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ADDENDUM

Phase transition in a nematic n -vector model: the large- n limit

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Abstract. The free energy of the RP^{n-1} model is rigorously computed in the $n = \infty$ limit. The system shows a first-order transition with latent heat, in two and three dimensions. The first correction in $1/n$ is also computed. Comparison of the results with numerical ones shows that whereas in three dimensions the large- n limit correctly reproduces the behaviour of the system for $n \geq 3$, it does not in two dimensions for some observables.

1. Introduction

Recently we have solved the RP^{n-1} model in the $n = \infty$ limit [1]. We found a first-order transition with latent heat in two and three dimensions. The result has been rederived by a different technique in [2]. The surprising nature of the results in two dimensions prompted us to see if it was an artifact of the $n = \infty$ limit, and if indeed such a phase transition would be present for finite but large n . The results of a numerical study were puzzling [3]. Whereas the value of the critical temperature was correctly reproduced, the detailed nature of the transition was not. By contrast, in three dimensions a genuine first-order transition occurred which can be reasonably described by the $n = \infty$ limit for any $n \geq 3$ [1].

These findings motivated us to rederive our previous results in a more rigorous way. By this we mean that we wanted to prove that under some conditions the $n = \infty$ and the thermodynamic limit can be exchanged. This is what we have succeeded in doing for the free energy. This result explains why the critical temperature is correctly reproduced in the $n = \infty$ limit, but leaves open the possibility that the nature of the singularity at T_c is not. This is what is happening in two dimensions but not in three dimensions. In order to detect some instability of the result, induced by the first correction in $1/n$, we have computed it for the free energy. No apparent instability was found in two dimensions. We think that these results show the subtlety and the importance of the question of the permutability of the $n = \infty$ and the thermodynamic limit.

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2. Bounds for the free energy and the limit $n = \infty$

Here we want to derive useful upper and lower bounds on the free energy of the model. They will be given in terms of the free energy of the Heisenberg model and appear useful for computing the free energy when the number of components n tends to infinity.

The volume will be taken to be a cube of size L and we will use periodic boundary conditions. First of all we express the partition function in terms of the partition function of an annealed Heisenberg model by means of the identity

$$Q = \left(\frac{n}{8\pi\beta}\right)^{dN/2} \int_{-\infty}^{+\infty} \prod_{\mu x} d\Lambda_{\mu}(x) \exp\left[-\frac{n}{4\beta} \sum_{\mu x} \Lambda_{\mu}^2(x)\right] Z(\{n\Lambda_{\mu}(x)\}) \tag{2.1}$$

where $Z(\{n\Lambda_{\mu}(x)\})$ is the partition function of a Heisenberg model, with inhomogeneous coupling constants $\Lambda_{\mu}(x)$

$$Z(\{\Lambda_{\mu}(x)\}) = \int dv(\sigma) \exp\left[\sum_{\mu x} \Lambda_{\mu}(x)(\sigma(x), \sigma(x + \mu))\right]. \tag{2.2}$$

The upper bound we are looking for will be given, essentially, by the maximum of the integrand in (2.1) which, as we will see, is reached when all the coupling $\Lambda_{\mu}(x)$ are the same.

We will prove that

$$\ln Z(\{\Lambda_{\mu}(x)\}) \leq \frac{1}{Nd} \sum_{\mu x} \ln Z(\Lambda_{\mu}(x)) \tag{2.3}$$

where $Z(\Lambda)$ is the partition function when all the coupling constants are equal to Λ . This bound might prove to be useful in the context of spin glasses.

From (2.3) we immediately get, for any $\beta' > \beta$

$$\frac{1}{nN} \ln Q \leq g(\beta') - \frac{d}{2n} \ln\left(1 - \frac{\beta}{\beta'}\right) \tag{2.4}$$

where

$$g(\beta) = \sup_{\Lambda} \left[\frac{-d\Lambda^2}{4\beta} + \frac{1}{nN} \ln Z(n\Lambda) \right]. \tag{2.5}$$

Let us now come to the proof of (2.3). First of all, we note that we can take all the $\Lambda_{\mu}(x)$ positive since

$$Z(\{\Lambda_{\mu}(x)\}) \leq Z(\{|\Lambda_{\mu}(x)|\}). \tag{2.6}$$

This can be seen easily by expanding the exponential in (2.2) and noting that all the coefficients of the $\{\Lambda_{\mu}(x)\}$ are positive.

