Two-Dimensional Heisenberg Model with Nonlinear Interactions

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Abstract

We investigate a two-dimensional classical $N$-vector model with a nonlinear interaction $(1 + \sigma_i \cdot \sigma_j)^p$ in the large-$N$ limit. As observed for $N = 3$ by Blöte et al. [Phys. Rev. Lett. 88, 047203 (2002)], we find a first-order transition for $p > p_c$ and no finite-temperature phase transitions for $p < p_c$. For $p > p_c$, both phases have short-range order, the correlation length showing a finite discontinuity at the transition. For $p = p_c$, there is a peculiar transition, where the spin-spin correlation length is finite while the energy-energy correlation length diverges.

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The two-dimensional Heisenberg model has been the object of extensive studies which mainly focused on the $O(N)$-symmetric Hamiltonian

$$H = -N\beta \sum_{(i,j)} \sigma_i \cdot \sigma_j,$$

where $\sigma_i$ is an $N$-dimensional unit spin and the sum is extended over all lattice nearest neighbors. The behavior of this system in two dimensions is well understood. It is disordered for all finite $\beta$ \cite{[1]} and it is described for $\beta \to \infty$ by the perturbative renormalization group \cite{[2–4]}. The square-lattice model has been extensively studied numerically \cite{[5–10]}, checking the perturbative predictions \cite{[11–15]} and the nonperturbative constants \cite{[16–18]}.

In this paper we study a more general Hamiltonian on the square lattice; more precisely, we consider

$$H = -N\beta \sum_{x\mu} W(1 + \sigma_x \cdot \sigma_{x+\mu}),$$

where $W(x)$ is a generic function such that $W(2) > W(x)$ for all $0 \leq x < 2$, in order to guarantee that the system orders ferromagnetically for $\beta \to \infty$. A particular case of the Hamiltonian (2) has been extensively studied in the years, the case in which $W(x)$ is a second-order polynomial. Such a choice of $W(x)$ gives rise to the so-called mixed $O(N)$-$\mathbb{R}P^{N-1}$ model \cite{[19–28]}, which is relevant for liquid crystals \cite{[29–34]} and for some orientational transitions \cite{[35]}.

In a recent Letter \cite{[36]}, the authors analyzed a model with $W(x) = ax^p + b$ and found an additional first-order transition for $p$ large enough. Here, we will study the same model, finding an analogous result: for $p > p_c \approx 4.537857$ a first-order transition appears, the correlation length—and in general, all thermodynamic quantities—showing a finite discontinuity. Note that the appearance of a first-order transition in nonlinear models is not a new phenomenon. Indeed, for $N = \infty$ it was already shown in Ref. \cite{[20]} that a first-order transition appears in mixed $O(N)$-$\mathbb{R}P^{N-1}$ models for some values of the couplings. It is of interest to understand the behavior for $p = p_c$. For such value of $p$, Ref. \cite{[30]} found a peculiar phase transition: while the spin-spin correlation length remains finite, the energy-energy correlation length diverges. Here, we will show that the same phenomenon occurs for $N = \infty$. However, at variance with what observed in Ref. \cite{[36]}, the critical theory shows mean-field—not Ising—behavior.

Let us consider the Hamiltonian (2) on a hypercubic $d$-dimensional lattice. We normalize $W(x)$ by requiring $W'(2) = 1$ so that in the spin-wave limit

$$H = \frac{N\beta}{2} \int dx \partial_\mu \sigma \cdot \partial_\mu \sigma. $$

(3)

We also fix $W(1) = 0$ so that $H = 0$ for a random configuration. Then, we introduce two new fields $\lambda_{x\mu}$ and $\rho_{x\mu}$ in order to linearize the dependence of the Hamiltonian on the spin coupling. We write

$$\exp[N\beta W(1 + \sigma_x \cdot \sigma_{x+\mu})] \sim \int d\rho_{x\mu} d\lambda_{x\mu} \exp \left[\frac{N\beta}{2} \lambda_{x\mu} (1 + \sigma_x \cdot \sigma_{x+\mu} - \rho_{x\mu}) + N\beta W(\rho_{x\mu})\right].$$

(4)
As usual in the large-$N$ expansion, we also introduce a field $\mu_x$ in order to eliminate the constraint $\sigma^2_x = 1$. Thus, we write

$$\delta (\sigma^2_x - 1) \sim \int d\mu_x \exp \left[ -\frac{N\beta}{2} \mu_x (\sigma^2_x - 1) \right].$$

(5)

With these transformations we can rewrite the partition function as

$$Z = \int \prod \left[ d\rho_{x\mu} d\lambda_{x\mu} \right] \prod \left[ d\mu_x d\sigma_x \right] e^{NA}$$

