Frustrated Spin Models and the q-Calculus

Andrea CAPPELLI and Filippo COLOMO

Abstract: We present the solution of the (gauged) frustrated Spherical Model, which is obtained by using q-polynomials. This is a first step towards the solution of the physically relevant frustrated XY model, a deterministic model which may behave as a spin glass. An analogy with the Matrix Models is also discussed, which suggests a physical picture for metastability in the frustrated models.

1. INTRODUCTION

In two recent papers [1], Parisi *et al.* have introduced and analysed the Spherical and XY Spin Models with frustration, but in the absence of quenched disorder. Their aim was to test the conjecture that the frustrated deterministic systems at low temperature behave as some suitably chosen spin-glass models with quenched disorder. They considered the frustrated models in the limit of large dimensionality D of the lattice, where the saddle-point approximation becomes exact.

The models are described by the Hamiltonian

$$H_0 = -\frac{1}{\sqrt{2D}} \sum_{\langle jk \rangle} \phi_j^\dagger U_{jk} \phi_k \ + \ \text{h.c.} \ . \tag{1}$$

The complex field $\phi_j \in \mathbf{C}$ is defined on the sites (labelled by j) of a D-dimensional hyper-cubic lattice, and there are nearest-neighbour interactions U_{ij}. Two different models can be obtained by constraining the field as follows:

$$\beta H_S = \beta H_0 + \mu \left(\sum_{j=1}^{N} |\phi_j|^2 - N \right) \ , \qquad \beta H_{XY} = \beta H_0 + \sum_{j=1}^{N} \mu_j \left(|\phi_j|^2 - 1 \right) \ , \tag{2}$$

where N is the number of sites of the lattice. The couplings U_{jk} are complex numbers of modulus one and satisfy the relation $U_{jk} = U_{kj}^*$; they are the link variables of a background Abelian lattice gauge field, which produces a static magnetic field. This is chosen in such a way as to give the same magnetic flux $\pm B$ for any plaquette of the lattice (the product of the four U's around the plaquette is $e^{\pm iB}$). Therefore, the magnetic field should have the same projection on all the axes of the lattice, modulo the sign: these signs are chosen randomly (this is the unique source of randomness in these models). Of course, setting $B = 0$ we recover the usual ferromagnetic models while setting $B = \pi$ we obtain the corresponding fully frustrated cases.

The main difficulty in studying these models consists in finding the spectrum of the lattice Laplacian in the presence of the magnetic field, which is defined as:

$$(\Delta f)_j = \sum_{k=1}^{2D} U_{jk} \ f_k \ . \tag{3}$$

However, there are simplifications due to the large D limit. The authors of Ref. [1] have approached the problem via the high-temperature expansion of the free energy. This is given by a sum over all closed loops with the weight given by the associated Wilson loop $W(\mathcal{C})$ made by the U_{ij}:

$$\beta F \equiv \sum_{k=0}^{\infty} \frac{\beta^{2k}}{2k} \ \text{Tr}[\Delta^{2k}] \ = \sum_{n=0, \ \text{even}}^{\infty} \ \frac{1}{n} \left(\frac{\beta}{\sqrt{2D}} \right)^n \ \mathcal{N}(n) \ \langle W(\mathcal{C}) \rangle_n \ . \tag{4}$$

These authors showed that the k^{th} term in this expansion is a polynomial in the variable $q = \cos B$, due to the average over all orientations of the magnetic field. Moreover, they found a recursion relation for the coefficients of this polynomial — a sort of Wick theorem — which can be nicely expressed by using the algebra of the q-oscillators $a_q, a_q^\dagger$:

$$a_q a_q^\dagger - q a_q^\dagger a_q = 1 \ . \tag{5}$$

These operators [2] act on the Hilbert space spanned by the vectors: $|m\rangle$, $m = 0,\ 1,\ ...,$ as follows,

$$a_q^\dagger|m\rangle = \sqrt{[m+1]_q}\ |m+1\rangle, \qquad a_q|m\rangle = \sqrt{[m]_q}\ |m-1\rangle, \qquad a_q|0\rangle = 0, \qquad [m]_q = \frac{1-q^m}{1-q} \ . \tag{6}$$

Using the recursion relation, the weighted multiplicities of the diagrams of eq. (4) were neatly written as an expectation value over the ground state of the q-oscillator [1]:

$$\mathrm{Tr}[\Delta^{2k}] \ = \ \langle 0|(a_q^\dagger + a_q)^{2k}|0\rangle \ . \tag{7}$$

