A Discrete Surface Theory
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Dedicated to Yumiko Naito

Abstract. In the present paper, we propose a new discrete surface theory on 3-valent embedded graphs in the 3-dimensional Euclidean space which are not necessarily “discretization” or “approximation” of smooth surfaces. The Gauss curvature and the mean curvature of discrete surfaces are defined which satisfy properties corresponding to the classical surface theory. We also discuss the convergence of a family of subdivided discrete surfaces of a given 3-valent discrete surface by using the Goldberg-Coxeter construction. Although discrete surfaces in general have no corresponding smooth surfaces, we may find one as the limit.

1 Introduction

The present paper discusses “discrete surface theory”. There are several proposals of discrete surface theory or “discrete differential geometry” by several authors from different viewpoints. For example, one of the big motivations of their studies is to visualize a given smooth surface and compute its geometric quantities, or to consider a series of simplex complex which approximates the surface and discuss convergence theories of the geometric quantities. This can be taken as a generalization of classical study of geometry of polyhedrons. Another direction is to study discrete integrable systems of the integer networks. See for example [1–5, 7, 19, 22], for references.

Our motivation is to develop a surface theory of embedded graphs. An embedded graph is a mathematical model of atomic configurations of a matter, where vertices represent atoms, edges interactions or bondings, respectively. A systematic study of chemical graphs is done by M. Deza and M. Dutour (see [8,10]) by applying combinatorics. Our approach is a little different. We would like to define discrete surfaces out of embedded graphs, and their differential geometric notions such as their Gauss curvature, and mean curvature, which are believed in materials science to indicate inner frustration and outer stress of the atomic configurations, respectively. For examples, A. L. Mackay and H. Terrones [18] proposed a carbon network, which is supposed to be a discrete Schwarzian surface (triply periodic minimal surface, negatively curved in particular) and caught much attentions in materials science, but there is no precise definitions of curvatures, as far as the authors know.

In the present paper, we define discrete surface as an “embedded” 3-valent graph equipped with the normal vector field $\mathbf{n}$ over its vertices, and the Gauss curvature $K$ and the mean curvature $H$ as the determinant and the trace and of the Weingarten map $\nabla \mathbf{n}$. We say a”graph” for an abstract graph and a 3-“discrete surface” for an embedded 3-valent graph. We show their properties in Section 3 corresponding to the classical surface theory, the variational formula of area (Theorem 3.13), and the relation between harmonic maps and

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minimal surfaces (Theorem 3.18). In Section 4, we compute the Gauss curvature and 
the mean curvature of some examples such as plane graphs, sphere-shaped graphs, car-
bon nanotubes (hexagonal graphs on a cylinder), and the Mackay-like crystals (spatial 
graphenes). We also discuss subdivision of discrete surfaces by using the subdivision 
theory for abstract 3-valent graphs, which is called the Goldberg-Coxeter construction, 
in Section 5. The Goldberg-Coxeter subdivision, which we discussed, keeps to be of 3-
valent. Moreover we discuss their convergence to smooth surfaces in Section 6. Topolog-
ical defects of the Mackay crystal can be detected by the Goldberg-Coxeter subdivisions. 

We here emphasize that we cannot apply the classical study of polyhedrons or simplex 
complex because there is no natural way to assign faces which bound a given 1-skeltons 
(graphs) and thus no associate complex so that we can apply known notions. We even treat 
graphs at each vertex of which graph the vector space spanned by the edges emerge from 
the vertex is of 2 dimensional (flat plane) but the whole graph lies as a surface in the 3-
dimensional Euclidean space. In that case, the classical definition of curvature defined by 
its angle defect is zero, but the surface looks like a negatively curved surface. We need a 
new definition of curvatures to take care of examples including the Mackay crystal, arising 
from materials sciences.

2 The classical surface theory in \( \mathbb{R}^3 \)

Prior to the introduction of a discrete surfaces theory in Section 3, in this section we 
briefly review basic facts of the classical surface theory in \( \mathbb{R}^3 \) for the readers. See [9] for 
example for details.

Let \( M \subset \mathbb{R}^3 \) be a regular surface (of class \( C^2 \)), which is (locally) parameterized by, 
say, \( p = p(u,v) : \Omega \to \mathbb{R}^3 \), where \( \Omega \subset \mathbb{R}^2 \). The tangent plane \( T_pM \) at \( p = p(u,v) \) is the 
vector space spanned by the partial derivatives \( \partial_u p \) and \( \partial_v p \) of \( p \) with respect to \( u \) and \( v \), 
respectively. It is equipped with the standard inner product \( \langle \cdot , \cdot \rangle \) in \( \mathbb{R}^3 \).

The first fundamental form \( I = I(u,v) \) of \( M \) at \( p(u,v) \) is a symmetric 2-tensor defined as

\[
I = dp \cdot dp = (\partial_u p, \partial_u p) du \cdot du + 2 (\partial_u p, \partial_v p) du \cdot dv + (\partial_v p, \partial_v p) dv \cdot dv,
\]

which is also expressed by the matrix-form:

\[
I = \begin{pmatrix} E & F \\ F & G \end{pmatrix} = \begin{pmatrix} \langle \partial_u p, \partial_u p \rangle & \langle \partial_u p, \partial_v p \rangle \\ \langle \partial_v p, \partial_u p \rangle & \langle \partial_v p, \partial_v p \rangle \end{pmatrix}.
\]

The matrix \( I(u,v) \) has rank 2 (positive definite) since we assume that \( M \) is regular. The unit normal vector field

\[
n = n(u,v) = \frac{\partial_u p \times \partial_v p}{|\partial_u p \times \partial_v p|}
\]

is well-defined at every point \( (u,v) \in \Omega \). The second fundamental form \( II = II(u,v) \) is then defined as

\[
II = -dp \cdot dn = \begin{pmatrix} L & M \\ M & N \end{pmatrix} = \begin{pmatrix} -\langle \partial_u p, \partial_u n \rangle & -\langle \partial_u p, \partial_v n \rangle \\ -\langle \partial_v p, \partial_u n \rangle & -\langle \partial_v p, \partial_v n \rangle \end{pmatrix},
\]

which is also a symmetric tensor.
Fact 2.1. The partial derivatives $\partial_u n$ and $\partial_v n$ of $n$, which is perpendicular to $n$, can be represented by $\{\partial_u p, \partial_v p\}$:

\[
\begin{align*}
\partial_u n &= \frac{FM - GL}{EF - F^2} \partial_u p + \frac{FL - EM}{EG - F^2} \partial_v p, \\
\partial_v n &= \frac{FN - GM}{EF - F^2} \partial_u p + \frac{FM - EN}{EG - F^2} \partial_v p.
\end{align*}
\]

We define the Weingarten map $S = \nabla n: T_p M \to T_p M$. By the symmetry of $\Pi$, $S$ is a symmetric operator in the sense that it satisfies $\langle SV, W \rangle = \langle V, SW \rangle$ for any $V, W \in T_p M$. The trace of $S$ is called the mean curvature $H(p)$ and the determinant of $S$ the Gauss curvature $K(p)$, respectively. Since the representation matrix of $S$ with respect to $\{\partial_u p, \partial_v p\}$ is $I^{-2}\Pi$.

Fact 2.2. The mean curvature $H(p)$ and the Gauss curvature $K(p)$ are defined by

\[
\begin{align*}
H(p) &= \frac{1}{2} \text{tr}(I^{-1}\Pi) = \frac{EN + GL - 2FM}{2(EG - F^2)}, \\
K(p) &= \det(I^{-1}\Pi) = \frac{LN - M^2}{EG - F^2}.
\end{align*}
\]

It is easy to see

\[S^2 - 2H(p)S + K(p)\text{Id} = 0.\]  

We also define the third fundamental form $\Pi = \Pi(u, v)$ as

\[\Pi = dn \cdot dn = \begin{pmatrix} \langle \partial_u n, \partial_u n \rangle & \langle \partial_u n, \partial_v n \rangle \\ \langle \partial_v n, \partial_u n \rangle & \langle \partial_v n, \partial_v n \rangle \end{pmatrix}.\]

Because of the symmetry of $S$, $\langle \partial_u n, \partial_u n \rangle = \langle S \partial_u p, S \partial_u p \rangle = \langle S^2 \partial_u p, \partial_u p \rangle$ and so on, from (2.3) we infer

\[K(p)I - 2H(p)\Pi + \Pi = 0.\]

We are ready to present several different meanings of the Gauss curvature. To do so let us consider the Gauss map $n: M \to \mathbb{S}^2$ from $M$ to the unit sphere $\mathbb{S}^2$. Then the Gauss curvature appears in its area element.

Fact 2.3. The Gauss curvature is written as the ratio of the infinitesimal area elements:

\[
|K(p(u_0, v_0))| = \lim_{\epsilon \to 0} \frac{A_{\Omega_\epsilon}(n)}{A_{\Omega_\epsilon}(p)}.
\]

Proof. It is easy by using (2.1) to have

\[
\partial_u n \times \partial_v n = \frac{LN - M^2}{EG - F^2} (\partial_u p \times \partial_v p) = K(p)(\partial_u p \times \partial_v p).
\]

If we take an $\epsilon$-neighborhood $\Omega_\epsilon \subseteq \Omega$ of $(u_0, v_0) \in \Omega$ for any $\epsilon > 0$, then since

\[
\begin{align*}
A_{\Omega_\epsilon}(p) &= \int_{\Omega_\epsilon} |\partial_u p \times \partial_v p| \, du dv, \\
A_{\Omega_\epsilon}(n) &= \int_{\Omega_\epsilon} |\partial_u n \times \partial_v n| \, du dv = \int_{\Omega_\epsilon} |K||\partial_u p \times \partial_v p| \, du dv
\end{align*}
\]

are the area of the image $p(\Omega_\epsilon) \subseteq M$ and $n(\Omega_\epsilon) \subseteq \mathbb{S}^2$, respectively. \qed
A variational approach is also available for the formulation of the curvatures as follows. Let \( p: \overline{\Omega} \rightarrow \mathbb{R}^3 \) be a regular surface of class \( C^2 \). The functional \( \mathcal{A}(p) \) defined as

\[
\mathcal{A}(p) := \int_\Omega |\partial_u p \times \partial_v p| \, du \, dv = \int_\Omega dA
\]

is called the area functional, whose first and second variation formulas are those we want. Let \( q_t = q(u, v, t): \overline{\Omega} \times (-\varepsilon, \varepsilon) \) be a variation of \( p \) with the variation vector field, say,

\[
V(u, v) = \varphi^1(u, v)\partial_u p(u, v) + \varphi^2(u, v)\partial_v p(u, v) + \psi(u, v)n(u, v),
\]

where \( \varphi^i, \psi \in C^1(\overline{\Omega}) \) (\( i = 1, 2 \)).

**Fact 2.4.** The first variation of \( \mathcal{A} \) at \( p \) is then given as

\[
d\mathcal{A}(p, V) = \left. \frac{d}{dt} \right|_{t=0} \mathcal{A}(q_t) = -2 \int_\Omega \psi \cdot H(p)|\partial_u p \times \partial_v p| \, du \, dv,
\]

independently of variations in the tangential direction.

While the second variation of \( \mathcal{A} \) at a general regular surface \( p \) with respect to the normal variation \( V = \psi n \) (that is, \( \varphi^1 = \varphi^2 = 0 \)) is given as

\[
d^2\mathcal{A}(p, \psi n) = \int_\Omega \left( |\nabla_M \psi|^2 + 2\psi^2 K(p) \right) \, dA,
\]

where the norm \( |\nabla_M \psi|^2 \) is taken with respect to \( I \), sometimes called the first Beltrami differentiator.

A surface \( M \subseteq \mathbb{R}^3 \) satisfying \( H(p) = 0 \) for any point \( p \in M \) is said to be minimal.

At the end of this section, we state a characterization of minimal surfaces as follows:

**Fact 2.5.** Let \( p = p(u, v): \Omega \rightarrow \mathbb{R}^3 \) be a regular surface of class \( C^2 \) and \( n: \Omega \rightarrow \mathbb{R}^3 \) be its Gauss map. Then

\[
\partial_u n \times \partial_v p - \partial_v n \times \partial_u p = 2H(p)|\partial_u p \times \partial_v p|n,
\]

or equivalently,

\[
d(n \times dp) = -2H(p)n \, dA,
\]

where \( n \times dp = (n \times \partial_u p) du + (n \times \partial_v p) dv \) is a differential 1-form on \( \Omega \) along \( p \). That is to say, \( p: \Omega \rightarrow \mathbb{R}^3 \) is a minimal surface if and only if \( n \times dp \) is closed.

### 3 A surface theory for graphs in \( \mathbb{R}^3 \)

#### 3.1 Definition of curvatures

Let \( X = (V, E) \) be a general graph, where \( V \) denotes the set of the vertices and \( E \) the set of the oriented edges. The oriented edge \( e \) is identified with a 1-dimensional cell complex. Thus we can assume that every edge \( e \in E \) is identified with the interval \([0, 1]\). The reverse edge is denoted by \( \overline{e} \), and \( E_1 \) is the set of edges which emerge from a vertex \( x \in V \).

A map \( \Phi: X \rightarrow \mathbb{R}^3 \) is said to be a piecewise linear realization if the restriction \( (\Phi|e)(t) \) on each edge \( e \in E \) is linear in \( t \in [0, 1] \) and \( (\Phi|\overline{e})(t) = (\Phi|e)(1 - t) \).

**Definition 3.1.** An injective piecewise linear realization \( \Phi: X \rightarrow \mathbb{R}^3 \) of a graph \( X = (V, E) \) is said to be a discrete surface if

(i) \( X = (V, E) \) is a 3-valent graph, that is a graph of degree 3,

(ii) for each \( x \in V \), at least two vectors in \( \{ \Phi(e) \mid e \in E_x \} \) are linearly independent as vectors in \( \mathbb{R}^3 \),
(iii) locally oriented, that is, the order of the three edges is assumed to be assigned to each vertex of $X$.

Let $\Phi: X = (V, E) \to M \subseteq \mathbb{R}^3$ be a discrete surface. For each vertex $x \in V$, we assume it is of 3-valent, namely the set $E_x = \{e_1, e_2, e_3\}$ of edges with origin $x$ consists of three oriented edges. In the sequel, we sometimes use the notation $\Phi(e) = \varepsilon \in M$ to denote the edge in $M$ which corresponds to $e \in E$. The tangent plane $T_x$ at $\Phi(x)$ is then the plane with $\underline{n}(x)$ as its oriented unit normal vector $n(x)$ at $\Phi(x)$ is defined as

$$\underline{n}(x) := \frac{(e_2 - e_1) \times (e_3 - e_1)}{|(e_2 - e_1) \times (e_3 - e_1)|} = \frac{e_1 \times e_2 + e_2 \times e_3 + e_3 \times e_1}{|e_1 \times e_2 + e_2 \times e_3 + e_3 \times e_1|}. \tag{3.1}$$

Note that we use the condition of graphs to be 3-valent to define its tangent plane.

For each $x \in V$ and $e \in E_x$, the vector

$$\nabla \varepsilon \Phi := \text{Proj}[\Phi(e)] = \varepsilon - \langle \varepsilon, \underline{n}(x) \rangle \underline{n}(x) \tag{3.2}$$

lies on $T_x$, where Proj is denoted by the orthogonal projection onto $T_x$ and $\langle \cdot, \cdot \rangle$ stands for the standard inner product of $\mathbb{R}^3$. Similarly, the directional derivative of $n$ along $e \in E$ is defined as

$$\nabla_e n := \text{Proj}[n(t(e)) - n(a(e))], \tag{3.3}$$

so that $\nabla_e n \in T_x$.

Before we define the curvature of a surface, we work with a triangle $\triangle = \triangle(x_0, x_1, x_2)$ of the graph in $\mathbb{R}^3$. Oriented unit vectors are assigned, say, $\underline{n}_0, \underline{n}_1$ and $\underline{n}_2$, respectively, at $x_0, x_1$ and $x_2$. Later they are taken as unit normal vectors, but we note they need not be perpendicular to the triangle $\triangle$.