(6)

where

$$A = \frac{\beta}{2} \sum_{x\mu} \left[ \lambda_{x\mu} + \lambda_{x\mu} \sigma_x \cdot \sigma_{x+\mu} - \lambda_{x\mu} \rho_{x\mu} + 2W(\rho_{x\mu}) \right] - \frac{\beta}{2} \sum_x \left( \mu_x \sigma^2_x - \mu_x \right).$$

(7)

We perform a saddle-point integration by writing

$$\lambda_{x\mu} = \alpha + \tilde{\lambda}_{x\mu},$$

$$\rho_{x\mu} = \tau + \tilde{\rho}_{x\mu},$$

$$\mu_x = \gamma + \tilde{\mu}_x.$$  

(8)

A standard calculation gives the following saddle-point equations [37]:

$$d\beta(1 - \tau) + \frac{1}{\alpha} \left[ (2d + m^2_0)I(m^2_0) - 1 \right] = 0,$$

$$\alpha - 2W''(\tau) = 0,$$

$$\frac{\beta}{2} - \frac{1}{\alpha} I(m^2_0) = 0,$$

(9)

where we set $\gamma = \alpha(2d + m^2_0)/2$,

$$I(m^2_0) = \int \frac{d^d p}{(2\pi)^d} \frac{1}{\tilde{p}^2 + m^2_0},$$

(10)

and $\tilde{p}^2 = 4 \sum_\mu \sin^2 p_\mu / 2$. The variable $m_0$ has a simple interpretation: it is related to the spin-spin correlation length by $\xi_\sigma = 1/m_0$. From Eq. (11) we obtain finally

$$\beta = \frac{I(m^2_0)}{W'(\tau)},$$

(11)

where

$$\tau = \tau(m_0) \equiv 2 + \frac{m_0^2}{2d} - \frac{1}{2d I(m^2_0)}.$$  

(12)

The corresponding free energy can be written as

$$F = -\beta dW(\tau) + \frac{1}{2} \log I(m^2_0) + \frac{1}{2} L(m^2_0),$$

(13)
Figure 1: Function $\beta(m_0) \equiv I(m_0)/W'(\tau)$ vs $m_0$, for $p = 4$, 4.5, 5, and 5.5. For any $p$, $\beta(m_0) \to \infty$ for $m_0 \to 0$.

where

$$L(m_0^2) = \int \frac{d^4p}{(2\pi)^d} \log(p^2 + m_0^2).$$

(14)

Focusing now on the two-dimensional case, let us show that, for any $W(x)$, the spin-spin correlation length is always finite, i.e. $\xi_\sigma = \infty$, i.e. $m_0 = 0$, only for $\beta = \infty$. Note first that $\tau = 2$ (resp. $\tau = 1$) for $m_0 = 0$ (resp. $m_0 = \infty$) and that $\tau(m_0)$ is a strictly decreasing function of $m_0$. Thus, $W'(\tau)$ is finite for all $m_0$. Then, since $I(0) = +\infty$, we find that $\xi_\sigma = \infty$ only if $\beta = \infty$, i.e. $\xi_\sigma$ is finite for all finite $\beta$.

We want now to discuss the behavior for $\beta \to \infty$. From Eq. (11), we see that $\beta \to \infty$ for $m_0 \to 0$ and possibly for $m_0 \to \bar{m}_i$, where $W'(\tau(\bar{m}_i)) = 0$. If there is more than one solution, the relevant one corresponds to the lowest free energy. Now, for $\beta \to \infty$, we can simply write $F \approx -2\beta W(\tau)$. Since $\tau(0) = 2$ and $W(2) > W(\tau)$ for all $0 \leq \tau < 2$ because of the ferromagnetic condition, the relevant solution is the one with $m_0 \to 0$. Then, using

$$I(m_0) = -\frac{1}{2\pi} \log \frac{m_0^2}{32} + O(m_0^2 \log m_0^2)$$

(15)

for $m_0 \to 0$, we obtain

$$m_0^2 = 32e^{-2\pi\beta+\pi W''(2)/2}[1 + O(\beta^{-1})],$$

(16)
in agreement with the standard perturbative renormalization-group predictions [39].