The proof will be based on the following inequality [4]:

$$|\text{tr}(T_1 \dots T_{2M})| \leq \prod_{i=1}^{2M} [\text{tr}(T_i T_i^{\dagger})^M]^{1/2M} \tag{2.7}$$

valid as long as, for example, all powers of $T_i T_i^{\dagger}$ are trace class.

The T_i in the following will be various transfer operators.

We begin by constructing transfer operators in the direction 1. Let A_i be the multiplication operator by

$$A_i(\sigma) = \exp\left[\sum_{\mu \neq 1x} \Lambda_{\mu}(ix)(\sigma(x), \sigma(x + \mu))\right] \tag{2.8}$$

x and μ now being vectors in \mathbb{Z}^{d-1} . The operator B_i is defined by the kernel

$$B_i(\sigma | \sigma') = \exp \left[\sum_{\mu \neq 1x} \Lambda_i(i\mu)(\sigma(x), \sigma'(x)) \right]. \tag{2.9}$$

This operator is compact, self-adjoint, and positive definite, on the space $L^2(S_{n-1}^{L^{d-1}})$.

The partition function can be written as

$$Z(\{\Lambda_\mu(x)\}) = \text{tr}(A_1 B_1 A_2 B_2 \dots A_{2M} B_{2M}) \tag{2.10}$$

if we choose $L = 2M$.

We can then define the operators

$$\begin{aligned} T_{2j-1} &= \sqrt{A_j} \sqrt{B_j} & j &= 1, \dots, 2M \\ T_{2j} &= \sqrt{B_j} \sqrt{A_{j+1}} & A_{2M+1} &\equiv A_1 \end{aligned} \tag{2.11}$$

and we see that

$$Z(\{\Lambda_\mu(x)\}) = \text{tr}(T_1 T_2 \dots T_{4M}). \tag{2.12}$$

Using (2.7) we conclude that

$$Z(\{\Lambda_\mu(x)\}) \leq \prod_{j=1}^{2M} [\text{tr}(\sqrt{A_j} B_j \sqrt{A_j})^{2M}]^{1/4M} [\text{tr}(\sqrt{B_j} A_{j+1} \sqrt{B_j})^{2M}]^{1/4M} \tag{2.13}$$

but

$$\text{tr}(\sqrt{A_j} B_j \sqrt{A_j})^{2M} = \text{tr}(A_j B_j)^{2M} \tag{2.14}$$

and

$$\begin{aligned} \text{tr}(A_j B_j)^{2M} &= \int d\nu(\sigma) \exp \left[\sum_{x_1 y} \Lambda_1(jy)(\sigma(x_1 y), \sigma(x_1 + 1y)) \right. \\ &\quad \left. + \sum_{\substack{\mu \neq 1 \\ x_1 y}} \Lambda_\mu(jy)(\sigma(x_1 y), \sigma(x_1 y + \mu)) \right]. \end{aligned} \tag{2.15}$$

Similarly

$$\begin{aligned} \text{tr}(\sqrt{B_j} A_{j+1} \sqrt{B_j})^{2M} &= \int d\nu(\sigma) \exp \left[\sum_{x_1 y} \Lambda_1(jy)(\sigma(x_1 y), \sigma(x_1 + 1y)) \right. \\ &\quad \left. + \sum_{\substack{\mu \neq 1 \\ x_1 y}} \Lambda_\mu(j+1y)(\sigma(x_1 y), \sigma(x_1 y + \mu)) \right]. \end{aligned} \tag{2.16}$$

In equality (2.13) can therefore be expressed as

$$Z(\{\Lambda_\mu(x)\}) \leq \prod_{\substack{i_1=1 \\ \sigma_1=0,1}}^L Z(\{\Lambda_1(i_1 \dots), \Lambda_\mu(i_1 + \sigma_1 \dots) \mu \neq 1\})^{1/2L}. \tag{2.17}$$

