Magnetic quantum phase transitions of the two-dimensional antiferromagnetic \( J_1-J_2 \) Heisenberg model

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Abstract – We obtain the complete magnetic phase diagram of the two-dimensional antiferromagnetic \( J_1-J_2 \) Heisenberg model, \( 0 \leq \alpha = J_2/J_1 \leq 1 \), within the framework of the \( O(N) \) nonlinear sigma model. We find two magnetically ordered phases, one with Néel order, for \( \alpha \leq 0.4 \), and another with collinear order, for \( \alpha \geq 0.6 \), separated by a nonmagnetic region, for \( 0.4 \leq \alpha \leq 0.6 \), where a gapped spin liquid is found. The transition at \( \alpha = 0.4 \) is of the second order while the one at \( \alpha = 0.6 \) is of the first order and the spin gaps cross at \( \alpha = 0.5 \). Our results are exact at \( N \to \infty \) and agree with numerical results from different methods.

Introduction. – Quantum phase transitions (QPTs) occur when the ground-state properties of a certain physical system undergo dramatic changes as one, or more, internal or external, parameters are varied [1]. Examples include, but are not restricted to, magnetic phase transitions between two distinct magnetic ground states or between a magnetic state and a nonmagnetic one, driven for example by an applied field, pressure, or the coupling to other degrees of freedom. QPTs are usually labelled according to the behaviour of some order parameter (OP) close to the quantum critical point (QCP) [2], and are said to be of the second order (2nd order) when the OP vanishes continuously as the QCP is approached, or of the first order (1st order) when the OP has a finite value near the QCP and jumps discontinuously to zero above it. Furthermore, knowledge of the range of the interactions, symmetries of the Hamiltonian and dimension of the OP, allow us to classify QPTs into universality classes [2], and help us to write down a Landau-Ginzburg free energy (LGFE) to describe such phase transitions (PTs). Typically, LGFEs up to the 4th power of the OP are enough to describe a 2nd-order PT, while LGFEs up to the 6th power of the OP are necessary to describe a 1st order PT.

The \( O(N) \) quantum nonlinear sigma model (NLSM) has long been acknowledged to be a very convenient framework to describe 2nd-order magnetic PTs in spin systems, such as, for example, the antiferromagnetic (AF) Heisenberg Hamiltonian, in two dimensions, with nearest-neighbour interactions on a square lattice [3]. Here the QPT occurs between a Néel ordered magnetic ground state, where the OP is the sublattice magnetization, \( \sigma \neq 0 \), and a nonmagnetic state \( (\sigma = 0) \) with a finite spin gap, \( \Delta \neq 0 \), as the OP at zero temperature. Such transition is driven by quantum fluctuations set by some coupling constant, \( g \), and is of the 2nd order, as both \( \sigma \) and \( \Delta \) vanish continuously at the QCP, \( g_c \). Despite being nonlinear, at the mean-field level \((N \to \infty)\) the model is quadratic, exactly solvable, and produces the usual mean-field values for the critical exponents of the Heisenberg universality class, \( \sigma \propto (g_c - g)^\beta \), for the ordered regime \((g < g_c)\), with \( \beta = 1/2 \), and \( \Delta \propto (g_c - g)^\nu \), for the nonmagnetic phase \((g > g_c)\), with \( \nu = 1 \) [4].

First-order PTs in spin systems occur whenever two magnetic phases cannot be continuously connected to one another by some order parameter. This is what happens, for example, already at the classical level, between the Néel- and collinear-type ordering phases of the \( J_1-J_2 \) Heisenberg model, at the border \( \alpha = 0.5 \). When quantum fluctuations are taken into account, a nonmagnetic region opens up around \( \alpha = 0.5 \) [5] and a gapped spin liquid phase is found for \( 0.4 \leq \alpha \leq 0.6 \) [6]. Although the precise nature of the nonmagnetic state is still under debate (typical candidates range from dimer to plaquette or VBS phases), the nature of the transition at \( \alpha = 0.4 \) is agreed to be of the 2nd order by both numerical and theoretical methods, like, for example, the NLSM [7]. For the transition at \( \alpha = 0.6 \), different numerical techniques, including series expansion [8], quantum Monte Carlo [9], exact diagonalization [10], and DMRG [11], strongly indicate it to be of the 1st order [12], but from the theoretical
point of view no conclusive statement has yet been presented. More importantly, this poses serious questions on the applicability of the NLSM to describe a 1st-order PT in frustrated magnetic systems [13], specially since no unusual powers of the OP are to be expected.

