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Théories statistique et thermodynamique des nombres

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Exposé dédié à Pierre Cartier qui, par son exceptionnelle ouverture d'esprit, a encouragé nombre de physiciens.

Physicists must compute the eigenstates and the dynamics of complex quantum hamiltonian systems. They resort most of the time to approximations, it is therefore extremely useful to be able to check them on simple examples. We shall discuss a number of explicit number theoretical Hamiltonians that lead to statistical mechanical equilibrium partition functions, some of which have been extensively studied in the past.

The Gibbs trick that ensures the extensivity of the entropy of a perfect classical gas of indistinguishable particles can be studied on two analogous examples of additive number theory.

The high energy asymptotic behavior of the density of states is related to the Hagedorn temperature singularity, and this is realized in a number of multiplicative number theoretical models. A "thermodynamic limit" of continuous spectrum leads to a suggestive approximation for the grand-canonical partition function of the "logarithmic gas". Some thermodynamical properties can be studied analytically.

A precise analogy is proposed between the two-dimensional lattice gas' (Ising model with magnetic field) partition function and a generalized Riemann zeta function of two complex variables. The overcritical temperatures must be treated differently.

We shall conclude in emphasizing the role ghosts may play in the study of the Riemann hypothesis.

1. Additive number theory and a remark on the indistinguishability of particles

For a dictionary we refer the reader to our original papers [1], a general knowledge of statistical mechanics should suffice to read on. Let us consider the generating function for the number $p(n)$ of unordered partitions of the integer n into a sum of integers. It is a classical result that it can be written :

$$\Xi_1^0 = \sum_{n=0}^{\infty} p(n)q^n = \prod_{k=1}^{\infty}(1/(1-q^k)).$$

More generally one can distinguish the number of terms of the partition and compute a two-variables generating function for it :

$$\Xi_1 = \prod_{k=1}^{\infty}(1/(1 - fq^k)).$$

Ξ_1^0 converges for $Re\beta > 0$ where we have put $q = e^{-\beta}$. It has a natural boundary at $Re\beta = 0$. Hardy and Ramanujan have estimated the singularity when β tends to 0^+, using the modular invariance of the Dedekind η function they could deduce the precise asymptotic behavior of $p(n)$. Let us recall the elementary dominant terms :

$$Log\Xi_1^0 \sim \pi^2/(6\beta)$$

corresponding to

$$Logp(n) \sim \pi\sqrt{2n/3}.$$

Had we considered ordered partitions, the analysis would have simplified greatly. The generating function for one summand is :

$$Z_{1,ordered} = q/(1 - q)$$

the full generating function for ordered partitions of n into N summands follows :

$$\Xi_{1,ordered} = \sum_{N=0}^{\infty}(fq/(1 - q))^N = (1 - q)/(1 - q(f + 1))$$

it converges for $Re\beta > Log(1 + f)$.

Let us now follow Gibbs and treat all partitions as if they had only unequal summands. The Gibbs approximation to the unordered generating function is obtained by dividing by $N!$ the term of order f^N of the ordered generating function. We obtain :

$$Log\Xi_1^G = fq/(1 - q)$$

so for $f = 1$ we find the correct location of the singularity at $q = 1$ but the wrong coefficient : 1 instead of $\pi^2/6$.

*Let us remain in the realm of additive number theory and consider now sums of squares. Again the simplest case is that of ordered partitions (with sign!). If we do keep track of the number of terms we find for one summand :

$$Z_{2,ordered} = \theta(\beta) = 1 + 2\sum_{n=1}^{\infty} q^{n^2},$$

or in Jacobi's notation

$$Z_{2,ordered} = \theta_3(z = 0; q).$$

Where θ_3 is given by the following series and product :

$$\theta_3 = 1 + 2\sum q^{n^2} cos2nz = \prod_{n=1}^{\infty}(1 - q^{2n})(1 + 2q^{2n-1}cos2z + q^{4n-2})$$

