Tropical Limit for Configurational Geometry in Discrete Thermodynamic Systems

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For classical discrete systems with constant composition (typically referred to substitutional alloys) under thermodynamically equilibrium state, macroscopic structure should in principle depend on temperature and many-body interaction through Boltzmann factor, \( \exp(-\beta E) \). Despite this fact, our recently find that (i) thermodynamic average for structure can be characterized by a set of special microscopic state whose structure is independent of energy and temperature, and (ii) bidirectional-stability character for thermodynamic average between microscopic structure and potential energy surface is formulated without any information about temperature or many-body interaction. These results strongly indicates the significant role of configurational geometry, where “anharmonicity in structural degree of freedom (ASDF)” that is a vector field on configuration space, plays central role, intuitively corresponding to nonlinearity in thermodynamic average depending only on configurational geometry. Although ASDF can be practically drawn by performing numerical simulation based on such as Monte Carlo simulation, it is still unclear how its entire character is dominated by geometry of underlying lattice. We here show that by applying limit in tropical geometry (i.e., tropical limit) with special scale-transformation to discrete dynamical system for ASDF, we find tropical relationships between how nonlinearity in terms of configurational geometry expands or shrinks and geometric information about underlying lattice for binary system with a single structural degree of freedom (SDF). The proposed tropical limit will be powerful procedure to simplify analysis of complicated nonlinear character for thermodynamic average with multiple SDF systems.

I. INTRODUCTION

When potential energy surface (PES) (or many-body interaction) is once given, structure (under prepared coordination \( \{q_1, \cdots, q_f\} \)) in thermodynamically equilibrium state with \( f \)-degree of freedoms in classical discrete system under constant composition (typically referred as substitutional crystalline solids) can be obtained through canonical average, whose summation is taken over all possible microscopic states on configuration space with weight of Boltzmann factor, \( \exp(-\beta U) \). Since number of microscopic states astronomically increases with increase of the system size and/or the number of components, theoretical techniques have been amply developed to effectively predict macroscopic properties including Metropolis algorithm, entropic sampling and Wang-Landau sampling. Although the current classical statistical mechanics successfully predict properties for given many-body interactions, it has been generally unclear how the canonical average can be (or cannot be) bidirectionally stable between PES and structure (i.e., stability from PES to structure, and from structure to PES).

Very recently, we show that without using any information about temperature or PES, the bidirectional stability relationship (BSR) is quantitatively formulated by newly-introduced vector field on configuration space, “anharmicity in structural degree of freedom (ASDF)” depending only on configurational geometry before applying many-body interaction to the system. More specifically, hyervolume correspondence between Euclid space of structure \( \{q_1, \cdots, q_f\} \) and of PES \( \langle U \mid q_1 \rangle, \cdots, \langle U \mid q_f \rangle \) is characterized by sum of divergence and Jacobian of ASDF. Here, potential energy \( U \) for any microscopic state \( Q \) under complete orthonormal basis is exactly given by

\[
U_p(Q) = \sum_{i=1}^{f} \langle U \mid q_i \rangle q_i(Q),
\]

where \( \langle \cdots \mid \cdots \rangle \) denotes inner product on configuration space, i.e., trace over all possible microscopic states, and subscript \( p \) denotes the choice of landscape of the PES. So far, although the ASDF intuitively corresponds to nonlinearity in the thermodynamic average in terms of configurational geometry, and can be estimated as time evolution of a special discrete dynamical system from numerical simulation, it is still unclear how its entire character is dominated by geometry of underlying lattice. We here show that by applying limit in tropical geometry (i.e., tropical limit) to the dynamical system, we clarify how configurational nonlinearity is characterized by lattice geometry for equiatomic binary system. Its derivation and the detailed discussions are shown below.

