Journal of Statistical Mechanics: Theory and Experiment
An IOP and SISSA journal

The ground state phase diagram of the quantum J_1–J_2 spin-1/2 Heisenberg antiferromagnet on an anisotropic square lattice

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Received 22 March 2010
Accepted 24 May 2010
Published 28 June 2010

Online at stacks.iop.org/JSTAT/2010/P06022
doi:10.1088/1742-5468/2010/06/P06022

Abstract. We have studied the ground state phase diagram of the quantum spin-1/2 frustrated Heisenberg antiferromagnet on a square lattice by using the framework of the differential operator technique. The Hamiltonian is solved by using an effective-field theory for a cluster with two spins (EFT-2). The model is described using the Heisenberg Hamiltonian with two competing antiferromagnetic interactions: nearest neighbor (NN) with different coupling strengths J_1 and J_1' along the x and y directions and next nearest neighbor (NNN) with coupling J_2. We propose a functional for the free energy (similar to the Landau expansion) and using Maxwell construction we obtain the phase diagram in the (λ, α) space, where $\lambda = J_1'/J_1$ and $\alpha = J_2/J_1$. We obtain three different states depending on the values of λ and α: antiferromagnetic (AF), collinear antiferromagnetic (CAF) and quantum paramagnetic (QP). For an intermediate

J. Stat. Mech. (2010) P06022

region $\lambda_1 < \lambda < 1$ we observe a QP state between the ordered AF and CAF phases, which disappears for λ above some critical value $\lambda_1 \simeq 0.51$. We find a second-order phase transition between the AF and QP phases and a first-order transition between the CAF and QP phases. The boundaries between these ordered phases merge at the *quantum triple point* (QTP). Below this QTP there is again a direct first-order transition between the AF and CAF phases, with a behavior approximately described by the classical line $\alpha_c \simeq \lambda/2$.

Keywords: phase diagrams (theory), quantum phase transitions (theory)

Over the last two decades there has been an intense effort to understand, theoretically, the phase diagram and thermodynamic properties of *frustration* in the two-dimensional (2D) quantum spin-1/2 Heisenberg model (known as the J_1–J_2 model) with competing nearest neighbor (NN) and next nearest neighbor (NNN) antiferromagnetic exchange interactions [1]–[14]. This J_1–J_2 model has been exhaustively studied by several methods, where the critical properties are relatively well known at $T = 0$. There are two magnetically long-range ordered phases at small and at large values of $\alpha = J_2/J_1$ separated by an intermediate quantum paramagnetic phase without magnetic long-range order in the region between $\alpha_{1c} \simeq 0.4$ and $\alpha_{2c} \simeq 0.6$. For $\alpha < \alpha_{1c}$ the system possesses antiferromagnetic (AF) long-range order with wavevector $\mathbf{Q} = (\pi, \pi)$ and for $\alpha > \alpha_{2c}$ we have two degenerate collinear states which are the helical states with pitch vectors $\mathbf{Q} = (\pi, 0)$ and $(0, \pi)$. These two collinear states are characterized by a parallel spin orientation of nearest neighbors in the vertical (or horizontal) direction and an antiparallel spin orientation of nearest neighbors in the horizontal (or vertical) direction, and therefore exhibit Néel order within the initial sublattices A and B.

The nature of the transition between the AF and quantum paramagnetic (QP) phases as well as the proprieties of the QP phase and the precise values of the transition points are still debated. Candidates for being the QP phase include homogeneous spin-liquid (SL) states of various types with no broken symmetry [15] and a valence-bond solid (VBS) with some broken symmetry [16, 17]. Other possible candidate SL states include a resonating-valence-bond (RVB) state, proposed by Anderson [18], which has been supported by quantum Monte Carlo simulation [19]. Other studies have indicated that this intermediate phase (QP) is a dimerized state with both broken translational and rotational symmetries [20, 9], while others have supported instead a plaquette state with only broken translational symmetry and keeping the rotational symmetry preserved [5]. The quantum disordered state is a singlet state with gapped excitations to the first triplet state [14]. In the cuprate compounds, antiferromagnetism and high temperature superconductivity are separated by a pseudo-gap regime and it has been conjectured that this regime is connected to a QCP with unusual properties [21]. The AF order may give way to a spin-liquid phase before the phase coherence of the Cooper pairs sets in at somewhat larger doping.

