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QUANTUM PHASE TRANSITIONS IN SPIN SYSTEMS

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We discuss the influence of strong quantum fluctuations on zero-temperature phase transitions in a two-dimensional spin-half Heisenberg system. Using a high-order coupled cluster treatment, we study competition of magnetic bonds with and without frustration. We find that the coupled cluster treatment is able to describe the zero-temperature transitions in a qualitatively correct way, even if frustration is present and other methods such as quantum Monte Carlo fail.

1 Introduction

Phase transitions have been a subject of great interest to physicists over many decades. Besides classical or thermal phase transitions, the so-called quantum phase transitions (or zero-temperature transitions) have started to attract a lot of attention (e.g., see Ref. 1). The study of a variety of simple models allows us to understand which aspects of thermal and zero-temperature phase transitions are common to classes of models and which are more special. For continuous order-disorder transitions we basically need the interplay between the interparticle interactions and fluctuations. For thermal transitions the Ising model may serve as the simplest model. The equilibrium state corresponds to a minimum of the free energy, and we have competition between energy and entropy controlled by the temperature. For zero-temperature transitions no thermal fluctuations are present, and the fluctuations arise due to Heisenberg's uncertainty principle. A corresponding basic model which has strong quantum fluctuations is the spin-half Heisenberg antiferromagnet (HAFM), particularly in low dimensions.

The subject of quantum spin-half Heisenberg antiferromagnetism in low-dimensional systems has attracted a great deal of interest in connection with the magnetic properties of the high-temperature superconductors. Although we know from the Mermin-Wagner theorem² that thermal fluctuations are strong enough to destroy magnetic long-range order (LRO) at any finite temperature in 1D and 2D, the role of quantum fluctuations is less understood. It is now clear that the ground-state of the HAFM in 1D is not long-range ordered, whereas the HAFM on the square lattice is long-range ordered (e.g., see Ref. 3). However, in 2D there are many other lattices with different coordination numbers and topologies, and there is no general statement concerning zero-temperature Néel-like LRO.

Anderson and Fazekas have suggested⁴ that additional competition between magnetic bonds may increase quantum fluctuations and can suppress the Néel-like LRO in 2D. Indeed, the strength of this competition may serve as the control parameter of a zero-temperature order-disorder transition. The competition between

magnetic bonds in quantum spin systems can be caused in various ways. As for classical spin systems, frustration can affect the magnetic ordering in quantum spin systems. In the classical HAFM the frustration often leads to canted (e.g., spiral) spin states which may or may not have counterparts in the quantum HAFM. Furthermore, due to frustration Marshall's sign rule need not be fulfilled.⁵ The violation of the sign rule in frustrated systems makes their theoretical investigation particularly difficult. For example, the quantum Monte Carlo (QMC) method suffers from the minus sign problem in frustrated spin systems.

A generic model of a frustrated HAFM is the spin-half J_1 - J_2 model on the square lattice, where the frustrating J_2 bonds plus quantum fluctuations yield a second-order transition from a Néel-ordered state to a disordered quantum spin liquid (see, e.g., Refs. 6–9). On the other hand, there are examples where frustration leads to a first-order transition in quantum spin systems in contrast to a second-order transition in the corresponding classical model (see, e.g., Refs. 10–13).

Besides frustration there is a second type of competition between bonds which favours a Néel-like distribution of spin correlations over the lattice and other bonds which favour the formation of local spin singlets. By contrast to frustration, which yields competition in quantum as well as in classical systems, this type of competition is present only in quantum systems. The formation of local singlets is accompanied by the 'melting' of the magnetic LRO. This mechanism for breaking magnetic LRO may be relevant for the quantum disordered state in bilayer systems^{14,15} as well as in CaV_4O_9 (see, e.g., Refs. 16,17). Of course both mechanisms can be mixed as, for instance, in $\text{SrCu}_2(\text{BO}_3)_2$ (see, e.g., Refs. 12,13,18,19).