We set $v_1 := x_1 - x_0$ and $v_2 := x_2 - x_0$ for simplicity, which corresponds to (3.2). The first fundamental form $I_\triangle$ of $\triangle$ is now defined as

$$I_\triangle := \begin{pmatrix} E & F \\ F & G \end{pmatrix} = \begin{pmatrix} \langle v_1, v_1 \rangle & \langle v_1, v_2 \rangle \\ \langle v_2, v_1 \rangle & \langle v_2, v_2 \rangle \end{pmatrix}. \tag{3.4}$$

As the directional derivative of $\underline{n}_0$ along $v_1$ and $v_2$ corresponding to (3.3), we set

$$\nabla_1 \underline{n} := \text{Proj}[\underline{n}_1 - \underline{n}_0]$$

for $i = 1, 2$, where Proj is the orthogonal projection onto $T_\triangle$, a plane on which $\triangle$ lies. As is straightforward to check, $\nabla_1 \underline{n}$ and $\nabla_2 \underline{n}$ are in fact written, respectively, as

$$\nabla_1 \underline{n} = \frac{FM_1 - GL}{EG - F^2} v_1 + \frac{FL - EM_1}{EG - F^2} v_2, \tag{3.5}$$

$$\nabla_2 \underline{n} = \frac{FN - GM_2}{EG - F^2} v_1 + \frac{FM_2 - EN}{EG - F^2} v_2,$$

where $E, F$ and $G$ are given by (3.4) and $L, M_1, M_2$ and $L$ are defined as

$$\Pi_\triangle := \begin{pmatrix} L & M_2 \\ M_1 & N \end{pmatrix} = \begin{pmatrix} -\langle v_1, \nabla_1 \underline{n} \rangle & -\langle v_1, \nabla_2 \underline{n} \rangle \\ -\langle v_2, \nabla_1 \underline{n} \rangle & -\langle v_2, \nabla_2 \underline{n} \rangle \end{pmatrix}. \tag{3.6}$$

in the second fundamental form of $\triangle$. Note here that $M_1 \neq M_2$ is possible in our case although the classical theory depends on the symmetry of $\Pi$. 

5
Now we can define the Weingarten-type map $S_{\triangle}: T_{\triangle} \rightarrow T_{\triangle}$ as $S_{\triangle} = -\nabla n$ and the mean curvature $H_{\triangle}$ and the Gauss curvature $K_{\triangle}$ of $\triangle$ as its trace and determinant as in the classical case.

The following result corresponds to (2.2).

**Proposition 3.2.** The mean curvature $H_{\triangle}$ and the Gauss curvature $K_{\triangle}$ have, respectively, the following representations:

\[
H_{\triangle} = \frac{1}{2} \text{tr}(I_{\triangle}^{-1}II_{\triangle}) = \frac{EN + GL - F(M_1 + M_2)}{2(EG - F^2)},
\]

\[
K_{\triangle} = \det(I_{\triangle}^{-1}II_{\triangle}) = \frac{LN - M_1M_2}{EG - F^2}.
\]

Since both the first fundamental form (3.4) and the third one (3.8) are symmetric, while it is not always the case with the second fundamental form (3.6), the same identity as (2.4) cannot be expected. But the next proposition shows that the symmetry of $II_{\triangle}$ is the only obstruction for (2.4) to be valid.

**Proposition 3.3.** Let $III_{\triangle}$ be the third fundamental form of $\triangle$ defined as

\[
III_{\triangle} := \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} = \begin{pmatrix} \langle \nabla_1 n, \nabla_1 n \rangle \\ \langle \nabla_2 n, \nabla_1 n \rangle \end{pmatrix} \begin{pmatrix} \langle \nabla_1 n, \nabla_2 n \rangle \\ \langle \nabla_2 n, \nabla_2 n \rangle \end{pmatrix}.
\]

Then

\[
K_{\triangle}I_{\triangle} - 2H_{\triangle}II_{\triangle} + III_{\triangle} = \frac{M_1 - M_2}{EG - F^2} \begin{pmatrix} EM_1 - FL & EN - FM_2 \\ FM_1 - GL & FN - GM_2 \end{pmatrix}.
\]

In particular, the second fundamental form $II_{\triangle}$ is symmetric if and only if

\[
K_{\triangle}I_{\triangle} - 2H_{\triangle}II_{\triangle} + III_{\triangle} = 0.
\]

**Proof.** A straightforward computation using (3.5) gives

\[
c_{11} = \frac{EM_1^2 - 2FLM_1 + GL^2}{EG - F^2},
\]

\[
c_{12} = c_{21} = \frac{EM_1N - FLN - FM_1M_2 + GLM_2}{EG - F^2},
\]

\[
c_{22} = \frac{EN^2 - 2FM_2N + GM_2^2}{EG - F^2}.
\]

This equalities combined with (3.4), (3.6) and (3.7) yield the required equality.

On the other hand, exactly same equality as (2.6) or (2.5) is obtained.

**Proposition 3.4.** The Gauss curvature $K_{\triangle}$ satisfies

\[
\nabla_1 n \times \nabla_2 n = \frac{LN - M^2}{EG - F^2} (v_1 \times v_2) = K_{\triangle} (v_1 \times v_2),
\]

Thus, in particular, the absolute value of the Gauss curvature $K_{\triangle}$ is given by

\[
|K_{\triangle}| = \frac{|\nabla_1 n \times \nabla_2 n|}{|v_1 \times v_2|}.
\]
Proof. The proof again follows from a direct computation using (3.5) as follows:

\[ \nabla_1 n \times \nabla_2 n = \left( \frac{FM_1 - GL}{EG - F^2} v_1 + \frac{FL - EM_1}{EG - F^2} v_2 \right) \times \left( \frac{FN - GM_2}{EG - F^2} v_1 + \frac{FM_2 - EN}{EG - F^2} v_2 \right) \]

\[ = \frac{v_1 \times v_2}{(EG - F^2)^2} \left[ (FM_1 - GL)(FM_2 - FN) - (FL - EM_1)(FN - GM_2) \right] \]

\[ = \frac{(LN - M_1 M_2)(EG - F^2)}{(EG - F^2)^2} (v_1 \times v_2) \]

\[ = \frac{LN - M_1 M_2}{EG - F^2} (v_1 \times v_2) \]

\[ = K_n (v_1 \times v_2), \]

as required. □

Figure 1.

Now we are ready to give the definitions of the mean curvature \( H \) and the Gauss curvature \( K \) of a discrete surface \( \Phi: X = (V, E) \to \mathbb{R}^3 \). Idea is to define them as the area-weighted average of those of the three triangles around the vertex.

Let \( x \in V \) be a vertex, \( E_x = \{e_1, e_2, e_3\} \) and \((\alpha, \beta) = (1, 2), (2, 3) \) or \((3, 1)\). If we choose the triangle \( \Delta_{\alpha\beta} = \Delta(x_0, x, x_\beta) \) as

\[ x_0 = \text{Proj}[\Phi(x)], \quad x_\alpha = \Phi(t(e_\alpha)) \quad \text{and} \quad x_\beta = \Phi(t(e_\beta)), \]

(see Figure 1) then the first, second and third fundamental form of \( \Delta_{\alpha\beta} \), are given as

\[ I_{\alpha\beta} = \left( \begin{array}{c}
\langle \nabla_{e_\alpha} \Phi, \nabla_{e_\beta} \Phi \rangle \\
\langle \nabla_{e_\beta} \Phi, \nabla_{e_\alpha} \Phi \rangle \\
\langle \nabla_{e_\beta} \Phi, \nabla_{e_\beta} \Phi \rangle
\end{array} \right), \]

\[ II_{\alpha\beta} = \left( \begin{array}{c}
-\langle \nabla_{e_\alpha} \Phi, \nabla_{e_\beta} n \rangle \\
-\langle \nabla_{e_\beta} \Phi, \nabla_{e_\alpha} n \rangle \\
-\langle \nabla_{e_\beta} \Phi, \nabla_{e_\beta} n \rangle
\end{array} \right). \]
The first asserts that we can forget about the projection \( \nabla \triangle \) every vertex. A discrete surface is said to be minimal if its mean curvature vanishes at every vertex.

Here we give two observations, which are useful in practical computations of \( H \) or \( K \). The first asserts that we can forget about the projection \( \nabla \nabla \triangle = \text{Proj}[\nabla \nabla \triangle] \) as seen below.

**Lemma 3.7.** The second fundamental form (3.6) of \( \triangle = \triangle(x_0, x_1, x_2) \) satisfies

\[
II_\triangle = \begin{pmatrix} -\langle e_1, n_1 - n_0 \rangle & -\langle e_1, n_2 - n_0 \rangle \\ -\langle e_2, n_2 - n_0 \rangle & -\langle e_2, n_3 - n_0 \rangle \end{pmatrix}.
\]

**Proof.** The assertion is obvious because \( v_i = x_i - x_0 \) \((i = 1, 2)\) lies on \( T_\triangle \), whereas \( \nabla v_i = \text{Proj}[n_i - n_0] \) is the orthogonal projection onto \( T_\triangle \). \( \square \)

The second asserts that the curvatures at \( x \) are equal to the corresponding curvatures of the triangle \( \triangle(x_1, x_2, x_3) \) with the adjacent vertices \( x_1, x_2 \) and \( x_3 \) of \( x \).

**Proposition 3.8.** Let \( \Phi: X = (V, E) \to \mathbb{R}^3 \) be a discrete surface. The mean curvature \( H(x) \) and the Gauss curvature \( K(x) \) at \( x \in V \) are represented, respectively, as

\[
H(x) = \sum_{\alpha, \beta} \sqrt{\det I_{\alpha\beta}(x)} H_{\alpha\beta}(x),
\]

\[
K(x) = \sum_{\alpha, \beta} \sqrt{\det I_{\alpha\beta}(x)} K_{\alpha\beta}(x),
\]

where the summations are taken over any \((\alpha, \beta)\) \(\in\{(1, 2), (2, 3), (3, 1)\}\) such that the Weingarten-type map \( S_{\alpha\beta}: T_x \to T_x \) is defined, also, \( A(x) \) is the denominator of (3.1):

\[
A(x) = |e_1 \times e_2 + e_2 \times e_3 + e_3 \times e_1|,
\]

twice the area of the triangle with \( \{\Phi(t(e_1)), \Phi(t(e_2)), \Phi(t(e_3))\} \) as its vertices.

**Definition 3.5.** For a discrete surface \( \Phi: X = (V, E) \to \mathbb{R}^3 \), the mean curvature \( H(x) \) and the Gauss curvature \( K(x) \) at \( x \in V \) are defined, respectively, as

\[
H(x) := \sum_{\alpha, \beta} \frac{\sqrt{\det I_{\alpha\beta}(x)}}{A(x)} H_{\alpha\beta}(x),
\]

\[
K(x) := \sum_{\alpha, \beta} \frac{\sqrt{\det I_{\alpha\beta}(x)}}{A(x)} K_{\alpha\beta}(x),
\]

where \( A(x) \) is defined, also, as

\[
A(x) = |e_1 \times e_2 + e_2 \times e_3 + e_3 \times e_1|,
\]

twice the area of the triangle with \( \{\Phi(t(e_1)), \Phi(t(e_2)), \Phi(t(e_3))\} \) as its vertices.

\[
II_\triangle = \begin{pmatrix} -\langle e_1, n_1 - n_0 \rangle & -\langle e_1, n_2 - n_0 \rangle \\ -\langle e_2, n_2 - n_0 \rangle & -\langle e_2, n_3 - n_0 \rangle \end{pmatrix}.
\]

**Proof.** The assertion is obvious because \( v_i = x_i - x_0 \) \((i = 1, 2)\) lies on \( T_\triangle \), whereas \( \nabla v_i = \text{Proj}[n_i - n_0] \) is the orthogonal projection onto \( T_\triangle \). \( \square \)

The second asserts that the curvatures at \( x \) are equal to the corresponding curvatures of the triangle \( \triangle(x_1, x_2, x_3) \) with the adjacent vertices \( x_1, x_2 \) and \( x_3 \) of \( x \).

**Proposition 3.8.** Let \( \Phi: X = (V, E) \to \mathbb{R}^3 \) be a discrete surface. The mean curvature \( H(x) \) and the Gauss curvature \( K(x) \) at \( x \in V \) are represented, respectively, as

\[
H(x) = \frac{1}{2} \text{tr}(I_{\triangle}(x) II_{\triangle}(x)),
\]

\[
K(x) = \text{det}(I_{\triangle}(x) II_{\triangle}(x)),
\]

where \( I_{\triangle}(x) \) and \( II_{\triangle}(x) \) are respectively the first and second fundamental forms of the triangle \( \triangle(x) \) with vertices \( \{\Phi(x_1), \Phi(x_2), \Phi(x_3)\} \), which is actually given as

\[
I_{\triangle}(x) = \begin{pmatrix} \langle e_2 - e_1, e_2 - e_1 \rangle & \langle e_2 - e_1, e_3 - e_1 \rangle \\ \langle e_3 - e_1, e_2 - e_1 \rangle & \langle e_3 - e_1, e_3 - e_1 \rangle \end{pmatrix},
\]

\[
II_{\triangle}(x) = \begin{pmatrix} -\langle e_2 - e_1, n(x_2) - n(x_1) \rangle & -\langle e_2 - e_1, n(x_3) - n(x_1) \rangle \\ -\langle e_3 - e_1, n(x_2) - n(x_1) \rangle & -\langle e_3 - e_1, n(x_3) - n(x_1) \rangle \end{pmatrix},
\]

where \( E_\triangle = \{e_1, e_2, e_3\} \) and \( x_i = t(e_i) \) for \( i = 1, 2, 3 \).
Proof. Let \( x \in V \) be fixed let \( E_x = \{ e_1, e_2, e_3 \} \) and \( x_i := t(e_i) \) for \( i = 1, 2, 3 \). Notice first that \( \Phi(e_j) \) itself needs not lie on the tangent plane \( T_x \) at \( \Phi(x) \), while does \( \Phi(e_j) - \Phi(e_i) \) \( (j = 1, 2) \). In the sequel, set \( n_{\alpha} := n(x) \), \( n_{\beta} := n(x_i) \) \( (i = 1, 2, 3) \) for simplicity and let \((\alpha,\beta) = (1, 2), (2, 3) \) or \((3, 1)\). Then we can write as

\[
\begin{pmatrix}
\nabla_{e_{\alpha}} \Phi \\
\nabla_{e_{\beta}} \Phi
\end{pmatrix} = \begin{pmatrix}
e_2 - e_1 \\
e_3 - e_1
\end{pmatrix} P_{\alpha\beta},
\]

with \( P_{\alpha\beta} = \frac{1}{A(x)} \begin{pmatrix}
+ \langle n_{\alpha} \times (e_3 - e_1) \rangle \\
- \langle n_{\alpha} \times (e_2 - e_1) \rangle
\end{pmatrix} \begin{pmatrix}
+ \langle n_{\beta} \times (e_3 - e_1) \rangle \\
- \langle n_{\beta} \times (e_2 - e_1) \rangle
\end{pmatrix} \). Under this transformation of frames, the first fundamental form \( I_{\alpha\beta} \) and second fundamental form \( \Pi_{\alpha\beta} \) of the triangle \( \Delta_{\alpha\beta} = \Delta(\Phi(x), \Phi(x_{\alpha}), \Phi(x_{\beta})) \) are transformed as

\[
I_{\alpha\beta} = \begin{pmatrix}
\nabla_{e_{\alpha}} \Phi \\
\nabla_{e_{\beta}} \Phi
\end{pmatrix} \begin{pmatrix}
\nabla_{e_{\alpha}} \Phi \\
\nabla_{e_{\beta}} \Phi
\end{pmatrix} = \begin{pmatrix}
e_2 - e_1 \\
e_3 - e_1
\end{pmatrix} P_{\alpha\beta}
\]

\[
\Pi_{\alpha\beta} = \begin{pmatrix}
- \langle n_{\alpha} \times (e_3 - e_1) \rangle \\
- \langle n_{\beta} \times (e_3 - e_1) \rangle
\end{pmatrix} \begin{pmatrix}
- \langle n_{\alpha} \times (e_3 - e_1) \rangle \\
- \langle n_{\beta} \times (e_3 - e_1) \rangle
\end{pmatrix} = \begin{pmatrix}
- \langle e_2 - e_1, n_{\alpha} \rangle \\
- \langle e_3 - e_1, n_{\alpha} \rangle
\end{pmatrix} \begin{pmatrix}
- \langle e_2 - e_1, n_{\beta} \rangle \\
- \langle e_3 - e_1, n_{\beta} \rangle
\end{pmatrix}.
\]

respectively. Therefore we obtain

\[
I_{\alpha\beta}^{-1} \Pi_{\alpha\beta} = P_{\alpha\beta}^{-1} I_{\Delta(x)} \begin{pmatrix}
- \langle e_2 - e_1, n_{\alpha} \rangle \\
- \langle e_3 - e_1, n_{\alpha} \rangle
\end{pmatrix} \begin{pmatrix}
- \langle e_2 - e_1, n_{\beta} \rangle \\
- \langle e_3 - e_1, n_{\beta} \rangle
\end{pmatrix}.
\]