For the nature of the phase transition between these two AF and SL phases some authors [22] have suggested a direct second-order quantum transition, which is not described by a Ginzburg–Landau-type critical theory, but is rather described in terms of a deconfined quantum critical point (QCP). This quantum phase transition, with different broken symmetries, is characterized by two seemingly independent order parameters (i.e.,

the staggered magnetization for the Néel phase and the dimer order parameter for the VBS phase or SL). These order parameters are represented in terms of the spinons (i.e., neutral spin-1/2 excitations which are confined in the two ordered phases), which themselves become deconfined physical degrees of freedom exactly at the QCP. Each of these phases has a different broken symmetry (i.e., spin-rotation symmetry for the AF phase and the lattice symmetry for the VBS phase). The deconfined phase transition theory [22] is still controversial and establishing the existence of the deconfined quantum criticality in an actual physical system is a non-trivial issue. Other authors, for example, Sirker *et al* [9], have argued by using spin wave theory and numerical results from series expansions that this transition is more likely to be a (weakly) first-order transition, where this quantum phase transition between the AF and SL phases must be due to a deconfinement of spinons. Also others have proposed perhaps less radical mechanisms for explaining such a second-order phase transition based on an effective-field theory (EFT) [23] within the standard Ginzburg–Landau critical theory.

An interesting phenomenon generated by frustration is the dimensional reduction recently observed in the Bose–Einstein condensation quantum phase transition in the $BaCuSi_2O_6$ compound [24]. Recently synthesis of layered magnetic materials [25]–[28], such as $SrZnVO(PO_4)_2$, Li_2VOSiO_4, Li_2VOGeO_4, $VOMoO_4$, and $BaCdVO(PO_4)_2$, which might be described by this frustrated model in the case of $J_2 \simeq J_1$ ($\alpha = J_2/J_1 \simeq 1$), has spurred a great deal of interest in the quantum spin-1/2 J_1–J_2 model. In these compounds a second-order phase transition to a long-range ordered magnetic phase has been observed. NMR spin–lattice relaxation measurements [25] below T_c show that the order is collinear. Due to the twofold degeneracy of the ground state for $\alpha > 0.7$ it is not possible to say *a priori* which will be the magnetic wavevector (i.e., $\mathbf{Q} = (\pi, 0)$ or $(0, \pi)$) below T_c. On the other hand, such a scenario can be changed by considering spin–lattice coupling which will lift the degeneracy of the ground state and will lower its energy [29]. Then, any structural distortion should inevitably reduce the competing interactions and thus reduce the frustration. In the case of this frustrated magnetic material, the competing interactions are inequivalent but their topology and magnitudes can be tuned so that the strong quantum fluctuations destroy the long-range ordering.

From the theoretical viewpoint, the isotropic J_1–J_2 model consists of a quantum spin-1/2 Heisenberg Hamiltonian with NN interaction J_1 running along the sides and NNN interaction J_2 running along the diagonals of the square lattice. The two interactions (J_1 and J_2) are equivalent along all directions of the square lattice. The ground state phase diagram reveals two ordered phases: antiferromagnetic—AF ($\alpha < \alpha_{1c}$) and collinear—CAF ($\alpha > \alpha_{2c}$), and an intermediate quantum paramagnetic (spin-liquid) phase without magnetic long-range order in the parameter region $\alpha_{1c} < \alpha < \alpha_{2c}$. A generalization of this frustrated model was introduced by Nersesyan and Tsvelik [30] and also studied by other groups [31]–[36]: the so-called J_1–J_1'–J_2 model, considering inequivalence of NN couplings J_1 and $J_1' = \lambda J_1$ in the two orthogonal spatial lattice dimensions with all the NNN bonds across the diagonals having the same strength J_2. This spatial anisotropy tends to narrow the critical region and destroys it completely at a certain value of the interchain parameter λ.

On the other hand, by using the continuum limit of the J_1–J_1'–J_2 spin-1/2 model Starykh and Balents [31] have shown that this transition splits into two, with the presence of an intermediate quantum paramagnetic (columnar dimer) phase for $\lambda \leq 1$.