In this paper we discuss the quantum order-disorder transition driven by local singlet formation as well as the influence of quantum fluctuations on zero-temperature transitions driven by frustration. To that end we study a spin-half model on the square lattice in which both mechanisms, frustration and singlet formation, are observed in different regions. High-order implementations of the coupled cluster method (CCM) are used to obtain a consistent description of both types of competition for this model. The CCM (see, e.g., Ref. 20) is one of the most powerful and most universal techniques in quantum many-body theory, and has previously been applied to quantum spin systems^{8,21–25} with great success. In particular, we shall study to what extent the CCM is able to describe zero-temperature transitions in spin systems.

2 The Model

We consider a spin-half Heisenberg model on a square lattice with two kinds of nearest-neighbour bonds J and J' , as shown in Fig. 1,

$$H = J \sum_{\langle ij \rangle_1} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle ij \rangle_2} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (1)$$

The expressions $\langle ij \rangle_1$, and $\langle ij \rangle_2$ indicate nearest-neighbour bonds arranged in a regular zigzag pattern, as shown in Fig. 1 by the dotted and solid lines, respectively. Each square-lattice plaquette consists of three J bonds and one J' bond. If J' and J have different signs, then the plaquettes are frustrated, whereas competition

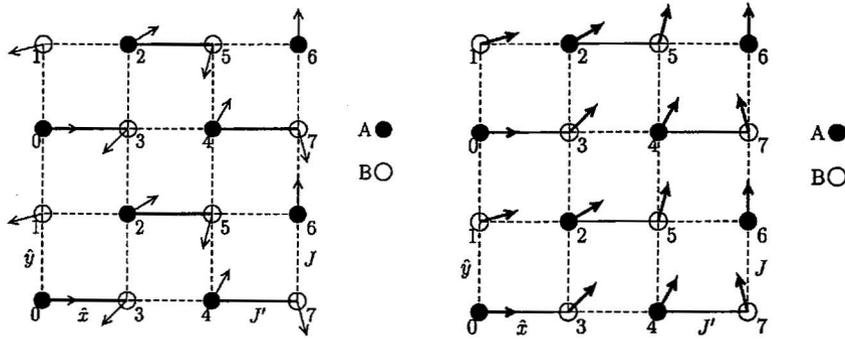


Figure 1. Illustration of the model (J -bonds correspond to dotted lines and J' -bonds to solid lines) and of the classical spiral state for antiferromagnetic $J = +1$ and ferromagnetic $J' < -1/3$ (left graph) and vice versa ($J = -1$, $J' > 1/3$) (right graph). As discussed in the text, both spiral states can be transformed into each other by reversing all of the spins on the B sublattice.

without frustration is realized for antiferromagnetic bonds $J' > J > 0$.

3 The Classical Ground State

To discuss the influence of quantum fluctuations on the ground-state (GS) properties of the model we need to know the classical GS of Eq. (1). We set $J = 1$. Without frustration ($J' > 0$), the classical GS is the Néel state, independent of the strength of J' . Frustration appears for (ferromagnetic) $J' < 0$. One finds that the Néel state remains the GS for small amounts of frustration, $0 \geq J' \geq -1/3$. At the critical point $J' = -1/3$, a second-order transition takes place from the Néel state to a spiral state characterized by a pitch angle $\Phi_{cl} = \arccos(\sqrt{1 - 1/J'}/2)$ (see left graph of Fig. 1). We note that $\Phi_{cl} = 0$ (for $J' > -1/3$) corresponds to the Néel state. The spin directions belonging to the A and B sublattices respectively, are given by $\mathbf{S}_A(\mathbf{R}) = e_x \cos \mathbf{Q} \cdot \mathbf{R} + e_y \sin \mathbf{Q} \cdot \mathbf{R}$ and $\mathbf{S}_B(\mathbf{R} + \hat{x}) = e_x \cos(\mathbf{Q} \cdot \mathbf{R} + \pi + 3\Phi) + e_y \sin(\mathbf{Q} \cdot \mathbf{R} + \pi + 3\Phi)$, where \mathbf{R} runs over the sites of the sublattice A, and $\mathbf{Q} = (2\Phi, 0)$. We note that this spiral state is incommensurate in the x -direction. By contrast to the quantum case, the classical model with $J = -1$ can be transformed into the model with $J = 1$ considered above by the simultaneous substitution $J \rightarrow -J$, $J' \rightarrow -J'$, $\mathbf{S}_{i \in B} \rightarrow -\mathbf{S}_{i \in B}$. Hence the physics for $J = -1$ is classically the same as for $J = +1$ (c.f., Fig. 1).

