Frustrated Heisenberg Magnets: A Nonperturbative Approach

M. Tissier,* B. Delamotte,† and D. Mouhanna‡

Laboratoire de Physique Théorique et Hautes Energies, Universités Paris VI-Pierre et Marie Curie-Paris VII-Denis Diderot, 2 Place Jussieu, 75252 Paris Cedex 05, France

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Frustrated magnets are a notorious example of where usual perturbative methods fail. Using a nonperturbative Wilson-like approach, we get a coherent picture of the physics of frustrated Heisenberg magnets everywhere between $d = 2$ and $d = 4$. We recover all known perturbative results in a single framework and find the transition to be weakly of first order in $d = 3$. We compute effective exponents that are in good agreement with numerical and experimental data.

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Understanding the effect of competing interactions in three-dimensional classical spin systems is one of the great challenges of condensed matter physics. However, after twenty five years of investigations, the nature of the universality class for the phase transition of the simplest frustrated model, the antiferromagnetic Heisenberg model on a triangular lattice (AFHT model), is still a strongly debated question [1]. Because of frustration, the ground state of the AFHT model is given by a canted configuration—the famous 120° structure—that implies a matrixlike order parameter [2] and, thus, the possibility of a new universality class. Experiments performed on materials which are supposed to belong to the AFHT universality class display indeed exponents different from those of the standard $O(N)$ universality class: for VCl_2 [3], $\beta = 0.20(2)$, $\gamma = 1.05(3)$, and $\nu = 0.62(5)$; for VBr_2 [4], $\alpha = 0.30(5)$; for CuFUD [5], $\beta = 0.22(2)$, for $Fe[S_2CN(C_2H_5)_2]_2Cl$ [6–8], $\beta = 0.24(1)$ and $\gamma = 1.16(3)$. These results, however, call for several comments. First, the exponents violate the scaling relations, at least by 2 standard deviations. Second, they differ significantly from those obtained by Monte Carlo (MC) simulations performed either directly on the AFHT model [$\nu \simeq 0.59(1)$, $\gamma \simeq 1.17(2), \beta \simeq 0.29(1), \alpha \simeq 0.24(2)$] or on models supposedly belonging to the same universality class: AFHT with rigid constraints [$\nu = 0.504(10), \gamma = 1.074(29), \beta = 0.221(9), \alpha = 0.488(30)$], dihedral (i.e., $V_{3,2}$ Stiefel) models [$\nu \simeq 0.51(1), \gamma \simeq 1.13(2), \beta \simeq 0.193(4), \alpha \simeq 0.47(3)$]. See Ref. [9] for a review, and references therein. Finally, the anomalous dimensions η obtained by means of scaling relations are found to be negative in experiments as well as in MC simulations, a result forbidden by first principles for second order phase transitions [10]. All of these results are hardly compatible with the assumption of universality. It has been proposed that the exponents are, in fact, effective exponents characterizing a very weak first order transition, the so-called "almost second order phase transition" [11–13].

From the theoretical point of view the situation is also very unsatisfactory since one does not have a coherent picture of the expected critical behavior of the AFHT model between two and four dimensions. On the one hand, the weak coupling expansion performed on the suitable Landau-Ginzburg-Wilson (LGW) model in the vicinity of $d = 4$ leads to a first order phase transition due to the lack of a stable fixed point [14–16]. On the other hand, the low temperature expansion performed around two dimensions on the nonlinear sigma (NLσ) model predicts a second order phase transition of the standard $O(4)/O(3)$ universality class [17]. Since there is no indication that these perturbative results should fail in their respective domain of validity, i.e., for small $\epsilon = 4 - d$ and small $\epsilon = d - 2$, this situation raises two problems. First, and contrary to what happens in the nonfrustrated case, one cannot safely predict the three-dimensional behavior from naive extrapolations of the perturbative results. Although a direct computation in three dimensions, possible on the LGW model [18,19], can circumvent this difficulty, such an approach misses a second fundamental problem: the incompatibility between the symmetries of the NLσ and LGW models. Indeed, the renormalization group flow drives the NLσ model action towards an $O(4)$ symmetric regime, more symmetric than the microscopical system, a phenomenon that *cannot* occur within all previous treatments of the LGW model (see Ref. [17] and below). The LGW model is therefore unable to find the $O(4)$ behavior which has been nevertheless observed numerically in $d = 2$ [20]. This raises serious doubts on the perturbative analysis of the LGW model away from $d = 4$. Reciprocally, the *perturbative* analysis of the NLσ model, based on a Goldstone mode expansion, predicts an $O(4)/O(3)$ fixed point everywhere between $d = 2$ and $d = 4$, as for the $N = 4$ ferromagnetic model, in contradiction with the perturbative LGW results and the experimental and numerical situation in $d = 3$. All of this suggests that nonperturbative features could play a major role and thus imposes one to go beyond the standard perturbative approaches.