Since \( \sqrt{\det I_{\alpha\beta}} = A(x) \det P_{\alpha\beta}\), it follows from the definition (3.11) of \( H(x) \) that

\[
2H(x) = \sum_{\alpha,\beta} \frac{\sqrt{\det I_{\alpha\beta}}}{A(x)} \text{tr}(I_{\alpha\beta}^{-1} \Pi_{\alpha\beta})
\]

\[
= \sum_{\alpha,\beta} \left[ I_{\Delta(x)}^{-1} (\det P_{\alpha\beta} \cdot P_{\alpha\beta}^{-1}) \begin{pmatrix}
- \langle e_2 - e_1, n_{\alpha} \rangle \\
- \langle e_3 - e_1, n_{\alpha} \rangle
\end{pmatrix} \begin{pmatrix}
- \langle e_2 - e_1, n_{\beta} \rangle \\
- \langle e_3 - e_1, n_{\beta} \rangle
\end{pmatrix} \right]
\]

\[
= \text{tr} \left[ I_{\Delta(x)}^{-1} \sum_{\alpha,\beta} (\det P_{\alpha\beta} \cdot P_{\alpha\beta}^{-1}) \begin{pmatrix}
- \langle e_2 - e_1, n_{\alpha} \rangle \\
- \langle e_3 - e_1, n_{\alpha} \rangle
\end{pmatrix} \begin{pmatrix}
- \langle e_2 - e_1, n_{\beta} \rangle \\
- \langle e_3 - e_1, n_{\beta} \rangle
\end{pmatrix} \right],
\]

where the summation are taken over \((\alpha,\beta) = (1, 2), (2, 3) \) and \((3, 1)\). We complete the proof of (3.13) by proving

\[
\text{tr}(\Pi_{\Delta(x)}) = \text{tr} \sum_{\alpha,\beta} (\det P_{\alpha\beta} \cdot P_{\alpha\beta}^{-1}) \begin{pmatrix}
- \langle e_2 - e_1, n_{\alpha} \rangle \\
- \langle e_3 - e_1, n_{\alpha} \rangle
\end{pmatrix} \begin{pmatrix}
- \langle e_2 - e_1, n_{\beta} \rangle \\
- \langle e_3 - e_1, n_{\beta} \rangle
\end{pmatrix},
\]

which follows from a simple direct computation.
Our next task is to prove (3.14). It again follows from the definition (3.12) of $K(x)$ that

$$K(x) = \sum_{\alpha, \beta} \frac{\sqrt{\det I_{\alpha\beta}}}{A(x)} \det (I_{\alpha\beta}^{-1} I_{\alpha\beta}) = \sum_{\alpha, \beta} \frac{\det (I_{\alpha\beta})}{A(x)^2 \det P_{\alpha\beta}}$$

$$= \frac{1}{A(x)^2} \sum_{\alpha, \beta} \det \left( -\left< e_2 - e_1, n_\alpha \right> - \left< e_2 - e_1, n_\beta \right> \right)$$

$$= \frac{1}{A(x)^2} \left( -\left< e_2 - e_1, n_2 - n_1 \right> - \left< e_2 - e_1, n_3 - n_1 \right> \right)$$

$$= \frac{1}{A(x)^2} \det (\Pi_{\alpha(x)}).$$

Thus we prove (3.14) because $A(x)^2 = \det (I_{\alpha(x)})$. □

We end this subsection by the following proposition, which corresponds to (2.9).

**Proposition 3.9.** Let $\Phi: X = (V, E) \to \mathbb{R}^3$ be a discrete surface, let $x \in V$ be fixed and let $E_x = \{e_1, e_2, e_3\}$. Then the mean curvature $H(x)$ at $\Phi(x)$ is written as

$$2H(x)A(x)\eta(x) = \sum_{\alpha, \beta} \left( \nabla_{e_\alpha} \Pi \times \nabla_{e_\beta} \Phi - \nabla_{e_\alpha} \Pi \times \nabla_{e_\beta} \Phi \right)$$

(3.15)

$$= \nabla_{e_{2-1}} n \times \nabla_{e_3-e_1} \Phi - \nabla_{e_{2-1}} n \times \nabla_{e_3-e_1} \Phi$$

$$= \nabla_{e_{2-1}} n \times \Phi(e_1) + \nabla_{e_{2-1}} n \times \Phi(e_2) + \nabla_{e_{2-1}} n \times \Phi(e_3),$$

where the summation is taken over all $(\alpha, \beta) = (1, 2), (2, 3)$ and $(3, 1)$, and $\nabla_{e_{2-1}} \Phi := \nabla_{e_2} \Phi - \nabla_{e_1} \Phi = \Phi(e_1) - \Phi(e_2)$ as well as $\nabla_{e_{2-1}} n := \nabla_{e_2} n - \nabla_{e_1} n$ denote the directional derivatives along $\Phi(e_1) - \Phi(e_2)$.

**Proof.** Set, for simplicity, $\eta_i = \Phi(e_i)$ and $n_i = n(t(e_i))$ $(i = 1, 2, 3)$ as usual. As a consequence of Proposition 3.8 we have

$$H(x) = \frac{1}{2A(x)^2} \left| e_2 - e_1 \right|^2 \left( e_3 - e_1, n_3 - n_1 \right) - \left| e_3 - e_1 \right|^2 \left( e_2 - e_1, n_2 - n_1 \right)$$

$$+ \left( e_2 - e_1, e_3 - e_1 \right) \left( \left< e_2 - e_1, n_3 - n_1 \right> + \left< e_3 - e_1, n_2 - n_1 \right> \right)$$

$$= \frac{-1}{2A(x)^2} \left| e_1 - e_2 \right|^2 \left( e_1, n_2 \right) + \left| e_2 - e_1 \right|^2 \left( e_1, n_3 \right) + \left| e_3 - e_1 \right|^2 \left( e_2, n_2 \right)$$

$$+ \left( e_1 - e_2, e_2 - e_3 \right) \left( \left< e_2, n_2 \right> + \left< e_3, n_2 \right> \right)$$

$$+ \left( e_2 - e_3, e_3 - e_1 \right) \left( \left< e_1, n_3 \right> + \left< e_2, n_1 \right> \right)$$

$$+ \left( e_3 - e_1, e_1 - e_2 \right) \left( \left< e_2, n_3 \right> + \left< e_3, n_3 \right> \right).$$

The terms involving $n_i$ are then summarized, using $\left< a, c \right> b - \left< b, c \right> a = (a \times b) \times c$ for $a, b, c \in \mathbb{R}^3$, as

$$\left< e_2 - e_1, (e_3 \times e_2 + e_2 \times e_3 + e_3 \times e_1) \times n_1 \right> = A(x) \left< e_2 - e_3, n(x) \times n_1 \right>,$$

and similarly for $n_2$ and $n_3$. Therefore,

$$H(x) = \frac{-1}{2A(x)} \left\{ \left< e_2 - e_3, n(x) \times n_1 \right> + \left< e_3 - e_1, n(x) \times n_2 \right> + \left< e_1 - e_2, n(x) \times n_3 \right> \right\}.$$
\[ \begin{align*}
&= -\frac{1}{2A(x)}(\langle n(x), n_1 \times (e_2 - e_3) + n_2 \times (e_3 - e_1) + n_3 \times (e_1 - e_2) \rangle) \\
&= \frac{1}{2A(x)}(\langle n(x), (n_1 - n_2) \times e_1 + (n_1 - n_3) \times e_2 + (n_1 - n_2) \times e_3 \rangle).
\end{align*} \]

Since \( \nabla_{e_2} n = \nabla_{e_3} n - \nabla_{e_1} n = \text{Proj}[n_1 - n_2, n_3] \in T_x \) is the orthogonal projection onto the tangent plane \( T_x \) whose normal vector is \( n(x) \), so that \( \nabla_{e_2} n \times e_2 \) is parallel to \( n(x) \) for \((\alpha, \beta, \gamma) = (1, 2, 3), (2, 3, 1) \) or \((3, 1, 2) \), we infer

\[ 2H(x)A(x)n(x) = \nabla_{e_2} n \times e_1 + \nabla_{e_3} n \times e_2 + \nabla_{e_1} n \times e_3. \]

The remaining two expressions in (3.15) are easily proved. \( \square \)

**Corollary 3.10.** Let \( X = (V, E) \) be a fixed graph, \( \Phi_0 : X = (V, E) \to \mathbb{R}^3 \) be a 3-valent discrete surface with \( n_0 : V \to \mathbb{R}^3 \) its oriented unit normal vector field, and \( H : V \to \mathbb{R} \) be a function. Assume that \( \{\nabla_{e_1} n_0, \nabla_{e_2} n_0, \nabla_{e_3} n_0\} \) is a pair of linearly independent vectors in \( \mathbb{R}^3 \), for every \( x \in V \), where \( E_x = \{e_1, e_2, e_3\} \). If a 3-valent discrete surface \( \Phi : X = (V, E) \to \mathbb{R}^3 \) solves

\[ (3.16) \quad 2H(x)m(x) = \nabla_{e_2} n_0 \times e_1 + \nabla_{e_3} n_0 \times e_2 + \nabla_{e_1} n_0 \times e_3, \]

the prescribed mean curvature equation, where \( m : V \to \mathbb{R}^3 \) is the unnormalized normal vector field, given as

\[ m(x) = \Phi(e_1) \times \Phi(e_2) + \Phi(e_1) \times \Phi(e_3) + \Phi(e_2) \times \Phi(e_3), \]

then, after switching the orientation of edges \( E_x = \{e_1, e_2, e_3\} \) at each \( x \in V \) if necessary, the mean curvature of \( \Phi \) coincides with \( H(x) \) at each \( x \in V \).

**Proof.** Let \( \Phi : X = (V, E) \to \mathbb{R}^3 \) solve (3.16). Taking the inner product of (3.16) with \( \Phi(e_2) - \Phi(e_1) \), which is perpendicular to \( m(x) \), gives

\[ 0 = \langle \Phi(e_2) - \Phi(e_1), \nabla_{e_2} n_0 \times \Phi(e_1) \rangle \]
\[ + \langle \Phi(e_2) - \Phi(e_1), \nabla_{e_3} n_0 \times \Phi(e_2) \rangle \]
\[ + \langle \Phi(e_2) - \Phi(e_1), \nabla_{e_1} n_0 \times \Phi(e_3) \rangle \]
\[ = \langle \nabla_{e_2} n_0 - \nabla_{e_1} n_0, \Phi(e_1) \times \Phi(e_2) \rangle \]
\[ - \langle \nabla_{e_3} n_0 - \nabla_{e_1} n_0, \Phi(e_2) \times \Phi(e_1) \rangle \]
\[ + \langle \nabla_{e_3} n_0 - \nabla_{e_2} n_0, \Phi(e_3) \times (\Phi(e_2) - \Phi(e_1)) \rangle \]
\[ = -\langle \nabla_{e_2} n_0, \Phi(e_1) \times \Phi(e_2) + \Phi(e_2) \times \Phi(e_3) + \Phi(e_3) \times \Phi(e_1) \rangle \]
\[ + \langle \nabla_{e_3} n_0, \Phi(e_1) \times \Phi(e_2) + \Phi(e_2) \times \Phi(e_3) + \Phi(e_3) \times \Phi(e_1) \rangle \]
\[ = \langle \nabla_{e_2} n_0 - \nabla_{e_3} n_0, m(x) \rangle \]
\[ = \langle \nabla_{e_2} n_0 - \nabla_{e_3} n_0, m(x) \rangle. \]

In a similar way, taking the inner product with \( \Phi(e_3) - \Phi(e_1) \) gives \( \langle \nabla_{e_2} n_0 - \nabla_{e_3} n_0, m(x) \rangle = 0 \).

Since our assumption guarantees that \( \{\nabla_{e_2} n_0, \nabla_{e_3} n_0\} \) spans the tangent plane to \( \Phi_0(x) \) at \( \Phi_0(x) \), we conclude that \( m(x) \) is perpendicular to the plane, or equivalently, parallel to \( n_0(x) \). The assumption that \( \Phi \) is a 3-valent discrete surface guarantees that \( m(x) \neq 0 \) for every \( x \in V \). \( \square \)
Notice that if we choose $H = 0$ as a function $H : V \to \mathbb{R}$ in Corollary 3.10, then the equation (3.16) is linear with respect to $\Phi$, so that, is always solvable, although a solution is not possibly a 3-valent discrete surface. Several examples obtained by solving such equations will be actually provided in Section 4.4.

### 3.2 Variational approach

Recall that both the mean curvature and the Gauss curvature of a smooth surface is formulated also by a variational approach of its area functional (2.7) and (2.8). This sub-section is devoted to derive a variation formula for the area functional defined as

\[
A[\Phi] := \sum_{x \in V} |\Phi(e_{x,1}) \times \Phi(e_{x,2}) + \Phi(e_{x,3}) \times \Phi(e_{x,1})|
\]

of a 3-valent discrete surface $\Phi : X = (V, E) \to \mathbb{R}^3$, where $E_x = \{e_{x,1}, e_{x,2}, e_{x,3}\}$ is the set of edges with origin $x$ such that the order of $e_i$’s is chosen to match the orientation.

As in the preceding subsection, we focus on a triangle $\triangle = \triangle(x_0, x_1, x_2)$ with vertices $\{x_1, x_2, x_3\} \subseteq \mathbb{R}^3$, to each $x_i$ of which the oriented unit normal vector $\vec{n}_i$ is assumed to be assigned, to derive the variation formulas of its area:

\[
A(x_1, x_2, x_3) := \{x_2 - x_1\} \times \{x_3 - x_1\}.
\]

For any triplet $\{u_i \mid i = 1, 2, 3\}$ of vectors in $\mathbb{R}^3$, we consider the variation of $\triangle(x_1, x_2, x_3)$ with $\vec{u}$ as the variation vector field, that is, a 1-parameter family of triangles $\triangle(x_1(t), x_2(t), x_3(t))$ with

\[
x_i(t) = x_i + tu_i \quad (i = 1, 2, 3)
\]

of its vertices for $t \in \mathbb{R}$.

