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The influence of Ising anisotropy on the zero-temperature phase transition in the square lattice spin- $\frac{1}{2}$ J - J' model

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Abstract

We use a variational mean-field-like approach, the coupled cluster method (CCM), and exact diagonalization to investigate the ground-state order–disorder transition for the square lattice spin-half XXZ model with two different nearest-neighbour couplings J and J' . On increasing $J' > J$ the model shows in the isotropic Heisenberg limit a second-order transition from semi-classical Néel order to a quantum paramagnetic phase with enhanced local dimer correlations on the J' bonds at about $J'_c \sim 2.5 \dots 3J$. This transition is driven by the quantum competition between J' and J . On increasing the anisotropy parameter $\Delta > 1$ we diminish the quantum fluctuations and thus the degree of competition. As a result the transition point J'_c is shifted to larger values. We find indications for a linear increase of J'_c with Δ , i.e. the transition disappears in the Ising limit $\Delta \rightarrow \infty$.

1. Introduction

The study of zero-temperature phase transitions driven by quantum fluctuations has been a subject of great interest to physicists during the last decade; see [1–4] and references therein. For order–disorder quantum phase transitions we basically need the interplay between the interparticle interactions and fluctuations. A canonical model to study quantum phase transitions is the spin-half Heisenberg model with competing interactions in two dimensions. Competition between bonds appears in frustrated systems. Besides frustration, there is another mechanism weakening the ground-state Néel order in Heisenberg antiferromagnets, namely the competition of non-equivalent nearest-neighbour (NN) bonds leading to the formation of local singlets of two (or even four) coupled spins. In contrast to frustration, which yields

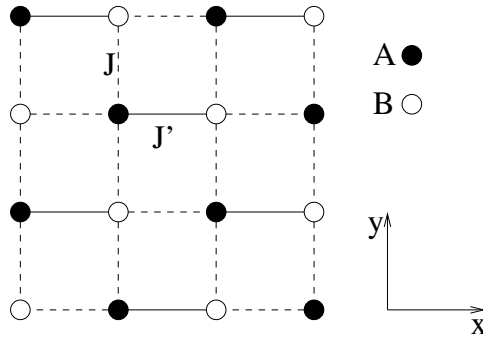


Figure 1. Illustration of the arrangement of bonds in the J – J' model on the square lattice (equation (1)): J —dashed lines; J' —solid lines; A and B characterize the two sublattices of the classical Néel ground state.

competition in quantum as well as in classical systems, this type of competition is present only in quantum systems.

Recent experiments on $\text{SrCu}_2(\text{BO}_3)_2$ [5, 6] and on CaV_4O_9 [7, 8] demonstrate the existence of gapped quantum paramagnetic ground states in (quasi-)two-dimensional Heisenberg systems, and have stimulated various theoretical studies of quantum spin lattices with competing interactions. A famous example for competition in a frustrated Heisenberg antiferromagnet is the spin-half J_1 – J_2 model on the square lattice, where the frustrating J_2 bonds plus quantum fluctuations lead to a second-order transition from Néel ordering to a disordered quantum spin liquid; see for example, [9–13]. On the other hand, it has been predicted that frustration may lead to a first-order transition in quantum spin systems in contrast to a second-order transition in the corresponding classical model [14–17]. An example for competition without frustration is the ‘melting’ of semi-classical Néel order by local singlet formation in Heisenberg systems with two non-equivalent nearest-neighbour bonds like the bilayer antiferromagnet [18, 19], the J – J' antiferromagnet on the square lattice [17, 20, 21], and on the depleted square (CaVO) lattice [22, 23].

In the above-mentioned papers [17–20, 22, 23] the strength of quantum fluctuations is tuned by variation of the exchange bonds. Alternatively, the strength of quantum fluctuations can be tuned by the anisotropy Δ in an XXZ model.

In this paper we study the influence of the Ising anisotropy on the zero-temperature magnetic order–disorder transition for the J – J' spin-half XXZ antiferromagnet on the square lattice. We use a variational mean-field-like approach (MFA), the coupled cluster method (CCM), and exact diagonalization (ED). We mention that the CCM, being one of the most powerful methods of quantum many-body theory, has previously been applied to various quantum spin systems with much success [12, 17, 21, 24–28].