It follows that the full generating function for the number of ordered partitions into a sum of squares is :

$$\Xi_{2,ordered} = 1/(1 - fZ_{2,ordered}).$$

We may recall that if we define $t = \beta/\pi$, θ_3 is solution of the heat equation

$$\partial_t\theta_3 = \pi/4\ \partial^2\theta_3/\partial z^2$$

with period π in the variable z and $t = 0$ initial condition :

$$\theta_3(t = 0) = \pi\delta(z).$$

So for vanishing β, $Z_{2,ordered} \sim \sqrt{\pi/\beta}$; let us apply Gibbs' trick again to find a lower bound for the generating function of the number of unordered partitions.

$$Log\Xi_2^G = f\theta(\beta).$$

This suggests following [2] that the number $p_2(n)$ of unordered partitions into sums of squares behaves asymptotically as $e^{An^{1/3}}$, we must just extremize the term of the series expansion of Ξ and fit the exponential behavior of $p_2(n)$ so as to match that of the partition function. As a matter of fact E. Wright [3] has proved the asymptotic formula :

$$Logp_2(n) \sim 3[\Gamma(3/2)\zeta(3/2)/2]^{2/3}n^{1/3}.$$

Once more Gibbs' trick provides us with the right qualitative behavior at high temperature (β is the inverse temperature for physicists).

It might be useful at this stage to recall [1] that the number of terms in a partition can be viewed as a number N of (quasi-)particles and that the Ξ generating functions are traces of $e^{-\beta(H-\mu N)}$. H is a free hamiltonian : a sum of harmonic oscillators of energies the allowed summands and $f = e^{\beta\mu}$ is the "fugacity". In other words the Ξ's are the equilibrium grand canonical partition functions.

*In the rest of this paper we shall mostly consider multiplicative number theory. The bridge between the additive and multiplicative worlds is the Euler Gamma function. It was natural to consider the power series $P(q) = \sum a_n q^n$ in the additive case, it is equally natural to consider the Dirichlet series $D(s) = \sum a_n/n^s$ in the multiplicative case. The product $\Gamma(s)D(s)$ is a Mellin transform of P, it is equal to : $\int_0^\infty d\beta\beta^{s-1}P(e^{-\beta})$. This Mellin transform is a bisided Laplace transform exchanging s and the logarithm of β. We must warn the reader that s will be also interpreted as the inverse of a temperature i.e. another β below.

Two examples are noteworthy : the case of the Riemann zeta function ($a_n = 1$) and more generally the case of Hecke modular eigenforms whose Mellin transforms are multiplicative Dirichlet series that obey a functional equation and admit a peculiar Euler product decomposition. Explicitly

$$\xi(s) = \zeta_R(s)\pi^{-s/2}\Gamma(s/2) = 1/2\int_O^\infty dtt^{s/2-1}(\theta(t)-1)$$

is symmetric with respect to $s = 1/2$ thanks to the modular covariance of θ.

If we were to apply the same transformation to the function θ_3 of two variables we would have to consider the more complicated transformation rules under the modular group, for example

$$\theta_3(z/it, 1/t) = \sqrt{t}e^{z^2/\pi t}\theta_3(z,t)$$

which mixes t and z variables. And the naive Mellin transform loses its appeal as one may have guessed from the form of the heat equation that is not adapted to it either.

2. Singularities of Laplace/Dirichlet transforms and Hagedorn catastrophes

Let us now concentrate on some multiplicative models. The additive theory occured in physics whenever the energy spectra where the integers (in string theory for example) or squares as in free motion in a box. Energy is usually additive in first approximation and to accomodate multiplicative number theory one must assume that the spectrum is logarithmic. At present this is an assumption but nobody can prevent us from studying the statistical mechanical properties of such a system and its thermodynamics. We shall in fact bring a large chunk of theoretical physics technology to bear on important mathematical problems and conversely one hopes to learn from a century of analytical number theory to understand better several issues of modern physics like the quark-gluon plasma transition and the Hagedorn critical temperature.

