# Entropy of Triangular Lattices

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## 1 Introduction

In this section we derive the free energy of triangular lattices at given macroscopic deformations. The method is the same as the one used in [1].

Suppose the bond before the deformation is $\vec{r}_i$, and the bond after the deformation is $\vec{R}_i$, where $i$ is an index number for bonds in the unit cell. We could express the deformation as

$$\vec{r}_i \to \vec{R}_i = \Lambda \cdot \vec{r}_i + \vec{u}_i, \tag{1}$$

where $\Lambda$ is the deformation gradient tensor of the (homogeneous) macroscopic deformation, and $\vec{u}_i$ is the fluctuation deviating from the macroscopic deformation.

To capture bulk and shear moduli we take

$$\Lambda = \begin{pmatrix} 1+s_1 & t \\ 0 & 1+s_2 \end{pmatrix}, \tag{2}$$

where $\gamma$ represents a shear change, and $s_1$, $s_2$ represents the change at the x-direction and y direction, respectively.

The lattice free energy at given $\Lambda$ can be obtained by integrating out fluctuations $\vec{u}$. To do this we first expand the Hamiltonian to second order in $\vec{u}$

$$H = H_0\left(\Lambda\right) + \frac{1}{V}\sum_q \vec{u}_q \cdot D_q\left(\Lambda\right) \cdot \vec{u}_{-q} + o(\vec{u}^3), \tag{3}$$

where $H_0$ is the energy of the uniformly deformed state, $\vec{u}_q$ is the Fourier transform of $\vec{u}_i$, and

$$D_q = \sum_i [1 - \cos(\vec{q} \cdot \vec{r}_i)] A_i \tag{4}$$

with

$$A_i = \frac{V_i^{'}}{|\Lambda \cdot \vec{r}_i|} I + \left(V_i^{''} - \frac{V_i^{'}}{|\Lambda \cdot \vec{r}_i|}\right) \Lambda \cdot \left(\frac{\vec{r}_i \vec{r}_i}{|\Lambda \cdot \vec{r}_i|^2}\right) \cdot \Lambda^T \tag{5}$$

and $\sum_i$ represents the sum over all the bonds in the unit cell. Thus the dynamic matrix $D_q$ could be expressed as

$$D_q(\Lambda) = v_q(\Lambda) I + \Lambda \cdot M_q(\Lambda) \cdot \Lambda^T. \tag{6}$$

We then integrate out fluctuations $\vec{u}$ to obtain the lattice free energy

$$F(\Lambda) = -T \ln \int \mathcal{D}\vec{u} e^{-H/T} = H_0(\Lambda) + \frac{T}{2} \ln \det D_q(\Lambda). \tag{7}$$

It was shown in [2] that $F(\Lambda)$ only depends on the uniform deformation through the combination of strain tensor $\epsilon = (\Lambda \cdot \Lambda^T - I)/2$, so it keeps the same symmetry as $H_0(\Lambda)$ and thus the Ward identity is satisfied.

# 2 Entropy of Regular Triangular Lattice

As $F = U - TS$, we could see a correspondence between the entropy and $\ln \det D_q(\Lambda)$. In this section, we would explore this second term under different types of lattices and different deformations.

First of all, we explore the case when the lattice is formed by regular triangles with side length 1. When we do a deformation on the lattice, we expect a change of the lattice entropy, and by doing numerical calculations, we could know the trend of changes.

There are four variables involved: $s_1$, $s_2$, $t$, and $S$, which forms a four-dimensional space. We would project this entropy function to two-dimensional and three-dimensional spaces and try to find the extreme values.

Case I: $s_1$ is a free variable, $s_2 = 0$, $t = 0$. When $s_1$ is small, we could see $-S$ is a linear function of $s_1$ with a 0.999976 coefficient of determination (Figure 1). The linear fit of the function is $-S = 10.4358 + 131.537 s_1$.