2. Model

We consider an anisotropic spin- $\frac{1}{2}$ Heisenberg (XXZ) model on the square lattice with two kinds of nearest-neighbour bonds J and J' , as shown in figure 1:

$$H = J \sum_{\langle ij \rangle_1} (s_i^x s_j^x + s_i^y s_j^y + \Delta s_i^z s_j^z) + J' \sum_{\langle ij \rangle_2} (s_i^x s_j^x + s_i^y s_j^y + \Delta s_i^z s_j^z). \quad (1)$$

The sums over $\langle ij \rangle_1$ and $\langle ij \rangle_2$ run over the two kinds of nearest-neighbour bonds, respectively (cf figure 1). Each square-lattice plaquette consists of three J bonds and one J' bond. We

consider antiferromagnetic bonds $J' \geq J > 0$, i.e. there is no frustration in the model. In what follows we set $J = 1$ and consider the Ising anisotropy $\Delta \geq 1$ and J' as the parameters of the model. Since there is no frustration the classical ground state is the two-sublattice Néel state.

3. Methods

3.1. The variational mean-field approach (MFA)

For the square-lattice antiferromagnet ($J = J'$) the ground state is Néel ordered. The corresponding uncorrelated mean-field state is the Néel state $|\phi_{\text{MF}_1}\rangle = |\uparrow\rangle|\downarrow\rangle|\uparrow\rangle|\downarrow\rangle\cdots$. In the limit $J' \rightarrow \infty$ and for finite Δ the ground state approaches a rotationally invariant product state of local pair singlets (valence-bond state) $|\phi_{\text{MF}_2}\rangle = \prod_{i \in A} \{|\uparrow_i\rangle|\downarrow_{i+\hat{x}}\rangle - |\downarrow_i\rangle|\uparrow_{i+\hat{x}}\rangle\}/\sqrt{2}$, where i and $i + \hat{x}$ correspond to those sites which cover the J' bonds. In order to describe the transition between both states, we consider an uncorrelated product state of the form [17, 19]

$$|\Psi_{\text{var}}\rangle = \prod_{i \in A} \frac{1}{\sqrt{1+t^2}} [|\uparrow_i\downarrow_{i+\hat{x}}\rangle - t|\downarrow_i\uparrow_{i+\hat{x}}\rangle]. \quad (2)$$

The trial function $|\Psi_{\text{var}}\rangle$ depends on the variational parameter t and interpolates between the valence-bond state $|\phi_{\text{MF}_2}\rangle$ realized for $t = 1$ and the Néel state $|\phi_{\text{MF}_1}\rangle$ realized for $t = 0$. By minimizing $E_{\text{var}} = \langle \Psi_{\text{var}} | H | \Psi_{\text{var}} \rangle$ with respect to the variational parameter t we obtain

$$\frac{E_{\text{var}}}{N} = \begin{cases} -\frac{1}{24\Delta}(J'^2 + 3\Delta^2 J' + 9\Delta^2) & \text{for } J' \leq 3\Delta \\ -\frac{1}{8}J'(\Delta + 2) & \text{for } J' > 3\Delta. \end{cases} \quad (3)$$

The relevant order parameter describing the Néel order is the sublattice magnetization

$$M_s = \langle \Psi_{\text{var}} | S_{i \in A}^z | \Psi_{\text{var}} \rangle = \begin{cases} \frac{1}{2}\sqrt{1 - (J'/3\Delta)^2} & \text{for } J' \leq 3\Delta \\ 0 & \text{for } J' > 3\Delta. \end{cases} \quad (4)$$

M_s vanishes at the critical value $J'_c = 3\Delta J$. The corresponding critical index is the mean-field index 1/2. Equation (3) may be rewritten in terms of M_s as

$$E_{\text{var}}/N = -\frac{1}{8}J'\Delta - \frac{1}{4}J'\sqrt{1 - 4M_s^2} - \frac{3}{2}\Delta M_s^2. \quad (5)$$