**Lemma 3.11.** The first variation of area (3.18) of the triangle $\triangle = \triangle(x_1, x_2, x_3)$ with respect to $\vec{u} = \{u_i \mid i = 1, 2, 3\}$ is given as

\[
\frac{d}{dt} \bigg|_{t=0} A(x_1(t), x_2(t), x_3(t)) = \left\langle V^1, u_1 \right\rangle + \left\langle V^2, u_2 \right\rangle + \left\langle V^3, u_3 \right\rangle,
\]

where, for $(i, j, k) = (1, 2, 3), (2, 3, 1) \text{ or } (3, 1, 2)$, $V^i$ is obtained by rotating $\vec{x}_j - \vec{x}_k$ by 90° on the plane on which $\triangle$ lie (in the counterclockwise direction as viewed facing the normal vector of $\triangle$). If in particular $u_i$ is the unit normal vector $\vec{n}_i$ which is assigned to $x_i$, it follows that

\[
\frac{1}{A(x_1, x_2, x_3)} \frac{d}{dt} \bigg|_{t=0} A(x_1(t), x_2(t), x_3(t)) = -2H_{\triangle},
\]

where $H_{\triangle}$ is the mean curvature of $\triangle$. Moreover, if we consider a normal variation of $\triangle$ (i.e. $u_i = n_i, i = 1, 2, 3$), then we have

\[
\frac{1}{A(x_1, x_2, x_3)} \frac{d^2}{dt^2} \bigg|_{t=0} A(x_1(t), x_2(t), x_3(t)) = 2K_{\triangle} + \text{tr}(I_{\triangle}^{-1}(\text{III}'_{\triangle} - \text{III}_{\triangle})),
\]

where $K_{\triangle}$ is the Gauss curvature of $\triangle$, $I_{\triangle}$ and $\text{III}_{\triangle}$ are, respectively, the first fundamental form (3.4) and the third fundamental form (3.8) of $\triangle$ with respect to the frame $\{u_2 - u_1, u_3 - u_1\}$, and

\[
\text{III}'_{\triangle} := \begin{pmatrix} c_{22} & c_{23} \\ c_{32} & c_{33} \end{pmatrix} = \begin{pmatrix} n_2 - n_1, n_2 - n_1 & n_2 - n_1, n_3 - n_1 \\ n_3 - n_1, n_2 - n_1 & n_2 - n_0, n_3 - n_1 \end{pmatrix}.
\]
\textbf{In particular, if }\nabla_n n = n_2 - n_1 \text{ (}i = 2, 3\text{), in other words, }\Delta(x_1(t), x_2(t), x_3(t)) \text{ is parallel to }\Delta(x_1, x_2, x_3) \text{ for some/any } t > 0, \text{ then we have}

\begin{equation}
\frac{1}{A(x_1, x_2, x_3)} \frac{d^2}{dt^2} A(x_1(t), x_2(t), x_3(t)) = 2K_\Delta.
\end{equation}

\textbf{Proof.} We discuss with the frame \{v_2 = u_2 - u_1, v_3 = u_3 - u_1\} and set

\[ g_{ij} := \langle v_i, v_j \rangle, \quad b_{ij} := -\langle v_i, \nabla u \rangle = -\langle v_i, u_j - u_i \rangle \quad (i, j = 2, 3). \]

By (3.19),

\[ g_{ij}(t) := \langle x_i(t) - x_0, x_j(t) - x_0 \rangle = g_{ij} - tb_{ij} - t^2 \langle u_j - u_i, u_j - u_i \rangle. \]

Note that the coefficient \( \langle u_j - u_i, u_j - u_i \rangle \) of \( t^2 \) is \( c_{ij} \) in the case \( u_i = n_i \).

We first consider the case that \( u_i = n_i \) for \( i = 1, 2, 3 \). Then, by using \( g_{ij} = g_{ij} \) and \( 2H_\Delta = g_{11}b_{11} + g_{22}b_{22} + g_{33}b_{33} + g_{12}b_{12} + g_{13}b_{13} + g_{23}b_{23}, \) where \( g_{ij} \) is the \( (i, j) \)-component of the inverse matrix of \( I_\Delta = (g_{ij})_{i,j}, \)

\begin{equation}
\begin{aligned}
\det(g_{ij}(t))_{i,j} &= g_{22}(t)g_{33}(t) - g_{23}(t)g_{32}(t) \\
&= \det(g_{ij})_{i,j} - 2t(g_{12}b_{12} - g_{13}b_{13} - g_{21}b_{21} - g_{23}b_{23}) \\
&+ t^2(g_{11}c_{11} - g_{12}c_{12}) \\
&= \det(g_{ij})_{i,j} \left\{ 1 - 4tH_\Delta + t^2 \left( \sum_{i,j=1}^{2} g_{ij}c_{ij} + \frac{4 \det \Pi_{sym}}{\det(g_{ij})_{i,j}} \right) \right\},
\end{aligned}
\end{equation}

where \( \Pi_{sym} := (\Pi_\Delta + \Pi_\Delta^T)/2 \) is the symmetrized matrix of the second fundamental form.

Using \( \sqrt{1 + \lambda + t^2\mu} = 1 + (\lambda/2)t + (\mu/2 - \lambda^2/8)t^2 + O(t^3) \) for \( |t| \ll 1, \)

\[ \frac{\sqrt{\det(g_{ij}(t))_{i,j}}}{\det(g_{ij})_{i,j}} = 1 - 2tH_\Delta + t^2 \left( \sum_{i,j=1}^{2} g_{ij}c_{ij} + \frac{2 \det \Pi_{sym}}{\det(g_{ij})_{i,j}} - 2H_\Delta^2 \right) + O(t^3). \]

Since \( A(x_1(t), x_2(t), x_3(t)) = \sqrt{\det(g_{ij}(t))_{i,j}}, \) this expansion shows (3.21).

To get (3.22) we continue with more computation of the term involving \( t^2 \). Using the equality

\[ \sum_{i,j=1}^{2} g_{ij}c_{ij} = 4H_\Delta^2 - 2K_\Delta + \frac{(M_1 - M_2)^2}{EG - F^2}, \]

which follows from (3.29), we have

\[ \sum_{i,j=1}^{2} g_{ij}c_{ij} + \frac{2 \det \Pi_{sym}}{\det(g_{ij})_{i,j}} = 2H_\Delta^2 - K_\Delta + \frac{(M_1 - M_2)^2}{2(EG - F^2)} + \frac{4LN - (M_1 + M_2)^2}{2(EG - F^2)} = 2H_\Delta^2 - K_\Delta + \frac{2(LN - M_1M_2)}{EG - F^2} = 2H_\Delta^2 + K_\Delta, \]

which completes the proof.
where the last equality follows from the definition of $K_\Delta$. Thus we infer
\[
\frac{\sqrt{\text{det}(g_{ij}(t))_{i,j}}}{\text{det}(g_{ij})_{i,j}} = 1 - 2tH_\Delta + t^2 \left( K_\Delta + \frac{1}{2} \text{tr}(I^1_\Delta (\text{III}_\Delta' - \text{III}_\Delta)) \right) + O(t^3).
\]
This proves (3.22). The latter assertion of the proposition immediately follows from (3.22).

We then consider for a general variation vector field $u$. A similar computation as (3.20) shows
\[
\frac{\sqrt{\text{det}(g_{ij}(t))_{i,j}}}{\text{det}(g_{ij})_{i,j}} = 1 - \frac{t}{\text{det}(g_{ij})_{i,j}}(g_{33}b_{22} + g_{22}b_{33} - g_{23}b_{32} - g_{32}b_{23}) + O(t^3).
\]
Therefore
\[
\left. \frac{d}{dt} \right|_{t=0} \sqrt{\text{det}(g_{ij}(t))_{i,j}} = \frac{1}{\text{det}(g_{ij})_{i,j}} \left( \langle v_3, v_3 \rangle \langle v_2, u_2 - u_1 \rangle + \langle v_2, v_2 \rangle \langle v_3, u_3 - u_1 \rangle - \langle v_2, v_3 \rangle (\langle v_2, u_3 - u_1 \rangle + \langle v_3, u_2 - u_1 \rangle) \right)
\]
\[
= \langle V^1, u_1 \rangle + \langle V^2, u_2 \rangle + \langle V^3, u_3 \rangle,
\]
where $V_i$ contains neither of $u_j$ and has the following expression:
\[
V^i = \frac{1}{A(x_1, x_2, x_3)} \left( \langle x_j - x_k, x_k - x_i \rangle \langle x_j - x_k, x_k - x_i \rangle \langle x_k - x_i \rangle \right)
\]
\[
= \frac{1}{A(x_1, x_2, x_3)} (x_j - x_k) \times \left( (x_j - x_k) \times (x_k - x_i) \right),
\]
where $(i, j, k) = (1, 2, 3), (2, 3, 1)$ or $(3, 1, 2)$. Since $(x_j - x_k) \times (x_k - x_i)$ divided by $A(x_1, x_2, x_3)$ is the (reversed) unit normal vector of $\triangle$, this expression shows that $V^i$ is perpendicular to both the normal vector and $x_j - x_k$, proving (3.20).

**Proposition 3.12** (general first variation formula for $\mathcal{A}$). Let $\Phi: X = (V, E) \to \mathbb{R}^3$ be a 3-valent discrete surface and $u = \{u_x\}_{x \in V}$ be any vector field on the surface, that is, each $u_x$ is a vector in $\mathbb{R}^3$ assigned to the vertex $x \in V$.

(i) The first variation formula for $\Phi + tu$ $(t \in \mathbb{R})$ is given of the form
\[
\left. \frac{d}{dt} \right|_{t=0} \mathcal{A}[\Phi + tu] = \sum_{x \in V} \langle V^1_{x_1}, u_{x_1} \rangle + \langle V^2_{x_2}, u_{x_2} \rangle + \langle V^3_{x_3}, u_{x_3} \rangle,
\]
where $E_x = \{e_1, e_2, e_3\}$ and $t(e_i) = x_i$.

(ii) The vector $V^i_{x_1}$ is obtained by rotating $x_{12} - x_{13}$ by $90^\circ$ on the tangent plane $T_{x_1}$ at $x_1$ in the counterclockwise direction as viewed facing the normal vector of $T_{x_1}$ (see Figure 1).

(iii) When the variation around a vertex $x \in V$ is given by the normal deformation, i.e. $u_{x_1} = n_{x_1}$ for the adjacent vertices $x_i \in V$ $(i = 1, 2, 3)$ of $x$, then
\[
\left( \langle V^1_{x_1}, n_{x_1} \rangle + \langle V^2_{x_2}, n_{x_2} \rangle + \langle V^3_{x_3}, n_{x_3} \rangle \right)
\]
is equal to the mean curvature $-2H(x)A(x)$, where $A(x) := |(e_2 - e_1) \times (e_3 - e_1)|$ is the area element at $x \in V$.

Now we restate the results on the variation formula in terms of 3-valent discrete surfaces.
Figure 2. Thick segments are the edges of the surface, and the four dashed triangles are on the tangent planes at \( x_i \) \( (i = 1, 2, 3) \). \( V_e \) is obtained by rotating \( x_{12} - x_{13} \) by 90° on the tangent plane at \( x_1 \), on which the gray-hued triangle lies.

**Theorem 3.13** (normal variation formula for \( \mathcal{A} \)). Let \( \Phi : X = (V, E) \to \mathbb{R}^3 \) be a 3-valent discrete surface with \( n : V \to \mathbb{R}^3 \) its oriented unit normal vector field. The normal variation \( \Phi + tn \) \( (t \in \mathbb{R}) \) of \( \Phi \) gives the following variation formulas:

\[
\frac{d}{dt}\bigg|_{t=0} \mathcal{A}[\Phi + tn] = -2 \sum_{x \in V} H(x)A(x),
\]

\[
\frac{d^2}{dt^2}\bigg|_{t=0} \mathcal{A}[\Phi + tn] = \sum_{x \in V} \left\{ 2K(x) + \text{tr}(I^{-1}_x (\Pi'_x - \Pi_x)) \right\} A(x),
\]

where \( \Delta(x) \) is the triangle with \( \{\Phi(t(e_{x,1})), \Phi(t(e_{x,2})), \Phi(t(e_{x,3}))\} \) as its vertices for \( x \in V, E_x = \{e_{x,1}, e_{x,2}, e_{x,3}\} \). If, in particular, \( \Phi + tn \) is actually a family of parallel surfaces (in the sense that each tangent plane of \( \Phi + tn \) is parallel to the corresponding one of \( \Phi + t'n \) for any \( t, t' \in \mathbb{R} \)), then the second variation is given as

\[
\mathcal{A}[\Phi + tn] = \sum_{x \in V} \left\{ 1 - 2tH(x) + t^2K(x) \right\} A(x),
\]

which is so-called the Steiner formula.

**Proof.** The former assertion is immediate from Proposition 3.11. Let us consider the case that \( \Phi_t = \Phi + tn \) gives a family of parallel surfaces for \( t \in \mathbb{R} \). Then, since \( \nabla_{e_{i-1}} \Phi_t = \nabla_{e_{i-1}} \Phi + t\nabla_{e_{i-1}} n \) for \( i = 2, 3 \), we obtain

\[
\nabla_{e_{2-1}} \Phi_t \times \nabla_{e_{3-1}} \Phi_t = \nabla_{e_{2-1}} \Phi \times \nabla_{e_{3-1}} \Phi + t(n \times \nabla_{e_{2-1}} \Phi) + t^2(\nabla_{e_{2-1}} n \times \nabla_{e_{3-1}} n) = A(x)n(x) - 2tH(x)A(x)n(x) + t^2K(x)A(x)n(x) = (1 - 2tH(x) + t^2K(x))A(x)n(x),
\]
which implies the unit normal vector \( \mathbf{n} \) of \( \Phi \), does not change for sufficiently small \( |t| \ll 1 \).

The area element \( A_i(x) \) of \( \Phi_i \) is then computed as

\[
A_i(x) = |\nabla e_{c_1}, \Phi_i \times \nabla e_{c_2}, \Phi_i| = (1 - 2tH(x) + t^2K(x))A(x),
\]

as required. \( \square \)

**Remark 3.14.** Unlike the classical surface theory, a tangential first variation of a discrete surface may not vanish, so that a surface with \( H = 0 \) is not always an extremum of area \( A \).

### 3.3 Harmonic and minimal surfaces

The area of a smooth regular surface \( p: \Omega \to \mathbb{R}^3 \), where \( \Omega \subseteq \mathbb{R}^2 \) is a domain, is dominated by its Dirichlet energy:

\[
(3.26) \quad \int_\Omega \sqrt{|\partial_u p|^2|\partial_v p|^2 - \langle \partial_u p, \partial_v p \rangle^2} \, dudv \leq \frac{1}{2} \int_\Omega (|\partial_u p|^2 + |\partial_v p|^2) \, dA,
\]

and the equality holds if and only if \( p \) is conformal in the sense that \( |\partial_u p|^2 = |\partial_v p|^2 \) and \( \langle \partial_u p, \partial_v p \rangle = 0 \). To solve the Plateau Problem, Douglas and Radó (1930s) came up with the idea to minimize the Dirichlet energy instead of the area functional itself for several advantageous reasons. In our settings, the corresponding Dirichlet energy is given as the sum of square norm of the edges. A (periodic) realization of a graph which minimizes such an energy is called a **harmonic realization** in \([16]\) or an **equilibrium placement** in \([6]\).

An elementary result, related with our settings, corresponding to (3.26) is described as follows.

**Proposition 3.15.** Let \( \triangle(x_1, x_2, x_3) \) be a triangle with vertices \( \{x_1, x_2, x_3\} \subseteq \mathbb{R}^3 \) and let \( A \) be its area. For any point \( \bar{x} \in \mathbb{R}^3 \), it follows

\[
\frac{4\sqrt{3}}{3} A \leq |x_1 - \bar{x}|^2 + |x_2 - \bar{x}|^2 + |x_3 - \bar{x}|^2.
\]

The equality holds if and only if \( \triangle(x_1, x_2, x_3) \) is an equilateral triangle and \( \bar{x} \) is located at its barycenter.

**Definition 3.16.** Let \( X = (V, E, m) \) be a weighted graph with weight \( m: E \to (0, \infty) \) satisfying \( m(e) = m(\bar{e}) \). A discrete surface \( \Phi: X = (V, E, m) \to \mathbb{R}^3 \) is said to be **harmonic with weight** \( m \) if it is a harmonic realization with weight \( m \), that is, if it satisfies

\[
(3.27) \quad m(e_{x,1})\Phi(e_{x,1}) + m(e_{x,2})\Phi(e_{x,2}) + m(e_{x,3})\Phi(e_{x,3}) = 0
\]

for every vertex \( x \in V \), where \( E_x = \{e_{x,1}, e_{x,2}, e_{x,3}\} \).

Exact representation of \( H \) and \( K \) in the case of discrete harmonic surfaces is given as follows.

**Proposition 3.17.** Let \( X = (V, E, m) \) be a weighted graph with weight \( m: E \to (0, \infty) \) satisfying \( m(e) = m(\bar{e}) \), and \( \Phi: X = (V, E, m) \to \mathbb{R}^3 \) be a 3-valent discrete harmonic surface, \( x \in V \) be fixed and \( E_x = \{e_1, e_2, e_3\} \). Then the mean curvature \( H(x) \) and the Gauss curvature \( K(x) \) are, respectively, written as

\[
(3.28) \quad H(x) = \frac{m_1 + m_2 + m_3}{2A(x)^2} \sum_{(\alpha, \beta, \gamma)} \langle e_\alpha, e_\beta \rangle \left( \frac{\langle e_\alpha, n_\beta \rangle + \langle e_\beta, n_\alpha \rangle}{m_\gamma} \right).
\]
\[
K(x) = -\frac{m_1 + m_2 + m_3}{2A(x)^2} \sum_{(\alpha, \beta, \gamma)} \frac{\langle e_{\alpha}, n_{\beta} \rangle \langle e_{\beta}, n_{\gamma} \rangle}{m_{\gamma}},
\]
where \( m_i = m(e_i) \), \( A(x) = |e_1 \times e_2 + e_2 \times e_3 + e_3 \times e_1| \). \( e_j = \nabla_{e_j} \Phi = \Phi(e_i) \in T_x \) is a tangent vector at \( \Phi(x) \), \( n_i = n(t(e_i)) \) is the oriented unit normal vector at each adjacent vertex of \( \Phi(x) \), for \( i = 1, 2, 3 \), and the summations are taken over any \( (\alpha, \beta, \gamma) \in \{(1, 2, 3), (2, 3, 1), (3, 1, 2)\} \).