Instead of partitioning integers into sums of "things" let us now factorize them into primes, or into integers, or into generalized (Beurling) primes. Again the object to be computed is a generating function for these numbers of factorizations, and as we mentioned above the natural thing to construct is a Dirichlet series. Let us first consider ordered factorizations into primes. If there is only one factor we find :

$$Z_P(s) = 1 + \sum p^{-s}$$

where the sum is over primes. It follows that the full (grand-canonical) partition function for any number of prime factors is

$$\Xi_{P,ordered}(s, f) = 1/(1 - f(Z_P - 1)).$$

A Gibbs approximation to the unordered prime factorization is

$$\Xi_P^G = e^{f(Z_P - 1)}.$$

The exact analog of Ξ_P in the unordered case is nothing but the Riemann zeta function $\zeta_R(s)$ for $f = 1$ and its 2-variables generalization proposed in [1] in the general case :

$$\Xi_{P,unordered} = \Xi_R = \sum n^{-s} f^{\Omega(n)}$$

where the sum is over integers and $\Omega(n)$ is the total number of prime factors (with multiplicity) in the factorization of n.

Finally the number of ordered factorizations into integers and its Gibbs approximation are obvious whereas the unordered case is more interesting :

$$\Xi_{Log} = \sum_{k,n} f^k F(n,k) n^{-s} = \prod 1/(1 - f n^{-s}).$$

$F(n,k)$ is the number of factorizations of n into k integer factors. The suffix Log stands for logarithmic gas, see [4].

Beurling considered an arbitrary increasing sequence of positive numbers as generalized primes. He then took their products and studied the relative densities of these two sets of real numbers in the spirit of the prime number theorem which estimates the density of ordinary primes. If we take primes $p'_n = p_n e^{-\mu}$ ζ_R becomes Ξ_R ; if we take $p_n = n$ it becomes $\Xi_{Log}(f = 1)$.

*The theory of Dirichlet series differs from that of power series in the possibility for the line of convergence not to contain any singular point, in fact the rightmost singularity can be a finite distance away from it. However in the case of positive coefficients this line does contain a singularity on the real axis. We may interpret $D(s) = \sum a_n / n^s$ as the Laplace transform of a density of states $\rho(E) = \sum a_n \delta(E - Log n)$.

In the case of power series one has Abel's theorem and one can deduce from the convergence on the boundary convergence in some neighborhoods. The converse requires a so-called tauberian condition. When a Dirichlet series diverges on the real axis at the convergence abscissa, the nature of the divergence of the series at $s = 0$ determines the s-behavior as one comes down to the convergence abscissa. In other words the behavior of the integrated density of states $N(E) = \sum_{Log n \leq E} a_n$ at infinity determines the rightmost singularity in s ($s = \beta = 1/T$ in standard physics conventions). Again the converse requires an additional assumption like regularity on the rest of the axis of convergence (Ikehara see [5]); note that typically the abscissa of convergence will be strictly positive (1 in the case of the zeta function) and we are not exactly in the framework of Abel's theorem.

We refer to [6] for more analogs of the theorems of Abel and Tauber in the theory of Dirichlet series. We shall indeed be interested in the integrated density of states $N(E) = \sum_{Log n \leq E} a_n$, its derivative is the density of states. With a mild additional assumption (Hardy, Littlewood and Karamata) one can show that the divergence $D(s) \sim (s-1)^r$ at the abscissa of convergence (1 for definiteness) implies the asymptotic behavior

$$\int^E \rho(E')e^{-E'}dE' \sim E^r/r!$$

at infinity. Let us note that a lot of work went into estimating the error in these estimates (actually this does not permit the evaluation of $\rho(E)$ itself) and that in the case of non necessarily positive real $a'_n s$ the absence of singularity on the real axis at the abscissa of convergence implies a lower bound on the oscillations of $N(E)$ which takes both signs [6].

*The case $r = 1$ is well known in physics in situations where the full spectrum is exponentially dense at infinity. It was studied in detail by Hagedorn and is thought to occur in the spectrum of hadronic resonances for example. In this situation the microcanonical Gibbs state cannot correspond to a canonical temperature higher than a critical value β_H defined by

$$\rho(E) \sim e^{\beta_H E}$$

at infinity. β_H was taken to be one above, so its inverse the "Hagedorn temperature" is also equal to one there.

