Arithmetical properties of dynamical zeta functions

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The zeta functions we have been considering share more than a formal resemblance to the Riemann zeta functions. It is possible to give an algebraic structure to the set of periodic orbits, strengthening the analogy between the thermodynamical zeta functions and the Riemann zeta functions. Except for the substitution of n^{-s} in the Riemann function by a more general form, most other properties can be translated. Upon correct interpretation many of the results of multiplicative number theory can be directly translated into equivalent statements about thermodynamical zeta functions. Also, the algebraic structure of the set of configurations is as rich as the algebraic structure of the non-negative integers ($\mathbf{Z}_{\geq}$), and can be further used. In particular there is an analog of the prime number decomposition of the integers.

In this section we take a combinatorial approach to the zeta function, which by employing different summation methods can lead to different forms of the zeta function. The usual approach is to sum the linearly periodic configurations, but other summations are possible. By investigating the formal structure of the zeta functions one finds the most general setting in which the formalism is applicable.

The Riemann zeta function

We will briefly review the arithmetic properties of the Riemann zeta function. A function of the integers f is said to be multiplicative if $f(1) = 1$ and for any two integers a and b one has

$$f(ab) = f(a)f(b) \quad \text{with } a \perp b\,. \tag{1}$$

$a \perp b$ indicates that a and b are relative primes. If relation (1) holds even if a and b are not relative primes, then F is said to be strongly multiplicative.

As any integer can be decomposed into a product of power of primes in a unique way, this tells us that all we have to know to evaluate a multiplicative function is its values at the primes and its powers. An example of a multiplicative function is $f(n) = n^{-s}$. Given two multiplicative functions one can build another one by considering their product. A textbook with these concepts is *Concrete mathematics*, by Graham, Knuth and Patashnik (Addison-Wesley, Reading, 1989).

Consider the sum

$$\zeta_f = \sum_{k \geq 1} f(k)\,, \tag{2}$$

assumed to be absolutely convergent. It can be expressed as an Euler product, of the form

$$\prod_{p \ \text{prime}} (1 + f(p) + f(p^2) + f(p^3) + \cdots)\,. \tag{3}$$

To see this, restrict the product to be over all primes smaller than a certain large prime P. By expanding out the product, one gets a sum of terms where each is a product of f evaluated at either one or a prime to a power. As all powers occur the resulting sum will consist of all the numbers that do not have a prime factor larger than P. The error between this product and the the sum in (2) goes to zero as we make P larger, establishing the equality of (2) and (3). In the case f is strongly multiplicative we have that $f(p^k) = f(p)^k$, and each term of the product can be simplified:

$$\zeta_f = \sum_{k \geq 1} f(k) = \prod_{p \ \text{prime}} (1 - f(p))^{-1}\,. \tag{4}$$

After the resummation of the geometric series we can apply the equality between (2) and (3) again and discover a new multiplicative function. From the "infinite" sum in the product

$$\zeta_f^{-1} = \prod_{p \ \text{prime}} (1 - 1 \cdot f(p) + 0 \cdot f(p^2) + 0 \cdot f(p^3) + \cdots) = \sum_{k \geq 1} \mu(k) f(k) \tag{5}$$

we discover another multiplicative function, the Möbius function $\mu(n)$. From the above relation we see that it has the value -1 when evaluated at a prime p

(to the power one) and zero when evaluated at a higher powers p^k with $k > 1$ of a prime. Because it is multiplicative, it can be extended to any other integer by factorization. For example

$$\begin{aligned}\mu(30) &= \mu(2\times 3\times 5) = \mu(2)\mu(3)\mu(5) = (-1)^3 = -1\\ \mu(12) &= \mu(2\times 2\times 3) = \mu(2^2)\mu(3) = 0\,.\end{aligned}$$

The Möbius function counts the parity of the number of distinct square-free factors of its argument. We will see that there is a close analogy between the number theoretical concepts we have considered and the thermodynamic zeta functions.