2. SPECTRUM OF THE LAPLACIAN

In our work [2] we made expression (7) more explicit by considering the coordinate representation for the q-oscillator. This is defined by $x_q|x\rangle = x|x\rangle$, where $x_q \equiv a_q^\dagger + a_q$, and is realized by the so-called continuous q-Hermite polynomials $H_n(x) = \langle x|n\rangle\ \mathcal{C}_n$, with the normalization constant $\mathcal{C}_n$ fixed by $H_0(x) = 1$ [2]. A convenient parametrisation is found to be $x = (2/\sqrt{1-q})\cos\theta$, with $\theta \in [0,\pi]$. The most important property for us is the orthogonalizing measure $\nu_q(x)$:

$$\int_{-2/\sqrt{1-q}}^{2/\sqrt{1-q}} \nu_q(x)\ dx\ H_n(x)\ H_m(x) \ = \ \delta_{n,m}\ [n]_q! \ , \tag{8}$$

$$\nu_q(x) \ = \ \frac{\sqrt{1-q}}{2\pi}\ q^{-1/8}\ \Theta_1\left(\frac{\theta}{\pi}, q\right) \ = \ \frac{\sqrt{1-q}}{\pi} \sum_{n=0}^{\infty} (-1)^n q^{n(n+1)/2}\ \sin[(2n+1)\theta] \ , \tag{9}$$

where $\Theta_1(z,q)$ is the first Jacobi theta function. Using these results, and (7), we can compute the trace of any function of the frustrated Laplacian:

$$\mathrm{Tr}\ \left[f\left(\Delta\right)\right] \equiv \langle 0|f(x_q)|0\rangle = \int\ dx\ \nu_q(x)\ f(x) \ . \tag{10}$$

Therefore, the Laplacian is diagonal in the coordinate representation of the q-oscillators: it has a continuous spectrum over the interval $[-2/\sqrt{1-q},\ 2/\sqrt{1-q}]$, with eigenvalue density given by ν_q in eq. (9).

In order to compute the free energy, it is convenient to introduce the resolvent $R(z)$ of the Laplace operator and obtain its explicit expression:

$$R(z) \equiv \mathrm{Tr}\left[\frac{1}{1-z\ \Delta}\right] = \int_{-2/\sqrt{1-q}}^{2/\sqrt{1-q}} dx\ \frac{\nu_q(x)}{1-z\ x} = \frac{\sqrt{1-q}}{z} \sum_{n=0}^{\infty} (-1)^n\ q^{n(n+1)/2} \left[K\left(\frac{2z}{\sqrt{1-q}}\right)\right]^{2n+1} , \tag{11}$$

where we introduced

$$K(\alpha) = \frac{1-\sqrt{1-\alpha^2}}{\alpha} \ . \tag{12}$$

The resolvent is originally well-defined for real z in the interval $|z| < z_c = (\sqrt{1-q})/2$ and is then analytically extended to the whole complex plane of z. Its singularities are completely determined by those of the simpler function $K(2z/\sqrt{1-q})$. Actually, the series is very well convergent for $|q|<1$ as any Jacobi theta function. Moreover, for $|q| = 1$, it is a geometric series, which still converges because $|K| < 1$ for $|z| < z_c$.

The high-temperature expansion of the internal energy of the Spherical Model can be obtained by expanding $R(\beta)$ in series; we verified that this expansion indeed matches the numerical results of Ref. [1].

3. SOLUTION OF THE SPHERICAL MODEL

Our approach essentially follows the original Berlin-Kac solution of the ferromagnetic model in $D = 1,2,3$: the mechanism of the phase transition is the same, only the form of the Laplacian is different [2]. The partition function is

$$Z_S = \int_{\mu_0 - i\infty}^{\mu_0+i\infty} d\mu \int \mathcal{D}\phi \; e^{\beta \sum \; \phi^\dagger \Delta \phi - \mu\left(\sum |\phi|^2 - N\right)} = \int_{\mu_0 - i\infty}^{\mu_0+i\infty} d\mu \;\; e^{-\mathrm{Tr}[\ln(\mu - \beta\Delta)] + \mu N} . \tag{13}$$

The integration path over μ is along a straight line which runs in the complex plane parallel to the imaginary axis; a positive real part should be added in order to make the integration over ϕ convergent. In the thermodynamic (large N) limit, we can apply the saddle point method to evaluate the integral over μ. The saddle point equation, which must be solved for real, positive values of μ, is:

$$\mathrm{Tr}\left[\frac{1}{\mu - \beta\Delta}\right] = 1 \qquad \longrightarrow \qquad \beta = zR(z) \; , \qquad z \equiv \frac{\beta}{\mu} \; . \tag{14}$$