In this work we derive and apply the $O(N)$ NLSM formalism for the $J_1$-$J_2$ Heisenberg model, for the whole range of parameters, $0 \leq \alpha \leq 1$. Up to the classical border, $0 \leq \alpha \leq 0.5$, the model describes smooth fluctuations of the staggered order parameter on top of a Néel ordered ground state and possesses a 2nd-order phase transition, at $\alpha = 0.4$, driven by quantum fluctuations, towards a nonmagnetic, gapped spin liquid phase. Beyond the classical border, $0.5 \leq \alpha \leq 1$, the model describes, instead, smooth fluctuations of the staggered order parameter on top of a collinearly ordered ground state. Remarkably, although at the mean-field ($N \to \infty$) level the model remains quadratic and exactly solvable, we show that its quantum dynamics is importantly modified by a term proportional to the AF order parameter, which causes significant changes on the behaviour of the OP at zero temperature. The nonmagnetic, gapped spin liquid and collinear phases can no longer be continuously connected and a 1st-order QPT is theoretically obtained.

**Derivation of the model.** — The $J_1$-$J_2$ Heisenberg spin-Hamiltonian is given by

$$\hat{H} = J_1 \sum_{\langle \langle i,j \rangle \rangle} \hat{S}_i \cdot \hat{S}_j + J_2 \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j,$$  

where $J_1 > 0$ and $J_2 > 0$ are, respectively, the AF superexchange between nearest-neighbors, $\langle \langle i,j \rangle \rangle$, and next-to-nearest-neighbors, $\langle i,j \rangle$, spins $\hat{S}_i$ on a two-dimensional square lattice. The Hamiltonian (1) exhibits two types of magnetic order: Néel order, with wave vector at $q = (\pi, \pi)$, for $\alpha \leq 0.4$, and collinear order, with wave vectors at $q = (\pi, 0)$ and/or $q = (0, \pi)$, for $\alpha > 0.6$ [14].

For the Néel ($\pi, \pi$) phase, different effective field theories, of the NLSM type, have been proposed [7], and they all succeed in describing the 2nd-order PT at $\alpha = 0.4$. For the collinear ($\pi, 0$) and/or ($0, \pi$) phase, instead, no such description has been provided yet, and we shall proceed as follows: we treat the collinear magnetic state as a result of two interpenetrated Néel ordered sublattices and introduce a double coherent spin-state basis, with spin operators labeled by indices $A$ and $B$, see fig. 1. We then associate the spins operators in eq. (1) to vector fields $\vec{n}_A(i)$ and $\vec{n}_B(i)$ that describe long wavelength deviations from the Néel state in each sublattice. As usual we parametrize the spin-1 fields into a smooth, $\vec{m}$, and a fast and uniform, $\vec{L}$, varying components, $\vec{n}_{A,B} = \theta_{A,B} \vec{m}_{A,B} \sqrt{1-(\hat{a}_{A,B})^2} + \vec{L}_{A,B}$, where $\theta_{A,B}(i) = +1$ for spin $\uparrow$ and $= -1$ for spin $\downarrow$, and $\hat{a} = a^d/S$. To satisfy $\vec{n}_{A,B} \cdot \vec{n}_{A,B} = 1$ we assume that $\vec{m}_{A,B} \cdot \vec{m}_{A,B} \approx 1$, while $\vec{m}_{A,B} \cdot \vec{L}_{A,B} \approx 0$, $\vec{a}^2 \vec{L}_{A,B} \cdot \vec{L}_{A,B} \ll 1$, and $\vec{m}_A \cdot \vec{L}_B = 0$. After integration over $\vec{L}$ the action for the smooth fields is

$$S = \frac{\rho_S}{2} \int \left[ (\nabla \vec{m}_A)^2 + (\nabla \vec{m}_B)^2 + (\partial_t \vec{m}_A)^2 + (\partial_t \vec{m}_B)^2 \right],$$

where $\rho_S = 2J_2S^2$ is the spin stiffness in two dimensions, $c_0 = \sqrt{2S \alpha \sqrt{16J_2^2 - J_1^2}}$ and $c_1 = \sqrt{2J_2/\sqrt{c_0}}$ are spin-wave velocities, and $\gamma_0 = J_2/c_0$. The first line in eq. (2) corresponds to the usual NLSM for the two Néel sub-structures of fig. 1, labelled $A$ and $B$, which are decoupled when $J_1 = 0$. For $J_1 \neq 0$, however, two couplings arise: the first one involves only gradient terms and produces different spin-wave velocities along the diagonals [15]; the second, and more important one, is a result of the coupled pression of magnetic moments on the two Néel sub-structures and modifies importantly the dynamics of the problem, ultimately leading to the first-order character of the phase transition at $\alpha = 0.6$.

