frac{\partial \rho_1}{\partial x} \right) \cdot \frac{\partial \lambda_1}{\partial y} + \frac{\partial}{\partial \lambda_2} \left( \frac{\partial \rho_1}{\partial x} \right) \cdot \frac{\partial \lambda_2}{\partial y} + \frac{\partial}{\partial \lambda_3} \left( \frac{\partial \rho_1}{\partial x} \right) \cdot \frac{\partial \lambda_3}{\partial y}, \\ \frac{\partial^2 \rho_1}{\partial x \partial y} &= \frac{\partial}{\partial \lambda_1} \left( \frac{\partial \rho_1}{\partial y} \right) \cdot \frac{\partial \lambda_1}{\partial x} + \frac{\partial}{\partial \lambda_2} \left( \frac{\partial \rho_1}{\partial y} \right) \cdot \frac{\partial \lambda_2}{\partial x} + \frac{\partial}{\partial \lambda_3} \left( \frac{\partial \rho_1}{\partial y} \right) \cdot \frac{\partial \lambda_3}{\partial x}.\end{aligned}$$

From (3.2, 3.3),

$$(5.1) \quad \frac{\partial^2 \rho_1}{\partial x^2} = \frac{1}{D_{xy}^2} \begin{cases} (5\lambda_1 - 1)y_{23}^2 + \\ 2\lambda_1 y_{31} y_{12} + 2\lambda_2 y_{12} y_{23} + 2\lambda_3 y_{23} y_{31} & \text{in } B_1 \\ (\lambda_3 - \lambda_2)y_{31}^2 + 2\lambda_2 y_{31} y_{12} & \text{in } B_2 \\ (\lambda_2 - \lambda_3)y_{12}^2 + 2\lambda_3 y_{31} y_{12} & \text{in } B_3 \end{cases}$$

$$(5.2) \quad \frac{\partial^2 \rho_1}{\partial x \partial y} = \frac{1}{D_{xy} D_{yx}} \begin{cases} (5\lambda_1 - 1)y_{23} x_{23} + \\ \lambda_1 (y_{31} x_{12} + x_{31} y_{12}) + \lambda_2 (y_{12} x_{23} + x_{12} y_{23}) + \lambda_3 (y_{23} x_{31} + x_{23} y_{31}) & \text{in } B_1 \\ (\lambda_3 - \lambda_2) y_{31} x_{31} + \lambda_2 (y_{31} x_{12} + x_{31} y_{12}) & \text{in } B_2 \\ (\lambda_2 - \lambda_3) y_{12} x_{12} + \lambda_3 (y_{31} x_{12} + x_{31} y_{12}) & \text{in } B_3 \end{cases}$$

$$(5.3) \quad \frac{\partial^2 \rho_1}{\partial y^2} = \frac{1}{D_{yx}^2} \begin{cases} (5\lambda_1 - 1)x_{23}^2 + \\ 2\lambda_1 x_{31} x_{12} + 2\lambda_2 x_{12} x_{23} + 2\lambda_3 x_{23} x_{31} & \text{in } B_1 \\ (\lambda_3 - \lambda_2)x_{31}^2 + 2\lambda_2 x_{31} x_{12} & \text{in } B_2 \\ (\lambda_2 - \lambda_3)x_{12}^2 + 2\lambda_3 x_{31} x_{12} & \text{in } B_3 \end{cases}$$

Formulas for the second derivatives of the two remaining correction functions  $\rho_2$  and  $\rho_3$  follow by cyclic substitution (1.2). It is readily verified that the second derivatives are continuous at the barycenter, that is, each subcubic yields the same value for  $\lambda_1 = \lambda_2 = \lambda_3 = 1/3$ . That continuity, however, does not generally extend along every common edge of two subtriangles. The same continuity pattern holds for the full element (2.10).



We now turn to the functions  $V_i$  defined in (2.8) whose first derivatives have been calculated in Section 3 (3.7). It follows by straightforward applications of the Chain Rule that

$$(5.4) \quad \begin{aligned} \frac{\partial^2 V_1}{\partial x^2} &= \frac{2}{D_{xy}^2} [\lambda_3 y_{31}^2 + (\lambda_2 - \lambda_3) y_{12} y_{31} - \lambda_2 y_{12}^2] + K_1 \frac{\partial^2 \rho_1}{\partial x^2} - \frac{\partial^2 \rho_2}{\partial x^2} + \frac{\partial^2 \rho_3}{\partial x^2}, \\ \frac{\partial^2 V_1}{\partial x \partial y} &= \frac{2}{D_{xy} D_{yx}} [\lambda_3 y_{13} x_{31} + (\lambda_2 - \lambda_3) (y_{12} x_{31} + x_{12} y_{31}) - \lambda_2 y_{21} x_{12} + \\ &\quad K_1 \frac{\partial^2 \rho_1}{\partial x \partial y} - \frac{\partial^2 \rho_2}{\partial x \partial y} + \frac{\partial^2 \rho_3}{\partial x \partial y}], \\ \frac{\partial^2 V_1}{\partial y^2} &= \frac{2}{D_{yx}^2} [\lambda_3 x_{31}^2 + (\lambda_2 - \lambda_3) x_{12} x_{31} - \lambda_2 x_{12}^2] + K_1 \frac{\partial^2 \rho_1}{\partial y^2} - \frac{\partial^2 \rho_2}{\partial y^2} + \frac{\partial^2 \rho_3}{\partial y^2}. \end{aligned}$$

The second derivatives of the two remaining functions  $V_2$  and  $V_3$  follow from the above by cyclic substitution (1.2). We can now express the second derivatives of the rHCT function  $z = z(x, y)$  in terms of the second derivatives of  $V_i$ ,  $i = 1, 2, 3$ .