In the case of $q = 0$, this equation can be easily solved:

$$\frac{1}{2z^2}(1 - \sqrt{1 - 4z^2}) = \frac{\beta}{z} \qquad \longrightarrow \qquad z(\beta) = \frac{\beta}{1 + \beta^2} \; , \tag{15}$$

which corresponds to $\mu = 1 + \beta^2$. This solution is valid for $z < z_c = 1/2$, namely it describes the high-temperature phase $\beta < \beta_c = 1$. Indeed, let us follow the saddle point in the z plane, starting from $\beta = 0$, where $z = 0$ too. Upon increasing β, z moves toward the critical value $z_c = 1/2$; for $\beta > 1$, z cannot increase anymore because it finds the square-root branch cut of $\mathrm{Tr}[\log(1 - z\Delta)]$, and therefore "it sticks to the singularity". Hence, for $\beta > 1$, the saddle point equation has no longer an acceptable solution; nevertheless, the leading contribution to the μ integral in (13) still comes from the neighbourhood of $z = 1/2$. Therefore, the low-temperature solution is $z(\beta) = 1/2$ independent of β, *i.e.* $\mu = 2\beta$. It turns out that the internal energy can be written in both phases as:

$$U(\beta) = (\partial_\beta + (\partial_\beta \mu)\partial_\mu)(\beta F) = \frac{1}{\beta} - \frac{1}{z(\beta)} \; . \tag{16}$$

More explicitly,

$$U(T) = \begin{cases} -\frac{1}{T} & T > 1 \\ T - 2 & T < 1 \end{cases} \qquad (q = 0) \; . \tag{17}$$

The internal energy is therefore continuous at the transition, and the specific heat presents a discontinuity in its first derivative (it is discontinuous for $q \neq 0$). These results are qualitatively very similar to those of the Berlin-Kac ferromagnetic model.

The solution for any $-1 < q < 1$ is a straightforward generalization of the $q = 0$ case. The discussion of the saddle-point equation (14) is analogous, because the singularities of $R(z)$ are still given by a square-root branch cut. The expression for $z(\beta)$ cannot be given in closed form as in (15); nevertheless, one can use z as a parameter for both $U(\beta)$ and $\beta = \beta(z)$, according to (14) and (16). In the high-temperature phase z grows form zero to the critical point $z_c = (\sqrt{1-q})/2$, where it sticks for $\beta > \beta_c$. A plot of the internal energy is shown in Fig.1.

In conclusion, the qualitative behaviour of the (infinite-dimensional) frustrated Spherical Model in the low-temperature phase is rather smooth and standard. The dynamics of the model is too simple to develop the potential features of: (i) glassy behaviour (many ground states), which is found in the corresponding systems with quenched disorder [1]; (ii) commensurability in the spectrum for $B = 2\pi r/s$ (r, s integers), which was observed in the $D = 2$ hopping model in a magnetic field [2].

A glassy behaviour is expected in the frustrated XY Model (2) [1]. Unfortunately, we have not been able so far to solve it by the same techniques: the saddle point condition for the *local* Lagrange multiplier μ_i in (2) is now a functional equation.

4. ANALOGY WITH THE MATRIX MODELS

The previous solution of the frustrated Spherical Model is very reminiscent of the large N solution of the Hermitean Random Matrix Model [2]. This analogy can be useful to import some technical tools as well as to gain a physical intuition for the less understood frustrated models. The Matrix Model is characterized by the $(N \times N)$ matrix variable $M = M^\dagger$ and by the Hamiltonian $\beta H = \mathrm{Tr}V(M) =$