**The large-$N$ limit.** — In the magnetically ordered phase we can write $\vec{m}_{A,B} = \pi_{x,(A,B)} \hat{x} + \pi_{y,(A,B)} \hat{y} + \sigma \hat{z}$. The $\pi$ fields are associated to the quantum fluctuations and the $\sigma$ field to the staggered OP. We introduce the Lagrange multiplier $S_{\text{vac}} \propto \int i\lambda(|\vec{m}_A|^2 - 1) + i\lambda(|\vec{m}_B|^2 - 1)$ and after integrating out transverse fluctuations we end up with the partition function $Z(\beta) = N^2 \int D[\phi] D[\sigma] e^{-N S_{\text{eff}}[\phi, \sigma]}$, where $S_{\text{eff}}[\phi, \sigma] = \frac{N - 1}{N} \text{Tr} \ln \left( A(\partial) + i\lambda \vec{l} \right) + \int \frac{2}{gc_0} i\lambda(\sigma^2 - 1)$.
is given in terms of

$$A(\partial) = \begin{pmatrix} a_1(\partial) & 0 & a_2(\partial) & 0 \\ 0 & a_1(\partial) & 0 & a_2(\partial) \\ a_2(\partial) & 0 & a_1(\partial) & 0 \\ 0 & a_2(\partial) & 0 & a_1(\partial) \end{pmatrix}, \quad (3)$$

with $a_1(\partial) = -c_0^2 \partial^2 - \partial^2$, $a_2(\partial, \sigma) = \gamma_0 c_0^2 \partial_x \partial_y + \frac{v^2}{2} \partial^2$, $v = c_0^2 / c_1^2$, and $g = \frac{\gamma_0 c_0^2}{\rho c_s} = 2 \sqrt{2} a_0^2 \sqrt{1 - \frac{1}{4m_0^2}}$ determines the strength of the coupling between quantum fluctuations (set by $1/S$) and frustration (set by $J_1/J_2$).

In the limit $N \to \infty$ we look for solutions of the type $\sigma(\vec{x}, \tau) = \sigma_0$ and $s(\vec{x}, \tau) = m_0^2$, where $\sigma_0$ and $m_0^2$ are given by $\frac{\partial S_{c\sigma}}{\partial \sigma} |_{\sigma=\sigma_0} = 0$, and $\frac{\partial S_{c\lambda}}{\partial \lambda} |_{\lambda=m_0^2} = 0$. The saddle point equations in the large-$N$ limit and for the magnetically ordered phase, where $\sigma_0 \neq 0$, then become

$$\begin{cases} \sigma_0^2 = f(m_0, \sigma_0), \\
\left( \frac{m_0}{c_0} \right)^2 = h(m_0, \sigma_0). \quad (4) \end{cases}$$

We are interested in the quantum phase transition in which case $\frac{1}{m_0} \sum_{\omega_n} \to \int \frac{dk}{2\pi}$, and thus [16]

$$f(m_0, \sigma_0) = 1 - g \int \frac{d^3k}{(2\pi)^3} \left[ G_k^+(m_0, \sigma_0) + G_k^-(m_0, \sigma_0) \right],$$

$$h(m_0, \sigma_0) = \frac{gv}{2} \int \frac{d^3k}{(2\pi)^3} k_z^2 \left[ G_k^-(m_0, \sigma_0) - G_k^+(m_0, \sigma_0) \right],$$

where $k_z = \omega/c_0$. The Green’s functions are $G_k^\pm(m_0, \sigma_0) = \frac{G_k^2(\sigma_0)}{\sigma_0 + \frac{m_0}{c_0}}$, where we have defined $D_k^2(\sigma_0) = k_x^2 + k_y^2 \pm \gamma_0 k_z^2 k_y + k_z^2(1 + \frac{m_0^2}{c_0^2})$. We should emphasise now that the unusual coupling between the order parameter, $\sigma_0$, and the frequencies, $k_z = \omega/c_0$, in $D_k^2(\sigma_0)$ will be responsible for the first-order character of the quantum phase transition.