II. DERIVATION AND APPLICATIONS

A. Preparation for derivation

Before formulating the nonlinearity in thermodynamic average in terms of lattice geometry, we first briefly explain the basic concept of the ASDF, BSR and related discrete dynamical system. In the present study, we employ generalized Ising model (GIM) providing a complete orthonormal basis function for any configuration on given lattice. For instance, in A-B binary system, occupation of a lattice site \( i \) is specified by spin variables, \( \sigma_i = +1 \) for A and \( \sigma_i = -1 \) for B. Using the spin variables, basis function is given by

\[
\phi_i^{(d)} = \left\langle \prod_{i \in s} \sigma_i \right\rangle_d.
\]

Here, \( \left\langle \cdots \right\rangle_d \) means taking average for microscopic state \( d \), taking over symmetry-equivalent figure \( s \). When structure \( Q \) is interpreted as \( f \)-dimensional vector \( Q = \{q_1, \cdots, q_f\} \) under
the orthonormal basis, ASDF is defined as the following vector field at $Q$:

$$A(Q) = \left\{ \phi_h(\beta) \circ (-\beta \cdot \Lambda)^{-1} \right\} \cdot Q - Q,$$

(3)

where $\phi_h$ denotes canonical average, $\beta$ inverse temperature, $\circ$ composite map, and $\Lambda$ is $f \times f$ real symmetric matrix of

$$\Lambda_k = \sqrt{\frac{\pi}{2}} \langle q_k \rangle_2 \langle q_k \rangle_k^{(+)} ,$$

(4)

where $\langle \quad \rangle_2$ denotes taking standard deviation for CDOS, and $\langle q_k \rangle_k^{(+)}$ represents taking partial linear average satisfying $q \geq 0$. Note that here and hereinafter, structure $Q$ is measured from center of gravity of CDOS. Important points here are that (i) these average and standard deviation are taken before applying many-body interaction to the system, and (ii) image of the composite map in Eq. (4) is independent of temperature and of many-body interaction: Therefore, we can know vector field of ASDF without any information about temperature or energy, i.e., it can be a priori known depending only on configurational geometry. Since we have shown that $\Lambda$ is a unique representation of linear part in canonical average in terms of configurational geometry, ASDF in Eq. (3) is a measure of nonlinearity in $\phi_h$ defined on individual configuration $Q$.

Next, we briefly describe the BSR in $\phi_h$. The BSR for structure $Q$ has been defined as

$$B(Q) = \log \left( \frac{R(Q)}{R(0)} \right),$$

(5)

with

$$R(Q) = \frac{dQ(Q)}{dU(Q)},$$

(6)

where $dQ(Q)$ and $dU(Q)$ respectively denotes hypervolume in $f$-dimensional $Q$- and PES-space defined above, and superscript $(0)$ denotes structure at center of gravity of CDOS (i.e., disordered structure). Therefore, this definition of BSR intuitively provides that $B > 0$ is $Q \rightarrow U$ stable for $\phi_h$ as a map, $B < 0$ is $U \rightarrow Q$ stable, and $B = 0$ is bidirectionally stable. We have shown that the BSR can be quantitatively formulated using only of the ASDF:

$$B = \log \left| 1 + \text{div}A + \sum F J F \left[ \frac{\partial A}{\partial Q} \right] + J \left[ \frac{\partial A}{\partial Q} \right] \right| ,$$

(7)

where $J$ denotes Jacobian, and summation $F$ is taken over all possible subspaces derived from configuration space considered. From Eq. (7), we can clearly see that the BSR can be characterized by information only about configurational geometry, and the BSR should be investigated through analyzing the trajectory of the following discrete dynamical system for ASDF:

$$Q_{a+1} = Q_a + A(Q_a) ,$$

(8)

since we see the BSR for $Q_{a+1}$ at $Q_a$. Note that $A(Q_a)$ is a scalar for a considered single coordination. We have previously shown that at center of gravity of CDOS, $\phi_h$ becomes a linear map, i.e.,

$$A(Q_0) = 0 .$$

(9)