**Proof.** We first make the following observations which are easily proved from (3.27):

(i) Every \( \Phi(e_i) \) lies on the tangent plane \( T_x \) at \( \Phi \), so that \( e_j = \nabla_{e_j} \Phi = \Phi(e_i) \in T_x \) for \( i = 1, 2, 3 \).

(ii) \( m_3^{-1}(e_1 \times e_2) = m_1^{-1}(e_2 \times e_3) = m_2^{-1}(e_3 \times e_1) \) and is parallel to \( n(x) \).

Let \( (\alpha, \beta) = (1, 2), (2, 3) \) or \( (3, 1) \) be fixed. The first fundamental form \( I_{\alpha\beta} \) and the second fundamental form \( II_{\alpha\beta} \) the triangle \( \triangle_{\alpha\beta} = \triangle(\Phi(x), t(e_\alpha), t(e_\beta)) \) are, respectively, written as

\[
I_{\alpha\beta} = \begin{pmatrix}
\langle e_{\alpha}, e_{\alpha} \rangle & \langle e_{\alpha}, e_{\beta} \rangle \\
\langle e_{\beta}, e_{\alpha} \rangle & \langle e_{\beta}, e_{\beta} \rangle
\end{pmatrix},
II_{\alpha\beta} = \begin{pmatrix}
0 & -\langle e_{\alpha}, n_{\beta} \rangle \\
-\langle e_{\beta}, n_{\alpha} \rangle & 0
\end{pmatrix}
\]

because \( \langle e_{\alpha}, n_{\alpha} \rangle = 0 = \langle e_{\beta}, n_{\beta} \rangle \) by (ii). Then we have

\[
H_{\alpha\beta} = \frac{\langle e_{\alpha}, e_{\beta} \rangle (\langle e_{\alpha}, n_{\beta} \rangle + \langle e_{\beta}, n_{\alpha} \rangle)}{2|e_{\alpha}|^2|e_{\beta}|^2 - |e_{\alpha} \times e_{\beta}|^2},
\]

\[
K_{\alpha\beta} = -\frac{\langle e_{\alpha}, n_{\beta} \rangle \langle e_{\beta}, n_{\alpha} \rangle}{|e_{\alpha}|^2|e_{\beta}|^2 - |e_{\alpha} \times e_{\beta}|^2}.
\]

Here we note that

\[
|e_{\alpha}|^2|e_{\beta}|^2 - |e_{\alpha} \times e_{\beta}|^2 = \det I_{\alpha\beta} = |e_{\alpha} \times e_{\beta}|^2 = \frac{A(x)^2 m_{\gamma}}{m_1 + m_2 + m_3},
\]

where \( \gamma \neq \alpha, \beta \). The desired expressions are now immediately obtained from

\[
\frac{\sqrt{\det I_{\alpha\beta}(x)}}{A(x)} H_{\alpha\beta} = \frac{1}{2A(x)} \frac{\sqrt{\det I_{\alpha\beta}(x)}}{A(x)} \frac{\langle e_{\alpha}, e_{\beta} \rangle (\langle e_{\alpha}, n_{\beta} \rangle + \langle e_{\beta}, n_{\alpha} \rangle)}{m_{\gamma}}
\]

\[
= \frac{m_1 + m_2 + m_3}{2A(x)^2} \cdot \frac{\langle e_{\alpha}, n_{\beta} \rangle \langle e_{\beta}, n_{\alpha} \rangle}{m_{\gamma}}.
\]

A discrete harmonic surface needs not be minimal in the sense of Definition [3.6] but we can provide a sufficient condition for a harmonic surface to be minimal, which is corresponding to the conformality of graphs.

**Theorem 3.18.** Let \( X = (V, E, m) \) be a weighted graph with weight \( m \): \( E \rightarrow (0, \infty) \) satisfying \( m(e) = m(e) \). A 3-valent harmonic discrete surface \( \Phi : X = (V, E, m) \rightarrow \mathbb{R}^3 \) is minimal if

\[
(\Phi(e_1), \Phi(e_2)) = (\Phi(e_2), \Phi(e_3)) = (\Phi(e_3), \Phi(e_1))
\]

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holds at every \( x \in V \), where \( E_x = \{e_1, e_2, e_3\} \). Moreover, if \( m : E \rightarrow (0, \infty) \) is constant, then the condition (3.32) is equivalent to
\[
|\Phi(e_1)| = |\Phi(e_2)| = |\Phi(e_3)|.
\]

**Proof.** We use the same notation as in Proposition 3.17. We then sort (3.28) by terms involving the common \( n_x \) to compute
\[
H(x) = \frac{m_1 + m_2 + m_3}{2A(x)^2m_1m_2m_3} \sum_{(a,b,c)} m_a m_b \langle e_a, e_b \rangle \left( \langle e_a, n_x \rangle + \langle e_b, n_x \rangle \right)
\]
\[
= \frac{m_1 + m_2 + m_3}{2A(x)^2} \sum_{(a,b,c)} m_a m_b \langle e_a, e_b \rangle \left( \langle e_a, n_x \rangle + m_a m_3 \langle e_3, n_x \rangle \right)
\]
\[
= \frac{m_1 + m_2 + m_3}{2A(x)^2} \sum_{(a,b,c)} m_a \langle e_a, e_b \rangle m_b e_3 + \langle e_3, e_a \rangle m_3 e_3 n_x,
\]
which equals zero provided (3.32); \( \langle e_1, e_2 \rangle = \langle e_2, e_3 \rangle = \langle e_3, e_1 \rangle \) holds because \( m_3 e_3 = -m_2 e_2 \) is perpendicular to \( n_x \).
Moreover, if the weight \( m : E \rightarrow (0, \infty) \) is constant, then the equation (3.27) becomes
\[
e_1 + e_3 + e_1 = 0,
\]
which gives
\[
|e_1|^2 = -\langle e_1, e_3 \rangle - \langle e_3, e_1 \rangle,
\]
\[
|e_3|^2 = -\langle e_3, e_1 \rangle - \langle e_1, e_3 \rangle,
\]
after taking the inner product with \( e_1 \) and \( e_3 \). This shows \( |e_1| = |e_3| \) if and only if \( \langle e_1, e_3 \rangle = \langle e_3, e_1 \rangle \).
\( \Box \)

## 4 Several examples

### 4.1 Plane graphs

A 3-valent discrete surface \( \Phi : X = (V, E) \rightarrow \mathbb{R}^3 \) is said to be a plane if its image \( \Phi(X) \) lies on a plane in \( \mathbb{R}^3 \). Since the second fundamental form of a plane vanishes identically, independently of the choice of its side at each point, so do both its mean curvature and Gauss curvature. Since its third fundamental form again vanishes, the second variation of the area functional also vanishes.

### 4.2 Sphere-shaped graphs

**Proposition 4.1.** Let \( X = (V, E) \) be a finite graph, \( S^2(r) \subseteq \mathbb{R}^3 \) be the round sphere with radius \( r > 0 \) and with center at the origin, and \( \Phi : X = (V, E) \rightarrow S^2(r) \) be a 3-valent discrete surface with the property that
\[
\Phi(x) = rn(x)
\]
for every vertex \( x \in V \), where \( n(x) \) is the oriented unit normal vector at \( x \in V \). Then the mean curvature \( H \) and the Gauss curvature \( K \) of \( \Phi \) are given, respectively, as
\[
H(x) = -\frac{1}{r}, \quad K(x) = \frac{1}{r^2}
\]
regardless of \( x \in V \).
Proof. Let \( x \in V \) be fixed and let \( E_x = \{ e_1, e_2, e_3 \} \). The assumption (4.1) implies for \( i = 2, 3 \) that

\[
\nabla_{e_{i-1}} n = \nabla_{e_i} n = 0,
\]

which is parallel to both \( \nabla_{e_{i-1}} \Phi = \Phi(e_2) - \Phi(e_1) \) and \( \nabla_{e_{i-1}} \Phi = \Phi(e_3) - \Phi(e_1) \) with factor \( r \). Therefore the first \( I_{\Delta(x)} \), second \( II_{\Delta(x)} \) and third \( III_{\Delta(x)} \) of the triangle \( \Delta(x) \) with vertices \( \{ \Phi(t(e_i)) \}, \Phi(t(e_2)), \Phi(t(e_3)) \) satisfy

\[
I_{\Delta(x)} = -rII_{\Delta(x)} = r^2III_{\Delta(x)},
\]

which proves (4.2). \( \square \)

Remark 4.2. Since (4.3) implies that \( II_{\Delta(x)} \) is symmetric, it follows

\[
K(x)I_{\Delta(x)} - 2H(x)II_{\Delta(x)} + III_{\Delta(x)} = 0.
\]

Moreover, since \( III_{\Delta(x)} = III_{\Delta(x)} \),

\[
A_t(x) = \left( 1 - 2tH(x) + t^2K(x) \right) A_t(x), \quad \text{for } |t| \ll 1
\]

holds as well, where \( A_t(x) (t \in \mathbb{R}) \) stands for area of the normal variation of \( \Delta(x) \).

Corollary 4.3. (1) a regular hexahedron, (2) a regular dodecahedron and (3) a regular truncated icosahedron (fullerene \( C_{60} \)) are all 3-valent discrete surfaces with constant curvatures:

\[
H(x) = -\frac{1}{r}, \quad K(x) = \frac{1}{r^2},
\]

where \( r > 0 \) is the radius of the round sphere on which these surfaces lie.

Proof. It is easily seen that all satisfy (4.1). \( \square \)

4.3 Carbon nanotubes

In this section we will calculate the mean curvature and the Gauss curvature of a carbon nanotube \( CNT(\lambda, c) \) which is, as will be more precisely defined below, a regular hexagonal lattice wound on the right circular cylinder.

First, let \( H(u, \xi) \) be the regular hexagonal lattice which is the planer graph with vertices \( \{ u \} \cup \{ u + \xi_i \sqrt{3} \} \) and with (unoriented) edges \( \{ u + \xi_i \sqrt{3} \} \) extended by translations via \( a_1 := \xi_2 - \xi_1 \) and \( a_2 := \xi_3 - \xi_1 \). For an arbitrary positive number \( \lambda > 0 \) called the scale factor, we set the regular hexagonal lattice \( X(\lambda) \) by

\[
X(\lambda) := H(u, \xi), \quad u := \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \xi := \lambda \begin{pmatrix} -\sqrt{3}/2 \\ -1/2 \end{pmatrix}.
\]

Let \( a_1 := \rho \sqrt{3} \xi - \xi \) and \( a_2 := \rho \sqrt{3} \xi - \xi \) be its lattice vector. Note then that a vertex of the hexagonal lattice \( X(\lambda) \) can be represented as

\[
\xi = \alpha_1 a_1 + \alpha_2 a_2, \quad (\alpha_1, \alpha_2) \in \mathbb{Z} \times \mathbb{Z} \text{ or } (\alpha_1 + 1/3, \alpha_2 + 1/3) \in \mathbb{Z} \times \mathbb{Z}
\]

and that \( \xi = \alpha_1 a_1 + \alpha_2 a_2 \) and \( \eta = \beta_1 a_1 + \beta_2 a_2 \) are mutually adjacent if and only if one of the following three conditions is satisfied.

(i) \( \alpha_1 - \beta_1 = \pm 1/3, \alpha_2 - \beta_2 = \pm 1/3 \),

(ii) \( \alpha_1 - \beta_1 = \mp 2/3, \alpha_2 - \beta_2 = \pm 1/3 \),

(iii) \( \alpha_1 - \beta_1 = \pm 1/3, \alpha_2 - \beta_2 = \mp 2/3 \),

where the double-sign corresponds in the same order.
Definition 4.4. For any pair of integers \( c = (c_1, c_2) \in \mathbb{Z} \times \mathbb{Z} \) satisfying \( c_1 > 0 \) and \( c_2 \geq 0 \), called a chiral index and \( \lambda > 0 \), a carbon nanotube CNT(\( \lambda, c \)) is a 3-valent discrete surface \( \Phi_{\lambda,c} : X(\lambda) = (V(\lambda), E(\lambda)) \to \mathbb{R}^3 \) defined by the map

\[
\mathbb{R}^2 \to \mathbb{R}^3 : \begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} r(\lambda, c) \cos \frac{x}{r(\lambda, c)} \\ r(\lambda, c) \sin \frac{x}{r(\lambda, c)} \\ y \end{pmatrix}
\]

composed with the counterclockwise rotation

\[
\rho_{-\theta(\lambda,c)} = \frac{\sqrt{3}}{2L_0(c)} \begin{pmatrix} 2c_1 + c_2 & \sqrt{3}c_2 \\ -\sqrt{3}c_2 & 2c_1 + c_2 \end{pmatrix}
\]

of angle \( -\theta(\lambda,c) \), where \( \theta(\lambda,c) \in [0, \pi/2) \) is the vector angle between \( \zeta := c_1a_1 + c_2a_2 \), called the chiral vector and \( (1,0)^T \), and \( r(\lambda,c) := |c|/(2\pi) \), called the radius. More precisely, CNT(\( \lambda, c \)) is the graph in \( \mathbb{R}^3 \) with \( \Phi_{\lambda,c}(V(\lambda)) \) as the set of vertices and with

\[
\{ \Phi_{\lambda,c}(t(e)) - \Phi_{\lambda,c}(o(e)) | e \in E(\lambda) \}
\]
as the set of edges.

Remark 4.5. (1) Let \( X(\lambda, c) = (V(\lambda, c), E(\lambda, c)) \) be defined as a fundamental region with respect to the translation in \( c \)-direction acting on the regular hexagonal lattice \( X(\lambda) = (V(\lambda), E(\lambda)) \). In other words, \( X(\lambda, c) \) is obtained by identifying \( x \) with \( x + nc \) and \( e \) with \( e + ne \), respectively, for any \( n \in \mathbb{Z}, x \in V(\lambda), \) and \( e \in E(\lambda) \). Then CNT(\( \lambda, c \)) is isomorphic to \( X(\lambda, c) \) as an abstract graph; indeed, \( x \) and \( x + nc \), where \( n \in \mathbb{Z} \), are mapped by \( \Phi_{\lambda,c} \) to the same point in \( \mathbb{R}^3 \).

(2) CNT(\( \lambda, c \)) has period in the direction \( t := t_1a_1 + t_2a_2 \), where \( d(c) := \gcd(c_1+2c_2,2c_1+c_2) \) and

\[
t(1,2) := \left( \frac{c_1 + 2c_2}{d(c)}, \frac{2c_1 + c_2}{d(c)} \right),
\]

that is, the image of \( \Phi_{\lambda,c} \) is invariant under a translation in \( t \)-direction acting on \( X(\lambda) \) (See [21]).

Now we come to grips with the calculation of the curvatures of CNT(\( \lambda, c \)). In what follows, fix \( \lambda > 0 \) and \( c = (c_1, c_2) \), which are sometimes abbreviated, such as \( r = r(\lambda,c) \) or \( L_0 = L_0(c) \).

Proposition 4.6. For any \((\alpha_1,\alpha_2) \in \mathbb{Z} \times \mathbb{Z}\), a vertex \( x(\alpha_1,\alpha_2) = \Phi_{\lambda,c}(\alpha_1a_1 + \alpha_2a_2) \) of CNT(\( \lambda, c \)) is represented as

\[
x(\alpha_1,\alpha_2) = R(\phi(\alpha_1,\alpha_2))x(0,0) - \sqrt{3}r\psi(\alpha_1,\alpha_2)(0,0,1)^T,
\]

where \( x(0,0) = (r,0,0)^T \),

\[
R(\tau) := \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

and

\[
(C_1, C_2) := \left( \frac{3\pi c_1}{L_0(c)^2}, \frac{3\pi c_2}{L_0(c)^2} \right), \quad (T_1, T_2) := \left( \frac{3\pi t_1d(c)}{L_0(c)^2}, \frac{3\pi t_2d(c)}{L_0(c)^2} \right),
\]

\[
\phi(\alpha_1,\alpha_2) = T_2\alpha_1 - T_1\alpha_2, \quad \psi(\alpha_1,\alpha_2) = C_2\alpha_1 - C_1\alpha_2.
\]
Figure 3. \((c_1, c_2) = (4, 2)\), and \((t_1, t_2) = (-4, 5)\). The rectangle is wound on the cylinder along the red line.