$$(5.5) \quad \begin{aligned} \frac{\partial^2 z}{\partial x^2} &= \frac{2}{D_{xy}^2} [Q_{23} y_{12} y_{31} + Q_{31} y_{23} y_{12} + Q_{12} y_{31} y_{23}] \\ &\quad + C_{23} \frac{\partial^2 V_1}{\partial x^2} + C_{31} \frac{\partial^2 V_2}{\partial x^2} + C_{12} \frac{\partial^2 V_3}{\partial x^2}, \\ \frac{\partial^2 z}{\partial x \partial y} &= \frac{2}{D_{xy} D_{yx}} [Q_{23} (y_{12} x_{31} + x_{12} y_{31}) + Q_{31} (y_{23} x_{12} + x_{23} y_{12}) + Q_{12} (y_{31} x_{23} + x_{31} y_{23})] \\ &\quad + C_{23} \frac{\partial^2 V_1}{\partial x \partial y} + C_{31} \frac{\partial^2 V_2}{\partial x \partial y} + C_{12} \frac{\partial^2 V_3}{\partial x \partial y}, \\ \frac{\partial^2 z}{\partial y^2} &= \frac{2}{D_{yx}^2} [Q_{23} x_{12} x_{31} + Q_{31} x_{23} x_{12} + Q_{12} x_{31} x_{23}] \\ &\quad + C_{23} \frac{\partial^2 V_1}{\partial y^2} + C_{31} \frac{\partial^2 V_2}{\partial y^2} + C_{12} \frac{\partial^2 V_3}{\partial y^2}. \end{aligned}$$

## 6. The Barycentric Integrals

The functions which form the integrand of the energy integral (1.1) have been expressed in terms of the barycentric coordinates, but the variables of the integration are still  $x$  and  $y$ .

More precisely, that integrand will be a quadratic polynomial in  $\lambda_1, \lambda_2, \lambda_3$ . The same holds for additive components of the integrand, if these were to be evaluated separately.

In view of the relation  $\lambda_1 + \lambda_2 + \lambda_3 = 1$ , various normalizations of such polynomials are possible. For instance, the polynomial can be required to be a homogeneous quadratic form, that is, contain only terms of degree 2. Or one of the barycentric coordinates, say,  $\lambda_3$ , can be expressed in terms of the remaining ones, yielding a nonhomogeneous quadratic polynomial in, say,  $\lambda_1$  and  $\lambda_2$ .

Similarly, the cartesian coordinates  $x, y$  can be expressed linearly in any two of the barycentric coordinates. For instance, eliminating  $\lambda_3$  in relations (2.1) will yield such an expression – and its cyclic permutations (1.2):

$$\begin{aligned}\begin{pmatrix} x \\ y \end{pmatrix} &= \begin{pmatrix} x_3 \\ y_3 \end{pmatrix} + \begin{pmatrix} x_{13} & x_{23} \\ y_{13} & y_{23} \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} \\ \begin{pmatrix} x \\ y \end{pmatrix} &= \begin{pmatrix} x_1 \\ y_1 \end{pmatrix} + \begin{pmatrix} x_{21} & x_{31} \\ y_{21} & y_{31} \end{pmatrix} \begin{pmatrix} \lambda_2 \\ \lambda_3 \end{pmatrix} \\ \begin{pmatrix} x \\ y \end{pmatrix} &= \begin{pmatrix} x_2 \\ y_2 \end{pmatrix} + \begin{pmatrix} x_{32} & x_{12} \\ y_{32} & y_{12} \end{pmatrix} \begin{pmatrix} \lambda_3 \\ \lambda_1 \end{pmatrix}.\end{aligned}$$

Note further, that the determinants of the above linear transformations agree with the previously encountered determinant  $D_{xy}$  (2.2) of the linear system (2.1):

$$\det \begin{vmatrix} x_{13} & x_{23} \\ y_{13} & y_{23} \end{vmatrix} = \det \begin{vmatrix} x_{21} & x_{31} \\ y_{21} & y_{31} \end{vmatrix} = \det \begin{vmatrix} x_{32} & x_{12} \\ y_{32} & y_{12} \end{vmatrix} = D_{xy}.$$

The area element  $dx dy$  is transformed under a linear transformation

$$\begin{pmatrix} \bar{x} \\ \bar{y} \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} + T \begin{pmatrix} x \\ y \end{pmatrix}$$

into the area element  $\det(T)d\bar{x} d\bar{y}$ . We thus have

$$(6.1) \quad dx dy = D_{xy}d\lambda_1 d\lambda_2 = D_{xy}d\lambda_2 d\lambda_3 = D_{xy}d\lambda_3 d\lambda_1.$$

In view of  $\lambda_3 = 1 - \lambda_1 - \lambda_2$ , the definition (2.4) of the subtriangle  $B_1$  can be altered. Up to differences of measure 0, we have

$$B_1 := \{(\lambda_1, \lambda_2, \lambda_3) : 0 \leq \lambda_1 \leq 1/3, \lambda_1 \leq \lambda_2 \leq 1 - 2\lambda_1\},$$

suggesting limits of integration over those subtriangles. Indeed, for any function  $f(\lambda_1, \lambda_2)$ , we have

$$\int_{B_1} f(\lambda_1, \lambda_2)d\lambda_2 d\lambda_1 = \int_0^{\frac{1}{3}} \left[ \int_{\lambda_1}^{1-2\lambda_1} f(\lambda_1, \lambda_2)d\lambda_2 \right] d\lambda_1.$$

Using this procedure, we find for the following six key integrals:

$$\begin{aligned}
\int_{B_1} 1 d\lambda_2 d\lambda_1 &= \int_0^{\frac{1}{3}} \left[ \int_{\lambda_1}^{1-2\lambda_1} 1 d\lambda_2 \right] d\lambda_1 = \frac{1}{6} \\
\int_{B_1} \lambda_1 d\lambda_2 d\lambda_1 &= \int_0^{\frac{1}{3}} \left[ \int_{\lambda_1}^{1-2\lambda_1} \lambda_1 d\lambda_2 \right] d\lambda_1 = \frac{1}{54} \\
\int_{B_1} \lambda_2 d\lambda_2 d\lambda_1 &= \int_0^{\frac{1}{3}} \left[ \int_{\lambda_1}^{1-2\lambda_1} \lambda_2 d\lambda_2 \right] d\lambda_1 = \frac{2}{27} \\
\int_{B_1} \lambda_1^2 d\lambda_2 d\lambda_1 &= \int_0^{\frac{1}{3}} \left[ \int_{\lambda_1}^{1-2\lambda_1} \lambda_1^2 d\lambda_2 \right] d\lambda_1 = \frac{1}{324} \\
\int_{B_1} \lambda_1 \lambda_2 d\lambda_2 d\lambda_1 &= \int_0^{\frac{1}{3}} \left[ \int_{\lambda_1}^{1-2\lambda_1} \lambda_1 \lambda_2 d\lambda_2 \right] d\lambda_1 = \frac{5}{648} \\
\int_{B_1} \lambda_2^2 d\lambda_2 d\lambda_1 &= \int_0^{\frac{1}{3}} \left[ \int_{\lambda_1}^{1-2\lambda_1} \lambda_2^2 d\lambda_2 \right] d\lambda_1 = \frac{13}{324}.
\end{aligned}$$

These key integrals and their cyclic equivalents are all that is needed for the energy formula to be derived in the next section.