Repeating the process in all the other directions, we get

$$Z(\{\Lambda_\mu(x)\}) \leq \prod_{\substack{i_1 \dots i_d \\ \sigma_1 \dots \sigma_d}}^L Z(\{\Lambda_1(i_1 i_2 + \sigma_2, i_3 + \sigma_3 \dots), \Lambda_2(i_1 + \sigma_1, i_2, i_3 + \sigma_3) \dots\})^{1/2^d L^d}. \tag{2.18}$$

However, in the right-hand side of this inequality there appears the partition function of the model with all couplings homogeneous in each direction, but different in these directions. We will prove the bound

$$Z(\{\Lambda_\mu\}) \leq \prod_{\mu=1}^d Z(\Lambda_\mu)^{1/d}. \tag{2.19}$$

This bound combined with (2.18) immediately gives the announced bound (2.3). In order to prove (2.19) we will use transfer operators along the diagonal. For simplicity of notation, we discuss the two-dimensional case. As discussed in Baxter [5], we can introduce a transfer operator by defining two operators

$$V_{\Lambda_1, \Lambda_2}(\sigma | \sigma') = \exp \left[\Lambda_1 \sum_{n=1}^L (\sigma(n), \sigma'(n)) + \Lambda_2 \sum_{n=1}^L (\sigma(n), \sigma'(n-1)) \right] \tag{2.20}$$

and

$$W_{\Lambda_1, \Lambda_2}(\sigma | \sigma') = \exp \left[\Lambda_2 \sum_{n=1}^L (\sigma(n), \sigma'(n)) + \Lambda_1 \sum_{n=1}^L (\sigma(n), \sigma'(n+1)) \right] \tag{2.21}$$

so that

$$W_{\Lambda_1, \Lambda_2}^T = V_{\Lambda_2, \Lambda_1} \tag{2.22}$$

and the partition function can be written as

$$Z(\Lambda_1, \Lambda_2) = \text{tr}(V_{\Lambda_1, \Lambda_2} W_{\Lambda_1, \Lambda_2})^M. \tag{2.23}$$

In equality (2.7) therefore gives

$$Z(\Lambda_1, \Lambda_2) \leq [\text{tr}(V_{\Lambda_1, \Lambda_2} V_{\Lambda_1, \Lambda_2}^T)^M]^{1/2} [\text{tr}(W_{\Lambda_1, \Lambda_2} W_{\Lambda_1, \Lambda_2}^T)^M]^{1/2}. \tag{2.24}$$

From (2.22) $V_{\Lambda_1, \Lambda_2} V_{\Lambda_1, \Lambda_2}^T = V_{\Lambda_1, \Lambda_2} W_{\Lambda_2, \Lambda_1}$. This transfer operator describes a model with alternating coupling constants along the directions perpendicular to those considered. Thus, if we now introduce a transfer operator along the perpendicular diagonal we get

$$\text{tr}(V_{\Lambda_1, \Lambda_2} V_{\Lambda_1, \Lambda_2}^T)^M = \text{tr}(V_{\Lambda_1, \Lambda_1} W_{\Lambda_2, \Lambda_2})^M. \tag{2.25}$$

and applying again inequality (2.7) we conclude, using (2.22), that

$$\text{tr}(V_{\Lambda_1, \Lambda_2} V_{\Lambda_1, \Lambda_2}^T)^M \leq [\text{tr}(V_{\Lambda_1, \Lambda_1} W_{\Lambda_1, \Lambda_1})^M]^{1/2} [\text{tr}(W_{\Lambda_2, \Lambda_2} V_{\Lambda_2, \Lambda_2})^M]^{1/2}. \tag{2.26}$$

Combining (2.24) and (2.26) we conclude that

$$Z(\Lambda_1, \Lambda_2) \leq Z(\Lambda_1, \Lambda_1)^{1/2} Z(\Lambda_2, \Lambda_2)^{1/2}. \tag{2.27}$$

In more than two dimensions, we can derive the corresponding inequality by introducing diagonal transfer operators in all the various planes (12), (23), (31), ...

In order to obtain a lower bound on the partition function, we simply translate $\Lambda_\mu(x)$ by Λ in expression (2.1).