In this Letter we accomplish this program by using the Wilson renormalization group framework [21]. We obtain a coherent picture of the physics of the AFHT model everywhere between $d = 2$ and $d = 4$. We find that the fixed point expected from the NLσ model approach exists indeed in the vicinity of $d = 2$ but disappears below, and close to, three dimensions. The transition for AFHT

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in $d = 3$ is thus *weakly* first order, contrary to the different predictions of both a new universality class [2] and an $O(4)/O(3)$ second order behavior [17]. We obtain effective exponents compatible with the numerical and experimental data quoted above. For generalization to $N > 4$ component spins, we find the transition in $d = 3$ to be second order with exponents in good agreement with recent extensive MC simulations—contrary to those found from three loop Padé-Borel resummed series [19].

Our approach relies on the concept of effective average action [22,23], $\Gamma_k[\phi]$, which is a coarse grained free energy where only fluctuations with momenta $q \geq k$ have been integrated out. The field ϕ corresponds to an average order parameter at scale k, the analog of a magnetization at this scale. At the scale of the inverse lattice spacing Λ, $\Gamma_{k=\Lambda}$ is the continuum limit of the lattice Hamiltonian obtained, for example, by means of a Hubbard-Stratonovich transformation. On the other hand, the usual free energy Γ, generating one particle-irreducible correlation function, is recovered in the limit $k \to 0$. The k dependence of Γ_k is controlled by an exact evolution equation [24,25]:

$$\frac{\partial \Gamma_k}{\partial t} = \frac{1}{2}\,\mathrm{Tr}\left\{(\Gamma_k^{(2)} + R_k)^{-1}\,\frac{\partial R_k}{\partial t}\right\}, \qquad (1)$$

where $t = \ln k/\Lambda$. The trace has to be understood as a momenta integral as well as a summation over internal indices. In Eq. (1), R_k is the effective infrared cutoff which suppresses the propagation of modes with momenta $q < k$. A convenient cutoff is provided by $R_k(q) = Zq^2/[\exp(q^2/k^2) - 1]$ [24,26], where Z is the field renormalization. In Eq. (1), $\Gamma_k^{(2)}$ is the *exact field-dependent* inverse propagator, i.e., the second derivative of Γ_k.

The effective average action Γ_k is a functional invariant under the symmetry group of the system and thus depends on all of the invariants built from the average order parameter. In our case, it is well known that the order parameter is a set of two vectors $\vec{\phi}_1$ and $\vec{\phi}_2$ which can be gathered in a real $N \times 2$ matrix ϕ_{ab} for N-component spins [2]. The symmetry of the system is the usual spatial rotation group $O(N)$ multiplied by an $O(2)$ corresponding to the symmetry of the underlying triangular lattice [17]. This $O(2)$ is realized on ϕ_{ab} as a right $O(2)$ "rotation" that turns the $\vec{\phi}_i$ into each other. There are two independent $O(N) \otimes O(2)$ invariants built out of ϕ_{ab}: $\rho = \mathrm{Tr}^t \phi\phi$ and $\tau = \frac{1}{2}\,\mathrm{Tr}({}^t\phi\phi)^2 - \frac{1}{4}\,(\mathrm{Tr}^t\phi\phi)^2$.