In general and for checking purposes, it may be useful to provide a complete list of barycentric integrals in subtriangles  $B_i$ . All the remaining integrals can be derived from the above key integrals using the relations  $\lambda_1 + \lambda_2 + \lambda_3$  and

$$(6.2) \quad d\lambda_1 + d\lambda_2 + d\lambda_3 = 0.$$

Since  $\lambda_3 = 1 - \lambda_1 - \lambda_2$ ,

$$\begin{aligned}
\int_{B_1} \lambda_3 d\lambda_2 d\lambda_1 &= \int_{B_1} 1 d\lambda_2 d\lambda_1 - \int_{B_1} \lambda_1 d\lambda_2 d\lambda_1 - \int_{B_1} \lambda_2 d\lambda_2 d\lambda_1 \\
&= \frac{1}{6} - \frac{1}{54} - \frac{2}{27} = \frac{2}{27}.
\end{aligned}$$

Analogous calculations yield the remaining integrals over subtriangle  $B_1$  based on the area element  $d\lambda_2 d\lambda_1$ . Integrals over the subtriangles  $B_2$  and  $B_3$  follow from integrals over  $B_1$  by cyclic substitution (1.2).

Suppose indices  $i, j, k$  are in cyclical order. Then substituting  $-d\lambda_j - d\lambda_k$  for  $d\lambda_i$  yields

$$d\lambda_j d\lambda_i = -d\lambda_j d\lambda_j - d\lambda_j d\lambda_k.$$

Since area elements change orientation when the sequence of the differentials is switched, and since consequently also  $d\lambda_j d\lambda_j = 0$ , it follows that

$$d\lambda_2 d\lambda_1 = d\lambda_3 d\lambda_2 = d\lambda_1 d\lambda_3.$$

As a result, it is immaterial which of the three area elements is specified, so that only the integrand is of interest. This permits the display of our barycentric integrals in Table (6.3).

(6.3) Barycentric integrals:

	$B_1$	$B_2$	$B_3$	$B$
1	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{2}$
$\lambda_1$	$\frac{1}{54}$	$\frac{2}{27}$	$\frac{2}{27}$	$\frac{1}{6}$
$\lambda_2$	$\frac{2}{27}$	$\frac{1}{54}$	$\frac{2}{27}$	$\frac{1}{6}$
$\lambda_3$	$\frac{2}{27}$	$\frac{2}{27}$	$\frac{1}{54}$	$\frac{1}{6}$
$\lambda_1^2$	$\frac{1}{324}$	$\frac{13}{324}$	$\frac{13}{324}$	$\frac{1}{12}$
$\lambda_2^2$	$\frac{13}{324}$	$\frac{1}{324}$	$\frac{13}{324}$	$\frac{1}{12}$
$\lambda_3^2$	$\frac{13}{324}$	$\frac{13}{324}$	$\frac{1}{324}$	$\frac{1}{12}$
$\lambda_1\lambda_2$	$\frac{5}{648}$	$\frac{5}{648}$	$\frac{17}{648}$	$\frac{1}{24}$
$\lambda_1\lambda_3$	$\frac{5}{648}$	$\frac{17}{648}$	$\frac{5}{648}$	$\frac{1}{24}$
$\lambda_2\lambda_3$	$\frac{17}{648}$	$\frac{5}{648}$	$\frac{5}{648}$	$\frac{1}{24}$

Additional symmetries are apparent. In subtriangle  $B_i$ , the roles of variables  $\lambda_j$  and  $\lambda_k$  are interchangeable as far as integration is concerned. That is at the root of relations

$$\int_{B_i} f(\lambda_i, \lambda_j) d\lambda_j d\lambda_i = \int_{B_i} f(\lambda_i, \lambda_k) d\lambda_j d\lambda_i, \quad j, k \neq i.$$

$$\int_B f(\lambda_1, \lambda_2) d\lambda_2 d\lambda_1 = \int_0^1 \left[ \int_0^{1-\lambda_1} f(\lambda_1, \lambda_2) d\lambda_2 \right] d\lambda_1.$$

Those results are also displayed in Table (6.3). They should be the sum of the integrals of the same integrand over the three subtriangles  $B_i$ .

## 7. Derivation of the rHCT Energy Formula

In this section, we will carry out the integration prescribed by the formula (1.1) for the surface energy of an almost flat thin plate for a single triangular rHCT element. That element is determined, as set forth in the previous sections, by the vertex data supplied at the corners of the given triangle  $B$ .

Let  $B = B_0 \cup B_1 \cup B_2 \cup B_3$  be the given triangle with its barycentric partition. The surface energy  $E$  of the surface element is then given by

$$(7.1) \quad E := \int \int_B \left[ \left( \frac{\partial^2 z}{\partial x^2} \right)^2 + 2 \left( \frac{\partial^2 z}{\partial x \partial y} \right)^2 + \left( \frac{\partial^2 z}{\partial y^2} \right)^2 \right] dx dy,$$

where  $z = z(x, y)$  is the rHCT function (2.10). Our goal is to express  $E$  in closed form in terms of the elevations and gradients at the triangle vertices as well as the triangle geometry.

Energy  $E$  is the sum of the energies  $E_i$  in the three subtriangles  $B_i$ ,  $i = 1, 2, 3$ ,

$$E = E_1 + E_2 + E_3,$$

and will be determined in that fashion. Once an expression for  $E_1$  has been obtained, energy expressions for  $E_2$  and  $E_3$  follow by cyclic substitution.

The second derivative expressions (5.1)–(5.5) for the  $\rho_i$ 's,  $V_i$ 's, and hence  $z$ , are linear in  $\lambda_1, \lambda_2$  and  $\lambda_3$ . Also, since  $\lambda_1 + \lambda_2 + \lambda_3 = 1$ , we can replace  $\lambda_3$  everywhere with  $1 - \lambda_1 - \lambda_2$ , resulting in second derivative expressions as follows which are linear in  $\lambda_1$  and  $\lambda_2$ .



$$\frac{\partial^2 z}{\partial x^2} = \frac{1}{D_{xy}^2} (c_{0xx} + c_{1xx}\lambda_1 + c_{2xx}\lambda_2)$$

$$\frac{\partial^2 z}{\partial x \partial y} = \frac{1}{D_{xy}^2} (c_{0xy} + c_{1xy}\lambda_1 + c_{2xy}\lambda_2)$$

$$\frac{\partial^2 z}{\partial y^2} = \frac{1}{D_{xy}^2} (c_{0yy} + c_{1yy}\lambda_1 + c_{2yy}\lambda_2) .$$

The coefficients  $c_{0xx}, c_{1xx}, \dots$  of the above linear form refer to subtriangle  $B_1$ , and are, of course, different for the other subtriangles  $B_i$  of the barycentric partition.