**First-order phase transition.** — Equations (4) determine the phase diagram of the model. By solving the above set of equations self-consistently we obtain the behaviour depicted in fig. 2. We observe that while for the Heisenberg model the OP goes smoothly to zero at $g_c$ (indicating a 2nd-order PT), frustration brings the system closer to the QCP and the OP jumps discontinuously to zero at $g_c$, indicating a 1st-order PT. The same is true for the spin gap (see the inset) when the transition is approached from the nonmagnetic side.

To further establish the 1st-order nature of the PT, we show, in fig. 3, the dependence of Log($\sigma_0$) as a function of Log$(1 - g/g_c)$. For $J_1 = 0$ the behaviour is of a straight line with slope given by $\beta = 1/2$, as expected for a mean-field behavior (large $N$) in a 2nd-order QPT (with the order parameter vanishing continuously at the quantum critical point). For $J_1 \neq 0$, however, we observe that, although away from the critical point the deviation from mean-field behaviour is very small, closer to $g_c$, the deviation is significant and characteristic of a first-order quantum phase transition, with $\sigma_0$ saturating as $g \to g_c$.

Let us now provide definitive analytical evidence that the transition is indeed 1st order and not a sharp 2nd-order PT. We note that the parameter values obtained from the self-consistent equations are such that we can write $m_0/c_0$ as a function of $\sigma_0$ [16],

$$\left( \frac{m_0}{c_0} \right)^2 (\sigma_0) = \frac{\omega v/2 b_1(\sigma_0)}{1 - \frac{\omega r}{2} b_2(\sigma_0)}, \quad (5)$$

![Fig. 2: (Colour online) Solutions to eqs. (4) for the OP $\sigma_0$ and the spin gap $m_0/c_0$ (inset), at $T = 0$, as a function of $g$, for different small ratios of $J_1/J_2$. For $J_1 = 0$ (black squares), the OP and the spin gap vanish continuously at $g_c$, and the PT is of the 2nd order (Heisenberg model). For $J_1 \neq 0$ (red, blue and green symbols), however, the OP and the spin gap jump discontinuously to zero at $g_c$, indicating a 1st-order PT.](image1.png)

![Fig. 3: (Colour online) Plot of Log($\sigma$) × Log$(1 - g/g_c)$ for different values of $J_1/J_2$. A 2nd-order PT, at the mean-field (large $N$) level, produces a straight line (black squares) with slope $\beta = 1/2$, where $\sigma_0 = 0$ as $g \to g_c$, as expected for $J_1 = 0$ (Heisenberg model). With frustration, $J_1 \neq 0$ (red, blue and green symbols), however, $\sigma_0 \neq 0$ as $g \to g_c$ (with increasing saturation value for $\sigma_0$ with increasing $J_1/J_2$) indicating a 1st-order PT.](image2.png)
For $g < g_c$ (green triangles and blue diamonds) there is only one stable equilibrium solution for $\sigma$ (inset: minimum of $U(\sigma)$). For $g = g_c$ (red circles), eq. (6) produces a nonzero value of $\sigma$, while for $g > g_c$ (pink squares) no solution is found and $\sigma$ jumps to zero discontinuously above $g_c$, as in a 1st-order PT.

where

$$b_1(\sigma_0) = \int \frac{d^3k}{(2\pi)^3} k^2 \left( \frac{e^{-D_k^z(\sigma_0)/\Lambda^2}}{D_k^z(\sigma_0)} - \frac{e^{-D_k^z(\sigma_0)/\Lambda^2}}{D_k^z(\sigma_0)} \right),$$

and

$$b_2(\sigma_0) = -\int \frac{d^3k}{(2\pi)^3} k^2 \left( \frac{e^{-D_k^z(\sigma_0)/\Lambda^2}}{(D_k^z(\sigma_0))^2} - \frac{e^{-D_k^z(\sigma_0)/\Lambda^2}}{(D_k^z(\sigma_0))^2} \right).$$

and within such approximation we can rewrite the system of self-consistent equations (4) in terms of a single self-consistent variable, namely