We expand E_{var} up to the fourth order in M_s near the critical point and we find a Landau-type expression, given by

$$E_{\text{var}}/N = -\frac{1}{8}J'(\Delta + 2) + \frac{1}{2}(J' - 3\Delta)M_s^2 + \frac{1}{2}J'M_s^4. \quad (6)$$

3.2. The coupled cluster method (CCM)

The CCM formalism is now briefly considered; for further details the interested reader is referred to [27, 28]. The starting point for the calculation of the many-body ground state is a normalized reference or model state $|\Phi\rangle$. For our model the appropriate reference state is the Néel state. To treat each site equivalently we perform a rotation of the local axis of the up spins such that all spins in the reference state align in the same direction, namely along the negative z axis. After this transformation we have $|\Phi\rangle = |\downarrow\rangle|\downarrow\rangle|\downarrow\rangle|\downarrow\rangle\cdots$. Now we define a set of multi-spin creation operators $C_I^\dagger = s_r^+, s_r^+ s_l^+, s_r^+ s_l^+ s_m^+, \dots$. The choice of the C_I^\dagger ensures that $\langle \Phi | C_I^\dagger = 0 = C_I | \Phi \rangle$, where C_I is the Hermitian adjoint of C_I^\dagger . The CCM parametrizations of the ket and bra ground states are then given by

$$|\Psi\rangle = e^S |\Phi\rangle, \quad S = \sum_{I \neq 0} S_I C_I^\dagger, \quad (7)$$

$$\langle \tilde{\Psi} | = \langle \Phi | \tilde{S} e^{-S}, \quad \tilde{S} = 1 + \sum_{I \neq 0} \tilde{S}_I C_I. \quad (8)$$

The correlation operators S and \tilde{S} contain the correlation coefficients S_I and \tilde{S}_I which have to be calculated. Using the Schrödinger equation, $H|\Psi\rangle = E|\Psi\rangle$, we can now write the ground-state energy as $E = \langle \Phi | e^{-S} H e^S | \Phi \rangle$. The order parameter is calculated by $M_s = -\langle \tilde{\Psi} | s_i^z | \Psi \rangle$.

To find the correlation coefficients S_I and \tilde{S}_I we have to require that the expectation value $\bar{H} = \langle \tilde{\Psi} | H | \Psi \rangle$ is a minimum with respect to S_I and \tilde{S}_I . This formalism is exact if we take into account all possible multispin configurations in the correlation operators S and \tilde{S} . Of course, this is impossible for our model. Thus we have to use approximation schemes to truncate the expansion of S and \tilde{S} in equations (7) and (8). The most common scheme is the LSUB n scheme, where we include only n or fewer correlated spins in all configurations (or lattice animals in the language of graph theory) which span a range of no more than n adjacent lattice sites.

To improve the results it is useful to extrapolate the ‘raw’ CCM-LSUB n results to the limit $n \rightarrow \infty$. Although no exact scaling theory for results of LSUB n approximations is available, there are empirical indications [17, 25, 27, 28] of scaling laws for the order parameter for antiferromagnetic spin models. In accordance with those findings we use $M_s(n) = M_s(\infty) + a_1(1/n) + a_2(1/n)^2$ to extrapolate to $n \rightarrow \infty$. Vanishing $M_s(\infty)$ determines the critical point J'_c . The values for J'_c obtained by extrapolation of the LSUB n results for M_s are, however, found to be slightly too large [17]. We may also consider the inflection points of the $M_s(J')$ curve for the LSUB n approximation, assuming that the true $M_s(J')$ curve will have a negative curvature up to the critical point. We might expect that (for increasing n) the inflection point J'_{inf} approaches the critical point J'_c . Thus determining the inflection points for the LSUB n approximation again we can extrapolate to the limit $n \rightarrow \infty$ using a scaling law $J'_{\text{inf}}(n) = J'_{\text{inf}}(\infty) + b_1(1/n) + b_2(1/n)^2$ and interpret $J'_{\text{inf}}(\infty)$ as the critical value J'_c .