The second derivative expressions also show that the coefficients  $c_{..}$  themselves are homogeneous quadratic forms in the coordinate differences  $x_{ij}, y_{ij}$ , all of which can be expressed linearly in  $x_{21}, x_{13}, y_{12}, y_{31}$  since  $x_{32} = -x_{13} - x_{21}$ , etc. Due to the structure of the derivative expressions only nine coefficients  $a_{ijk}$  occur as coefficients of those quadratic forms. For  $i = 1, 2, 3$ ,

$$\begin{aligned} c_{ixx} &= a_{i22}y_{12}^2 + 2a_{i23}y_{12}y_{31} + a_{i33}y_{31}^2 \\ c_{ixy} &= a_{i22}x_{21}y_{12} + a_{i23}(x_{21}y_{31} + x_{13}y_{12}) + a_{033}x_{13}y_{31} \\ c_{iyy} &= a_{i22}x_{21}^2 + 2a_{i23}x_{21}x_{13} + a_{i33}x_{13}^2 , \end{aligned}$$

where

$$\begin{aligned} a_{022} &= -2Q_{31} + 2C_{12} - (K_1 + 1)C_{23} + (K_2 - 7)C_{31} \\ a_{023} &= -Q_{12} + Q_{23} - Q_{31} + 3C_{12} - (2K_1 + 3)C_{23} + (K_2 - 6)C_{31} \\ a_{033} &= -2Q_{12} + 4C_{12} - (3K_1 - 1)C_{23} + (K_2 - 5)C_{31} \\ a_{122} &= -(K_3 + 9)C_{12} + (5K_1 + 3)C_{23} - (4K_2 - 18)C_{31} \\ a_{123} &= -(2K_3 + 12)C_{12} + (7K_1 + 3)C_{23} - (3K_2 - 15)C_{31} \\ a_{133} &= -(3K_3 + 15)C_{12} + (7K_1 - 3)C_{23} - (2K_2 - 12)C_{31} \\ a_{222} &= +(K_3 + 3)\check{C}_{12} - 2K_1C_{23} - (K_2 - 3)C_{31} \\ a_{223} &= +(K_3 + 3)C_{12} + 6C_{23} - (K_2 - 3)C_{31} \\ a_{233} &= +(K_3 + 3)C_{12} + 2K_1C_{23} - (K_2 - 3)C_{31} \end{aligned}$$

Note that the coefficients are homogeneous linear forms in the quantities  $Q_{i,j}, C_{ij}$  whose coefficients depend only on geometric information,  $K_1 = 3(L_2^2 - L_3^2)/L_1^2, \dots$ , independent of the choice of the coordinate system.

The coefficients  $a_{..}$  above, as well as the subsequent results reported here, were mostly determined with the help of Mathematica [16] and verified by comparison with hand calculations.

So, the integrand in the energy integral (7.1) can be expressed over subtriangle  $B_1$  in barycentric coordinates as a quadratic polynomial in the barycentric coordinates  $\lambda_1, \lambda_2$ :

$$\begin{aligned}
& \left( \frac{\partial^2 z}{\partial x^2} \right)^2 + 2 \left( \frac{\partial^2 z}{\partial x \partial y} \right)^2 + \left( \frac{\partial^2 z}{\partial y^2} \right)^2 \\
= & \frac{1}{D_{xy}^4} (c_{0xx} + c_{1xx}\lambda_1 + c_{2xx}\lambda_2)^2 + \\
& \frac{2}{D_{xy}^4} (c_{0xy} + c_{1xy}\lambda_1 + c_{2xy}\lambda_2)^2 + \\
& \frac{1}{D_{xy}^4} (c_{0yy} + c_{1yy}\lambda_1 + c_{2yy}\lambda_2)^2 \\
:= & \frac{1}{D_{xy}^4} (q_{00} + 2q_{01}\lambda_1 + 2q_{02}\lambda_2 + q_{11}\lambda_1^2 + 2q_{12}\lambda_1\lambda_2 + q_{22}\lambda_2^2) .
\end{aligned}$$

The coefficients

$$q_{ij} = c_{ixx}c_{jxx} + 2c_{ixy}c_{jxy} + c_{iyy}c_{jyy}, \quad 0 \leq i \leq j \leq 2,$$

of that quadratic function are themselves quadratic forms in the nine coefficients  $a_{...}$  with coefficients that are homogeneous biquadratic forms in coordinate differences. To prepare for that evaluation, we calculate the three products in the above formula separately.

$$\begin{aligned}
c_{ixx}c_{jxx} = & a_{i22}a_{j22}y_{12}^4 + a_{i22}a_{j23}2y_{12}^3y_{31} + a_{i22}a_{j33}y_{12}^2y_{31}^2 + \\
& a_{i23}a_{j22}2y_{12}^3y_{31} + a_{i23}a_{j23}4y_{12}^2y_{31}^2 + a_{i23}a_{j33}2y_{12}y_{31}^3 + \\
& a_{i33}a_{j22}y_{12}^2y_{31}^2 + a_{i33}a_{j23}2y_{12}y_{31}^3 + a_{i33}a_{j33}y_{31}^4
\end{aligned}$$

$$\begin{aligned}
c_{ixy}c_{jxy} = & a_{i22}a_{j22}x_{21}^2y_{12}^2 + a_{i22}a_{j23}(x_{21}^2y_{12}y_{31} + x_{21}x_{13}y_{12}^2)a_{i22}a_{j33}x_{21}x_{13}y_{12}y_{31} + \\
& a_{i23}a_{j22}(x_{21}^2y_{12}y_{31} + x_{21}x_{13}y_{12}^2) + \\
& a_{i23}a_{j23}(x_{21}^2y_{31}^2 + 2x_{21}x_{13}y_{12}y_{31} + x_{13}^2y_{12}^2) + \\
& a_{i23}a_{j33}(x_{21}x_{13}y_{31}^2 + x_{13}^2y_{12}y_{31}) \\
& a_{i33}a_{j22}x_{21}x_{13}y_{12}y_{31} + a_{i33}a_{j23}(x_{21}x_{13}y_{31}^2 + x_{13}^2y_{12}y_{31}) + a_{i33}a_{j33}x_{13}^2y_{31}^2
\end{aligned}$$