The exact effective average action involves all of the powers of ρ, τ and of derivative terms, and so Eq. (1) is a nonlinear functional equation, too difficult to be solved exactly in general. We therefore need to truncate it. One possibility is to keep in Γ_k only the momentum (i.e., derivative)-independent part, an approximation called the local potential approximation (LPA). In the case of frustrated magnets, this has been considered by Zumbach [11–13]. This approximation however misses the field renormalization and worse, as described below, the phenomenon of enlarged symmetry around $d = 2$ found perturbatively in the NLσ model [17]. This does not mean that this approximation is not useful: it is simply, in essence, unable to answer the question of the matching of the different perturbative approaches. Another truncation is, however, possible which preserves this possibility: it consists of an expansion of Γ_k around its minimum in order to keep a finite number of monomials in the invariants ρ and τ while including the derivative terms which allow one to recover the different perturbative results. We choose the simplest such truncation:

$$\Gamma_k = \int d^d x \left\{\frac{Z}{2}\,\nabla\phi_{ab}\nabla\phi_{ab} + \frac{\omega}{4}\,(\epsilon_{ab}\phi_{ca}\nabla\phi_{cb})^2 + \frac{\lambda}{4}\left(\frac{\rho}{2} - \kappa\right)^2 + \frac{\mu}{4}\,\tau\right\}, \qquad (2)$$

where $\{\omega, \lambda, \kappa, \mu, Z\}$ are the coupling constants which parametrize the model. All terms but one—the "current term" $(\epsilon_{ab}\phi_{ca}\nabla\phi_{cb})^2$—are very natural and correspond to those appearing in the usual LGW action that realizes the symmetry breaking scheme of frustrated magnets. Indeed for λ and $\mu \geq 0$, the minimum of the action is realized by a configuration of the form $\phi_{ab}^{\min} = \sqrt{\kappa}\,R_{ab}$, where R_{ab} is a matrix built with two orthonormal N-component vectors. The symmetry of this minimum is a product of a diagonal $O(2)$ group and a residual $O(N-2)$ group. The symmetry breaking scheme is thus $O(N) \otimes O(2) \to O(N-2) \otimes O(2)_{\mathrm{diag}}$ [17]. Note that, for $\phi_{ab} = \phi_{ab}^{\min}$, one has $\rho = 2\kappa$ and $\tau = 0$ so that Eq. (2) corresponds indeed to a quartic expansion around the minimum. The spectrum in the low temperature phase consists of $2N - 3$ Goldstone modes and three massive modes: one singlet of mass $m_1 = \kappa\lambda$ and one doublet of mass $m_2 = \kappa\mu$ which correspond to fluctuations of the relative angle and of the norms of the two vectors $\vec{\phi}_1$ and $\vec{\phi}_2$.

Without the current term, the truncation Eq. (2) is, however, not sufficient in our case. This term plays a crucial role since, for $N = 3$, it allows the model to enlarge its symmetry from $O(3) \otimes O(2)$ to $O(3) \otimes O(3) \sim O(4)$ at the fixed point around $d = 2$, leading to the well-known $O(4)/O(3)$ behavior [17]. The current term is systematically discarded in the perturbative treatment of the LGW model around four dimensions, for the—correct—reason that it is power-counting irrelevant. Here we can include it in our *ansatz* since it is, in any case, present in the full effective action Γ_k and, in fact, we *must* include it since it becomes relevant somewhere between two and four dimensions. The formalism we use is in charge to decide where it is important.

Let us emphasize that the effective average action method leads to nontrivial and/or new results even within a quartic truncation of Γ_k. One can mention the Kosterlitz-Thouless phase transition [27], low energy quantum chromodynamics [28], the Abelian Higgs model and superconductivity [29,30], matrix models [31], etc. The accuracy of the results thus obtained depends on two main features: (i) the smallness of the anomalous dimension η

and (ii) the fact that the thermodynamics of the system is controlled by a unique minimum of Γ_k.

The flow equations for the different coupling constants κ, λ, μ, ω, and Z are derived by using Eqs. (1) and (2) along the same lines as in [28]. The explicit recursion equations are too long to display and not particularly illuminating (see [32]). Moreover, they require a numerical analysis, apart in $d = 2 + \epsilon$ and in $d = 4 - \epsilon$, where, as we now see, they get analytically tractable.