Figure 4. CNT\((\lambda, (4, 2))\)

**Lemma 4.7.** The value of the mean curvature as well as the Gauss curvature of CNT\((\lambda, c)\) at \(x(\alpha_1, \alpha_2)\) coincide with those at \(x(0, 0)\), respectively.

**Proof.** For any \(a_1a_1 + a_2a_2 \in V(\lambda)\), let \(T(\alpha_1, \alpha_2) \subseteq X(\lambda)\) be the tree consisting of \(a_1a_1 + a_2a_2\) as well as all the chains of length 2 starting with \(a_1a_1 + a_2a_2\), which completely determines the curvatures at \(x(\alpha_1, \alpha_2)\). Then \(T(\alpha_1, \alpha_2)\) is obtained from the translation either (i) of \(T(0, 0)\) or (ii) of \(T(-1/3, -1/3)\) by \(\beta_1a_1 + \beta_2a_2\) for some \((\beta_1, \beta_2) \in \mathbb{Z} \times \mathbb{Z}\).

In the case of (i), \(x(T(\alpha_1, \alpha_2)) \subseteq \text{CNT}(\lambda, c)\) is the rotation of angle \(\phi(\beta_1, \beta_2)\) around \(z\)-axis composed with the translation by \((0, 0, -\sqrt{3}r\psi(\beta_1, \beta_2))\) of \(x(T(0, 0))\). Thus the mean curvature as well as the Gauss curvature at \(x(\alpha_1, \alpha_2)\) clearly coincides with those at \(x(0, 0)\), respectively.

While, in the case of (ii), \(x(T(\alpha_1, \alpha_2))\) is the rotation of \(x(T(\beta_1, \beta_2))\) of angle 180° around the axis which intersects orthogonally with \(z\)-axis and through the point \(\frac{1}{2}(x(\alpha_1, \alpha_2) + x(\beta_1, \beta_2)) = \frac{1}{2}(x(\beta_1 - 1/3, \beta_2 - 1/3) + x(\beta_1, \beta_2))\).

Therefore again the curvatures at \(x(\alpha_1, \alpha_2)\) coincide with those at \(x(\alpha_1, \alpha_2)\) and thus coincides with those at \(x(0, 0)\). \(\Box\)
Let 
\[ x_1 := x(-1/3, -1/3), \quad x_2 := x(2/3, -1/3), \quad x_3 := x(-1/3, 2/3) \]
in the sequel. A normal vector of CNT(\(\lambda, c\)) is computed as follows.

**Proposition 4.8.** For \((\alpha_1, \alpha_2) \in \mathbb{Z} \times \mathbb{Z}\), the outer unit normal vector \(n(\alpha_1, \alpha_2)\) at \(x(\alpha_1, \alpha_2)\) is given as the rotation \(n(\alpha_1, \alpha_2) = R(\phi(\alpha_1, \alpha_2))n_0\) of the outer unit normal vector \(n_0 = n(0, 0)\) at \(x(0, 0)\), where \(n_0 = m_0 / |m_0|\), \(m_0 = x_1 \times x_2 + x_2 \times x_3 + x_3 \times x_1\) having the coordinates

\[
m_0 = 2 \sqrt{3} r^2 \begin{pmatrix} C_1 \cos \frac{C_2}{2} \sin \frac{T_2}{2} - C_2 \cos \frac{C_1}{2} \sin \frac{T_1}{2} \\ -C_1 \sin \frac{C_2}{2} \sin \frac{T_2}{2} + C_2 \sin \frac{C_1}{2} \sin \frac{T_1}{2} \\ \frac{2}{\sqrt{3}} \frac{T_1}{2} \sin \frac{T_2}{2} \sin \frac{T_1 + T_2}{2} \end{pmatrix} =: 2 \sqrt{3} r^2 \begin{pmatrix} \frac{m_1(c)}{m_1(c)} \\ \frac{m_2(c)}{\sqrt{3} m_1(c)} \end{pmatrix}.
\]

While for \((\beta_1 + 1/3, \beta_2 + 1/3) \in \mathbb{Z} \times \mathbb{Z}\), the outer unit normal vector \(n(\beta_1, \beta_2)\) at \(x(\beta_1, \beta_2)\) is given as the rotation \(n(\beta_1, \beta_2) = R(\phi(\beta_1 + 1/3, \beta_2 + 1/3))n_1\) of the outer unit normal vector \(n_1 = n(-1/3, -1/3)\) at \(x(-1/3, -1/3)\), where \(n_1 = m_1 / |m_1|\), \(m_1\) satisfies \(|m_1| = |m_0|\) and has the coordinates

\[
m_1 = 2 \sqrt{3} r^2 \begin{pmatrix} C_1 \sin \frac{T_2}{2} \cos \frac{T_2}{2} - C_2 \sin \frac{T_1}{2} \cos \frac{T_1}{2} \\ -C_1 \sin^2 \frac{T_2}{2} - C_2 \sin^2 \frac{T_1}{2} \\ \frac{2}{\sqrt{3}} \frac{T_1}{2} \sin \frac{T_2}{2} \sin \frac{T_1 + T_2}{2} \end{pmatrix} =: 2 \sqrt{3} r^2 \begin{pmatrix} \frac{m_{1,z}(c)}{m_{1,z}(c)} \\ \frac{m_{1,y}(c)}{\sqrt{3} m_{1,z}(c)} \end{pmatrix}.
\]

Using Proposition 4.6, Lemma 4.7 and Proposition 4.8 we can obtain the following result.

**Theorem 4.9.** The carbon nanotube CNT(\(\lambda, c\)) with scale factor \(\lambda > 0\) and with chiral index \(c = (c_1, c_2)\) has the constant mean curvature

\[
H(\lambda, c) = -\frac{m_2(c)}{2 \lambda(c)} \cdot \frac{m_2(c)^2 + m_3(c)^2 + (8/3) m_5(c)^2}{(m_2(c)^2 + m_3(c)^2 + (4/3) m_5(c)^2)^{3/2}}
\]

and has the constant Gauss curvature

\[
K(\lambda, c) = \frac{4 m_5(c)^2 (m_2(c)^2 + m_3(c)^2)}{3 \lambda(c)^2 (m_2(c)^2 + m_3(c)^2 + (4/3) m_5(c)^2)^2},
\]

where \(\lambda(c)^2 = |\varpi|/(2\pi) > 0\) is the radius of the circular cylinder on which CNT(\(\lambda, c\)) winds, and

\[
m_2(c) = C_1 \cos \frac{C_2}{2} \sin \frac{T_2}{2} - C_2 \cos \frac{C_1}{2} \sin \frac{T_1}{2},
\]
\[
m_3(c) = -C_1 \sin \frac{C_2}{2} \sin \frac{T_2}{2} + C_2 \sin \frac{C_1}{2} \sin \frac{T_1}{2},
\]
\[
m_5(c) = \sin \frac{T_1}{2} \sin \frac{T_2}{2} \sin \frac{T_1 + T_2}{2},
\]
\[
(C_1, C_2) = \left( \frac{3 \pi c_1}{L_0(c)^2}, \frac{3 \pi c_2}{L_0(c)^2} \right),
\]
\[
(T_1, T_2) = \left( \frac{3 \pi (c_1 + 2 c_2)}{L_0(c)^2}, \frac{3 \pi (2 c_1 + c_2)}{L_0(c)^2} \right).
\]
\[ L_0(c) = \frac{|c^i|}{\lambda} = \sqrt{3(c_1^2 + c_1 c_2 + c_2^2)}. \]

If, in particular, \( c_1 = c_2 \), then, \( m_z(c) = 0 \), so that \( H(\lambda, c) \) and \( K(\lambda, c) \) respectively have the following representations

\[ H(\lambda, c) = -\frac{1}{2r(\lambda, c)} \cos \frac{C_1}{2}, \quad K(\lambda, c) = 0. \]

**Proof.** By Lemma [4.7], it suffices to determine the value of the mean curvature and the Gauss curvature of \( \text{CNT}(\lambda, c) \) only at \( x(0,0) \). We will make use of Proposition [3.8] rather than calculate according to the original definition (Definition [3.5]). Namely, we choose the frame

\[ \nu_1 := x_2 - x_1, \quad \nu_2 := x_3 - x_1 \]

to determine the first fundamental form \( I \) and the second fundamental form \( II \) of \( \text{CNT}(\lambda, c) \) at \( x(0,0) \) The results are follows.

\[
I = \begin{pmatrix}
|\nu_1|^2 & \langle \nu_1, \nu_2 \rangle \\
\langle \nu_2, \nu_1 \rangle & |\nu_2|^2
\end{pmatrix}, \quad
II = \begin{pmatrix}
-\langle \nu_1, n_2 - n_1 \rangle & -\langle \nu_1, n_3 - n_1 \rangle \\
-\langle \nu_2, n_2 - n_1 \rangle & -\langle \nu_2, n_3 - n_1 \rangle
\end{pmatrix},
\]

where \( n_i \) is the outer unit normal vector at \( x_i \) \((i = 1, 2, 3)\) and

\[
|\nu_1|^2 = r^2 \left( 4 \sin^2 \frac{T_2}{2} + 3c_1^2 \right),
\]
\[
|\nu_2|^2 = r^2 \left( 4 \sin^2 \frac{T_1}{2} + 3c_2^2 \right),
\]
\[
\langle \nu_1, \nu_2 \rangle = -r^2 \left( 4 \sin \frac{T_1}{2} \sin \frac{T_2}{2} \cos \frac{T_1 + T_2}{2} + 3c_1 c_2 \right),
\]
\[
-\langle \nu_1, n_2 - n_1 \rangle = -\frac{8 \sqrt{3} \rho^3 m_z}{|m_0|} \sin^2 \frac{T_2}{2},
\]
\[
-\langle \nu_1, n_3 - n_1 \rangle = -\frac{8 \sqrt{3} \rho^3 m_z}{|m_0|} \sin^2 \frac{T_1}{2},
\]
\[
-\langle \nu_2, n_2 - n_1 \rangle = \frac{8 \sqrt{3} \rho^3 m_z}{|m_0|} \sin \frac{T_1}{2} \sin \frac{T_2}{2} \left( m_z \cos \frac{T_1 + T_2}{2} - m_z \sin \frac{T_1 + T_2}{2} \right),
\]
\[
-\langle \nu_2, n_3 - n_1 \rangle = \frac{8 \sqrt{3} \rho^3 m_z}{|m_0|} \sin \frac{T_1}{2} \sin \frac{T_2}{2} \left( m_z \cos \frac{T_1 + T_2}{2} + m_z \sin \frac{T_1 + T_2}{2} \right).
\]

The rest of the proof is also a direct computation of

\[ H(\lambda, c) = \frac{1}{2} \text{tr}(I^{-1}II), \quad K(\lambda, c) = \det(I^{-1}II). \]

\[ \square \]

### 4.4 Mackay-like crystals

The Schwarzian surface of type \( P \) and \( D \) and Gyroid are well known example of triply periodic minimal surfaces in \( \mathbb{R}^3 \). Examples of 3-valent discrete surfaces which is claimed to lie on the Schwarzian surface of \( P \)-type have been known since 1990s. In 1991, A. L. Mackay and H. Terrones [18] proposed a \( sp^2 \) bonding (hence a 3-valent discrete surface) carbon crystal, now called the Mackay crystal, consists of 6- and 8-membered rings (see Figure 8). There is no proof for it actually lies on the Schwarzian surface but it has
the same symmetries as those of the Schwarzian surface of type \( P \). T. Lenosky et al. \cite{17} introduced another 3-valent discrete surfaces consisting of 6- and 7-membered rings. More recently, the first and second author et al. \cite{26} systematically investigated carbon crystals of \( sp^2 \)-bonding (i.e. 3-valent) with the octahedral symmetry and the dihedral symmetry, and listed up all the possible structures with small number of vertices. They are called Mackay-like crystals.

In \cite{26}, a standard realization of a Mackay-like crystal in \( \mathbb{R}^3 \) is obtained by solving a solvable linear system and that the lattice vectors form an orthogonal basis all with equal length. Thus the Gauss curvature as well as the mean curvature of them are computed explicitly. Please see Figure 5 for the Gauss curvature and Figure 6 for the mean curvature how the curvatures are distributed on them. The classical Mackay crystal \cite{18} has, as an abstract graph, the octahedral symmetry, whose fundamental region is shown in Figure 7. It has further symmetry and its smallest patch is a subgraph with three vertices lying on the green-hued domain in Figure 7.

A standard realization \( \Phi_0: X = (V, E) \to \mathbb{R}^3 \) for the classical Mackay crystal, whose lattice vectors \( \{e_x, e_y, e_z\} \) form an orthogonal frame of \( \mathbb{R}^3 \), say, \( e_x = (2, 0, 0)^T \), \( e_y = (0, 2, 0)^T \)

---

**Figure 5.** The Gauss curvature of Mackay-like crystals founded in \cite{26}. The Gauss curvature attain smallest (negative, largest absolutely) values at the most blue points in the respective pictures. while zero at the white points. The color on the faces are linearly interpolated between vertices.
Figure 6. The mean curvature of Mackay-like crystals founded in [26]. The mean curvature attain smallest (negative, largest absolutely) values at the most blue points in the respective pictures, while zero at the white points. The color on the faces are linearly interpolated between vertices.

Figure 7. The fundamental region for the octahedral symmetry.
and \( e_z = (0, 0, 2)^T \). Then \( \Phi_0 \) is the unique solution of the system

\[
\begin{align*}
0 &= \Phi_0(x_1) + R_{xy}(L(\Phi_0(x_0))) + L(\Phi_0(x_0)) - 3\Phi_0(x_0), \\
0 &= \Phi_0(x_0) + \Phi_0(x_2) + R_{xy}(\Phi_0(x_2)) - 3\Phi_0(x_1), \\
0 &= \Phi_0(x_1) + L(\Phi_0(x_2)) + R_{z1}(\Phi_0(x_2)) - 3\Phi_0(x_2),
\end{align*}
\]

where \( R_{xy}(x, y, z) := (y, x, z) \), \( L(x, y, z) := (1 - z, 1 - y, 1 - x) \), which is the reflection over the line through \((1/2, 1/2, 1/2)\) and \((0, 1/2, 1)\), and \( R_{z1}(x, y, z) := (x, y, 2 - z) \). Its figure is shown in the left-side of Figure 8.