B. Tropical limit of discrete dynamical system

From above discussions, we can see that although BSR is characterized by ASDF, i.e., geometrical nonlinearity, it is still unclear how entire character of BSR is dominated by geometry of underlying lattice, since drawing vector field ASDF for large systems typically requires numerical simulation clearly seen from Eq. (3). To overcome this problem, some special limit for ASDF would be naturally suggested, to focusing on relationships between lattice geometry and the nonlinearity. Here, our strategy is to apply tropical limit to the discrete dynamical system in order to magnify relationships to be interested. Briefly, tropical limit for multi-order real polynomials is interpreted as map from $\mathbb{R}_{>0}, +, \times$ to $\mathbb{R}_{>0}, \oplus, \otimes$ through the following:

$$\mathbb{R}_{>0} \ni x, y : \begin{align*}
    x &\mapsto t^x , \quad y \mapsto t^y \\
    X \oplus Y &:= \lim_{t \to 0} \log \left( t^X + t^Y \right) = \max \{ X, Y \} \\
    X \otimes Y &:= \lim_{t \to 0} \log \left( t^X \cdot t^Y \right) = X + Y ,
\end{align*}$$

(10)

where $\oplus$ and $\otimes$ respectively corresponds to tropical sum and tropical product, naturally inducing max-plus algebra. Note that the tropical limit has been naturally adopted in statistical mechanics, e.g., free energy $F = -kT \sum \exp(-\beta E)$ with $\beta \to \infty$ induces tropical limit, where $F$ merely equals to minimum energy. However, we emphasize here that the present tropical limit is completely different from such adoption. Because of the above character, we cannot simply apply tropical limit to the discrete dynamical system because (i) domain of $Q$ includes negative value, and (ii) $A(Q)$ can take positive, zero or negative sign, depending on $Q$. Problem (i) can be straightforwardly solved by variable transformation of $Q' = Q + B$ where e.g., $B \geq 1$ such that range of $Q'$ takes positive sign. Therefore, nontrivial problem is (ii). One straightforward approach for the problem (ii) is to take square for both sides of Eq. (8) after the variable transformation, leading to

$$(Q_{a+1}')^2 + (Q_a')^2 = 2Q_{a+1}'Q_a' + A^2.$$

(11)

Then corresponding tropical limit becomes

$$\max \{ 2\Omega_{a+1}, \Omega_a \} = \max \{ \Omega_{a+1} + \Omega_a, 0 \} ,$$

(12)

which has solution of

$$\Omega_{a+1} = \Omega_a \quad (\Omega_a \geq 0)$$

$$\Omega_{a+1} = 0 \quad (\Omega_a < 0) .$$

(13)

However, above dynamical system of Eq. (11) has several essential problems: Taking square of both sides can lose part
of information about original dynamical system of Eq. (8), resultant solution of Eq. (13) exhibit completely different behavior of practical vector field which is now ready to be applied to tropical limit. These facts strongly suggest that do not take square of both sides, and A should not be treated merely as scalar since A is a function both of $Q_a$ and $B$. Therefore, to explicitly apply tropical limit for ASDF, A should be represented by polynomial in terms of $Q_a$ and $B$. To achieve this, we start from series expansion of A in terms of moments of CDOS, given by

$$A = \sum_{k=2}^{\infty} \frac{1}{k!} \frac{1}{(Q')^k} \left\{ \langle Q^{(k+1)} \rangle + \sum_j c_j \cdot \prod_{\{w_j\mid \sum w_j = (k+1)\}} (Q')^{w_j} \right\} \cdot Q^k,$$

where $\langle \cdot \rangle$ denotes taking linear average on CDOS, and $c_j$ corresponds to coefficient for the expansion. We here focus on a single $Q$ as pair correlation on equicompositional binary system, where only diagrams for moments, with number of odd-time occupation by lattice points taking zero, dominantly contribute to A at thermodynamic limit. Under this condition, expression of A is greatly simplified to

$$A \simeq \sum_{k=2}^{\infty} \left[ (k+1) \frac{J_{k+1}}{D} \sum_{m=0}^{k} \left\{ kC_m Q^m (-B)^{(k-m)} \right\} \right], \quad (15)$$