Pseudoconfigurations

Consider a one dimensional lattice where each site can be in a finite number of states. We wish to compute the zeta function for this system. The partition function for a system with N sites is given by

$$Z_N(\beta) = \sum_{\Omega(\Lambda_N)} e^{-\beta H_N(\sigma)}\,,$$

where the sum is over all the configurations $\Omega(\Lambda_N)$ of the system inside of a box Λ_N with N sites labeled 0 through $N-1$. The Hamiltonian $H_N(\sigma)$ computed for a configuration σ is written as a sum of potentials to ensure that it is translational invariant,

$$H_N(\sigma) = \sum_{i\in\Lambda_N} \Phi(\sigma_i, \sigma_{i+1}, \ldots) \tag{6}$$

The potentials are usually due to pairwise interactions $\phi(\sigma_i, \sigma_j)$. In this case the potentials Φ used above could be expressed in terms of the interactions as

$$\Phi(\sigma_1, \sigma_2, \ldots) = \sum_{j\,>\,1} \delta(\sigma_1, \sigma_j)\phi(1, j)\,. \tag{7}$$

For the thermodynamic limit we must have that

$$\sup_\sigma \Phi(\sigma) < \infty\,.$$

In the case the potential is of infinite range, one must specify the values of the spins outside the box Λ_N, that is, the boundary conditions must be specified. The combination of the sum in (6) and the restricted sum in (7) ensures that each interacting pair is counted only once. The boundary conditions we use are equivalent to periodic boundary conditions: all sites along $\mathbf{Z}$ are determined by tiling it with repeated copies of Λ_N. This is equivalent to assuming $\sigma_k = \sigma_{k \bmod N}$ in equation (6).

We are going to compute the thermodynamical properties of this system using the grand-canonical ensemble. In this ensemble one introduces a new parameter, the fugacity z, which plays for the particle number N the same role that β plays for the energy H in the canonical ensemble. The grand-partition function $\Xi(z,\beta)$ is given by

$$\Xi(z,\beta) = \sum_{m\geq 0} \frac{z^m Z_m(\beta)}{m}\,. \tag{8}$$

As we have done before, we modified the grand-partition function by dividing each term by n. This is no longer a technical simplification, but a necessity for the development of the formalism. The thermodynamics follows from the logarithm of the grand-partition function,

$$p(\beta) = -\lim \frac{1}{N} \log \Xi_N(z,\beta)\,.$$

The other thermodynamical quantities follow from the pressure p.

To simplify the notation we are going to introduce the Gibbs factor t_σ of a configuration σ with $|\sigma|$ sites,

$$t_\sigma = z^{|\sigma|} e^{-\beta H_{|\sigma|}(\sigma)}\,. \tag{9}$$

Notice that the (inverse) temperature β and the fugacity z have been absorbed into the symbol t_σ and are no longer explicitly indicated. We can now write

$$z^n Z_n(\beta) = \sum_{\sigma\in\Omega(\Lambda_n)} t_\sigma\,,$$

the sum running over all the configurations $\Omega(\Lambda_n)$ in the box Λ_n. Then for example,

$$z^2 Z_2(\beta) = t_{(00)} + t_{(01)} + t_{(10)} + t_{(11)}\,.$$

We will be grouping the symbols in a given configuration with parenthesis, as in (011).

There are two useful properties of the Gibbs factors t_σ. One is the invariance of the factors under rotations of the configurations, that is,

$$t_{(101)} = t_{(011)} = t_{(110)}\,.$$

This follows from the definition of the factors and the use of periodic boundary conditions. One expands the Hamiltonian in terms of the potentials, as in (6),

$$\begin{aligned}
H(\sigma) &= H(\sigma_1,\sigma_2,\ldots,\sigma_n) \\
&= \sum_{1\leq i\leq n} \Phi(\sigma_i,\sigma_{i+1},\ldots,\sigma_{i+n-1}) \\
&= \sum_{2\leq i\leq n+1} \Phi(\sigma_i,\sigma_{i+1},\ldots,\sigma_{i+n-1}) \\
&= H(\sigma_2,\sigma_3,\ldots,\sigma_n,\sigma_1)\,.
\end{aligned}$$

Because of the periodic boundary conditions $\sigma_{n+1} = \sigma_1$, and by rearranging the sum one gets the equality of the Hamiltonians under rotations of the configurations, and therefore of the Gibbs factors t_σ.