In this way we get

$$Q = \left(\frac{n}{8\pi\beta} \right)^{dN/2} Z(n\Lambda) \int_{-\infty}^{+\infty} \prod_{\mu x} d\Lambda_\mu(x) \exp \left[-\frac{n}{4\beta} \sum_{\mu x} (\Lambda + \Lambda_\mu(x))^2 \right] \times \left\langle \exp \left[n \sum_{\mu x} \Lambda_\mu(x) (\sigma(x), \sigma(x+\mu)) \right] \right\rangle (\Lambda) \tag{2.28}$$

where the expectation value in the integrand is with respect to the Heisenberg model with coupling constant $n\Lambda$. Jensen's inequality gives

$$\left\langle \exp \left[n \sum_{\mu x} \Lambda_{\mu}(x) (\sigma(x), \sigma(x + \mu)) \right] \right\rangle \geq \exp \left[n \sum_{\mu x} \Lambda_{\mu}(x) \langle (\sigma(x), \sigma(x + \mu)) \rangle \right] \quad (2.29)$$

and we get the lower bound

$$\frac{1}{nN} \ln Q \geq \left[-\frac{d}{4\beta} \Lambda^2 + \frac{1}{nN} \ln Z(n\Lambda) \right] + d\beta \left(\langle (\sigma(0), \sigma(\mu)) \rangle - \frac{\Lambda}{2\beta} \right)^2. \quad (2.30)$$

Finally, making the optimal choice for Λ , we get

$$\frac{1}{nN} \ln Q \geq g(\beta). \quad (2.31)$$

In conclusion we have proven that

$$g_{n,N}(\beta) \leq \frac{1}{nN} \ln Q \leq g_{n,N}(\beta') - \frac{d}{2n} \log \left(1 - \frac{\beta}{\beta'} \right) \quad (2.32)$$

valid for any $\beta' > \beta$, where we recall that

$$g_{n,N}(\beta) = \sup_{\Lambda} \left[-\frac{d\Lambda^2}{4\beta} + f_{n,N}(\Lambda) \right] \quad (2.33)$$

where $f_{n,N}(\Lambda) = (1/nN) \ln Z(n\Lambda)$ is the free energy of the Heisenberg model.

These bounds are optimal when $n \rightarrow \infty$, after or before the thermodynamic limit. Indeed, since for those Λ giving a maximum to the expression in (2.33), we have

$$\frac{d\Lambda}{2\beta} = f'_{n,N}(\Lambda) = \langle (\sigma(0), \sigma(\mu)) \rangle \leq 1$$

therefore

$$|\Lambda| \leq \frac{2\beta}{d}. \quad (2.34)$$

Hence the supremum in (2.33) has to be taken on the compact interval given by (2.34). We can prove that the convergence to the spherical model of the free energy of the Heisenberg model is uniform both in N and n . Unfortunately the proof by Kac and Thompson [4] of this result is incorrect although the final result is of course correct. A correct proof has been given by Shcherbina [8]. Hence we can replace the expression for $f_{n,N}(\Lambda)$ appearing in (2.33) by its thermodynamic limit, and this limit when n tends to infinity. And since $g(\beta)_{\infty, \infty}$ is continuous in β , we obtain the final result

$$\beta p = \lim_{n \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{nN} \ln Q = \lim_{N \rightarrow \infty} \lim_{n \rightarrow \infty} \frac{1}{nN} \ln Q \quad (2.35)$$

with

$$\beta p = \sup_{\Lambda} \left[-\frac{d\Lambda^2}{4\beta} + f_{\infty}(\Lambda) \right] \quad (2.36)$$

with the well known result for $f_{\infty}(\Lambda)$:

$$f_{\infty} = -\frac{1}{2} + \inf_{\varepsilon \geq 0} \left[\frac{\varepsilon}{2} - \frac{1}{2} \int_0^{2\pi} \frac{d^d \theta}{(2\pi)^d} \ln \left(\varepsilon + 2\Lambda \sum_{\mu} \cos \theta_{\mu} \right) \right]. \quad (2.37)$$

In this way we have given a rigorous justification for the results obtained in [1].

An analysis [1] of the equations (2.36) and (2.37) shows that the model has a first-order transition, in any dimension $d \geq 2$ when $n = \infty$.