The physics around two dimensions.—Around two dimensions, one expects that the perturbative "Goldstone mode" expansion of the NLσ model works well. In the Goldstone regime, the fluctuations of the modulus of $\vec{\phi}_1$ and $\vec{\phi}_2$ and of their relative angle are frozen. This corresponds to the large mass limit $m_{1r}, m_{2r} \to \infty$. In this limit, our equations greatly simplify since the coupling constants divide into two sets $\{\kappa, \omega, Z\}$ and $\{\lambda, \mu\}$ that do not mix. We only quote here the flow equations for the renormalized coupling constants of the first set:

$$\begin{cases} \dfrac{d\kappa_r}{dt} = -(d - 2 + \eta)\kappa_r + \dfrac{N-2}{2\pi} + \dfrac{1}{4\pi(1 + \kappa_r\omega_r)} \\ \dfrac{d\omega_r}{dt} = (-2 + d + 2\eta)\omega_r + \dfrac{1 + \kappa_r\omega_r + (N-1)\kappa_r^2\omega_r^2 + (N-2)\kappa_r^3\omega_r^3}{2\kappa_r^2\pi(1 + \kappa_r\omega_r)} \\ \eta = -\dfrac{d\ln Z}{dt} = \dfrac{3 + 4\kappa_r\omega_r + 2\kappa_r^2\omega_r^2}{4\kappa_r\pi(1 + \kappa_r\omega_r)} \end{cases} \tag{3}$$

These equations admit a fixed point for any $N > 2$ of coordinates $\kappa_r^* \simeq 1/\epsilon$, $\omega_r^* \simeq \epsilon$, while $\lambda_r^*, \mu_r^* \simeq$ cst. The masses m_{1r}^*, m_{2r}^* are thus very large, proving the consistency of the limit. In fact, with respect to the change of variables: $\eta_1 = \kappa_r$ and $\eta_2 = 2\kappa_r(1 + \kappa_r\omega_r)$, the equations for κ_r and ω_r are exactly those obtained at one loop in the perturbative analysis of the NLσ model [17]. For $N = 3$, they admit a fixed point for which the model is $O(4)$ symmetric.

Let us now recall how this phenomenon of enlarged symmetry for $N = 3$ can be understood directly on the partition function. At the fixed point, the potential gets infinitely deep so that one recovers the hard constraints of the NLσ model: $\vec{\phi}_1 \perp \vec{\phi}_2$ and $\vec{\phi}_1^2 = \vec{\phi}_2^2 = \kappa_r^*$. For $N = 3$, this allows us to rewrite the current term as the kinetic term of a third vector, the cross product of two others: $(\epsilon_{ab}\phi_{ca}\nabla\phi_{cb})^2 \propto (\nabla\vec{\phi}_3)^2$ with $\vec{\phi}_3 = \vec{\phi}_1 \wedge \vec{\phi}_2$. The order parameter of the system is then a trihedral of orthogonal vectors $(\vec{\phi}_1, \vec{\phi}_2, \vec{\phi}_3)$. Thus, contrary to what could be expected from a naive expansion in powers of the fields, the current term plays a role as important as the usual kinetic terms. At the fixed point, ω_r takes a value such that the three vectors play a symmetric role and the symmetry breaking scheme is $O(3) \otimes O(3)/O(3) \sim O(4)/O(3)$ instead of $O(3) \otimes O(2)/O(2)$. Such a result is of course missed within the LPA [11–13]. Therefore, the presence of the current term not only improves the accuracy of the calculation but it is necessary for its consistency.

The physics around four dimensions.—Around four dimensions, we have expanded our equations at leading order in the coupling constants λ_r and μ_r. At this order the current term decouples and we are left with the following equations for the quartic coupling constants:

$$\begin{cases} \dfrac{d\lambda_r}{dt} = (-4 + d)\lambda_r + \dfrac{1}{16\pi^2}\left[4\lambda_r\mu_r + 4\mu_r^2 + \lambda_r^2(4 + N)\right], \\ \dfrac{d\mu_r}{dt} = (-4 + d)\mu_r + \dfrac{1}{16\pi^2}\left(6\lambda_r\mu_r + N\mu_r^2\right). \end{cases} \tag{4}$$

They are those obtained at one loop from the LGW approach [14]. These flow equations admit a stable fixed point for $N > N_c \simeq 21.8$, attesting that the phase transition is second order. For $N < N_c$ the transition is first order since no fixed point is found.