The other useful property is the decomposition of periodic configurations. Because of the choice of periodic boundary conditions, the Gibbs factor of a periodic configuration can be expressed in terms of its fundamental period. That is, if we are given the configuration (100100100), the its Gibbs factor is a function of the Gibbs factor of (100). If the period of a configuration σ is p, so that $|\sigma| = kp$, for a positive integer k, one has

$$\begin{aligned} H_{kp}(\sigma) &= \sum_{1\le i\le kp} \Phi(\sigma_i, \sigma_{i+1}, \ldots) \\ &= \sum_{j=1}^{k} \sum_{i=(j-1)p+1}^{jp} \Phi(\sigma_i, \sigma_{i+1}, \ldots) \end{aligned} , \tag{10}$$

and due to the periodicity, all sums in the second line of (10) have the same value independent of j and are equal to the H of the repeating period. We have then

$$t_{\underbrace{\sigma\sigma\cdots\sigma}_{k \text{ times}}} = (t_\sigma)^k . \tag{11}$$

For the example considered

$$t_{(100100100)} = t^3_{(100)} .$$

A configuration is said to be *irreducible* if it is not periodic. The irreducible configurations play the role of the prime numbers in the arithmetic of configurations. We will now define an operation on configurations, the concatenation. If we multiply two Gibbs factors t_σ and t_ω we say that there is a *pseudoconfiguration* $\sigma\omega$ whose weight is exactly the product of the weight of its parts. One has

$$t_{\sigma\omega} = t_\sigma t_\omega ,$$

by definition. An example of a pseudoconfiguration would be (101) (0011), with Gibbs factors

$$t_{(101)\,(0011)} = t_{(101)} t_{(0011)} ,$$

and in analogy with the decomposition of an integer into its prime factors we call (101) and (0011) the factors or configurations of the pseudoconfiguration. A difference between pseudoconfigurations and the integers is that for pseudoconfigurations we do not have a compact notation to write the product of factors. Using pseudoconfigurations is like using integers in their prime factor decomposition. As with the integers, two pseudoconfigurations that differ by the order of their factors are the same pseudoconfiguration. So in the example we used, (101) (0011) = (0011)(101). Notice that by construction a pseudoconfiguration has a unique decomposition in terms of its configurations. This is the equivalent of the prime factor decomposition of the integers for pseudoconfigurations.

There is one relation between pseudoconfigurations and a configuration. A periodic configuration can be decomposed into a concatenation of pseudoconfigurations while preserving the Gibbs factor. This is expressed in equation (11), and results in the Gibbs factor being a strongly multiplicative function. An example is

$$t_{(100100)} = t_{(100)\,(100)}\,.$$

We can summarize by stating that the Gibbs factor t is a strongly multiplicative function from the set P of all pseudoconfigurations. The null configuration is in the set P and the value of t on it is one.

Thermodynamical zeta functions

The grand-partition (8) can be written as the sum

$$\Xi(z, \beta) = \sum_{n \geq 1} \frac{z^n}{n} Z_n(\beta) = \sum_{\sigma \in \Omega} \frac{1}{|\sigma|} t_\sigma$$

with the sum being over all possible configurations (*not* pseudo-configurations) without any length restrictions. The terms in this sum have the property of not being multiplicative functions due to lack of structure of the set Ω of all configurations. This leads us to consider the exponential of the grand-partition, as exponentials of generating functions tend to count only once things that differ by permutations. Let us consider

$$\zeta = e^{\Xi} = \exp(\sum_{\sigma} t_\sigma/\sigma)$$

The claim is that the exponential of Ξ can be written as the sum over all possible pseudoconfigurations:

$$\zeta = e^{\Xi} = \sum_{\sigma \in P} t_\sigma\,.$$

We shall prove this in a later section, and here we will just show a few examples of how it works. First we expand the exponential into a sum of terms

$$\exp(\Xi) = \sum_{n \geq 0} \frac{\Xi^n}{n!} = \sum_{\sigma \in P} t_\sigma\,. \tag{12}$$