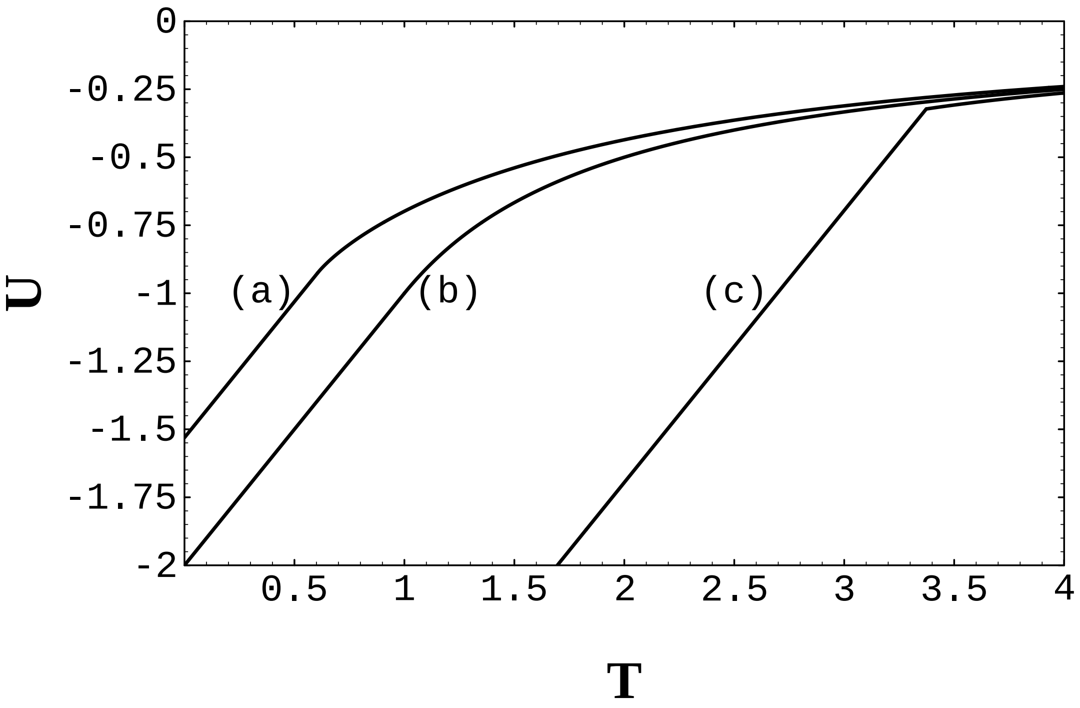

Figure 1: Internal energy of the Spherical Model versus temperature for the three values: (a) $q = -0.707$; (b) $q = 0$; (c) $q = 0.707$.

$\mathrm{Tr}\,(M^2/2 + \cdots)$. After diagonalization of the matrix, one is left with the partition function over the eigenvalues λ_i, $i = 1, \ldots, N$:

$$Z_M = \int \prod_{i=1}^{N} d\lambda_i \ \mathrm{e}^{-\sum_i V(\lambda_i)} \ \prod_{i<j} (\lambda_i - \lambda_j)^2 \ . \tag{18}$$

This can be thought of as being the statistical mechanics of N charges with coordinates λ_i in one dimension, which repel each other logarithmically and are kept together by the external potential $V(\lambda)$. In the large N limit, the partition sum is dominated by the contribution of the saddle point, which corresponds to the equilibrium configuration of the charges, neglecting fluctuations. The rescaled charge density becomes a continuous function $\nu(\lambda)$ which satisfies the equation:

$$\frac{1}{2}\ V'(\lambda) = P \int_{-a}^{a} dx\ \frac{\nu(x)}{\lambda - x}\ , \qquad \lambda \in (-a, a)\ , \qquad \int_{-a}^{a} dx\ \nu(x) = 1\ , \tag{19}$$

where P stands for the principal value of the integral. Here, $\nu(\lambda)$ is the unknown and $V(\lambda)$ is given. The solution of this integral equation is rather well known [2]: one introduces the function

$$F(\lambda) = \int_{-a}^{a}\ dx\ \frac{\nu(x)}{\lambda - x}\ , \tag{20}$$

which is analytic outside the segment of the real axis $(-a, a)$ corresponding to the spectrum. For λ inside the spectrum, we have

$$\mathrm{Re}\ F(\lambda) = \frac{1}{2} V'(\lambda)\ , \qquad \mathrm{Im}\ F(\lambda) = -\pi \nu(\lambda)\ , \qquad \lambda \in (-a, a)\ . \tag{21}$$

The function $F(\lambda)$ can be found by analyticity arguments and determines the density $\nu(\lambda)$.