A 3-valent discrete minimal surface of the Mackay crystal is constructed by deforming the standard realization \( \Phi_0 \) by solving (3.16) on the smallest patch \( \{x_0, x_1, x_2\} \) (see Figure 7) so as to have symmetry with respect to folding along the boundary of the green-hued domain. The system is as follows:

\[
\begin{align*}
0 &= \text{Proj}_{x_0}(n_{x0} - n_{x1}) \times (\Phi(x_1) - \Phi(x_0)) \\
&\quad + \text{Proj}_{x_0}(n_{x1} - n_{x0}) \times (R_{xy}(L(\Phi(x_0))) - \Phi(x_0)), \\
0 &= \text{Proj}_{x_1}(n_{x2} - n_{x3}) \times (\Phi(x_0) - \Phi(x_1)) \\
&\quad + \text{Proj}_{x_1}(n_{x3} - n_{x2}) \times (\Phi(x_2) - \Phi(x_1)), \\
0 &= \text{Proj}_{x_2}(n_{x3} - n_{x0}) \times (\Phi(x_1) - \Phi(x_2)) \\
&\quad + \text{Proj}_{x_2}(n_{x0} - n_{x3}) \times (R_{z1}(\Phi(x_2)) - \Phi(x_2)), \\
0 &= \Phi(x_0) - R_{xy}(\Phi(x_0)), \\
0 &= \Phi(x_1) - R_{xy}(\Phi(x_1)),
\end{align*}
\]

(4.7)

where \( n_i \) stands for the unit normal vector of \( \Phi_0 \) at \( x_i \), \( n_i^* \) for the one at \( R_{z1}(x_2) \), and \( \text{Proj}_{x_i} \) for the orthogonal projection onto the tangent plane \( T_{x_i} \) of \( \Phi_0 \). The actual coordinates are given as follows:

\[
\begin{align*}
\Phi(x_0) &= \frac{1}{18190160132} \begin{pmatrix} 7635077341 + 4959792 \sqrt{187} \\ 7635077341 + 4959792 \sqrt{187} \\ 12286671541 - 10842192 \sqrt{187} \end{pmatrix}, \\
\Phi(x_1) &= \frac{1}{18190160132} \begin{pmatrix} 6537796891 + 8687376 \sqrt{187} \\ 6537796891 + 8687376 \sqrt{187} \\ 15629549191 - 22198320 \sqrt{187} \end{pmatrix}, \\
\Phi(x_2) &= \frac{1}{18190160132} \begin{pmatrix} 3663967141 + 18450096 \sqrt{187} \\ 8262094741 + 2829744 \sqrt{187} \\ 17302810741 - 27882576 \sqrt{187} \end{pmatrix}.
\end{align*}
\]

By symmetry of \( \Phi_0 \), the first three equations in (4.7) actually gives 7 linearly independent equations, which is less than the number of unknown variables by 2. The last two equations in (4.7) is needed for \( \Phi \) to have the same symmetry as the Mackay crystal. The figure of the minimal discrete surface \( \Phi \) is shown in the right-side of Figure 8.
4.5 \( K_4 \) lattice

The \( K_4 \) lattice is the maximal abelian cover of the complete 3-valent graph (the \( K_4 \) graph) (c.f. [16, 20, 23]). The standard realization of the \( K_4 \) lattice has edges with uniform length, so the mean curvature of it vanishes at every vertex (by Proposition 3.18) while its Gauss curvature is positive at every vertex. Thus the eigenvalues of the Weingarten-type map (the principal curvatures) are not real numbers.

5 Goldberg-Coxeter construction

For a given 3-valent discrete surface, we would like to construct a sequence of its subdivisions which gets finer and finer, and converges to a smooth surface. An idea for this is the Goldberg-Coxeter construction, which can be applied to 3-valent abstract planer graph to increase only 6-membered rings. The Goldberg-Coxeter construction is a generalization of simplicial subdivision considered by Goldberg [11], and originally discussed by M. Deza and M. Dutour [8,10]. Here, we recall the definition of it for readers’ convenience, and calculate subdivisions of the regular hexagonal lattice.

**Definition 5.1** ([8 Section 2.1]). Let \( X = (V, E) \) be a 3-valent planer graph and \( k > 0, \ell \geq 0 \) be integers. The graph \( GC_{k,\ell}(X) \) is built in the following steps.

1. Take the dual graph \( X^* \) of \( X \). Since \( X \) is 3-valent, \( X^* \) is a triangulation, namely, a planer graph whose faces are all triangles.
2. Every triangle in \( X^* \) is subdivided into another set of faces in accordance with Figure 9. If we obtain a face which are not triangle, then it can be glued with other neighboring non-triangle faces to form triangles.
3. By duality, the triangulation of (2) is transformed into \( GC_{k,\ell}(X) \).
Example 5.2. The following figures (Figure 10) give the steps of the construction for $GC_{2,0}(X)$ of a regular hexagonal lattice $X$ (i.e. $X(4)$ in Section 4.3).

Example 5.3. Here are the figures of $GC_{k,\ell}(X)$ of a regular hexagonal lattice $X$ for several $(k, \ell)$.

A basic result on the iterating subdivisions is stated as follows.

Theorem 5.4 ([8, Theorem 2.1.1]). For any 3-valent planer graph $X$, it follows

$$GC_{z_2}(GC_{z_1}(X)) = GC_{z_2z_1}(X),$$

where $GC_z(X) := GC_{k,\ell}(X)$ for $z = k + \ell \omega$, $\omega = (1 + \sqrt{3}i)/2$.

The rest of this section is devoted to the computation of the actual coordinates of $GC_{k,\ell}(X)$ of a hexagonal lattice $X$. To this end, we fix the following notation:

Let $p_0$ be the counterclockwise rotation in $\mathbb{R}^2$ of angle $\theta$ around the origin. For given $u, \xi \in \mathbb{R}^2$, set $\xi_1 := \xi$, $\xi_2 := \rho_{2\pi/3}\xi$ and $\xi_3 := \rho_{-2\pi/3}\xi$. Recall the regular hexagonal lattice $H(u, \xi)$ as in Section 4.3, and let $T(u, \xi)$ be the triangular lattice which is also the planer
graph with vertices \(v, a_1 + v, a_2 + v\) and with (unoriented) edges \((v, v + a_1), (v, v + a_2), (v + a_1, v + a_2)\) extended by translations via \(a_1\) and \(a_2\).

**Lemma 5.5.**

1. The dual lattice \(X^*\) of \(X = H(u, \xi)\) is given as \(X^* = T(v, a)\), where, for example,

\[
y = u - \frac{\xi}{3} = u - \rho_{-2\pi/3} \xi,
\]

\[
a = \rho_{\pi/3} (\frac{\xi}{3} - \frac{\xi}{3}) = -\xi - \rho_{\pi/3} \xi = -\sqrt{3} \rho_{\pi/3} \xi.
\]

2. The dual lattice \(X^*\) of \(X = T(v, a)\) is given as \(X^* = H(u, \xi)\), where, for example,

\[
u = v + \frac{1}{3}(a + \rho_{\pi/3} a),
\]

\[
\xi = \frac{1}{3}(\rho_{\pi/3} a - a) = (\rho_{-2\pi/3} - \text{Id})^{-1} a = -\frac{1}{\sqrt{3}} \rho_{-\pi/6} a.
\]

**Proof.** The proof is immediate by noting that the respective base vertices \(v\) and \(u\) of the dual lattices \(X^*\) are barycenters of a hexagon and a triangle of \(X\), respectively. \(\square\)

**Proposition 5.6.** Let \(X = H(u, \xi)\) be a hexagonal lattice, \(k > 0\) and \(l \geq 0\) be integers. Then \(\text{GC}_{k,l}(X)\) is the hexagonal lattice \(H(w, \zeta)\) with

\[
w = u - \rho_{-2\pi/3} \xi - \frac{1}{3(k^2 + kl + \ell^2)} \left\{ (k + 2\ell) \xi + (2k + \ell) \rho_{\pi/3} \xi + (k - \ell) \rho_{2\pi/3} \xi \right\},
\]

\[
\zeta = \frac{1}{3(k^2 + kl + \ell^2)} \left\{ (2k + \ell) \xi + (k - \ell) \rho_{\pi/3} \xi - (k + 2\ell) \rho_{2\pi/3} \xi \right\}
\]

**Proof.** The dual graph \(X^* = T(v, a)\) as is given in Lemma 5.5. The \((k, \ell)\)-subdivision \((X^*)_{k,\ell}\) of \(X^*\) is by definition \(T(v, b)\) for some \(b \in \mathbb{R}^2\). Since the set of vertices of \((X^*)_{k,\ell}\) is given as \(\{v + \beta_1 b_1 + \beta_2 b_2 \mid \beta_1, \beta_2 \in \mathbb{Z} \times \mathbb{Z}\}\), where \(b_1 = b\) and \(b_2 = \rho_{\pi/3} b\), the definition of subdivision implies

\[
a_1 = k b_1 + \ell b_2,
\]

\[
a_2 = \rho_{\pi/3} a = k \rho_{\pi/3} b_1 + \ell \rho_{\pi/3} b_2 = -\ell b_1 + (k + \ell) b_2,
\]

so that

\[
b_1 = \frac{1}{k^2 + kl + \ell^2} \left( (k + \ell) a_1 - \ell a_2 \right),
\]

\[
b_2 = \frac{1}{k^2 + kl + \ell^2} \left( \ell a_1 + k a_2 \right).
\]

So far we have

\[(X^*)_{k,\ell} = T(v, b) = T \left( u - \rho_{-2\pi/3} \xi, \frac{1}{k^2 + kl + \ell^2} \left( (k + \ell) a_1 - \ell a_2 \right) \right).\]

The dual of \((X^*)_{k,\ell} = T(v, b)\), say \(H(w, \zeta)\), is \(\text{GC}_{k,l}(X)\) and we already know from Lemma 5.5 how to find \((w, \zeta)\) from \((v, b)\). \(\square\)

**Example 5.7.** Table 1 is a table for \(X = H((0,0), (-\sqrt{3}/2, 1/2))\).
6 Convergence of the GC-subdivisions

This section provides several examples of the convergence of GC-subdivisions. We start with a simple observation on the convergence of general sequence of 3-valent discrete surfaces.

GC-subdivisions of a dodecahedron, a hexahedron, or a tetrahedron are called Goldberg polyhedra. In particular, fullerene $C_{60}$ (a truncated octahedron) is GC$_{1,1}$ of a dodecahedron (see [12]).

6.1 Convergence theorem

Here, a GC-subdivision of discrete surfaces is a discrete surface, which is a GC-construction as an abstract graph and is embedded as suitable way.

Proposition 6.1. Let $\{\Phi_k: X_k = (V_k, E_k) \to \mathbb{R}^{3\,\text{dim}}_{k=1} \}$ be a sequence of 3-valent discrete surfaces with the following properties.

(i) The sequence of sets of points $\{\Phi_k(V_k)\}_{k=1}^{\infty}$ converges to a smooth surface $M$ in $\mathbb{R}^3$ in the Hausdorff topology.

(ii) For any $p \in M$, the unit normal vector $n_p(x_k)$ of $\Phi_k$ at $x_k \in V_k$ converges to the unit normal vector $n(p)$ of $M$ at $p$, independently of the choice of $\{x_k\}_{k=1}^{\infty}$ with $\Phi_k(x_k) \to p$ as $k \to \infty$.

(iii) The Weingarten map $S_k: T_{x_k} \to T_{x_k}$ of $\Phi_k$ converges to the Weingarten map $S: T_pM \to T_pM$ of $M$ in the following sense: for $\{x_k\}_{k=1}^{\infty}$ with $\Phi_k(x_k) \to p$ as $k \to \infty$ and for $\{v_k \in T_{x_k}\}_{k=1}^{\infty}$ converging to some $v \in T_pM$, it follows

$$S_k(v_k) \to S(v)$$

in $\mathbb{R}^3$ as $k \to \infty$.

Then both the mean curvature $H_k(x_k)$ and the Gauss curvature $G_k(x_k)$ of $\Phi_k$ respectively converge to the mean curvature $H(p)$ and the Gauss curvature $G(p)$ of $M$ for $\{x_k\}_{k=1}^{\infty}$ with $\Phi_k(x_k) \to p$ as $k \to \infty$.

Proof. Let $p \in M$ be a point and $\{x_k\}_{k=1}^{\infty}$ be a sequence of points $x_k \in V_k$ such that $\Phi_k(x_k)$ converges to $p$ in $\mathbb{R}^3$. For any tangent vector $\dot{v} \in T_pM$, as is easily seen using (ii), it follows that the sequence $\{\dot{v}_k\}_{k=1}^{\infty}$, where $\dot{v}_k$ is the orthogonal projection of $\dot{v}$ onto $T_{x_k}$, converges to $\dot{v}$. If we take a pair of linearly independent vectors $\{v_k, w_k\} \subseteq T_pM$ so that $v \times w$ has the same direction as $n(p)$, then, the vectors $\{v_k, w_k\} \subseteq T_{x_k}$ which are respectively obtained from $\{v, w\} \subseteq T_pM$ as in the above manner are also linearly independent as well as $v_k \times w_k$.

\[
\begin{array}{|c|c|c|c|}
\hline
(k, \ell) & w & \zeta & |\zeta|/|\ell| \\
\hline
(2, 0) & (0, 1/2) & (-\sqrt{3}/4, 1/4) & 1/2 \\
(3, 0) & (0, 2/3) & (-\sqrt{3}/6, 1/6) & 1/3 \\
(4, 0) & (0, 3/4) & (-\sqrt{3}/8, 1/8) & 1/4 \\
(2, 1) & (-\sqrt{3}/14, 9/14) & (-\sqrt{3}/7, 2/7) & 1/\sqrt{7} \\
(3, 1) & (-\sqrt{3}/26, 19/26) & (-3\sqrt{3}/26, 5/26) & 1/\sqrt{13} \\
\hline
\end{array}
\]
has the same direction as \( n_k(x_k) \) for sufficiently large \( k \in \mathbb{N} \). Then, by (iii),
\[
\begin{pmatrix}
\langle \nu_k, \nu_k \rangle & \langle \nu_k, \nu_k \rangle \\
\langle w_k, \nu_k \rangle & \langle w_k, w_k \rangle
\end{pmatrix}^{-1}
\begin{pmatrix}
\langle \nu_k, S_k (\nu_k) \rangle & \langle \nu_k, S_k (w_k) \rangle \\
\langle w_k, S_k (\nu_k) \rangle & \langle w_k, S_k (w_k) \rangle
\end{pmatrix},
\]
whose trace is equal to \( H_k(x_k) \) (resp. determinant is equal to \( G_k(x_k) \)), converges, as \( k \to \infty \), to
\[
\begin{pmatrix}
\langle \nu, \nu \rangle & \langle \nu, w \rangle \\
\langle w, \nu \rangle & \langle w, w \rangle
\end{pmatrix}^{-1}
\begin{pmatrix}
\langle \nu, S (\nu) \rangle & \langle \nu, S (w) \rangle \\
\langle w, S (\nu) \rangle & \langle w, S (w) \rangle
\end{pmatrix},
\]
whose trace is equal to \( H(\nu) \) (resp. determinant is equal to \( G(\nu) \)). \( \square \)

The following examples shows that the condition of the preceding proposition is optimal in the most general settings.

**Example 6.2.** Let \( X_k \) be the regular hexagonal lattice in the plane with exception at a vertex, say, \((0, 0)\), which is located at \((0, 0, h_k)\), where \( h_k > 0 \). If the distance of adjacent vertices becomes small with order \( 1/k \), then
(i) \( X_k \) does not converge to the plane in the Hausdorff sense unless \( h_k \) converges to 0 as \( k \to \infty \).
(ii) The normal vector does not converge provided \( kh_k \) is bounded away from 0 as \( k \to \infty \).
(iii) The Weingarten map does not converge provided \( k^2h_k \) is bounded away from 0 as \( k \to \infty \).

### 6.2 Convergence of carbon nanotubes

Here we consider a sequence of subdivisions of a carbon nanotube \( \text{CNT}(\lambda, c) \) via Goldberg-Coxeter construction. Namely, GC-subdivisions of a carbon nanotube are GC-construction of the regular hexagonal lattice and then are rolled up to a tube with suitable radius. For convenience, we put no assumptions on the index \( c \) other than \( c \neq 0 \). Even then (unless \( c_1 > 0 \) and \( c_2 \geq 0 \)), \( \text{CNT}(\lambda, c) \) is well-defined in the exactly same manner, although two carbon nanotubes with different indexes may have just the same structure.

**Proposition 6.3.** \( \text{GC}_{k,\ell}(X(\lambda)) = H(w, \xi) \) of \( X(\lambda) = H(0, \xi) \) as in (4.4) satisfies
\[
(6.1) \quad \frac{1}{|\zeta|} = \frac{1}{\sqrt{k^2 + k\ell + \ell^2}} |\xi|, \quad \frac{\langle \zeta, \xi \rangle}{|\zeta| |\xi|} = \frac{2k + \ell}{2 \sqrt{k^2 + k\ell + \ell^2}}.
\]

In particular, the angle between \( \zeta \) and \( \xi \) is same as that between the chiral vector \( \zeta = k a_1 + \ell a_2 \) in \( X(\lambda) \) and \( \xi_1 = (1, 0)^T \).

**Proof.** The expressions (6.1) are consequences of straightforward computation using Proposition 5.6. Recall that the chiral vector \( \zeta = k a_1 + \ell a_2 \) in \( X(\lambda) \) is given as
\[
\zeta = \sqrt{3} \frac{2k + \ell}{2 \sqrt{k^2 + k\ell + \ell^2}}.
\]
Since \( |\zeta| = \lambda \sqrt{3(k^2 + k\ell + \ell^2)} \), a simple computation shows that \( \langle \zeta, \xi_1 \rangle / (|\zeta| |\xi_1|) \) is exactly same as the latter of (6.1). \( \square \)
Example 6.6. Here are simple examples of \( \text{CNT}(\lambda, c) \). This observation suggests that any \( \text{GC}_{k,\ell}(X(\lambda)) \) is nothing less than a subdivision of \( X(\lambda) \) in consideration of \( \text{CNT}(\lambda, c) \).