Consider a term from the right hand side of (12), say $t_{(1)(01)}$. This term can only come from factors involving Z_1 which contain the term $t_{(1)}$ and Z_2 which contains the terms $t_{(01)}$ and $t_{(10)}$ which are equivalent when viewed as pseudoconfigurations. The combination of Z_1 and Z_2 is of two terms and can only occur in the factor $\Xi^2/2!$ of the left-hand side of (12). There we have

$$\frac{1}{2!} 2 \frac{Z_1}{1} \frac{Z_2}{2} = \frac{1}{2} \left(t_{(1)} t_{(01)} + t_{(1)} t_{(10)} \right) = t_{(1)(01)}\,,$$

that is, the pseudoconfiguration occurs only once on the right-hand side. As another example let us consider the term $t_{(0)(1)(001)}$. It can only come from the product $Z_1 Z_1 Z_3$. This product only occurs in the term $\Xi^3/3!$. It occurs with a coefficient 3 as there are three different ways of arranging two Z_1 and one Z_3. Each factor Z_n is divided by n so we get a factor 1/3 and finally there are six combinations that are equivalent to $t_{(0)(1)(001)}$, as $t_{(001)}$ can occur in three different rotations and the other two can appear in two different orders. Collecting all these terms we have

$$\frac{1}{3!} \cdot 3 \cdot \frac{1}{1 \cdot 1 \cdot 3} \cdot 6 = 1 \,.$$

We can use the theorem we proved at the beginning of this chapter, expression (4), to express the exponential of the grand-partition as an Euler product.

$$\zeta(z, \beta) = e^{\Xi(z,\beta)} = \sum_{\sigma \in P} t_\sigma = \prod_p (1 - t_p)^{-1} \,, \tag{13}$$

where the product is over all “prime” pseudoconfigurations. A pseudoconfiguration is prime if it cannot be decomposed into a product of other configurations. Notice that periodic configurations can be written as a product, so no repeating configuration appears in the right-hand side product.

Matrix form

In many cases we can consider the partition function as being generated by a transfer matrix. If we have that

$$Z_n = \mathrm{tr} T^n \,,$$

then the expression for the generating function Ξ can be written in matrix form

$$\Xi = \sum_{n>0} \frac{z^n}{n} \mathrm{tr} T^n = -\mathrm{tr} \ln (1 - zT) \,.$$

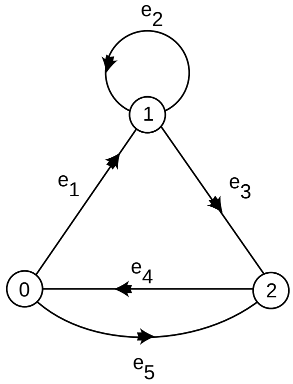
In this case the relation 13 allows one to relate the ζ function to a matrix determinant using the relation $\ln \det = \mathrm{tr} \ln$. The only difficulty is that we have an extra negative sign. We want to determine $e^{-\Xi}$ rather than e^{Ξ}. That means that in equation 12 we would have

$$\sum_{n \geq 0} \frac{(-1)^n \Xi^n}{n!} = \sum_{\sigma \in P} (-1)^{|\sigma|} t_\sigma \,.$$

The notation $|\sigma|$ means the sum of the length of all the prime orbits making up the pseudo-configuration. For example, $(-1)^{|(0)(01)|} = (-1)^{1+2} = -1$. With this notation:

$$\zeta^{-1} = e^{-\Xi} = \exp\left(\mathrm{tr} \ln (1 - zT)\right) = \det (1 - zT) = \sum_{\sigma \in P} (-1)^{|\sigma|} t_\sigma \,.$$

This means that the determinant of $1 - zT$ can be expressed as a sum over all pseudo-configurations with appropriate sign for each pseudo-configuration. For example, if we have the diagram



with the weight matrix

$$T = \begin{bmatrix} 0 & 0 & e_4 \\ e_1 & e_2 & 0 \\ e_5 & e_3 & 0 \end{bmatrix}$$

the expansion for the determinant reads:

$$\begin{aligned} \det(1 - zT) &= 1 - t_{(1)} - t_{(02)} - t_{(012)} + t_{(1)(02)} \\ &= 1 - ze_2 - z^2 e_4 e_5 - z^3 \left(e_1 e_3 e_4 - (e_2)(e_4 e_5)\right) . \end{aligned}$$

The longest loop in the graph is the (012) loop, so the expansion only goes up to terms in z^3.