J. Stat. Mech. (2010) P06022

Bishop *et al* [34], by using the coupled cluster treatment, found the surprising and novel result that there exists a quantum triple point (QTP) with coordinates at ($\alpha_t = 0.33 \pm 0.02$, $\lambda_t = 0.60 \pm 0.03$), below which there is a second-order phase transition between the AF and CAF phases while above this QTP there are two ordered phases separated by the intermediate magnetically disordered phase (VBS or RVB). The order parameters of both the AF and CAF phases vanish continuously both below and above the QTP, which is typical of second-order phase transitions. There is some evidence that the transition between the CAF and intermediate phases is a first-order one. Using exact diagonalization [32] with a small lattice of $N \leq 36$ (6×6) size, the intermediate QP phase for all intervals of $\lambda \in [0, 1]$ has been obtained for the pure spin-1/2 J_1–J_2 model on a square lattice. These results are in accordance with results obtained by Starykh and Balents [31], that predicted no QTP in the ground state phase diagram recently observed by Bishop *et al* [34].

Experimentally the ground state phase diagram of frustrated compounds, described by the J_1–J_2 model, can be explored continuously from the high to the low $\alpha = J_2/J_1$ regime by applying high pressures (P), which modify the bonding lengths and angles. Recent results from x-ray diffraction measurements [37] on the Li_2VOSiO_4 compound have shown that the ratio α decreases by about 40% when the pressure increases from 0 to 7.6 GPa. Studies of extensive band structure calculations [36] for the vanadium phosphates $ABVO(PO_4)_2$ (AB = Pb_2, SrZn, BaZn, and BaCd) have indicated four inequivalent exchange couplings: J_1 and J_1' between NN and J_2 and J_2' between NNN. For example, for $SrZnVO(PO_4)_2$, $J_1'/J_1 \simeq 0.7$ and $J_2'/J_2 \simeq 0.4$ were estimated, causing a spin–lattice distortion.

In previous studies [23], [38]–[41], effective-field theory (EFT) was developed and used to treat a few frustrated models (classical and quantum) on two- and three-dimensional lattices. In this work we will apply EFT to study the ground state phase diagram of the quantum spin-1/2 J_1–J_1'–J_2 model in the α–λ plane (where $\alpha = J_2/J_1$ and $\lambda = J_1'/J_1$). The objective of this work is to investigate the existence of a QTP (*quantum triple point*) at non-zero values of α and λ, as well as the nature of the phase transitions (first or second order?)

The critical behavior of the quantum spin-1/2 J_1–J_2 Heisenberg model has been studied for many years, but very little has been done in the anisotropic square lattice case, which is described by the following Hamiltonian:

$$\mathcal{H} = \sum_{\langle i,j \rangle} \left(J_1 \boldsymbol{\sigma}_{i,j} \cdot \boldsymbol{\sigma}_{i+1,j} + J_1' \boldsymbol{\sigma}_{i,j} \cdot \boldsymbol{\sigma}_{i,j+1} \right) + J_2 \sum_{\langle\langle i,j \rangle\rangle} \left(\boldsymbol{\sigma}_{i,j} \cdot \boldsymbol{\sigma}_{i+1,j+1} + \boldsymbol{\sigma}_{i+1,j} \cdot \boldsymbol{\sigma}_{i,j+1} \right), \qquad (1)$$

where $\boldsymbol{\sigma}_{i,j} = (\sigma_{i,j}^x, \sigma_{i,j}^y, \sigma_{i,j}^z)$ are the spin-1/2 Pauli spin operators, and the index (i, j) labels the x (row) and y (column) components of the lattice sites. The first sum runs over all NN and the second sum runs over all NNN pairs. We denote the Hamiltonian (1) as the J_1–J_1'–J_2 model, with strength J_1 along the row direction, J_1' along the column direction, and J_2 along the diagonals, and we assume all couplings to be positive with $J_1' < J_1$. In our EFT calculations we set $\alpha = J_2/J_1$ and $\lambda = J_1'/J_1$ to obtain the ground state ($T = 0$) phase diagram in the α–λ plane.