The following result is a theorem: let $f_n(\beta)$ be a sequence of convex functions, which have a limit $f(\beta)$. Then

$$\lim_{n \rightarrow \infty} \frac{df_n(\beta)}{d\beta} = \frac{df}{d\beta}$$

for all values of β at which $f(\beta)$ is differentiable. If we apply this theorem to the free energy of the RP^{n-1} model, we can conclude that the internal energy of the RP^{n-1} model approaches, when n tends to infinity, that computed from equations (2.36) and (2.37), except possibly at β_c , the inverse critical temperature found in the limit $n = \infty$. From our result we can therefore conclude that near β_c the internal energy of the RP^{n-1} should vary very suddenly when n is large, but it leaves open the possibility either that there is no true phase transition or that, if it exists, it is not first-order.

3. First order in a $1/n$ expansion for the free energy

We can now proceed to an expansion in the parameter $1/n$. In the expression for the partition function

$$Q = \left(\frac{n}{8\pi\beta}\right)^{Nd/2} \int_{-\infty}^{+\infty} d\Lambda_\mu \exp\left[-\frac{n}{4\beta} \sum_{\mu x} \Lambda_\mu^2(x)\right] \times \int d\nu(\sigma) \exp\left[n \sum_{x\mu} \Lambda_\mu(x)(\sigma(x), \sigma(x+\mu))\right] \tag{3.1}$$

we are justified in developing around a uniform saddle point. We therefore define

$$\Lambda_\mu(x) = \Lambda + \frac{1}{\sqrt{n}} A_\mu(x) \tag{3.2}$$

so that

$$Q = \left(\frac{n}{8\pi\beta}\right)^{Nd/2} Q_H(n\Lambda) \exp\left[-\frac{nN d \Lambda^2}{4\beta}\right] \bar{Q} \tag{3.3}$$

where

$$\bar{Q} = \int_{-\infty}^{+\infty} dA \exp\left[-\frac{1}{4\beta} \sum_{x\mu} A_\mu^2(x) - \frac{\sqrt{n}}{2\beta} \sum_{x\mu} A_\mu(x)\Lambda\right] \times \left\langle \exp\left[\sqrt{n} \sum_{x\mu} A_\mu(x)(\sigma(x), \sigma(x+\mu))\right] \right\rangle_H \tag{3.4}$$

and $Q_H(n\Lambda)$ is the partition function of the usual Heisenberg model with inverse temperature $n\Lambda$. $\langle \dots \rangle_H$ refers to an average with respect to this model. Although it may not look obvious, we have not violated gauge invariance by choosing the saddle point (3.2). Indeed, all the saddle points

$$\{\Lambda \epsilon_x \epsilon_{x+\mu}\} \tag{3.5}$$

with $\epsilon_x = \pm 1$, obtained by letting the gauge group Z_2 act on the uniform saddle point, would give the same result. This can be seen by noting that

$$Q = \frac{1}{2^N} \sum_{\epsilon_x} Q_\epsilon \tag{3.6}$$

where in Q_ϵ we develop around the saddle point (3.5). Using gauge invariance we can stay with equation (3.2).

We can now develop in cumulants the average of the exponential appearing in equation (3.4), and we get to second order:

$$\bar{Q} = \int_{-\infty}^{+\infty} dA \exp \left\{ -\frac{1}{2} \sum_{\substack{\mu x \\ \nu y}} A_\mu(x) A_\nu(y) C_{\mu\nu}(xy) + \sqrt{n} \sum_{x\mu} A_\mu(x) \left[\frac{\Lambda}{2\beta} - \langle e_\mu(x) \rangle_H \right] \right\} \quad (3.7)$$

where

$$e_\mu(x) = (\sigma(x), \sigma(x + \mu)) \quad (3.8)$$

is the local energy in the direction μ for the Heisenberg model and the matrix C is defined by

$$C_{\mu\nu}(xy) = \frac{1}{2\beta} \delta_{\nu,\mu} \delta_{x,y} - n [\langle (e_\mu(x) e_\nu(y)) \rangle_H - \langle e_\mu(x) \rangle_H \langle e_\nu(y) \rangle_H]. \quad (3.9)$$