$$\begin{aligned}
c_{iyy}c_{jyy} = & a_{i22}a_{j22}x_{21}^4 + a_{i22}a_{j23}2x_{21}^3x_{13} + a_{i22}a_{j33}x_{21}^2x_{13}^2 + \\
& a_{i23}a_{j22}2x_{21}^3x_{13} + a_{i23}a_{j23}4x_{21}^2x_{13}^2 + a_{i23}a_{j33}2x_{21}x_{13}^3 + \\
& a_{i33}a_{j22}x_{21}^2x_{13}^2 + a_{i33}a_{j23}2x_{21}x_{13}^3 + a_{i33}a_{j33}x_{13}^4 .
\end{aligned}$$

By substituting into the additive expression for coefficient  $q_{ij}$  and collecting terms,

$$\begin{aligned}
q_{ij} = & a_{i22}a_{j22} (x_{21}^2 + y_{12}^2)^2 + \\
& a_{i22}a_{j23} 2(x_{21}^2 + y_{12}^2)(x_{21}x_{13} + y_{12}y_{31}) + \\
& a_{i22}a_{j33}(x_{21}x_{13} + y_{12}y_{31})^2 + \\
& a_{i23}a_{j22} 2(x_{21}^2 + y_{12}^2)(x_{21}x_{13} + y_{12}y_{31}) + \\
& a_{i23}a_{j23} 2 \left[ (x_{21}x_{13} + y_{12}y_{31})^2 + (x_{21}^2 + y_{12}^2)(x_{13}^2 + y_{31}^2) \right] + \\
& a_{i23}a_{j33} 2(x_{13}^2 + y_{31}^2)(x_{21}x_{13} + y_{12}y_{31}) + \\
& a_{i33}a_{j22}(x_{21}x_{13} + y_{12}y_{31})^2 + \\
& a_{i33}a_{j23} 2(x_{13}^2 + y_{31}^2)(x_{21}x_{13} + y_{12}y_{31}) + \\
& a_{i33}a_{j33}(x_{13}^2 + y_{31}^2)^2 .
\end{aligned}$$

Since

$$x_{21}x_{13} + y_{12}y_{31} = \frac{L_1^2 - L_2^2 - L_3^2}{2} ,$$

we find

$$\begin{aligned}
q_{ij} = & a_{i22}a_{j22} (L_3^4) + \\
& 2a_{i22}a_{j23} \left( \frac{L_1^2 - L_2^2 - L_3^2}{2} \right) L_3^2 + \\
& a_{i22}a_{j33} \left( \frac{L_1^2 - L_2^2 - L_3^2}{2} \right)^2 + \\
& 2a_{i23}a_{j22} \left( \frac{L_1^2 - L_2^2 - L_3^2}{2} \right) L_3^2 + \\
& 2a_{i23}a_{j23} \left[ \left( \frac{L_1^2 - L_2^2 - L_3^2}{2} \right)^2 + L_2^2 L_3^2 \right] + \\
& 2a_{i23}a_{j33} \left( \frac{L_1^2 - L_2^2 - L_3^2}{2} \right) L_2^2 + \\
& a_{i33}a_{j22} \left( \frac{L_1^2 - L_2^2 - L_3^2}{2} \right)^2 + \\
& 2a_{i33}a_{j23} \left( \frac{L_1^2 - L_2^2 - L_3^2}{2} \right) L_2^2 + \\
& a_{i33}a_{j33} (L_2^4) .
\end{aligned}$$

Note that the coefficients  $q_{..}$  thus represent purely geometric information independent of the choice of coordinate system, because the coefficients  $a_{..}$ , too, are independent of the choice of the coordinate system, as seen earlier. This indicates that the expression for the surface energy is independent of the choice of the coordinate system, as we would expect. (Note also that the  $q_{..}$ 's will be different for each subtriangle  $B_i$  in the partition of triangle  $B$ , since the coefficients  $c_{..}$  are.)

It remains to substitute the values of the key barycentric integrals. So, the energy integral over subtriangle  $B_1$  is

$$E_1 = \frac{1}{D_{xy}^3} \left( \frac{1}{6}q_{00} + \frac{1}{27}q_{01} + \frac{4}{27}q_{02} + \frac{1}{324}q_{11} + \frac{5}{324}q_{12} + \frac{13}{324}q_{22} \right),$$

where the  $q_{..}$ 's are those appropriate for  $B_1$ . This, finally, results in a homogeneous quadratic form in the derivative quantities  $Q_{ij}, C_{ij}$

$$\begin{aligned} E_1 = & ( g_{1c_1c_1} C_{23}C_{23} + g_{1c_1c_2} C_{23}C_{31} + g_{1c_1c_3} C_{23}C_{12} \\ & + g_{1c_1q_1} C_{23}Q_{23} + g_{1c_1q_2} C_{23}Q_{31} + g_{1c_1q_3} C_{23}Q_{12} \\ & + g_{1c_2c_2} C_{31}C_{31} + g_{1c_2c_3} C_{31}C_{12} + g_{1c_2q_1} C_{31}Q_{23} \\ & + g_{1c_2q_2} C_{31}Q_{31} + g_{1c_2q_3} C_{31}Q_{12} + g_{1c_3c_3} C_{12}C_{12} \\ & + g_{1c_3q_1} C_{12}Q_{23} + g_{1c_3q_2} C_{12}Q_{31} + g_{1c_3q_3} C_{12}Q_{12} \\ & + g_{1q_1q_1} Q_{23}Q_{23} + g_{1q_1q_2} Q_{23}Q_{31} + g_{1q_1q_3} Q_{23}Q_{12} \\ & + g_{1q_2q_2} Q_{31}Q_{31} + g_{1q_2q_3} Q_{31}Q_{12} + g_{1q_3q_3} Q_{12}Q_{12} ) / D_{xy}^3 \end{aligned}$$

with coefficients  $g_{1...}$  that are homogeneous rational functions – as displayed below – in the squares  $L_i^2$  of the side lengths of triangle  $B$ . The coefficients of these rational functions are rational numbers.