All of the above multiplicative models do exhibit this type of singularity or simple generalizations thereof. The Riemann zeta function's pole at $s = 1$ is known to be exactly that. Let us now consider the Dirichlet series Z_P, it diverges logarithmically at $s = 1$, this is the singularity of $Log\zeta_R$ as one may check from the Euler product formula and an expansion of the logarithm. This corresponds to the integrated density of states

$$N_P(E) = \pi(e^E) \sim e^E/E$$

according to the prime number theorem for the number of primes less than e^E. There are fewer primes than integers, but if one counts factorizations of integers into integers one finds an exponential divergence at $s = 1$! Let us expand $Log\Xi_{Log}$ at $f = 1$ and near $s = 1$. Its singularity is the same as that of ζ_R. Alternatively we can recover this singularity from the Gibbs' trick

$$Log\Xi^G_{Log}(f=1) = \zeta_R - 1 \sim 1/(s-1).$$

*We shall now replace the discrete sum by an integral to estimate Ξ_{Log} at large temperatures, the idea is to consider that near the Hagedorn temperature the partition function is dominated by large energies which are practically continuous. Let us introduce a parameter v and replace the energies $Logn$ of the oscillators by $Log(1+(n-1)/v)$. The model has $v=1$, but we shall develop the partition function in $1/v$. The spectrum is discrete for the finite volume situation, but we shall let v tend to infinity in such a way that the spectrum becomes continuous. Indeed the spacing becomes

$$Log(1+(n+1)/v) - Log(1+n/v) = Log(1+1/(v+n)) \sim 1/(v+n)$$

and tends to zero when v or n is large; we may remark that this approximation is slightly better than a naive thermodynamic type limit where one would have kept only the lowest order terms in v. Hence the density of oscillator levels reads :

$$\rho^{osc}_{L,v}(E) \sim ve^{E}.$$

If we take v large, the system becomes extensive and we can think of v as a volume. We then find for the pressure P :

$$P \sim (1/vs) Log\Xi^{v}_{Log}(s,f)$$

where the subscript v stands for the replacement of the true energy levels by their interpolating form in the grand canonical partition function. In the large volume limit :

$$Log\Xi^{v}_{Log} = -\int_0^\infty dE\rho^{osc}_{L,v}(E) Log(1-fe^{-sE})$$

and it follows after integrating by parts and transforming the boundary term that

$$P = fT\int_0^\infty dE'(e^{-rE'} - e^{-E'})/(1-fe^{-E'})$$

for $\sigma = Re(s) > 1$ and $|f| < 1$ and after changing variables $E' = sE$, $T = 1/s$ and $r = (s-1)/s = 1-T$. P becomes a Laplace transform to be found p. 145 in [7]. We deduce :

$$P = fT\{1/(1-T)F_G(1, 1-T; 2-T; f) - (idem T = 0)\}$$

where the Gauss hypergeometric series F_G is doubly degenerate and is a special case of the incomplete Beta function. We have obtained the equation of state in the thermodynamic limit of the Log gas.

F_G has a logarithmic singularity at $f = 1$. One can show that this logarithm is cancelled in P by the $T = 0$ term. On the other hand let us now investigate the blow up at $T = 1$. We expect it to be more serious than for the Riemann gas. In fact we find a pole $1/(1-T)$ again but in the pressure instead of in the partition function. It can be extracted from the series expansion

$$F_G = \sum_{n=0}^{\infty} f^n(1-T)/(1-T+n)$$

its residue is f which corresponds to $\Xi_1 \sim e^{f/(1-T)}$ near $T = 1$. For $f \sim 1$ we find

$$P/T \sim 1/(1-T) + Log(1-f) + \sum_{n=1}^{\infty} f^n/(1-T+n)$$

hence

$$P/T \sim 1/(1-T) - (1-T)\sum 1/(n^2 + n(1-T)).$$

This is precisely the singularity obtained by the other methods.

We can finally study the thermodynamics of this approximate Log gas. Some of the computations can be carried out analytically thanks to our [8,9] deep knowledge of the hypergeometric functions. Firstly one can compute the density of particles as a function of temperature and fugacity. This can be greatly simplified by using three facts : the fact that the derivative of the pressure with respect to the fugacity is again a combination of hypergeometric series, the Gauss contiguous relations and the degeneracy conditions. One can express the density in terms of the pressure itself.

$$P = T^2 \sum_{n=1}^{\infty} f^n/n(n-T)$$

and assuming the Legendre transforms are regular one has :

$$V/N = \partial\mu/\partial P \mid_T$$

so one finds

$$N/V(f,T) = P(f,T) - TLog(1-f).$$

One finds for example that the fugacity tends to one only for infinite density ! Then one may check the validity of one thermodynamic inequality ensuring stability of the system

$$\partial(N/V)/\partial P \mid_T > 0.$$

But the explicit computation of the entropy and of the specific heat is more subtle.