The classical ($S = \infty$) model (1) has only two ordered ground states: AF (or Néel) for $\alpha > \lambda/2$ and columnar stripe (CAF) for $\alpha < \lambda/2$, separated by a first-order line at $\alpha_c = \lambda/2$. In the $S = 1/2$ case (quantum limit), the line splits into two phase

J. Stat. Mech. (2010) P06022

transitions, where the ordered states (AF and CAF) are separated by an intermediate quantum paramagnetic (QP) phase, also on a square lattice. Exact diagonalization [11] has estimated a critical line at $\alpha_{\rm CAF} = \alpha_{\rm c} + 5\lambda^2/8\pi^2$ for the transition between the CAF and QP states, and at $\alpha_{\rm AF} = \alpha_{\rm c} - \lambda^2/8\pi^2$ between the AF and QP states. The phase diagram in the α–λ plane obtained is in accordance with Starykh and Balents [31]. However, the existence of the QTP (*quantum triple point*) that was predicted by Bishop *et al* [34] is not present in their phase diagram. Moreover, they found only the presence of second-order phase transitions in the phase diagram. These contradictory qualitative results (existence or absence of the QTP) is the primary motivation behind this present work. Our goal is to study this anisotropic J_1–J_1'–J_2 model using our EFT-2 technique. Mean-field theory works fairly well for small frustration. For large frustration one must take into account quantum fluctuations especially in two dimensions, where they are quite large.

The effective-field theory technique is briefly described below (for more details see [23], [38]–[41]). The starting point is to calculate the averages of a general function involving spin operator components, the order parameter (the magnetization of sublattice A is m_A), that are obtained from the generic expression

$$\langle \mathcal{O}(\{n\})\rangle = \left\langle \frac{{\rm Tr}_{\{n\}}\left\{\mathcal{O}(\{n\}){\rm e}^{-\beta\mathcal{H}_{\{n\}}}\right\}}{{\rm Tr}_{\{n\}}\left\{{\rm e}^{-\beta\mathcal{H}_{\{n\}}}\right\}}\right\rangle . \tag{2}$$

Above, the partial trace ${\rm Tr}_{\{n\}}\{\cdots\}$ is taken over the set $\{n\}$ of spin variables (*finite cluster*) specified by the multisite spin Hamiltonian $\mathcal{H}_{\{n\}}$ and $\langle\cdots\rangle$ indicates the usual canonical thermal average. The interactions within the cluster are exactly treated and the effect of the remaining lattice spins is treated by means of a suitable approximation which forms the basis of the *effective-field theory* technique.

The EFT provides a hierarchy of approximations for obtaining thermodynamic properties of magnetic models. On can continue this series of approximations to consider larger and larger clusters and as a consequence, better results are obtained. The exact solution would be obtained by considering an infinite cluster. In practice it is necessary to use systematic approximation schemes to truncate them to some finite cluster. However, as shown below, by using relatively small clusters which contain the topology of the lattice, one can obtain a reasonable description of the thermodynamic properties. The EFT is an effective tool for studying highly frustrated quantum models [23], [38]–[41], where, for example, the quantum Monte Carlo simulation is not applicable due to the negative-sign problem.

As in our previous work on frustrated models [23], [38]–[41], we use here the EFT for a cluster with $N = 2$ spins (EFT-2) to investigate the effect of the interchain coupling (J_1') in the ground state phase diagram in the λ–α plane. We chose a cluster with two spins in the vertical direction (see figure 1), and the Hamiltonian (1) for this cluster is given by

$$\mathcal{H}_2 = J_1'\boldsymbol{\sigma}_a\cdot\boldsymbol{\sigma}_b - A\sigma_a^z - B\sigma_b^z, \tag{3}$$

with

$$A = -\left[J_1'\sigma_3^z + J_1\left(\sigma_1^z+\sigma_5^z\right) + J_2\left(\sigma_2^z+\sigma_4^z+\sigma_6^z+\sigma_{10}^z\right)\right], \tag{4}$$

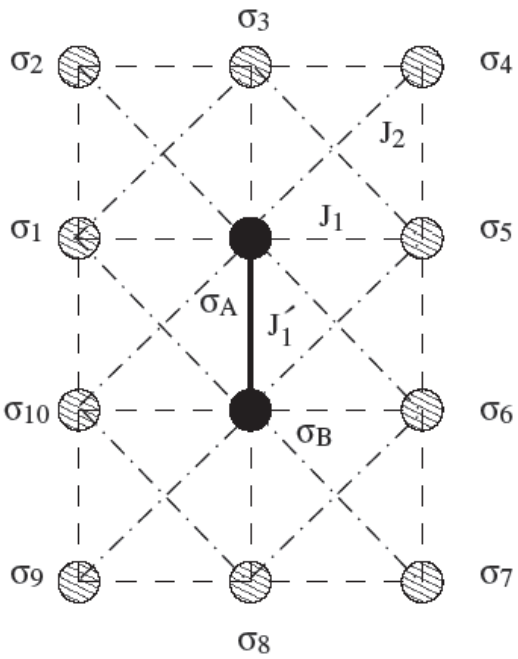

Figure 1. Configuration of the cluster with $N = 2$ spins used to treat the model (1) by using EFT-2.