Let us now discuss the possibility of first-order phase transitions, which may arise from the presence of multiple solutions to Eq. (11). As in Ref. [36], we consider

$$W(x) = \frac{2}{p} \left( \frac{x}{2} \right)^p - \frac{2^{1-p}}{p}.$$  \hfill (17)

In Fig. 1 we report the function $\beta(m_0) \equiv I(m_0^2)/W'(\tau)$, for $p = 4, 4.5, 5, 5.5$. For $p = 4, 4.5$, for each $\beta$ there is a unique solution $m_0$ and thus there are no phase transitions. On the other hand, for $p = 5, 5.5$ there is the possibility of multiple solutions, in which case the most relevant is the one that gives the lowest free energy. For $p = 5$, we report the free energy in Fig. 2. We observe a first-order transition for $\beta \approx 1.543$ with a finite discontinuity of the correlation length, $\Delta \xi_\sigma \approx 16.2$, and of all thermodynamic quantities. A numerical analysis of the gap equation (11) shows that a first-order transition exists for all $p > p_c \approx 4.537857$. For $p = p_c$, the thermodynamic functions are nonanalytic for $\beta = \beta_c \approx 1.33472$. In this case, $\beta - \beta_c \approx -0.035726(m_0 - m_{0c})^3 + O[(m_0 - m_{0c})^4], \hfill (18)$

where $m_{0c} \approx 0.387537$. Consequently, repeating the discussion of Ref. [20],

$$\xi_\sigma(\beta) \approx 2.5804 + 7.8682(\beta - \beta_c)^{1/3} + \cdots.$$  \hfill (19)
\[ E(\beta) \approx 0.162274 + 0.314385(\beta - \beta_c)^{1/3} + \cdots, \]  
\[ C(\beta) \approx 0.104795(\beta - \beta_c)^{-2/3} + \cdots, \]

where \( E \) and \( C \) are respectively the energy and the specific heat per site. Note that \( C(\beta) \) diverges at the critical point, indicating that, although spin-spin correlations are not critical, criticality is observed for energy-energy correlations. Indeed, consider

\[ D_Q(k) = \sum_{\mu \nu} e^{ik \cdot (x-y)} \langle Q(1 + \sigma_x \cdot \sigma_{x+\mu}); Q(1 + \sigma_y \cdot \sigma_{y+\nu}) \rangle, \]

where \( Q(x) \) is an arbitrary regular function. For \( N \to \infty \),

\[ D_Q(k) = [Q'(\tau)]^2 \sum_{\mu \nu} \langle \tilde{\rho}_\mu(-k); \tilde{\rho}_\nu(k) \rangle, \]

so that

\[ ND_Q(0) = \left( \frac{Q'(\tau)}{W''(\tau)} \right)^2 C(\beta). \]

It follows \( D_Q(0) \sim (\beta - \beta_c)^{-2/3} \) for any function \( Q(x) \). Thus, all correlation functions of the energy show a critical behavior. In order to compute the associated correlation length, we determine \( D_Q(k) \) for arbitrary \( k \). We obtain

\[ ND_Q(k) = \frac{2[Q'(\tau)]^2[A_2(k)A_0(k) - A_1(k)^2]}{\beta^2[W''(\tau)]^2A_0(k) - \beta W''(\tau)[A_2(k)A_0(k) - A_1(k)^2]}, \]

where

\[ A_n(k) = \int \frac{d^2q}{(2\pi)^2} \frac{\left( \sum_{\mu} \cos q_\mu \right)^n}{\left( (q + k/2)^2 + m_0^2 \right)^{n/2} \left( (q - k/2)^2 + m_0^2 \right)^{n/2}}. \]

For \( \beta \to \beta_c \) and \( k \to 0 \), we have

\[ D_Q(k)^{-1} = a(\beta - \beta_c)^{2/3} + bk^2 + O(k^4), \]

with \( a, b \neq 0 \). Thus, the energy-energy correlation length \( \xi_E(\beta) \) behaves as

\[ \xi_E(\beta) \sim (\beta - \beta_c)^{-1/3}, \]

i.e. \( \nu_E = 1/3 \). We thus confirm the results of Ref. [36] on the existence of the critical theory for \( p = p_c \), although we disagree on the nature of the critical behavior. Indeed, Ref. [36] suggested \( \alpha = 1 - 1/\delta \), with \( \delta \) assuming the Ising value \( \delta = 15 \). Instead, we find the mean-field value \( \delta = 3 \). It is unclear how our large-\( N \) result is compatible with what observed for \( N = 3 \). Indeed, the universality argument of Ref. [36] would predict Ising behavior for any value of \( N \). This issue deserves further investigations.

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[37] If $W'(1) = 0$, there is an additional solution with $\tau = 1, \alpha = 0, \gamma = \beta^{-1}$.

[38] This is obvious for $m_0 \to \bar{m}_i$, since $I(\bar{m}_i)$ and $L(\bar{m}_i)$ are finite. For $m_0 \to 0$, it is enough to observe that $L(0)$ is finite, while $\log I(m_0^2) \approx \log \beta$ because of the gap equations.

[39] The large-$\beta$ behavior of $\xi_\sigma$ for any $N \geq 3$ and any potential $W(x)$ is given in Ref. [12].