$$\sigma_0 = \sqrt{f(\sigma_0, m_0(\sigma_0))}. \quad (6)$$

Figure 4 shows the plots of eq. (6) for $J_1/J_2 = 0.2$ and for different values of the coupling constant $g$. For $g = g_1 < g_c$ (green triangles) $y_1(\sigma_0) = \sqrt{f(\sigma_0, m_0(\sigma_0))}$ crosses the straight line $y_2(\sigma_0) = \sigma_0$ at only one point, giving the value of the staggered magnetisation for this value of the coupling constant. For $g_1 < g = g_2 < g_c$ (blue diamonds), however, we see that $y_1(\sigma_0)$ and $y_2(\sigma_0)$ cross twice. The first (smaller) value of the magnetisation, however, corresponds to a local maximum of the free energy $U(\sigma)$ (inset: unstable fixed point) and shall be discarded, while the magnetisation is then determined by the second (higher) crossing point solely. By further increasing the coupling constant $g = g_3 = g_c$ (red circles) we find a single critical solution to eq. (6) giving a finite, nonzero and sizeable value for the staggered magnetisation, which, however, ceases to exist for $g = g_4 > g_c$ (pink squares). The fact that the sublattice magnetisation jumps to zero discontinuously for $g > g_c$ indicates the 1st-order nature of the QPT.

It is important to emphasise that the magnon dispersion along the collinear directions $k_x = k_y = k$ is given by

$$\omega_{\text{NL}}(k) = c - \sqrt{2 - \gamma_0 |k|}, \quad \text{with} \quad c_2 = c_0^2 - c_1^2/2 \quad \text{[14,15]},$$

and thus acquires an imaginary part beyond the border at $\alpha < 0.5$ when $\gamma_0 > 2$, showing that the magnetic excitations of the collinear state move from $q = (\pi, 0)$ and/or $q = (0, \pi)$ towards the one of the Néel state at $q = (\pi, \pi)$, as expected. The complete phase diagram obtained within the NLSM formalism, for the whole range $0 \leq \alpha \leq 1$ is given in fig. 5.

**Conclusions.** – We have obtained the complete phase diagram of the antiferromagnetic $J_1$-$J_2$ Heisenberg model within the framework of the $O(N)$ nonlinear sigma model. We have found that the two magnetically ordered phases, Néel order for $\alpha \leq 0.4$, and collinear order for $\alpha \geq 0.6$, are separated by a nonmagnetic region at $0.4 \leq \alpha \leq 0.6$ where a gapped spin liquid is found. The transition at $\alpha = 0.4$ is of the second order while the one at $\alpha = 0.6$ is of the first order and the spin gaps cross linearly at $\alpha = 0.5$. Although our formalism does not allow us to make statements about what sort of spin liquid lies within $0.4 \leq \alpha \leq 0.6$, the universal behaviour of the correlation length (inverse spin gap) at zero temperature is captured correctly, as can be seen in fig. 5, in agreement with DMRG [11]. Finally, when finite temperature is considered, the magnetic order parameter of such $SU(2)$ invariant Hamiltonian should be vanishing, $\sigma_0(T \neq 0) = 0$, as dictated by the Hohenberg-Mermin-Wagner’s theorem, and, as a consequence, the finite-temperature correlation length, $\xi$, behaves analogously as the one obtained for the ordinary Heisenberg model [4], diverging exponentially as $T \to 0$ for $\alpha \leq 0.4$ and $\alpha \geq 0.6$, and becoming constant as $T \to 0$ for $0.4 \leq \alpha \leq 0.6$. Our results are exact at $N \to \infty$. 

Fig. 4: (Colour online) Solution of eq. (6) for fixed $J_1/J_2 = 0.2$. For $g < g_c$ (green triangles and blue diamonds) there is only one stable equilibrium solution for $\sigma$ (inset: minimum of $U(\sigma)$). For $g = g_c$ (red circles), eq. (6) produces a nonzero value of $\sigma$, while for $g > g_c$ (pink squares) no solution is found and $\sigma$ jumps to zero discontinuously above $g_c$, as in a 1st-order PT.

Fig. 5: (Colour online) Complete phase diagram of the $J_1$-$J_2$ model generated by the NLSM for both Néel and collinear orders, $0 \leq \alpha \leq 1$. The Néel order parameter $\sigma$ (filled black squares) vanishes continuously indicating a 2nd-order PT while the collinear order parameter $\sigma$ (filled red circles) jumps to zero at the critical point, indicating a 1st-order PT. The spin gaps $m_0/u$ (empty black squares and empty red circles, scaled up by a factor 5 for clarity and $u = \sqrt{2S\alpha J_1}$) cross linearly at the classical border at $\alpha = 0.5$, in agreement with DMRG [11].
and agree with numerical results from different methods, such as DMRG, series expansion, exact diagonalization and quantum Monte Carlo.

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