and

$$B = -\left[J_1'\sigma_8^z + J_1\left(\sigma_6^z + \sigma_{10}^z\right) + J_2\left(\sigma_1^z + \sigma_5^z + \sigma_7^z + \sigma_9^z\right)\right]. \tag{5}$$

Substituting equation (3) in (2), we obtain the magnetization per spin in sublattice A (i.e., $m_A = \langle\sigma_a^z\rangle$) which is given by

$$m_A = \left\langle \frac{\sinh\left[\beta(A+B)\right] + \left(\mathrm{e}^{2K_1'}/W(A,B)\right)\sinh\left[W(A,B)\right]}{\cosh\left[\beta(A+B)\right] + \mathrm{e}^{2K_1'}\cosh\left[W(A,B)\right]} \right\rangle, \tag{6}$$

where $W(A,B) = \sqrt{4K_1'^2 + \beta^2(A-B)^2}$ and $K_1' = \beta J_1'$.

We now define the function $g(x,y)$ by

$$g(x,y) = \frac{\sinh(x+y) + \left(\mathrm{e}^{2K_1'}/W(x,y)\right)\sinh\left[W(x,y)\right]}{\cosh(x+y) + \mathrm{e}^{2K_1'}\cosh\left[W(x,y)\right]}, \tag{7}$$

where $W(x,y) = \sqrt{4K_1'^2 + (x-y)^2}$. Next using the identity $\mathrm{e}^{aD_x+bD_y}g(x,y) = g(x+a, y+b)$ where $D_\mu = (\partial/\partial\mu)$ is the differential operator, equation (6) can be rewritten as

$$m_A = \left\langle \mathrm{e}^{\beta(AD_x+BD_y)} \right\rangle g(x,y)\big|_{x,y=0}. \tag{8}$$

Now using the van der Waerden identity $\mathrm{e}^{\theta\sigma_i^z} = \cosh\theta + \sigma_i^z\sinh\theta$, equation (8) can be exactly written in terms of the multiple-spin-correlation function occurring on the right-hand side. However, is clear that if we try to treat exactly all boundary spin–spin correlation functions, the problem becomes unmanageable. The simplest and most frequently used approximation is to decouple them according to

$$\left\langle \sigma_i^z \cdot \sigma_j^z \cdots \sigma_l^z \right\rangle \simeq \left\langle \sigma_i^z \right\rangle \cdot \left\langle \sigma_j^z \right\rangle \cdots \left\langle \sigma_l^z \right\rangle (i \neq j \neq \cdots \neq l), \tag{9}$$

which means that the NN and NNN of site i are assumed to be completely independent of each other. It should be noted that the above decoupling scheme (equation (9)) is a better approximation than the approximations used in standard mean-field theory (MFT). This is because within the present framework (EFT-2) the kinematics relation is treated exactly (i.e., $(\sigma_i^z)^2 = 1$) through the van der Waerden identity and as a consequence it neglects correlations only between different spin variables. On the other hand in the usual MFT all the self-spin and multi-spin correlations are neglected.

For treatment of the model (1) by using EFT-2, we use the classical ground state (AF or Néel at small J_2 and CAF at large J_2). To obtain the equation of state in the AF phase, we use the following boundary conditions: (i) $\langle\sigma_i^z\rangle = -m_{\rm AF}$ for $i = 1, 3, 5, 7, 9$ and (ii) $\langle\sigma_i^z\rangle = m_{\rm AF}$ for $i = 2, 4, 6, 8, 10$, as given by

$$m_{\rm AF} = \Omega_{\rm AF}(m_{\rm AF}, t, \alpha, \lambda) = \sum_{r=0}^{4} A_{2r+1}^{\rm AF}(t, \alpha, \lambda) m_{\rm AF}^{2r+1}, \tag{10}$$

where $t = k_B T/J_1$, $\alpha = J_2/J_1$, $\lambda = J_1'/J_1$ and the coefficients $A_p^{\rm AF}(t, \alpha, \lambda)$ are determined analytically by applying the identity $\mathrm{e}^{aD_x + bD_y} g(x, y) = g(x+a, y+b)$. The final expression is too lengthy and will therefore be omitted.