3. 2-variables generalized Riemann zeta function and Lee-Yang theorem

Let us now return to the study of the function $\Xi_R(f,s)$ and take stock of the features seen so far. $\Xi_R(1,1/T)$ has a symmetry with respect to the inversion $T'-1 = 1/(\overline{T-1})$ up to a factor (ξ is truly symmetric). The Riemann hypothesis states that all the zeros of ξ lie on the invariant circle of the complex T plane. It is natural to recall that the 2-dimensional square Ising model has a Kramers-Wannier "duality" symmetry of the same type for the following transformation of the product of the coupling constant of nearest neighbours by the temperature

$$sinh 2K/T = 1/sinh 2K'/T'.$$

Furthermore Fisher [10] has shown that the zeroes of the corresponding canonical partition function all lie on the invariant set $\mid sinh 2K/T \mid = 1$. One even knows [11] that this duality can be proved using a Poisson summation formula as in the case of the functional equation above. In fact this result of Fisher presents some analogy with the Lee-Yang theorem [12].

The Lee-Yang theorem is of a much wider applicability and states that for "ferromagnetic interactions" (and positive temperature) the Ising model partition function in the presence of a magnetic field can only vanish if the latter is pure imaginary. The magnetic field is the analog of our chemical potential μ. Let us see whether the analog statement is true for the Riemann gas. In other words is it true that Ξ_R vanishes only for

$\mid f \mid = 1$? Upon my request G. Tenenbaum produced a beautiful formula inspired by the works of [13] :

$$\Xi_R = \prod_{n=1}^{\infty} \zeta_R(ns)^{P_n(f)}$$

where the polynomials P_n are defined by the Moebius relations :

$$f^m = \sum_{n|m} nP_n.$$

One finds the well known singularity exponent at $s = 1$

$$P_1 = f$$

and

$$2P_2 = f^2 - f$$

$$3P_3 = f^3 - f$$

$$4P_4 = f^4 - f^2$$

$$5P_5 = f^5 - f$$

$$6P_6 = f^6 - f^3 - f^2 + f$$

and so on. We refer to [14] for a detailed analysis. But the danger for real (positive) temperature comes from the poles at $s = 1/n$ if $ReP_n < 0$. It must be emphasized that we are above the Hagedorn temperature there. We find that for small f all inverse squarefree numbers are zeroes of order f of Ξ_R (as a function of s) if they have an odd number of factors. This suffices to ruin the analogy.

In the case of the logarithmic gas the pressure reads :

$$P/T^2 = \sum_{n=1}^{\infty} f^n/n(n-T)$$

defined for complex f in the unit disc but real T comprised between 0 and 1. A zero of the partition function would correspond to a singularity of the pressure so we must study the analytic continuation in the temperature. Again the integer temperatures will be singularities.

4. Prospects

We would like to conclude by elaborating on the connection between the zeroes of generating ("partition") functions and the asymptotic behavior of the density of states. In fact the general connection is between the singularities and the integrated density of states as we have seen in section 2. Yet in a multiplicative setting one can take the inverse of a partition function and exchange the role of the poles and zeroes while having related densities of states. In [1] we have realized that the Riemann hypothesis can be rephrased by saying that the critical temperature of fermionic (or bosonic) ghost oscillators (i.e. with fugacity -1) is equal to 2. In the fermionic case it is the statement that $1/\zeta_R$ should have abscissa of convergence 1/2 and not 1. There are sophisticated zero-free regions of ζ_R but it is not known whether the abscissa of convergence of its inverse is strictly less than 1 or not. The introduction of ghosts is exceptional in physics but one may try to find a symmetry that would explain the cancellations required for the Riemann hypothesis to be true.

Another path to be explored is motivated by the occurrence of the hypergeometric function in the thermodynamic limit of the logarithmic gas. The Riemann zeta function does not obey any known differential equation of finite order, how about its 2-variable generalization Ξ_R?

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