where $J_{k+1}$ denotes number of simple cycle per site consisting only of considered pair type, and $D$ number of pair per site. Since number of simple cycle cannot be simply formulated in terms of lattice geometry, we here perform numerical simulation to *exactly* count $N_k = kJ_k/D$ up to $k = 14$ for e.g., fcc with 1 nearest-neighbor (1-NN) and 2-NN pair, shown in Fig. 1. We can clearly see that $N_k \simeq e^{Mk}$ where $M$ depends on pair type except for $N_k = 0$ with $k$ taking odd number in 2-NN pair. Hereinafter, we focus on the case of $N_k \simeq e^{Mk}$, while the following derivation can be straightforwardly extended to other cases including 2-NN pair. Then coefficient for $(Q')^g$ in Eq. (15) can be geometric sequence with geometric ratio of $\sim e^{-M} \cdot (-B) > 1$ for large $k$, leading to

$$A \simeq \lim_{n \to \infty} \left\{ e^{(n+2)M} B^n (-1)^n Q' + \sum_{g=0}^{n+1} e^{(n+2)M} c_g \right\},$$

$$c_g = (-B)^{n+1-g} (Q')^g. \quad (16)$$

This transformation indicates that we naturally include coefficient for $Q'^m$ contributed from all possible $k \geq m$ ($k \leq k_{max} \to \infty$) in Eq. (15), while we terminate maximum power of $Q$ up to condition of $m_{max} \ll k_{max}$ so that

$$\lim_{k_{max} \to \infty} \frac{k_{max}}{M_{max}} = 0$$

is satisfied. Since a set of $c_g$ also forms geometric sequence with its ratio of $(-B) Q'$, dynamical system of Eq. (8) can be rewritten as

$$Q_{n+1}' = Q_n' + e^{(n+2)M} \left[ (-B)^{n+1} \frac{1 - (BO')^{n+2}}{1 + BO'} \right], \quad (18)$$

which is now ready to be applied to tropical limit.

It is clear that Eq. (18) should be analyzed individually by conditions of (i) parity of $n$ and (ii) whether or not absolute of geometric ratio $|(-B) Q'|$ exceeds 1: There results in 4 conditions.

We first start from $n$ is even with $|(-B) Q'| < 1$. In this case, since

$$\lim_{n \to \infty} (BO')^{n+2} = 0, \quad (19)$$

we have
We note here that by simply applying tropical limit to Eq. (20), geometric information of lattice is clearly dissapeared. Since we take \( n \to \infty \), we can overcome this problem by introducing following transformation:

\[
e^{\gamma n} = g(t) \cdot t,
\]

where \( g(t) > 0 \) (note: \( g(t) \) can be constant independent of \( t \)). Since at tropical limit, we take \( t \to \infty \) in log, under taking \( n \to \infty \), \( g(t) \) corresponds to parameter to control divergence magnitude between \( n \) and \( t \), which will be naturally determined from physical insight in the following discussions. Substituting Eq. (21) and setting artificial translation for \( Q \) of \( B = 1 \), we obtain tropical limit for Eq. (20) as

\[
BQ'_{a+1}Q'_a + Q'_{a+1} + B^{n+1}e^{(n+2)M} = \left( B^{n+1}e^{(n+2)M} + B \right) (Q'_a)^2 + \left( B^n e^{(n+2)M} + 1 \right) Q'_a.
\]  

(20)

This derived tropical limit of dynamical system exhibit diffferent behavior w.r.t. sign of \( M(1+\gamma) \). The exception is Eq. (22), which always results in

\[
n: \text{even}, \Omega_a < 0:
\max \{ \Omega_{a+1} + \Omega_a, \Omega_{a+1}, M(1+\gamma) \} = \max \{ (n+2)\Omega_a + M(1+\gamma), \Omega_a + M(1+\gamma), 2\Omega_a \} \quad (n: \text{even}, \Omega_a \geq 0)
\]

\[
n: \text{odd}, \Omega_a < 0:
\max \{ \Omega_{a+1} + \Omega_a, \Omega_{a+1}, 2\Omega_a + M(1+\gamma), \Omega_a + M(1+\gamma) \} = \max \{ 2\Omega_a, \Omega_a, M(1+\gamma) \} \quad (n: \text{odd}, \Omega_a < 0)
\]

\[
n: \text{odd}, \Omega_a \geq 0:
\max \{ \Omega_{a+1} + \Omega_a, 2\Omega_a + M(1+\gamma) \} = \max \{ (n+2)\Omega_a + M(1+\gamma), 2\Omega_a \} \quad (n: \text{odd}, \Omega_a \geq 0).
\]  