3.3. Exact diagonalization (ED)

In addition to the variational mean-field approach and the CCM we use ED to calculate the order parameter. We consider finite square lattices of $N = 8, 10, 16, 18, 20, 26, 32$ sites and employ periodic boundary conditions. The relevant order parameter for finite systems is the square of the sublattice magnetization M_s^2 , here defined as $M_s^2 = \langle [\frac{1}{N} \sum_{i=1}^N \tau_i s_i]^2 \rangle$ with the staggered factor $\tau_{i \in A} = +1$, $\tau_{i \in B} = -1$. For the finite-size scaling of M_s^2 we use the standard three-parameter formula [29–32]: $M_s^2(N) = M_s^2(\infty) + c_1 N^{-1/2} + c_2 N^{-1}$. The critical value J'_c is that point where $M_s^2(\infty)$ vanishes.

4. Results

To illustrate the behaviour of the order parameter’s dependence on J' we present $M_s(J')$ calculated by the CCM (figure 2) and by ED (figure 3) and the resulting extrapolated values for a particular value of Ising anisotropy $\Delta = 2$. Notice that corresponding results for the isotropic Heisenberg case ($\Delta = 1$) can be found in [17].

From the extrapolated order parameters one gets the critical values for $\Delta = 2$: $J'_c = 6.46$ (CCM) and $J'_c = 4.97$ (ED). The mean-field value is $J'_c = 6$. The inflection points of the $M_s(J')$ curves in figure 2 are $J'_{\text{inf}}(n) = 5.57$ (LSUB2), 5.42 (LSUB4), 5.26 (LSUB6), 5.11 (LSUB8) leading to an extrapolated value of $J'_c = J'_{\text{inf}}(\infty) = 4.66$. As mentioned above, the extrapolation of the CCM results of the order parameter tends to overestimate the critical value and yields the largest J'_c . This is connected with the change of the curvature in the M_s – J' curve in the vicinity of the critical point; cf figure 2. Therefore the critical value J'_c taken from the inflection points seems to be more realistic. Obviously, the difference in J'_{inf} between the LSUB n approximations is small and the extrapolated value is quite close to the

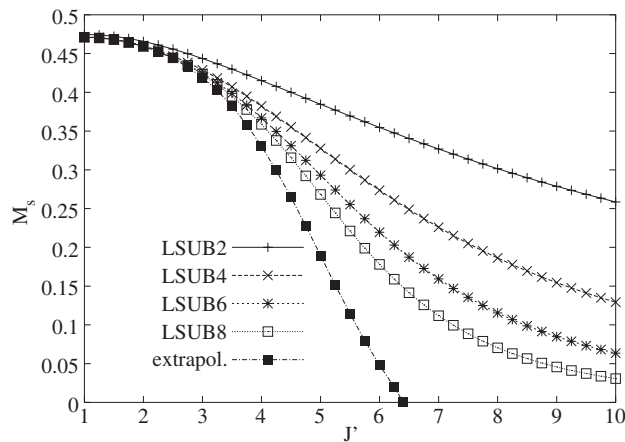


Figure 2. Sublattice magnetization M_s versus J' for $\Delta = 2$ using the coupled cluster method (CCM); see the text.

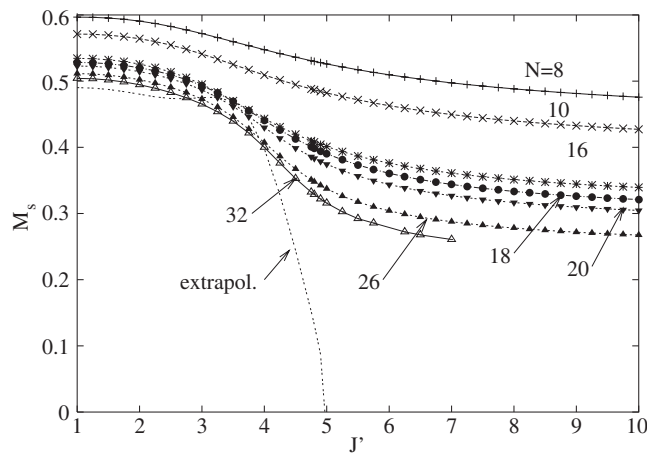


Figure 3. Order parameter versus J' for $\Delta = 2$ using exact diagonalization of finite lattices of different sizes N ; see the text.