4 Competition Without Frustration

In this section we restrict our attention to the region where $J = +1$ and $J' > 0$. The terms within the Hamiltonian now compete, because the first term favours Néel LRO on the "honeycomb" lattice, whereas the second term favours an uncorrelated product state of local pair singlets (see below). Again, we emphasize that there is no competition in the classical model.

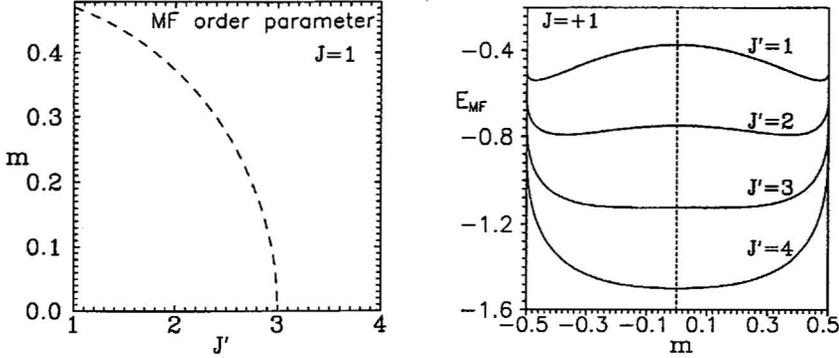


Figure 2. Sublattice magnetization versus J' (for $J = 1$) (left graph) and energy versus sublattice magnetization (right graph) using a mean field approach (2).

Mean Field Approach: We start with a simple mean-field (MF) like description of the order-disorder transition. The corresponding uncorrelated MF state for Néel LRO is the Néel state $|\phi_{\text{MF}_1}\rangle = |\uparrow\downarrow\uparrow\dots\rangle$, and for the dimerized singlet state it is the rotationally-invariant product state of local pair singlets $|\phi_{\text{MF}_2}\rangle = \prod_{i \in A} [|\uparrow_i\downarrow_{i+\hat{x}}\rangle - |\downarrow_i\uparrow_{i+\hat{x}}\rangle]/\sqrt{2}$, 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 interpolating between $|\phi_{\text{MF}_1}\rangle$ and $|\phi_{\text{MF}_2}\rangle$ of the form^{15,25}

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

We have $|\Psi_{\text{MF}}(t=0)\rangle = |\phi_{\text{MF}_1}\rangle$ and $|\Psi_{\text{MF}}(t=1)\rangle = |\phi_{\text{MF}_2}\rangle$. We minimize $\langle\Psi_{\text{MF}}|H|\Psi_{\text{MF}}\rangle$ with respect to t and obtain

$$\frac{E_{\text{MF}}}{N} = \frac{\langle\Psi_{\text{MF}}|H|\Psi_{\text{MF}}\rangle}{N} = \begin{cases} -\frac{3J'}{8} - \frac{1}{24J}(3J - J')^2 & J' \leq 3J \\ -\frac{3J'}{8} & J' > 3J, \end{cases} \quad (3)$$