$$g_{1c_1c_1} = (3L_1^8 - 6L_1^6L_2^2 + 88L_1^4L_2^4 - 12L_1^2L_2^6 + 11L_2^8 - 6L_1^6L_3^2 - 140L_1^4L_2^2L_3^2 + 12L_1^2L_2^4L_3^2 - 40L_2^6L_3^2 + 88L_1^4L_3^4 + 12L_1^2L_2^2L_3^4 + 58L_2^4L_3^4 - 12L_1^2L_3^6 - 40L_2^2L_3^6 + 11L_3^8) / (36L_1^4)$$

$$g_{1c_1c_2} = (11L_1^8 + 68L_1^6L_2^2 + 300L_1^4L_2^4 - 48L_1^2L_2^6 + 5L_2^8 - 84L_1^6L_3^2 - 368L_1^4L_2^2L_3^2 + 72L_1^2L_2^4L_3^2 - 28L_2^6L_3^2 + 100L_1^4L_3^4 + 38L_2^4L_3^4 - 24L_1^2L_3^6 - 12L_2^2L_3^6 - 3L_3^8) / (72L_1^2L_2^2)$$

$$g_{1c_1c_3} = (11L_1^8 - 84L_1^6L_2^2 + 100L_1^4L_2^4 - 24L_1^2L_2^6 - 3L_2^8 + 68L_1^6L_3^2 - 368L_1^4L_2^2L_3^2 - 12L_2^6L_3^2 + 300L_1^4L_3^4 + 72L_1^2L_2^2L_3^4 + 38L_2^4L_3^4 - 48L_1^2L_3^6 - 28L_2^2L_3^6 + 5L_3^8) / (72L_1^2L_3^2)$$

$$\begin{aligned}
g_{1c1q1} &= (-7L_1^4L_2^2 - 6L_1^2L_2^4 + 13L_2^6 + 7L_1^4L_3^2 - 31L_2^4L_3^2 + 6L_1^2L_3^4 \\
&\quad + 31L_2^2L_3^4 - 13L_3^6)/(18L_1^2) \\
g_{1c1q2} &= (-2L_1^6 + 23L_1^4L_2^2 - 20L_1^2L_2^4 - L_2^6 - 15L_1^4L_3^2 + 40L_1^2L_2^2L_3^2 \\
&\quad - L_2^4L_3^2 - 20L_1^2L_3^4 + 5L_2^2L_3^4 - 3L_3^6)/(18L_1^2) \\
g_{1c1q3} &= (2L_1^6 + 15L_1^4L_2^2 + 20L_1^2L_2^4 + 3L_2^6 - 23L_1^4L_3^2 - 40L_1^2L_2^2L_3^2 \\
&\quad - 5L_2^4L_3^2 + 20L_1^2L_3^4 + L_2^2L_3^4 + L_3^6)/(18L_1^2) \\
g_{1c2c2} &= (13L_1^8 + 78L_1^6L_2^2 + 124L_1^4L_2^4 - 50L_1^2L_2^6 + 3L_2^8 - 26L_1^6L_3^2 - 92L_1^4L_2^2L_3^2 \\
&\quad + 62L_1^2L_2^4L_3^2 - 4L_2^6L_3^2 + 14L_1^4L_3^4 + 14L_1^2L_2^2L_3^4 - 2L_1^2L_3^6 + L_3^8)/(72L_2^4) \\
g_{1c2c3} &= (-6L_1^8 - 18L_1^6L_2^2 + 39L_1^4L_2^4 - 16L_1^2L_2^6 + L_2^8 - 18L_1^6L_3^2 - 168L_1^4L_2^2L_3^2 + 28L_1^2L_2^4L_3^2 \\
&\quad + 2L_2^6L_3^2 + 39L_1^4L_3^4 + 28L_1^2L_2^2L_3^4 - 6L_2^4L_3^4 - 16L_1^2L_3^6 + 2L_2^2L_3^6 + L_3^8)/(36L_2^2L_3^2) \\
g_{1c2q1} &= (-2L_1^6 - 11L_1^4L_2^2 + 8L_1^2L_2^4 + 5L_2^6 + 4L_1^4L_3^2 - 6L_1^2L_2^2L_3^2 \\
&\quad - 22L_2^4L_3^2 - 2L_1^2L_3^4 + 17L_2^2L_3^4)/(18L_2^2) \\
g_{1c2q2} &= (5L_1^6 + 12L_1^4L_2^2 - 19L_1^2L_2^4 + 2L_2^6 - 5L_1^4L_3^2 + 32L_1^2L_2^2L_3^2 \\
&\quad - 3L_2^4L_3^2 - L_1^2L_3^4 + L_3^6)/(18L_2^2) \\
g_{1c2q3} &= (3L_1^6 + 28L_1^4L_2^2 + 11L_1^2L_2^4 - 2L_2^6 - 7L_1^4L_3^2 - 28L_1^2L_2^2L_3^2 \\
&\quad + 3L_2^4L_3^2 + 5L_1^2L_3^4 - L_3^6)/(18L_2^2) \\
g_{1c3c3} &= (13L_1^8 - 26L_1^6L_2^2 + 14L_1^4L_2^4 - 2L_1^2L_2^6 + L_2^8 + 78L_1^6L_3^2 - 92L_1^4L_2^2L_3^2 + 14L_1^2L_2^4L_3^2 \\
&\quad + 124L_1^4L_3^4 + 62L_1^2L_2^2L_3^4 - 50L_1^2L_3^6 - 4L_2^2L_3^6 + 3L_3^8)/(72L_3^4) \\
g_{1c3q1} &= (2L_1^6 - 4L_1^4L_2^2 + 2L_1^2L_2^4 + 11L_1^4L_3^2 + 6L_1^2L_2^2L_3^2 - 17L_2^4L_3^2 \\
&\quad - 8L_1^2L_3^4 + 22L_2^2L_3^4 - 5L_3^6)/(18L_3^2) \\
g_{1c3q2} &= (-3L_1^6 + 7L_1^4L_2^2 - 5L_1^2L_2^4 + L_2^6 - 28L_1^4L_3^2 + 28L_1^2L_2^2L_3^2 \\
&\quad - 11L_1^2L_3^4 - 3L_2^2L_3^4 + 2L_3^6)/(18L_3^2)
\end{aligned}$$