In the case of the CAF state, we use the following boundary conditions: (i) $\langle\sigma_i^z\rangle = -m_{\rm CAF}$ for $i = 1, 2, 4, 5, 6, 7, 9, 10$ and (ii) $\langle\sigma_i^z\rangle = m_{\rm CAF}$ for $i = 3, 8$, and the equation of state is given by

$$m_{\rm CAF} = \Omega_{\rm CAF}(m_{\rm CAF}, t, \alpha, \lambda) = \sum_{r=0}^{4} A_{2r+1}^{\rm CAF}(t, \alpha, \lambda) m_{\rm CAF}^{2r+1}, \tag{11}$$

where the expressions for the coefficients $A_p^{\rm CAF}(t, \alpha, \lambda)$ are again omitted here.

We observe first-order or second-order transitions, depending on the values of the parameters α and λ. We note that it is not possible to calculate the first-order transition line on the basis of just the equations of state (equations (10), and (11)). To solve this problem one needs to calculate the free energy for each state (AF, CAF and QP). Assuming that these equations of state are obtained by the minimization of a given free energy functional like $\Psi_\mu(m_\mu)$, i.e., $(\mathrm{d}\Psi_\mu(m_\mu)/\mathrm{d}m_\mu) = 0$, we obtain after integration

$$\Psi_\mu(m_\mu) = \Delta_1(t, \alpha, \lambda) + \Delta_2(t, \alpha, \lambda) \left[1 - \sum_{r=0}^{4} A_{2r+1}^{\mu}(t, \alpha, \lambda) \frac{m_\mu^{2r}}{r+1}\right] \frac{m_\mu^2}{2}, \tag{12}$$

where $\Delta_p(t, \alpha, \lambda)$ are arbitrary functions which turn out to be irrelevant for searching for the second-order and first-order transitions.

The zero-temperature phase diagram in the λ–α plane contains first-order and second-order lines. To obtain these phase transitions we have used a Maxwell construction that corresponds to the intersection point where the free energies of the phases are equal. In the case of the transitions between the AF (CAF) ordered and QP ($m = 0$) disordered phases we obtain the point of intersection $\Psi_\mu(m_\mu) = \Psi_{\rm QP}(m = 0)$ from equation (12):

$$\sum_{r=0}^{4} A_{2r+1}^{\mu}(t, \alpha, \lambda) \frac{m_\mu^{2r}}{r+1} = 1. \tag{13}$$

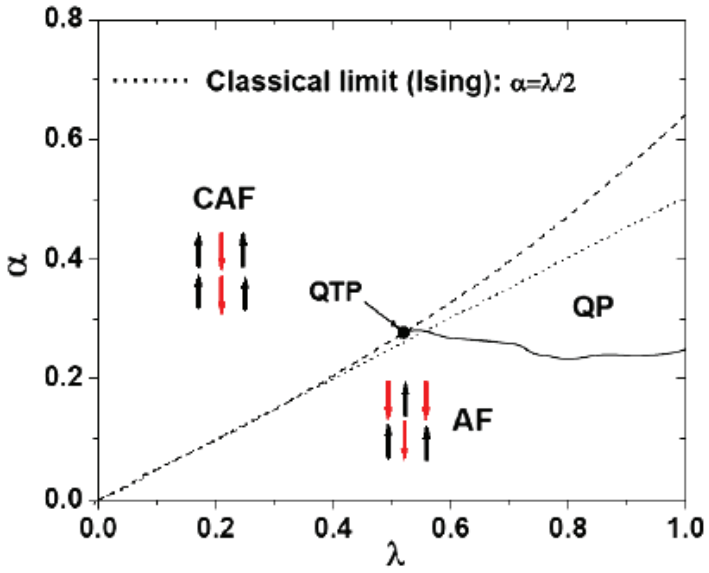

Figure 2. Ground state phase diagram in the λ–α plane for the quantum spin-1/2 J_1–J_1'–J_2 model on a square lattice, where $\alpha = J_2/J_1$ and $\lambda = J_1'/J_1$. The dashed and solid lines correspond to the first-order and second-order transition lines, respectively. The black point represents the *quantum triple point* (QTP). AF, CAF and QP correspond to the antiferromagnetic, collinear antiferromagnetic and quantum paramagnetic phases, respectively.