The saddle-point equation is now

$$\frac{\Lambda}{2\beta} = \langle e_\mu(x) \rangle_H \quad (3.10)$$

and we get, for the free energy in the thermodynamic limit,

$$\beta p = \beta p_H - \frac{d}{2} \ln 2\beta - \frac{1}{2} \int dk \operatorname{tr} \ln \hat{C}(k) - \frac{n\Lambda^2 d}{4\beta} \quad (3.11)$$

with

$$\hat{C}_{\mu\nu}(k) = \sum_r C_{\mu\nu}(0, r) \exp[i(k, r)] \quad (3.12)$$

and $\int dk$ means

$$\int_0^{2\pi} \prod_{\mu=1}^d \frac{dk_\mu}{2\pi}.$$

What remains to do is to compute the free energy of the Heisenberg model to first order in $1/n$ and the correlation function

$$n [\langle e_\mu(x) e_\nu(y) \rangle - \langle e_\mu(x) \rangle \langle e_\nu(y) \rangle] \equiv n \langle e_\mu(x); e_\nu(y) \rangle \quad (3.13)$$

in the limit $n = \infty$.

The equation for the saddle point will be given by

$$\frac{\Lambda}{2\beta} = \frac{1}{n} \frac{\partial}{\partial \Lambda} \beta p_H(n\Lambda). \quad (3.14)$$

The free energy to order $1/n$ has been calculated with the result [6]:

$$\beta p_H = \ln 2 + \frac{n\alpha}{2} + \frac{n}{2} \int dk \ln G(k) - \frac{1}{2} \int dk \ln \Pi(k) \quad (3.15)$$

where

$$G(k) = (\epsilon_k + \alpha)^{-1} \quad (3.16)$$

with

$$\epsilon_k = 2\Lambda \sum_{\mu} \cos k_{\mu} \quad (3.17)$$

$$\Pi(k) = \int dp G(p)G(p+k). \quad (3.18)$$

The parameter α is determined by the stationarity of βp_H with respect to it, i.e. by the equation

$$1 = \int dk \left[G(k) + \frac{1}{n} \frac{\partial}{\partial \alpha} \ln \Pi(k) \right]. \quad (3.19)$$

This condition also means that the constraint $\langle \sigma_x^2 \rangle = 1$ is satisfied to order $1/n$. We have also computed $\hat{C}_{\mu\nu}(k)$. After some lengthy computation, one finds

$$\hat{C}_{\mu\nu}(k) = \frac{1}{2\beta} \delta_{\mu\nu} + 2 \left[\frac{\Pi_{\mu}(k)\Pi_{\nu}(k)}{\Pi(k)} - \text{Re} \Pi_{\mu-\nu}(k) \exp[i(k_{\mu} - k_{\nu})] \right] \quad (3.20)$$

where

$$\Pi_{\mu}(k) = \int dp G(p)G(p+k) \exp[i(p, e_{\mu})] \quad (3.21)$$

e_{μ} being the unit vector in the direction μ . Equations (3.14), (3.15), (3.19) and (3.20) allow us, in principle, to compute the free energy given in equation (3.11). This set of equations is rather complicated to analyse in a quantitative way since it is difficult to get closed form expressions for the quantities $\Pi(k)$ and $\Pi_{\mu}(k)$, for example.

We can, however, draw the following qualitative conclusions. We have different solutions for the saddle point equation (3.10) besides the trivial one, $\Lambda = 0$. If we take the solution Λ' which coincides in the limit $n = \infty$ with the one Λ'_0 which minimizes the free energy when $\beta \geq \beta_c$, we will get $\Lambda' = \Lambda'_0 + \Lambda'_1/n$. We will therefore apparently add a smooth contribution to the free energy obtained in the limit $n = \infty$. This quantity possesses a jump in its derivative which the $1/n$ contribution cannot suppress unless the matrix $\hat{C}(k)$ possesses an eigenvalue which vanishes at the critical point $\beta_c(\infty)$, which would indicate an instability of the $1/n$ expansion. The numerical results indicate that in three dimensions, no stability of this kind occurs and the transition remains first order, even when $1/n$ corrections are taken into account. But in two dimensions where the Heisenberg model itself shows no transition when n is large, the numerical results indicate an instability in the $1/n$ expansion. In order to see if this is really the case a more detailed analysis, probably numerical, of the $1/n$ corrections is needed. We have left this for further study.

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