$$g_{1c3q3} = (-5L_1^6 + 5L_1^4L_2^2 + L_1^2L_2^4 - L_2^6 - 12L_1^4L_3^2 - 32L_1^2L_2^2L_3^2 + 19L_1^2L_3^4 + 3L_2^2L_3^4 - 2L_3^6)/(18L_3^2)$$

$$g_{1q1q1} = (L_1^4 - 2L_1^2L_2^2 + L_2^4 - 2L_1^2L_3^2 + 6L_2^2L_3^2 + L_3^4)/12$$

$$g_{1q1q2} = (-L_1^4 + 2L_1^2L_2^2 - L_2^4 - 2L_1^2L_3^2 - 2L_2^2L_3^2 + 3L_3^4)/6$$

$$g_{1q1q3} = (-L_1^4 - 2L_1^2L_2^2 + 3L_2^4 + 2L_1^2L_3^2 - 2L_2^2L_3^2 - L_3^4)/6$$

$$g_{1q2q2} = (L_1^4 - 2L_1^2L_2^2 + L_2^4 + 6L_1^2L_3^2 - 2L_2^2L_3^2 + L_3^4)/12$$

$$g_{1q2q3} = (3L_1^4 - 2L_1^2L_2^2 - L_2^4 - 2L_1^2L_3^2 + 2L_2^2L_3^2 - L_3^4)/6$$

$$g_{1q3q3} = (L_1^4 + 6L_1^2L_2^2 + L_2^4 - 2L_1^2L_3^2 - 2L_2^2L_3^2 + L_3^4)/12$$

The above coefficients  $g_{1\dots}$  reflect inherent symmetries with respect to interchanging the indices 2 and 3. Some coefficients are invariant with respect to this transposition. Others become the positive or negative of the coefficient whose subscripts have been interchanged. The negative outcome occurs for the coefficients associated with mixed products  $C_{ij}Q_{kl}$ , and is due to the fact that the derivative quantities  $C_{ij}$  switch signs as indices  $i$  and  $j$  are interchanged, whereas the derivative quantities  $Q_{kl}$  remain unchanged under index transposition. The following transitions are generated by the interchange  $2 \leftrightarrow 3$ :

$$(7.2) \quad \begin{aligned} g_{1c1c1} &\rightarrow +g_{1c1c1}, & g_{1c1c2} &\rightarrow +g_{1c1c3}, & g_{1c2c2} &\rightarrow +g_{1c3c3}, & g_{1c2c3} &\rightarrow +g_{1c2c3}, \\ g_{1c1q1} &\rightarrow -g_{1c1q1}, & g_{1c1q2} &\rightarrow -g_{1c1q3}, & g_{1c2q1} &\rightarrow -g_{1c3q1}, & g_{1c2q2} &\rightarrow -g_{1c3q3}, \\ g_{1q1q1} &\rightarrow +g_{1q1q1}, & g_{1q1q2} &\rightarrow +g_{1q1q3}, & g_{1q2q2} &\rightarrow +g_{1q3q3}, & g_{1q2q3} &\rightarrow +g_{1q2q3}. \end{aligned}$$

The remaining energy expressions  $E_2$  and  $E_3$  follow from the above one for  $E_1$  by cyclic substitution. Adding those three yields the complete energy expression

$$\begin{aligned} E = & ( g_{c_1c_1}C_{23}C_{23} + g_{c_1c_2}C_{23}C_{31} + g_{c_1c_3}C_{23}C_{12} \\ & + g_{c_1q_1}C_{23}Q_{23} + g_{c_1q_2}C_{23}Q_{31} + g_{c_1q_3}C_{23}Q_{12} \\ & + g_{c_2c_2}C_{31}C_{31} + g_{c_2c_3}C_{31}C_{12} + g_{c_2q_1}C_{31}Q_{23} \\ & + g_{c_2q_2}C_{31}Q_{31} + g_{c_2q_3}C_{31}Q_{12} + g_{c_3c_3}C_{12}C_{12} \\ & + g_{c_3q_1}C_{12}Q_{23} + g_{c_3q_2}C_{12}Q_{31} + g_{c_3q_3}C_{12}Q_{12} \end{aligned}$$

$$\begin{aligned}
& + g_{q_1 q_1} Q_{23} Q_{23} + g_{q_1 q_2} Q_{23} Q_{31} + g_{q_1 q_3} Q_{23} Q_{12} \\
& + g_{q_2 q_2} Q_{31} Q_{31} + g_{q_2 q_3} Q_{31} Q_{12} + g_{q_3 q_3} Q_{12} Q_{12} ) / D_{xy}^3,
\end{aligned}$$