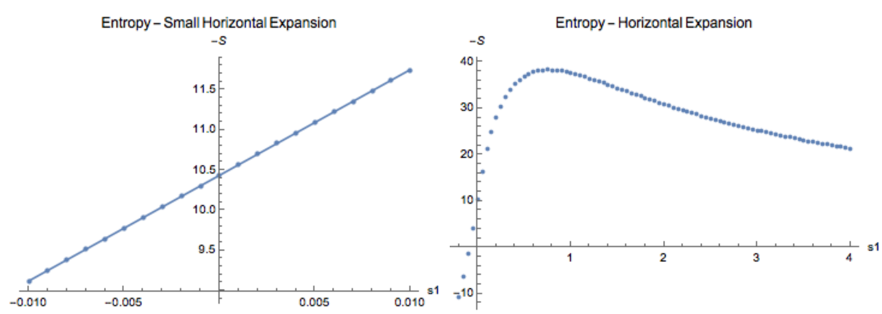



Figure 1

When $s_1 < -0.295$, the result of the integral has a large imagination part due to a negative $\det D_q$, which suggests an unstable lattice, so we could not horizontally shrink the lattice much. The function reaches an maximum value 38.2816 at $s_1 = 0.755$, which suggests a minimum entropy at $s_1 = 0.755$. Thus, when we expand the lattice isothermally, the entropy of the lattice first decreases and then increases.

Case II: $s_2$ is a free variable, $s_1 = 0$, $t = 0$. Similar to Case I, when $s_2$ is small, we could see $-S$ is a linear function of $s_2$ with a 0.999913 coefficient of determination (Figure 2). The linear fit of the function is $-S = 10.4306 + 131.966s_2$.

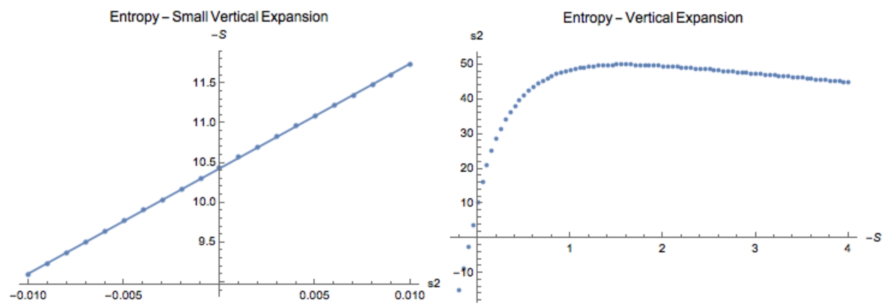



Figure 2

When $s_2 < -0.340$, the result of the integral has a large imagination part due to a negative $\det D_q$, which suggests an unstable lattice, so we could not horizontally shrink the lattice much. The function reaches an maximum value 49.9854 at $s_2 = 1.575$, which suggests a minimum entropy at $s_2 = 1.575$. Thus, when we expand the lattice isothermally, the entropy of the lattice first decreases and then increases.

Case III: $s_1$ and $s_2$ are free variables, and $t = 0$. When $s_1$ and $s_2$ are small, if we define $s_2 = ks_1$ with $k = const$, the $-S - s_1$ and $-S - s_2$ plots are similar to those in Case I and Case II, so the three dimensional plot of $-S - s_1 - s_2$ is a plane (Figure 3).

Case IV: $t$ is a variable, $s_1$ and $s_2$ are constants.

When there is no volume change ($s_1 = 0$,$s_2 = 0$), the simple shear could increase $-S$ parabolically when it is small, while the influence would be smaller as $t$ becomes larger (Figure 4).

What if $s1$ and $s2$ are nonzero? Figure 5 and Figure 6 show the relations between $-S$ and $t$ with different ranges of $t$ and different values of $s_1$, $s_2$. Generally speaking, since $s_1$ represents the expansion at the x-direction and $t$ represents the shear at the x-direction, and both represent similar actions on the lattice, so the change of $s_1$ would not really affect the pattern of the $-S - t$ diagram. However, $s_2$ represents a vertical expansion, which dramatically affects the results of a simple shear.