value for LSUB8. This statement holds for all values of Δ . As an example, for $\Delta = 4$ one finds $J'_{\text{inf}} = 10.37$ (LSUB2), 10.29 (LSUB4), 10.13 (LSUB6), 9.94 (LSUB8), leading to an extrapolated value of $J'_c = J'_{\text{inf}}(\infty) = 9.41$.

Our results for the critical point $J'_c(\Delta)$ obtained by MFA, CCM and ED are collected in figure 4. We find that the CCM results obtained by the extrapolation of the order parameter are in good agreement with the MFA data. On the other hand, there is an excellent agreement between the CCM results obtained by the extrapolation of the inflection points and the ED results obtained by the extrapolation of the order parameter. Clearly we see indications for a linear increase in J'_c as predicted by mean-field theory.

We mention that the curves shown in figure 4 cannot be extrapolated to $\Delta < 1$. Similar to the effect of the Ising anisotropy ($\Delta > 1$) one rather expects an increase of J'_c due to XY anisotropy, i.e. for $0 \leq \Delta < 1$. Indeed for the pure XY $J-J'$ model ($\Delta = 0$) the critical value was estimated as $J'_c = 4.56J$ [33].

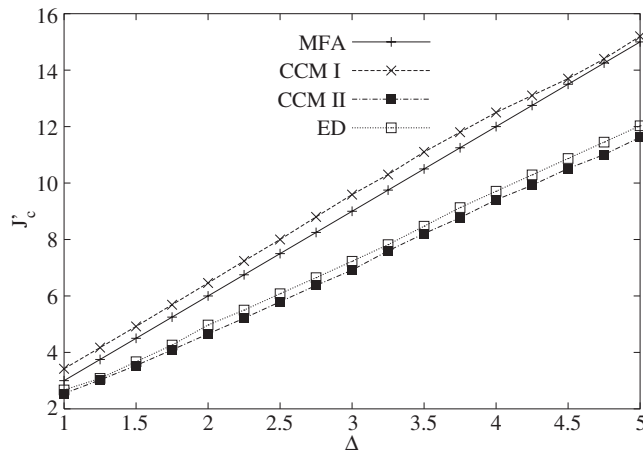


Figure 4. The critical points J'_c versus anisotropy parameter Δ using the mean-field approach (MFA), CCM with extrapolation of the order parameter (CCM I), CCM with extrapolation of the inflection points (CCM II), and exact diagonalization (ED).

5. Summary

We have studied the zero-temperature magnetic ordering in a square-lattice spin-half anisotropic Heisenberg (XXZ) model with two kinds of nearest-neighbour exchange bonds J and J' ; see figure 1. In particular we discuss the influence of the Ising anisotropy Δ on the position of the quantum critical point J'_c separating the phase with semi-classical Néel order ($J' < J'_c$) and the quantum paramagnetic phase without magnetic long-range order ($J' > J'_c$). For this we calculate the order parameter within a variational mean-field approach, the coupled cluster method, and exact diagonalization of finite lattices up to $N = 32$ sites. We find to a good approximation a linear relation $J'_c(\Delta) \propto \alpha \Delta$ ($\Delta \geq 1$) with $\alpha \sim 2.3 \dots 3.0$. This result can be attributed to the reduction of quantum spin fluctuations with increasing Ising anisotropy. In the pure Ising limit ($\Delta \rightarrow \infty$) the only remaining z - z terms in the Hamiltonian (1) commute with each other, i.e. no quantum spin fluctuations are present, and consequently the critical point disappears in the pure Ising limit.