**Proposition 6.4.** The lattice vectors \( \mathbf{a}_1, \mathbf{a}_2 \) of \( X(\lambda) \) belong to the set of vertices of \( \text{GC}_{k,\ell}(X(\lambda)) \) for any \( k > 0, \ell \geq 0 \). In particular, the chiral vector \( \mathbf{c} = c_1\mathbf{a}_1 + c_2\mathbf{a}_2 \) is also a vertex of \( \text{GC}_{k,\ell}(X(\lambda)) \) for any \( k > 0, \ell \geq 0 \), and the chiral index with respect to the lattice vectors of \( \text{GC}_{k,\ell}(X(\lambda)) \) is given as \( (kc_1 - \ell c_2, \ell c_1 + (k + \ell)c_2) \).

**Proof.** Since the lattice vectors of \( \text{GC}_{k,\ell}(X(\lambda)) \) are just \( \mathbf{b}_1, \mathbf{b}_2 \) of (5.1) and \( a_1 = kb_1 + \ell b_2, a_2 = -\ell b_1 + (k + \ell)b_2 \), the former assertion follows.

\[
\mathbf{c} = c_1\mathbf{a}_1 + c_2\mathbf{a}_2 = (kc_1 - \ell c_2)b_1 + (\ell c_1 + (k + \ell)c_2)b_2
\]

proves the latter assertion. \( \square \)

**Definition 6.5.** Let \( \text{CNT}(\lambda, c) \) be the carbon nanotube with chiral index \( c = (c_1, c_2) \). Then \( \text{CNT}(\mu, d) \) is said to be a \((k, \ell)-\text{subdivision}\) of \( \text{CNT}(\lambda, c) \) if there exist \( k > 0 \) and \( \ell \geq 0 \) such that

\[
\mu = \frac{\lambda}{\sqrt{k^2 + \ell^2 + \ell^2}},
\]

\[
d = (kc_1 - \ell c_2, \ell c_1 + (k + \ell)c_2).
\]

If this is the case, we write as

\[
\text{CNT}(\mu, d) = \text{GC}_{k,\ell}(\text{CNT}(\lambda, c)).
\]

**Example 6.6.** Here are simple examples of \((k, \ell)-\text{subdivisions}\).

\[
\text{GC}_{1,0}(\text{CNT}(\lambda, c)) = \text{CNT}(\lambda, c),
\]

\[
\text{GC}_{k,0}(\text{CNT}(\lambda, (c_1, c_2))) = \text{CNT} \left( \frac{\lambda}{k}, (kc_1, kc_2) \right),
\]

\[
\text{GC}_{k,k}(\text{CNT}(\lambda, (c_1, 0))) = \text{CNT} \left( \frac{\lambda}{\sqrt{3}k}, (kc_1, kc_1) \right),
\]

\[
\text{GC}_{k,k}(\text{CNT}(\lambda, (c_1, c_1))) = \text{CNT} \left( \frac{\lambda}{\sqrt{3}k}, (0, 3kc_1) \right).
\]

**Theorem 6.7.** Let \( \{\text{CNT}(\lambda(n), c(n))\}_{n=1}^{\infty} \) be a sequence of strictly monotone subdivisions \( \text{CNT}(\lambda, c) = \text{CNT}(\lambda^{(1)}, c^{(1)}) \) in the sense that \( \text{CNT}(\lambda^{(n+1)}, c^{(n+1)}) \) is a \((k_n, \ell_n)\)-subdivision of \( \text{CNT}(\lambda(n), c(n)) \) for some \( k_n \geq 2 \) and \( \ell_n \geq 0 \) for each \( n \in \mathbb{N} \). Then

\[
(6.2) \quad \lim_{n \to \infty} H^{(n)} = -\frac{1}{2r(\lambda, c)}, \quad \lim_{n \to \infty} K^{(n)} = 0,
\]

where \( H^{(n)} = H(\lambda(n), c^{(n)}) \) and \( K^{(n)} = K(\lambda^{(n)}, c^{(n)}) \) are, respectively, the mean curvature and the Gauss curvature of \( \text{CNT}(\lambda(n), c(n)) \) and

\[
r(\lambda, c) = \frac{\lambda}{2\pi} \sqrt{3(c_1^2 + c_1c_2 + c_2^2)}
\]

is the radius of \( \text{CNT}(\lambda, c) \).

To prove Theorem 6.7, we need the following lemma.
Lemma 6.8. If $\text{CNT}(\mu, d) = \text{GC}_{k,\ell}(\text{CNT}(\lambda, c))$, then

$$\mu = \frac{\lambda}{|k + \omega\ell|},$$

$$\omega d_1 + d_2 = (\omega c_1 + c_2)(k + \omega\ell),$$

where $\omega = (1 + \sqrt{3}i)/2$, $c = (c_1, c_2)$ and $d = (d_1, d_2)$.

Proof of Theorem 6.7. Note that any $(k, \ell)$-subdivision $\text{GC}_{k,\ell}(\text{CNT}(\lambda, c))$ of $\text{CNT}(\lambda, c)$ does not change the radius $r = r(\lambda, c) > 0$. From the consequence of Theorem 4.9 by noting that $m_n(c) \geq 0$ for any $c = (c_1, c_2) \in \mathbb{Z} \times \mathbb{Z} \setminus \{(0, 0)\}$, we further compute

$$H^{(n)} = -\frac{1}{2r} \left\{ \frac{m_n(c^{(n)})}{(m_n(c^{(n)})^2 + m_n(c^{(n)})^2 + (4/3)m_n(c^{(n)})^2)^{1/2}} \right. \right.$$

$$\left. \left( (4/3)m_n(c^{(n)})^2m_n(c^{(n)}) - (m_n(c^{(n)})^2 + m_n(c^{(n)})^2 + (4/3)m_n(c^{(n)})^2)^{1/2} \right) \right\},$$

and

$$0 \leq K^{(n)} = \frac{4m_n(c^{(n)})}{3r^2(m_n(c^{(n)})^2 + m_n(c^{(n)})^2 + (4/3)m_n(c^{(n)})^2)^2} \cdot \frac{m_n(c^{(n)})}{m_n(c^{(n)})^2 + m_n(c^{(n)})^2} \cdot \frac{1}{1 + m_n(c^{(n)})^2m_n(c^{(n)})^{-2}}.$$

Hence, to obtain (6.2), it suffices to see

$$(6.3) \quad \lim_{n \to \infty} \frac{m_n(c^{(n)})^2}{m_n(c^{(n)})^2} = 0, \quad \text{and} \quad \lim_{n \to \infty} \frac{m_n(c^{(n)})^2}{m_n(c^{(n)})^2} = 0.$$

It follows by Lemma 6.8 that

$$\omega c_1^{(n+1)} + c_2^{(n+1)} = (\omega c_1^{(n)} + c_2^{(n)})(k_n + \omega\ell_n)$$

for some $k_n \geq 2$ and $\ell_n \geq 0$, which implies $|\omega c_1^{(n)} + c_2^{(n)}| \geq (\sqrt{2})^{n-1}$. Since $L_0(c^{(n)}) = |\omega c_1^{(n)} + c_2^{(n)}|$ is the length of chiral vectors divided by $\lambda^{(n)}$, $C_i^{(n)}$ and $T_i^{(n)} (i = 1, 2)$ corresponding to (4.6) are estimated as

$$|C_i^{(n)}| = \frac{3\pi c_i^{(n)}}{L_0(c^{(n)})} \leq \frac{3\pi}{L_0(c^{(n)})} \quad (i = 1, 2),$$

$$|T_1^{(n)}| = \frac{3\pi(c_1^{(n)} + 2c_2^{(n)})}{L_0(c^{(n)})^2} \leq \frac{9\pi}{L_0(c^{(n)})^2}, \quad |T_2^{(n)}| = \frac{3\pi(2c_1^{(n)} + c_2^{(n)})}{L_0(c^{(n)})^2} \leq \frac{9\pi}{L_0(c^{(n)})^2},$$

all of which converge to 0 as $n$ tends to infinity.
We are now ready to prove (6.3). If either $C_i^{(n)} = 0$ or $C_2^{(n)} = 0$ (then $T_1^{(n)} \neq 0$ and $T_2^{(n)} \neq 0$ in either case), then $m_x(e^{(n)})/m_x(e^{(n)}) = 0$ as well as

$$m_x(e^{(n)}) = \frac{\sin(T_2^{(n)}/2) \sin((T_1^{(n)} + T_2^{(n)})/2)}{-C_2^{(n)} \cos(C_1^{(n)}/2)},$$

or

$$m_x(e^{(n)}) = \frac{\sin(T_1^{(n)}/2) \sin((T_1^{(n)} + T_2^{(n)})/2)}{C_1^{(n)} \cos(C_2^{(n)}/2)},$$

respectively, whose absolute values are both arbitrarily small for any sufficiently large $n \in \mathbb{N}$. If either $T_1^{(n)} = 0$, $T_2^{(n)} = 0$ or $T_1^{(n)} + T_2^{(n)} = 0$ (then $C_1^{(n)} \neq 0$ and $C_2^{(n)} \neq 0$ in either case), then this time $m_x(e^{(n)})/m_x(e^{(n)}) = 0$ as well as

$$m_x(e^{(n)}) = \tan \frac{C_2^{(n)}}{2}, \quad = \tan \frac{C_1^{(n)}}{2}, \quad \text{or} \quad = - \tan \frac{C_1^{(n)}}{2},$$

respectively, whose absolute values are also both arbitrarily small. If neither $C_i^{(n)}$, $T_i^{(n)}$ ($i = 1, 2$) nor $T_1^{(n)} + T_2^{(n)}$ are zero,

$$m_x(e^{(n)}) = \frac{-T_2^{(n)} \sin(C_1^{(n)/2} \sin(T_2^{(n)}/2)}{C_1^{(n)} \cos(C_1^{(n)/2})} + \frac{T_1^{(n)} \sin(C_1^{(n)/2} \sin(T_1^{(n)/2})}{C_1^{(n)} \cos(C_2^{(n)/2})},$$

as well as

$$m_x(e^{(n)}) = \frac{\sin(T_1^{(n)/2} \sin(T_2^{(n)/2}) \sin(T_1^{(n)+T_2^{(n)}/2})}{C_1^{(n)} \cos(C_2^{(n)/2})} - \frac{\sin(T_1^{(n)/2} \sin(T_2^{(n)/2}) \sin(T_1^{(n)+T_2^{(n)}/2})}{C_1^{(n)} \cos(C_2^{(n)/2})},$$

whose absolute value again becomes arbitrarily small. We then complete the proof of Theorem 6.7

\[ \square \]

6.3 Numerical computations for convergence of the Mackay crystal

We construct GC-subdivisions of the Mackay crystal as follows. First we construct GC-construction of the abstract graph of the fundamental region of the Mackay crystal (See Figure 7), and then construct the standard realization of the GC-constructed abstract graph. By using numerical computations, we obtain distributions of the curvatures of several steps of GC$k,0$-subdivisions of the Mackay crystal are shown in Figure 12 for the Gauss curvature and Figure 13 for the mean curvature.

The sequence of the GC-subdivisions of the Mackay crystal seems convergent to the Schwarzian surface of type $P$, however, mean curvatures of vertices around octagonal rings may not converges (see Figure 13). Table 2 shows min/max values of the mean curvature and the Gauss curvature for each subdivision. The maximum value of $|H|$ attains on vertices of octahedral rings. Table 3 also shows the min/max values of the length of edges, and the maximum value of the length of edges attains on edges of octahedral rings. Actually the octagonal rings, which are considered as topological defects, of the Mackay crystals seem to be obstructions of the convergence.
The translation vector of each discrete surface is $e_x = (1, 0, 0)$, $e_y = (0, 1, 0)$ and $e_z = (0, 0, 1)$.

| 1 | $-0.000000$ | $+0.029880$ | $+0.586578$ | $-3.771350$ | $+0.000000$ |
| 2 | $+0.000000$ | $+0.000646$ | $+0.679771$ | $-0.737990$ | $+0.000000$ |
| 3 | $+0.000000$ | $+0.000077$ | $+0.727594$ | $-0.305908$ | $+0.000000$ |
| 4 | $+0.000000$ | $+0.000018$ | $+0.751009$ | $-0.167605$ | $+0.000000$ |
| 5 | $+0.000000$ | $+0.000006$ | $+0.764183$ | $-0.105835$ | $+0.000000$ |
| 6 | $+0.000000$ | $+0.000002$ | $+0.772395$ | $-0.072912$ | $+0.000000$ |
| 7 | $+0.000000$ | $+0.000001$ | $+0.777901$ | $-0.053290$ | $+0.000000$ |
| 8 | $+0.000000$ | $+0.000001$ | $+0.781799$ | $-0.040653$ | $+0.000000$ |
| 9 | $-0.000000$ | $+0.000000$ | $+0.784674$ | $-0.032036$ | $+0.000000$ |
| 10 | $+0.000000$ | $+0.000000$ | $+0.786866$ | $-0.025898$ | $+0.000000$ |
| 12 | $+0.000000$ | $+0.000000$ | $+0.789952$ | $-0.017935$ | $+0.000000$ |
| 14 | $+0.000000$ | $+0.000000$ | $+0.791993$ | $-0.013153$ | $+0.000000$ |
| 16 | $+0.000000$ | $+0.000000$ | $+0.793424$ | $-0.010057$ | $+0.000000$ |
| 18 | $-0.000000$ | $+0.000000$ | $+0.794472$ | $-0.007939$ | $+0.000000$ |
| 20 | $-0.000000$ | $+0.000000$ | $+0.795268$ | $-0.006426$ | $+0.000000$ |

Table 2. The table of values of the mean curvature and the Gauss curvature, if the translation vector of each discrete surface is $e_x = (1, 0, 0)$, $e_y = (0, 1, 0)$ and $e_z = (0, 0, 1)$.

| min. length | max. length | ratio |
| 1 | $+0.08861403$ | $+0.10810811$ | $+1.2200$ |
| 2 | $+0.04511223$ | $+0.06204098$ | $+1.3753$ |
| 3 | $+0.03022620$ | $+0.04543279$ | $+1.5031$ |
| 4 | $+0.02271783$ | $+0.03650569$ | $+1.6069$ |
| 5 | $+0.01819462$ | $+0.03083187$ | $+1.6946$ |
| 6 | $+0.01517240$ | $+0.02686634$ | $+1.7707$ |
| 7 | $+0.01301066$ | $+0.02391848$ | $+1.8384$ |
| 8 | $+0.01138784$ | $+0.02162994$ | $+1.8994$ |
| 9 | $+0.01012480$ | $+0.01979505$ | $+1.9551$ |
| 10 | $+0.00911387$ | $+0.01828677$ | $+2.0065$ |
| 12 | $+0.00759670$ | $+0.01594444$ | $+2.0989$ |
| 14 | $+0.00651247$ | $+0.01420059$ | $+2.1805$ |
| 16 | $+0.00569903$ | $+0.01284540$ | $+2.2540$ |
| 18 | $+0.00506621$ | $+0.01175807$ | $+2.3209$ |
| 20 | $+0.00455986$ | $+0.01086381$ | $+2.3825$ |

Table 3. The table of length of edges. In each subdivision, edges of hexagons of center of dihedral action attain minimums of length, and two edges of tetrahedron attain maximums of length.
Figure 12. The Gauss curvature of $\text{GC}_{(k,0)}$ of Mackay crystals for $k = 1, \ldots, 9$. The Gauss curvature attain the smallest (negative, largest absolutely) values in the respective pictures at the most red points, while white points are those where the mean curvature is zero, and colors are linearly interpolated between blue and white.
Figure 13. The mean curvature of $GC_{(k,0)}$ of Mackay crystals for $k = 1, \ldots, 9$. The mean curvature attain the smallest (negative, largest absolutely)/largest (positive) values in the respective pictures at the most blue/red points, while white points are those where the mean curvature is zero, and colors are linearly interpolated between blue/white/red.

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