Möbius function

One can also introduce a Möbius function just as was done for the Euler product of the zeta function (5). The thermodynamical Möbius function is a multiplicative function that assumes the value -1 for all prime pseudoconfigurations and zero on any periodic configuration. Using its multiplicative character it can be extended to all pseudoconfigurations. For example

$$\mu((100)(1011)) = \mu((100))\mu((1011)) = 1 .$$

With it we can obtain the cycle expansion for the system described by the interaction Φ (from which one computes the Gibbs factors t). Applying the Euler product relation for the multiplicative function $\mu(c)t_c$ one gets

$$\zeta^{-1}(z, \beta) = \prod_p (1 - t_p) = \sum_{c \in P} \mu(c) t_c .$$

The sum is over all possible pseudoconfigurations. Notice that in the sum any pseudoconfiguration that has a repeated term does not contribute to the sum; also, only terms with prime sub-configurations contribute, as the periodic configurations get eliminated by the μ function.

Equality

Here we will prove the relation between the exponential of all configurations and the sum of all pseudoconfigurations. Let us say that Z_n is the sum of all Gibbs factors for the configurations with n elements, so for example

$$Z_2 = t_{(00)} + t_{(01)} + t_{(10)} + t_{(11)} .$$

Notice that in Z_n the configurations, and not the pseudoconfigurations, are summed up. For more on the definitions of configuration and pseudoconfigurations see section . A factor as $t_{(01)}$ means the exponential of the energy per two sites when the infinite configuration of the system is a repetition of the pattern 01. For a configuration the Gibbs factor t was defined as

$$t_\sigma = z^{|\sigma|} e^{H(\sigma)} ,$$

where by H of a configuration it is meant the average energy. For details in the definition of the Gibbs factor see expressions (6) and (9). This definition is extended to pseudoconfigurations by factoring t over the factors of the pseudoconfiguration. We want to show the identity

$$\exp\left(\sum_{n\geq 1} \frac{Z_n}{n}\right) = \sum_{\sigma\in P} t_\sigma \tag{14}$$

holds. The sum is over all the pseudoconfigurations, which means that a σ can be the concatenation of any set of configurations, up to rotations within the symbols of the configurations. So (011), and (110), and (101) are all the same pseudoconfiguration. Also (001)(01) and (01)(001) are the same pseudoconfiguration, as they only differ by the order of their component configurations.

The proof of the relation in (14) follows from the basic properties of exponentials of Dirichlet generating functions, and here we follow a proof given by J. Lowenstein. We begin by separating the right and left hand sides of the relation (14), and set

$$r = \sum_{\sigma\in P} t_\sigma$$

and

$$l = \exp\left(\sum_{n\geq 1} \frac{Z_n}{n}\right) .$$

Now we would like to think of the functions r and l as being functions of all the possible prime pseudoconfigurations or their powers. This means that we will think of the configurations in l as pseudoconfigurations. If we substitute all pseudoconfigurations by zero, we will be left just the null configuration in the sum of r which contributes with 1, and e^0 for l, so $r(0) = l(0)$. We will now show that for any prime pseudoconfiguration p we have that

$$\frac{1}{r}\frac{\partial r}{\partial p} = \frac{1}{l}\frac{\partial l}{\partial p} \tag{15}$$

and hence $r = l$. The derivative of l is

$$\frac{\partial l}{\partial p} = l \sum_{n \geq 1} \frac{1}{n}\frac{\partial Z_n}{\partial p}\,.$$

Because l is formed of either prime pseudoconfigurations or their powers, the term p can only appear in Z_n in a term of the form ap^k/n. If the configuration is prime then its length is n, and it will appear in Z_n a total of n times, once for each site in the configuration; in this case $a = n$. If the configuration is not prime and its prime period is $|p|$, which is repeated k times, it will only appear $|p|$ times; in this case $a = |p|$. In both cases we have that $n = ak$. We then get

$$\frac{\partial l}{\partial p} = l \sum_{k \geq 1} \frac{1}{ak} akp^{k-1} = \frac{l}{1-p}\,. \tag{16}$$

For r we re-write it by factoring out the term p from the sum. Denote by r_p the function obtained by substituting r in p by zero. Then

$$r = r_p + pr_p + p^2 r_p + \cdots = \frac{r_p}{1-p}\,. \tag{17}$$

This allows us to compute the derivative as

$$\frac{\partial r}{\partial p} = \frac{r_p}{(1-p)^2} = \frac{r}{1-p} \tag{18}$$

where we used the identity in (17) in going to the last equality. Comparing (18) and (16) we have the equality in (15).