Studies on discrete differential geometry and non-steady state nucleation in terms of the elliptic theta functions

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論　文　名	Studies on discrete differential geometry and non-steady state nucleation in terms of the elliptic theta functions （楕円テータ函数による離散微分幾何学と非定常核形成に関する研究）
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論　文　審　査　の　結　果　の　要　旨

The theta functions are known to appear in various areas of mathematics, and interestingly, the solutions to integrable systems are expressed in terms of the theta functions. In this connection, the theta functions are also used in the study of geometric objects associated with integrable systems. It is also known that integrable systems can be discretized preserving the structure of solutions. The methods of integrable systems are often applied in discrete differential geometry, which considers the discretization of various concepts that appear in differential geometry. Thus, the theta functions have also been used to construct explicit formulas for discrete curves and surfaces. On the other hand, it is well known that the theta functions appear in physics, such as fluid mechanics and statistical mechanics. In the last part of this thesis, the candidate focused on a phenomenon called non-steady state nucleation, in which the properties of the theta functions have not been utilized so far.

In this thesis, the candidate exploits various properties of the theta functions to construct explicit formulas for some smooth and discrete curves and to derive equations that can be used in experimental studies of non-steady state nucleation. The former is a part of the stream of studies of deformations of curves based on the methods of integrable systems and was originally inspired by Hashimoto (1972) and deepened by Lamb (1976) and Goldstein-Petrich (1991). Subsequently, deformations of discrete curves and discrete surfaces based on semi-discrete or discrete integrable systems have been studied (for example, Hirose, Inoguchi, Kajiwara, Matsuura and Ohta (2019)). The connection between nucleation theory and the elliptic theta functions was suggested by Kashchiev (1969) and Shneidman (1988), and the results have since been used in various experimental studies (for example, Kelton, Falster, Gambaro (1999)).

In Chapter 2, explicit formulas for isoperimetric deformations of smooth and discrete elasticae are constructed. Elastica is a well-known class of planar curves that describes the shape of thin elastic rods. Mathematically, it is characterized by the differential equation for its curvature. On the other hand, it is well known that the modified KdV (mKdV) equation describes an isoperimetric deformation of planar curves. Since the traveling wave solutions to the mKdV equation satisfy the equation for elastica, it is possible to construct an explicit formula for the isoperimetric deformation of elastica. Thanks to its integrability, it is also possible to construct explicit formulas for isoperimetric deformations of discrete analogue of elastica characterized by the integrable discrete analogue of the mKdV equation. The formulas can be regarded as the extended versions of the results by Mumford (1994) and Matsuura (2020).

In Chapter 3, by utilizing the explicit formulas for smooth and discrete space curves in terms of τ functions, the explicit formulas for curves with constant torsion are first constructed in terms of the elliptic theta functions. The closure conditions are also explicitly obtained. Then, their discrete analogues are also constructed in terms of the elliptic theta functions, and the closure conditions are also written down explicitly.

In Chapter 4, an explicit construction of Kaleidocycles is presented. Kaleidocycle is a linkage mechanism consisting of tetrahedra and hinges connecting them. It is known that this mechanism has various unique properties. In particular, numerical experiments have shown that special Kaleidocycles, called Möbius Kaleidocycles, have been numerically confirmed to possess a single degree of freedom regardless of the number of tetrahedra that consist of a Kaleidocycle. There is also prior research modeling Kaleidocycles as deformations of discrete curves with constant torsion angle described by the semi-discrete mKdV or the semi-discrete sine-Gordon equations, but the explicit formula has not been obtained so far. In this chapter, an explicit formula for the Kaleidocycle is constructed by applying and extending some of the results of the previous chapter. The deformation of Kaleidocycle corresponds to the continuous deformation of discrete curves such that the segment length and the torsion angle are preserved. It has also been proved that the potential function satisfies an alternate version of the semi-discrete mKdV equation simultaneously. This result is consistent with the conjecture that Möbius Kaleidocycles have single degrees of freedom, which is highly significant.

In Chapter 5, the candidate derives non-trivial relations for the non-steady state nucleation rate and discusses their applications by using the properties of the elliptic theta functions. Nucleation is a non-equilibrium process in which a different thermodynamic phase precipitates at a very localized region in response to supersaturation of a certain chemical species in the original phase. This physical phenomenon is universal and has been described by the classical nucleation theory, which is based on equilibrium thermodynamics. The non-steady state nucleation rate is a physical quantity characterizing nucleation, meaning the flux of molecular clusters that grow beyond a critical cluster size per unit time and unit volume. Although the relation between the non-steady state nucleation rate and the elliptic theta functions has been pointed out in previous studies, there have been no results that take advantage of rich mathematical properties of the elliptic theta functions. On the other hand, based on the classical nucleation theory. In this chapter, the candidate shows that the rich mathematical properties of the elliptic theta functions may help overcome various difficulties in experimental studies.

The above results are recognized as valuable achievements in the field of discrete differential geometry and the classical nucleation theory. Therefore, the candidate is worthy of being awarded the Doctor of Functional Mathematics degree.