where

$$\begin{aligned}
g_{c_1 c_1} &= (2L_1^8 - 11L_1^6 L_2^2 + 50L_1^4 L_2^4 + 9L_1^2 L_2^6 + 6L_2^8 - 11L_1^6 L_3^2 - 26L_1^4 L_2^2 L_3^2 - 9L_1^2 L_2^4 L_3^2 \\
& - 18L_2^6 L_3^2 + 50L_1^4 L_3^4 - 9L_1^2 L_2^2 L_3^4 + 24L_2^4 L_3^4 + 9L_1^2 L_3^6 - 18L_2^2 L_3^6 + 6L_3^8) / (12L_1^4) \\
g_{c_1 c_2} &= (3L_1^8 + 4L_1^6 L_2^2 + 98L_1^4 L_2^4 + 4L_1^2 L_2^6 + 3L_2^8 - 24L_1^6 L_3^2 - 40L_1^4 L_2^2 L_3^2 - 40L_1^2 L_2^4 L_3^2 \\
& - 24L_2^6 L_3^2 + 36L_1^4 L_3^4 - 56L_1^2 L_2^2 L_3^4 + 36L_2^4 L_3^4 - 12L_1^2 L_3^6 - 12L_2^2 L_3^6 - 3L_3^8) / (12L_1^2 L_2^2) \\
g_{c_1 c_3} &= (3L_1^8 - 24L_1^6 L_2^2 + 36L_1^4 L_2^4 - 12L_1^2 L_2^6 - 3L_2^8 + 4L_1^6 L_3^2 - 40L_1^4 L_2^2 L_3^2 - 56L_1^2 L_2^4 L_3^2 \\
& - 12L_2^6 L_3^2 + 98L_1^4 L_3^4 - 40L_1^2 L_2^2 L_3^4 + 36L_2^4 L_3^4 + 4L_1^2 L_3^6 - 24L_2^2 L_3^6 + 3L_3^8) / (12L_1^2 L_3^2) \\
g_{c_1 q_1} &= (L_1^4 L_2^2 - 2L_1^2 L_2^4 + L_2^6 - L_1^4 L_3^2 - 3L_2^4 L_3^2 + 2L_1^2 L_3^4 + 3L_2^2 L_3^4 - L_3^6) / (2L_1^2) \\
g_{c_1 q_2} &= (-L_1^4 + 2L_1^2 L_2^2 - L_2^4 + 2L_1^2 L_3^2 + 2L_2^2 L_3^2 - L_3^4) / 2 \\
g_{c_1 q_3} &= (L_1^4 - 2L_1^2 L_2^2 + L_2^4 - 2L_1^2 L_3^2 - 2L_2^2 L_3^2 + L_3^4) / 2 \\
g_{c_2 c_2} &= (6L_1^8 + 9L_1^6 L_2^2 + 50L_1^4 L_2^4 - 11L_1^2 L_2^6 + 2L_2^8 - 18L_1^6 L_3^2 - 9L_1^4 L_2^2 L_3^2 - 26L_1^2 L_2^4 L_3^2 \\
& - 11L_2^6 L_3^2 + 24L_1^4 L_3^4 - 9L_1^2 L_2^2 L_3^4 + 50L_2^4 L_3^4 - 18L_1^2 L_3^6 + 9L_2^2 L_3^6 + 6L_3^8) / (12L_2^4) \\
g_{c_2 c_3} &= (-3L_1^8 - 12L_1^6 L_2^2 + 36L_1^4 L_2^4 - 24L_1^2 L_2^6 + 3L_2^8 - 12L_1^6 L_3^2 - 56L_1^4 L_2^2 L_3^2 - 40L_1^2 L_2^4 L_3^2 \\
& + 4L_2^6 L_3^2 + 36L_1^4 L_3^4 - 40L_1^2 L_2^2 L_3^4 + 98L_2^4 L_3^4 - 24L_1^2 L_3^6 + 4L_2^2 L_3^6 + 3L_3^8) / (12L_2^2 L_3^2) \\
g_{c_2 q_1} &= (L_1^4 - 2L_1^2 L_2^2 + L_2^4 - 2L_1^2 L_3^2 - 2L_2^2 L_3^2 + L_3^4) / 2 \\
g_{c_2 q_2} &= (-L_1^6 + 2L_1^4 L_2^2 - L_1^2 L_2^4 + 3L_1^4 L_3^2 + L_2^4 L_3^2 - 3L_1^2 L_3^4 - 2L_2^2 L_3^4 + L_3^6) / (2L_2^2) \\
g_{c_2 q_3} &= (-L_1^4 + 2L_1^2 L_2^2 - L_2^4 + 2L_1^2 L_3^2 + 2L_2^2 L_3^2 - L_3^4) / 2 \\
g_{c_3 c_3} &= (6L_1^8 - 18L_1^6 L_2^2 + 24L_1^4 L_2^4 - 18L_1^2 L_2^6 + 6L_2^8 + 9L_1^6 L_3^2 - 9L_1^4 L_2^2 L_3^2 - 9L_1^2 L_2^4 L_3^2 \\
& + 9L_2^6 L_3^2 + 50L_1^4 L_3^4 - 26L_1^2 L_2^2 L_3^4 + 50L_2^4 L_3^4 - 11L_1^2 L_3^6 - 11L_2^2 L_3^6 + 2L_3^8) / (12L_3^4)
\end{aligned}$$

$$g_{c_3q_1} = (6L_1^8 - 18L_1^6L_2^2 + 24L_1^4L_2^4 - 18L_1^2L_2^6 + 6L_2^8 + 9L_1^6L_3^2 - 9L_1^4L_2^2L_3^2 - 9L_1^2L_2^4L_3^2 + 9L_2^6L_3^2 + 50L_1^4L_3^4 - 26L_1^2L_2^2L_3^4 + 50L_2^4L_3^4 - 11L_1^2L_3^6 - 11L_2^2L_3^6 + 2L_3^8)/(12L_3^4)$$

$$g_{c_3q_2} = (L_1^4 - 2L_1^2L_2^2 + L_2^4 - 2L_1^2L_3^2 - 2L_2^2L_3^2 + L_3^4)/2$$

$$g_{c_3q_3} = (L_1^6 - 3L_1^4L_2^2 + 3L_1^2L_2^4 - L_2^6 - 2L_1^4L_3^2 + 2L_2^4L_3^2 + L_1^2L_3^4 - L_2^2L_3^4)/(2L_3^2)$$

$$g_{q_1q_1} = (L_1^4 - 2L_1^2L_2^2 + L_2^4 - 2L_1^2L_3^2 + 6L_2^2L_3^2 + L_3^4)/4$$

$$g_{q_1q_2} = (-L_1^4 + 2L_1^2L_2^2 - L_2^4 - 2L_1^2L_3^2 - 2L_2^2L_3^2 + 3L_3^4)/2$$

$$g_{q_1q_3} = (-L_1^4 - 2L_1^2L_2^2 + 3L_2^4 + 2L_1^2L_3^2 - 2L_2^2L_3^2 - L_3^4)/2$$

$$g_{q_2q_2} = (L_1^4 - 2L_1^2L_2^2 + L_2^4 + 6L_1^2L_3^2 - 2L_2^2L_3^2 + L_3^4)/4$$

$$g_{q_2q_3} = (3L_1^4 - 2L_1^2L_2^2 - L_2^4 - 2L_1^2L_3^2 + 2L_2^2L_3^2 - L_3^4)/2$$

$$g_{q_3q_3} = (L_1^4 + 6L_1^2L_2^2 + L_2^4 - 2L_1^2L_3^2 - 2L_2^2L_3^2 + L_3^4)/4$$

Again the symmetries of the problem are reflected in transformations of the above coefficients under permutations of the indices  $i = 1, 2, 3$ . The relationships (7.2) obtain here, too, for the index interchange  $2 \leftrightarrow 3$ . In addition, the corresponding relationships are observed for the other two transpositions  $3 \leftrightarrow 1$  and  $1 \leftrightarrow 2$ . Those transpositions can be combined to generate all other permutations. Note that all coefficients of the form  $g_{c_jq_k}$ ,  $j \neq k$ , are symmetric functions in the squares  $L_i^2$  and are equal up to their sign.

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