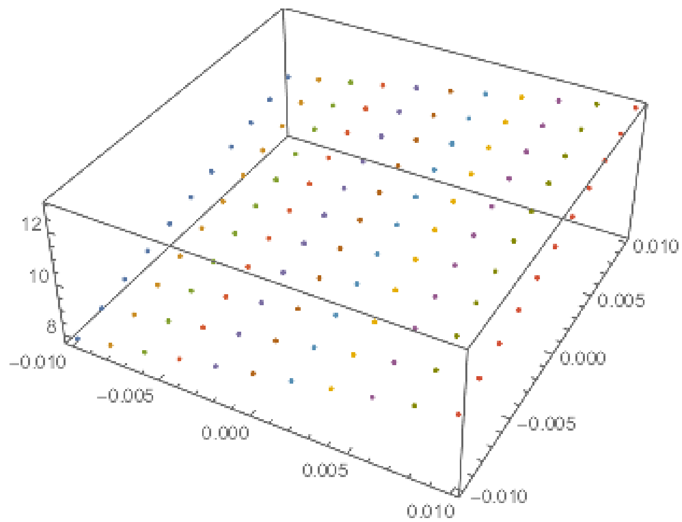



Figure 3

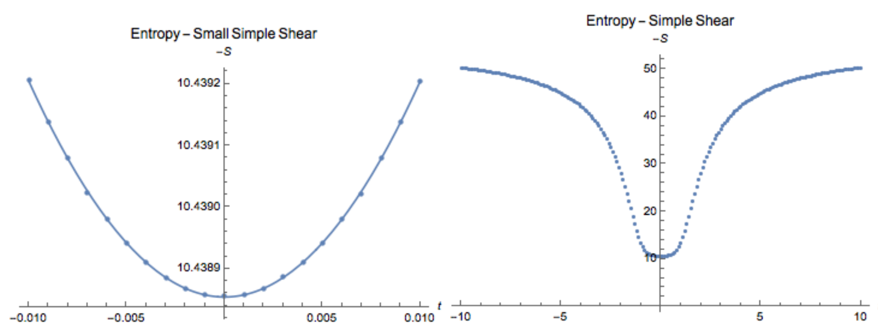



Figure 4

# 3 Entropy of Triangular Lattice with Different Shapes

As we have discussed the case of regular triangular lattices, we may be interested in the case when the unit cell is not a regular triangle.

it is easy to show that given the same shape of triangular lattices and same deformation, the entropy would be the same. So we could conveniently fix one side of the triangle on the x-axis and make it length 1.

Figure 7 shows the series of triangles we explore. We fix the height of the triangle, and change the $x$ so that the shape of the triangle changes. $x$ could be positive, negative or zero. The results corresponding to $x$ and $1-x$ are identical due to symmetry.

Figure 1 shows the relationship of the entropy and horizontal expansion

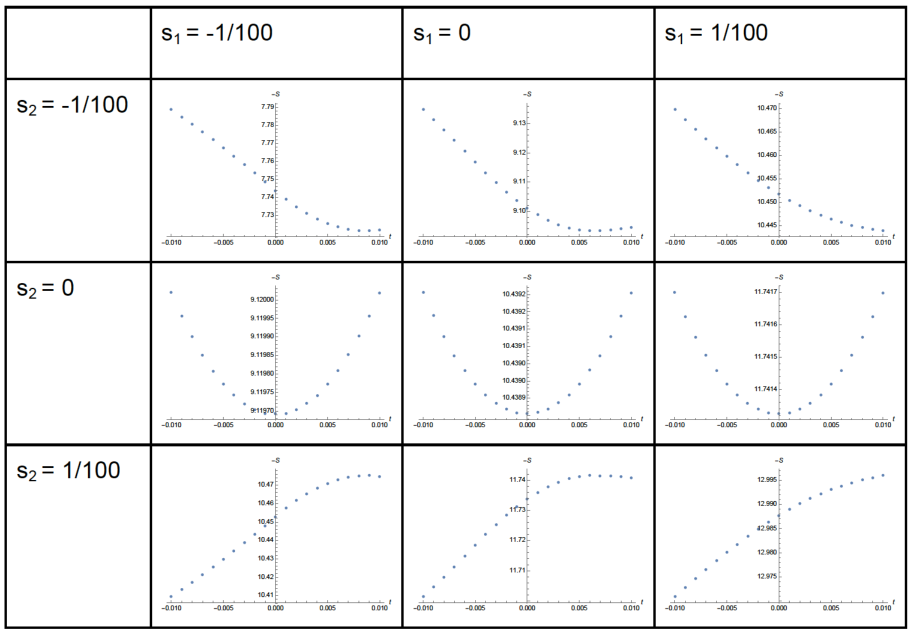



Figure 5

factor, and we could see that there is a low limit of $s1$ such that the lattice would be unstable if we shrink the lattice too much, and there is a point corresponds to the maximum of the negative entropy (minimum of the entropy). As we change $x$, this trend holds, but the value of the low limit and the maximum point change (Figure 8). There should be some interesting physics behind that, and we are still exploring.