(23)

Although these two time evolution is continuous at \( \Omega_a = 0 \), \( \Omega_{a+1} = M(1+\gamma) \) at \( \Omega_a = 0 \): This means that at center of gravity of CDOS, \( \phi_0 \) is not a linear map since \( \Omega_{a+1} - \Omega_a = M(1+\gamma) \), which loses important information about original dynamical system of Eq. (9). The exception is \( M(1+\gamma) = 0 \), corresponding to \( \gamma = -1 \). However, \( \gamma = -1 \) should not be allowed since in this case, we get from Eq. (21) that

\[
e^{\gamma n} = t^{-1} \cdot t = 1
\]  

(26)

regardless of the value of \( t \). Therefore, in order to keep the dynamical system linear at center of gravity of CDOS, \( M(1+\gamma) \geq 0 \) should not be allowed. Then we consider another condition of \( M(1+\gamma) < 0 \). In this case, dynamical system is also independent of parity of \( n \), resulting in

\[
\Omega_{a+1} = \begin{cases} 
M(1+\gamma) & (\Omega_a \leq M(1+\gamma)) \\
\Omega_a & (M(1+\gamma) < \Omega_a < -M(1+\gamma)/n) \\
(n+2)\Omega_a + M(1+\gamma) & (-M(1+\gamma)/n \leq \Omega_a)
\end{cases}
\]  

(27)
FIG. 2: Simulated discrete dynamical system of Eq. (8) for fcc equiatomic binary system with 1-NN pair correlation.

FIG. 3: Value of ASDF near center of gravity of CDOS.

We can now clearly see that $\Omega_{a+1} = \Omega_a$ at $\Omega_a = 0$ is satisfied. Therefore, to reasonably keep $\phi_b$ as linear map at center of gravity of CDOS, $M (1 + \gamma) < 0$ should be required. This condition means that $g(t)$ is an explicit function of $t$ (i.e., not constant), and

$$\lim_{t \to \infty} \frac{e^n}{t} = 0, \quad (28)$$

i.e., $e^n$ should also be zero at tropical limit, which is a naturally-adopted condition. Moreover, dynamical system of Eq. (27) exhibit several important character of original dynamical system: (i) At $\Omega_a = M (1 + \gamma) < 0$, divergence of the tropical vector field $\Omega$ becomes singular, which agrees with vertex of configurational polyhedra at negative sign of $Q_a$ behaves as adsorption point as shown in Fig. 2 and (ii) linear region is asymmetric (linearity in $\phi_b$ is stronger for $Q_a < 0$ than that for $Q_a > 0$), which also capture the asymmetric nonlinearity magnitude around center of gravity of CDOS as shown in Fig. 3. Especially, character of (i) should be exact only at $\beta \to \infty$ where ASDF is not well-defined for original dynamical system. Therefore, it is indicated that tropical limit of dynamical system would exhibit special relationships between ground-state at $\beta \to \infty$ and ideally disordered state at $\beta = 0$, which should be investigated in detail including other systems with higher-degree of SDF. Additional important point for Eq. (27) is that region for $\phi_b$ as linear map with increase of $M$: This can be intuitively interpreted that at limit of reducing spatial-constraint to constituents (by lattice) becoming free (i.e., continuous space with no constraint of lattice), linear map region naturally increases due to increase of $M$, which is consistent that deviation in landscape of CDOS from gaussian can typically reduces with reducing the spatial constraint, where we have shown that $\phi_b$ exactly becomes linear map if and only if CDOS takes Gaussian.

III. CONCLUSIONS

By introducing special scale transformation, we construct tropical limit of dynamical system for representing nonlinearity in thermodynamic average coming from configurational geometry, for classical discrete systems. The tropical dynamical system explicitly reveals how entire character of vector field of anharmonicity in the structural degree of freedom (corresponding to geometrical nonlinearity) is dominated by geometry of underlying lattice.

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