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References

- [1] Sachdev S 1999 *Quantum Phase Transitions* (Cambridge: Cambridge University Press)
- [2] Richter J, Krüger S, Farnell D and Bishop R 2001 Quantum phase transitions in spin systems *Series on Advances in Quantum Many-Body Theory* vol 3, ed R F Bishop, K A Gernoth and N R Walet (Singapore: World Scientific) pp 239–46
- [3] Shopova D V and Uzunov D I 2003 *Phys. Rep.* **379** 1
- [4] Richter J, Schulenburg J and Honecker A 2004 Quantum magnetism in two dimensions: from semi-classical Néel order to magnetic disorder *Quantum Magnetism (Springer Lecture Notes in Physics)* ed U Schollwöck, J Richter, D J J Farnell and R F Bishop (Berlin: Springer) at press

- [5] Taniguchi S, Nishikawa T, Yasui Y, Kobayashi Y, Sato M, Nishioka T, Kontani M and Sano K 1995 *J. Phys. Soc. Japan* **64** 2758
- [6] Troyer M, Kontani H and Ueda K 1996 *Phys. Rev. Lett.* **76** 3822
- [7] Kageyama H, Yoshimura K, Stern R, Mushnikov N V, Onizuka K, Kato M, Kosuge K, Slichter C P, Goto T and Ueda Y 1999 *Phys. Rev. Lett.* **82** 3168
- [8] Koga A and Kawakami N 2000 *Phys. Rev. Lett.* **84** 4461
- [9] Chandra P and Doucot B 1988 *Phys. Rev. B* **38** 9335
- [10] Richter J 1993 *Phys. Rev. B* **47** 5794
- [11] Oitmaa J and Zheng W 1996 *Phys. Rev. B* **54** 3022
- [12] Bishop R F, Farnell D J J and Parkinson J B 1998 *Phys. Rev. B* **58** 6394
- [13] Capriotti L and Sorella S 2000 *Phys. Rev. Lett.* **84** 3173
- [14] Xian Y 1995 *Phys. Rev. B* **52** 12485
- [15] Niggemann H, Uimin G and Zittartz J 1997 *J. Phys.: Condens. Matter* **9** 9031
- [16] Richter J, Ivanov N B and Schulenburg J 1998 *J. Phys.: Condens. Matter* **10** 3635
- [17] Krüger S E, Richter J, Schulenburg J, Farnell D J J and Bishop R F 2000 *Phys. Rev. B* **61** 14607
- [18] Sandvik A W and Scalapino D J 1994 *Phys. Rev. Lett.* **72** 2777
- [19] Gros C, Wenzel W and Richter J 1995 *Europhys. Lett.* **32** 747
- [20] Singh R R P, Gelfand M P and Huse D A 1988 *Phys. Rev. Lett.* **61** 2484
- [21] Krüger S E and Richter J 2001 *Phys. Rev. B* **64** 024433
- [22] Troyer M, Kontani H and Ueda K 1996 *Phys. Rev. Lett.* **76** 3822
- [23] Troyer M, Imada M and Ueda K 1997 *J. Phys. Soc. Japan* **66** 2957
- [24] Roger M and Hetherington J H 1990 *Phys. Rev. B* **44** 200
- [25] Bishop R F, Hale R G and Xian Y 1994 *Phys. Rev. Lett.* **73** 3157
- [26] Bishop R F, Parkinson J B and Xian Y 1991 *Phys. Rev. B* **44** 9425
- [27] Zeng C, Farnell D J J and Bishop R F 1998 *J. Stat. Phys.* **90** 327
- [28] Bishop R F, Farnell D J J, Krüger S E, Parkinson J B and Richter J 2000 *J. Phys.: Condens. Matter* **12** 6877
- [29] Neuberger H and Ziman T 1989 *Phys. Rev. B* **39** 2608
- [30] Hasenfratz P and Niedermayer F 1993 *Z. Phys. B* **92** 91
- [31] Oitmaa J, Hamer C J and Zheng W 1994 *Phys. Rev. B* **50** 3877
- [32] Sandvik A W 1997 *Phys. Rev. B* **56** 11678
- [33] Tomczak P and Richter J 2001 *J. Phys. A: Math. Gen.* **34** L461