In the ground state ($T = 0$), the quantum phase transitions in the λ–α plane between the AF (CAF) and QP states are found by simultaneously solving two transcendental expressions, equation (13) and the equation of state $m_\mu = \Omega_\mu(m_\mu, 0, \alpha, \lambda)$. For the second-order transition between the AF and QP phases, we obtain $m_{\rm AF} = 0$, while for the first-order transitions between the CAF and QP phases we have $m_{\rm CA} \neq 0$ which corresponds to the discontinuity of the staggered magnetization $m^*_{\rm CAF}(\alpha)$ at $\alpha_{\rm c}(\lambda)$.

For the case of the quantum phase transition between the two ordered phases (AF and CAF), using Maxwell construction, we obtain

$$\sum_{r=0}^{4} A^{\rm AF}_{2r+1}(t,\alpha,\lambda)\frac{m^{2r+2}_{\rm AF}}{r+1} - m^2_{\rm AF} = \sum_{r=0}^{4} A^{\rm CAF}_{2r+1}(t,\alpha,\lambda)\frac{m^{2r+2}_{\rm CAF}}{r+1} - m^2_{\rm CAF}. \qquad (14)$$

By simultaneously solving three transcendental expressions, equations (10), (11) and (14), we obtain a direct first-order transition.

The ground state phase diagram in the λ–α plane of the quantum spin-1/2 J_1–J_1'–J_2 model on a square lattice is shown in figure 2. It is dependent on the values of α and λ. We observe three phases: AF (antiferromagnetic), CAF (collinear antiferromagnetic), and QP (quantum paramagnetic). For $\lambda > \lambda_1 \simeq 0.51$ there exists a disordered (QP) intermediate region between the AF and CAF phases. The order parameters of the AF ($m_{\rm AF}$) and CAF ($m_{\rm CAF}$) phases vanish continuously and discontinuously, respectively, both below and above the correspondingly *quantum triple point* (QTP). The presence of the interchain parameter λ has the general effect of suppressing the QP phase. The QP phase region decreases gradually with the decrease of the parameter λ, and it disappears

completely at the QTP $\equiv (\lambda_1, \alpha_1)$ where the boundaries between phases merge. Below this QTP, which is for $\lambda < \lambda_1$, there is a direct first-order transition between the AF and CAF phases, with a transition line $\alpha_c \simeq \lambda/2$ (like the classical line).

In summary, we have studied the ground state phase diagram of the anisotropic quantum spin-1/2 J_1–J_1'–J_2 model on a square lattice in the λ–α plane. The influence of quantum fluctuations, frustration (α) and interchain coupling (λ) has been discussed. Using the differential operator technique within the so-called effective-field theory for a cluster with $N = 2$ spins (EFT-2), we obtain a closed set of analytical equations for the free energy ($\Psi_\mu(m_\mu)$) and order parameters ($m_{\rm AF}$ and $m_{\rm CAF}$) which can be used to determine the phase transition lines. The phase diagram is equivalent (qualitatively) to the one obtained by the coupled cluster method (CCM) [34], where a QTP was observed at $\lambda_1 \simeq 0.60$. With EFT-2 we find the QTP at $\lambda_1 \simeq 0.51$. On the other hand, the results on the nature of the phase transitions analyzed by using the CCM were inconclusive, indicating that the transitions are all continuous (second-order ones), while with our method we have obtained that the CAF–AF and CAF–QP transitions are first-order ones. In the isotropic limit ($\lambda = 1$), our calculations reproduce the results obtained by Viana and de Sousa [23]. However, our estimated values for the quantum critical points are underestimated in comparison with the values obtained by other methods [1]–[14]. Using linear spin wave theory (see, for example, [1, 2] for the isotropic case), the results do not show the existence of a QTP in the phase diagram. Our result, that there exists a QTP along with first-order phase transitions between the different phases, is in conflict with results obtained using other methods such as the linear spin wave theory, CCM, and exact diagonalization approaches. It may be worthwhile to investigate the existence of a QTP and to characterize the true ground state phase diagram of the J_1–J_1'–J_2 model on a square lattice using other analytical or numerical methods, such as using quantum Monte Carlo simulations and higher order spin wave theory calculations.

Acknowledgments

This work was partially supported by CNPq and CAPES (Brazilian agencies).

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J. Stat. Mech. (2010) P06022

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