# 4 References

[1]Zhang, Leyou, and Mao, Xiaoming. "Finite-temperature mechanical instability in disordered lattices." Physical Review E 93.2 (2016): 022110.

[2]Mao, Xiaoming, et al. "Mechanical instability at finite temperature." Nature communications 6 (2015).

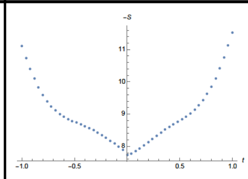
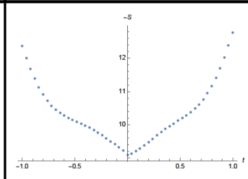
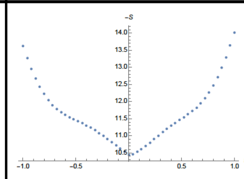
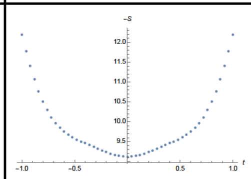
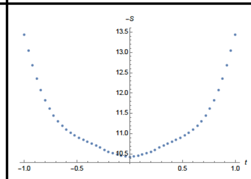
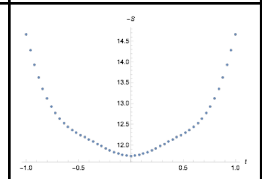
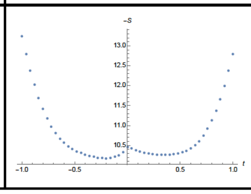
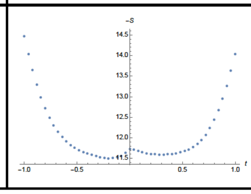
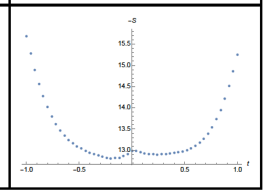
| | $s_1$ = -1/100 | $s_1$ = 0 | $s_1$ = 1/100 |
|---|---|---|---|
| $s_2$ = -1/100 |  |  |  |
| $s_2$ = 0 |  |  |  |
| $s_2$ = 1/100 |  |  |  |

Figure 6

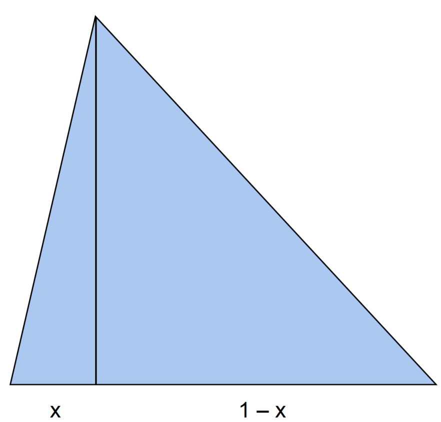



Figure 7

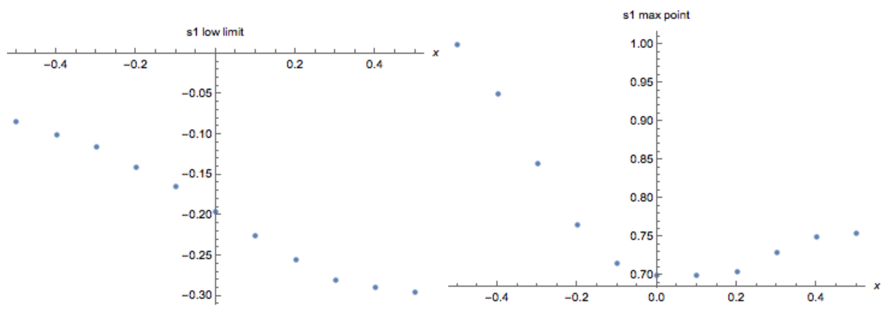

s1 low limit
−0.4
−0.2
0.2
0.4
x
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
s1 max point
1.00
0.95
0.90
0.85
0.80
0.75
0.70
−0.4
−0.2
0.0
0.2
0.4
x

Figure 8