To higher orders, N_c depends on the dimension. In $d = 3$, three loop calculations resummed in the manner of Padé-Borel predict $N_c(d = 3) = 3.91$ [18]. Note, however, that this calculation exhibits unusual behaviors compared to the $O(N)$ case: the coefficients of the series do not decrease monotonically and the series themselves are not alternate [19]. These features reveal the poor summability of the series. Finally, in the $N = 6$ case, for which the transition is second order, the predictions based on a Padé-Borel resummation, which provides $\nu = 0.575$ and $\gamma = 1.121$ [19], are in clear disagreement with recent numerical simulations, for which $\nu = 0.700(11)$ and $\gamma = 1.383(36)$ [19].

From this point of view our approach has several advantages: first, since it matches with the one loop perturbative results in $d = 2$ and $d = 4$ it is likely that the error does not vary much with the dimension—a fact that has been confirmed in the $O(N)$ case for which the precision for a given truncation is almost uniform with d. Second, it does not rely on a Padé-Borel resummation and therefore is free of the above-mentionned problems of convergence.

Of course, our results will change while improving the *ansatz* Eq. (2) by incorporating terms of higher order in fields and derivatives. However, all cases already treated within the average action method suggest that the lowest order approximation gives fairly good results, even with this crude approximation.

The physics between two and four dimensions.—Let us first study the fate of the fixed point found analytically in $d = 2 + \epsilon$ for $N = 3$. By numerically integrating the flow equations, we find that this stable $O(4)/O(3)$ fixed point describes a smooth trajectory in the coupling constant space while d is increased. Our flow equations actually admit another—but unstable—fixed point, which moves toward the stable fixed point as the dimension is increased. At a critical dimension $d_c \simeq 2.87$, the two fixed points collapse and disappear. Above d_c, no other stable fixed point is found and we conclude that the transition is first order in $d = 3$. We thus show that the $O(4)/O(3)$ fixed point obtained from the NLσ model plays no role in the three-dimensional physics of frustrated magnets, as conjectured, for example, by David and Jolicœur [33] and Dobry and Diep [34]. We also discard the possibility of a new universality class conjectured on the basis of a naive extrapolation of the $\epsilon = 4 - d$ calculation [1,2]. The proximity of d_c with $d = 3$, however, lets open the possibility of a very weak first order phase transition with effective critical exponents. This behavior manifests itself in our equations by the existence of a minimum around which the flow slows down. This characterizes a very large, although finite, correlation length ξ. A rough estimate of this correlation length—a few hundred lattice spacings—indicates that a pseudoscaling behavior can be observed although ξ is not large enough to ensure a true universality. This could explain the broad spectrum of effective critical exponents found in experiments and numerical simulations. Although the flow equations do not have a fixed point, we are able to compute effective exponents by linearizing the flow equations around the minimum. We recover here the phenomenon of almost second order phase transition first introduced by Zumbach [11–13] within the LPA. To get accurate results we have to take into account the ϕ^6-like terms in our *ansatz*. We find $\nu = 0.53$, $\gamma = 1.03$, and $\beta = 0.28$, which lie in between the various sets of exponents found experimentally and numerically (see above). For comparison, Zumbach found $\nu \simeq 0.63$ in the LPA [11–13], the difference being mainly due to the anomalous dimension.

Finally, we find a true fixed point in $d = 3$ for N larger than a critical value $N_c(d = 3) \simeq 4$. For $N = 6$, we get $\nu = 0.74$ and $\gamma = 1.45$ which compare well with the Monte Carlo data $\nu = 0.700(11)$ and $\gamma = 1.383(36)$ [19]. They are close to the LPA results, where $\nu = 0.76$ [12], and much better than those obtained by a three loop calculation in $d = 3$ [19] (see above). We have checked that our exponents do not vary significantly when monomials of order 6 in the fields are included in the *ansatz* Eq. (2).

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*Email address: tissier@lpthe.jussieu.fr
†Email address: delamotte@lpthe.jussieu.fr
‡Email address: mouhanna@lpthe.jussieu.fr

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