Our main observation is that this saddle point equation is similar to those encountered in the Spherical model. More precisely, we can identify $F(\lambda)$ in (20) with the resolvent (11): $F(\lambda) = zR(z)$, $z = 1/\lambda$. Therefore we can define the Matrix Model corresponding to the frustrated Spherical Model, as the one which possesses the same eigenvalue density $\nu_q(\lambda)$ in (9), in the large N limit. By using eqs.(20) and (21), we can determine its potential by the following expression:

$$V'(\lambda) = 2\mathrm{Re}\ F(\lambda) = 2\sqrt{1-q}\ \sum_{n=0}^{\infty} (-1)^n q^{n(n+1)/2} \cosh\left[(2n+1)\chi\right]\ ; \tag{22}$$

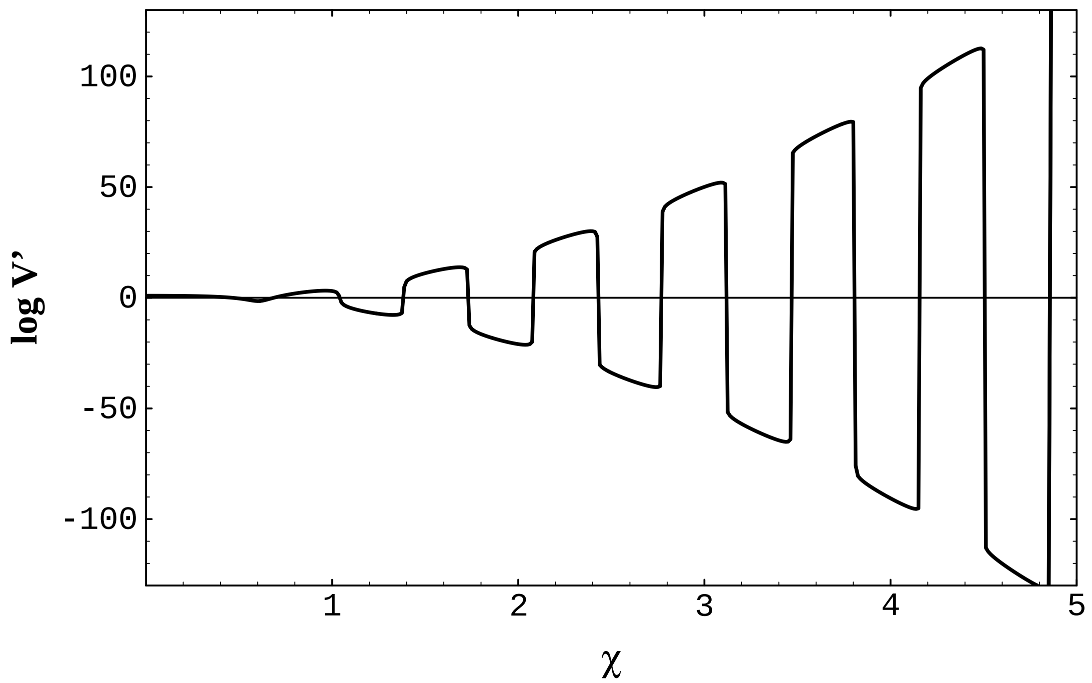

Figure 2: The first derivative of the Matrix Model potential in eq. (23) as a function of χ, for $q = -0.707$.

here, we introduced the convenient parametrisation $\lambda = (2/\sqrt{1-q})\cosh\chi$ for λ outside the cut $(-2/\sqrt{1-q}, 2/\sqrt{1-q})$ (see Fig.2). The Gaussian Matrix Model with $V(\lambda) = \lambda^2/2$ indeed corresponds to the $q = 0$ frustrated model [1].

The Spherical Model in the high-temperature phase and the Matrix Model in the large N limit have corresponding saddle point equations but rather different free energies, so they are not quite the same physical problem. Nevertheless, it is interesting to discuss the properties of this Matrix Model, whose potential $V(\lambda)$ has a peculiar widely oscillating behaviour at infinity. This potential satisfies a difference equation for translations by q (typical of q-polynomials), which can be called *q-periodicity* [2]. Such approximate periodicity implies the presence of metastable states in the Matrix Model. Actually, for large N the charge density forms an equilibrium configuration determined by the minimum of $V(\lambda)$ at the origin, and the tunnelling of charges to lower nearby minima is suppressed; thus the q-periodicity of the potential is not felt. Beyond this approximation, tunnelling switches on and the states in the spectrum can become metastable. This may lead to a complex pattern of metastability, which is a characteristic of the glass phase. This behaviour is not found in the Spherical Model, owing to its simplified dynamics involving the single variable μ. On the other hand, it may show up in the low-temperature phase of the frustrated XY model.

In conclusion, we believe that study of the frustrated deterministic spin models, like the XY Model, can shed new light on the glassy phenomena. Moreover, the techniques of q-calculus and Matrix Models seem to be ready for tackling these problems.

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