for the energy per site. For the sublattice magnetization $m \equiv \langle\Psi_{\text{MF}}|S_{i \in A}^z|\Psi_{\text{MF}}\rangle$ we get $m = \sqrt{(3J - J')(3J + J')}/(6J)$ for $J' \leq 3J$ and $m = 0$ otherwise. Note that m vanishes at a critical point $J'_c = 3J$, and that the critical index is the MF index $1/2$. Eq. (3) may be rewritten in terms of m as $E_{\text{MF}}/N = -\frac{1}{8}J' - \frac{1}{4}J'\sqrt{1 - 4m^2} - \frac{3}{2}Jm^2$, and Fig. 2 illustrates that the dependence of E_{MF} on m corresponds to a typical scenario of a second-order transition. We can expand E_{MF} up to the fourth order in m near the critical point and find a Landau-type expression, given by $E_{\text{MF}}/N = -\frac{3}{8}J' + \frac{1}{2}(J' - 3J)m^2 + \frac{1}{2}J'm^4$. However, as discussed elsewhere for a similar magnetic model for CaV_4O_9 ,¹⁷ MF theory probably does not describe the critical behaviour correctly.

CCM: Let us now apply a high-order CCM approach (for details see Refs. 23,25) to this model. We set the classical collinear Néel state to be the reference state $|\Phi\rangle$. We calculate the GS wave function, $|\Psi\rangle = e^S|\Phi\rangle$ within the LSUB n approximation scheme up to $n = 8$ and extrapolate to $n \rightarrow \infty$. The CCM results for the order

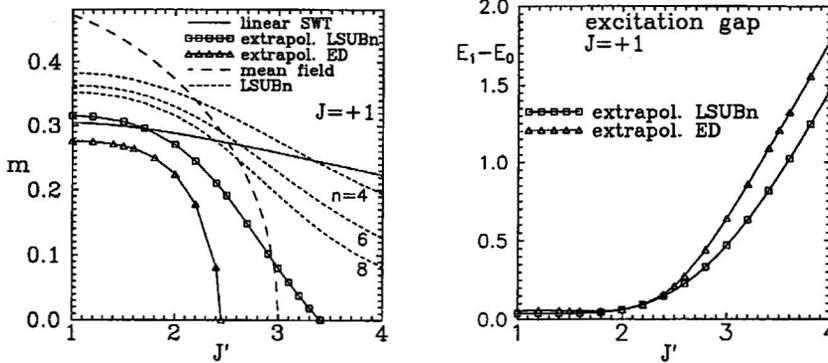


Figure 3. Sublattice magnetization (left graph) and excitation gap (right graph) versus J' .

parameter are shown in the left graph of Fig. 3 and they are compared to results of linear spin wave theory (SWT), exact diagonalization (ED) of $N=16,18,20,26,32$ sites, and the MF theory. The CCM is able to describe correctly the order-disorder transition, whereas conventional SWT cannot (for more details concerning the SWT and ED results see Ref. 25). The critical value predicted by extrapolation of the LSUB n results is, however, found to be slightly too large. We may also consider the inflection points of m versus J' for the LSUB n approximations. It is assumed that the true $m(J')$ -curve will have a negative curvature up to the critical point. Thus we might expect that (for increasing n) the inflection point approaches the critical point. We find the corresponding inflection points at $J' = 3.1$ ($n=2$), $J' = 3.0$ ($n=4$), $J' = 2.9$ ($n=6$), and $J' = 2.85$ ($n=8$), indicating a critical value J'_c somewhere between $2.5J$ and $3J$. Notice, that the estimation of $2.5 \lesssim J'_c/J \lesssim 3$ is consistent with results of series expansions and exact diagonalizations.^{25,26} The breakdown of Néel LRO due to singlet formation is also accompanied by the opening of an excitation gap between the singlet GS and the first triplet excitation. This behaviour is well described by the CCM (right graph of Fig. 3) which predicts that the gap opens in the range $2J < J' < 3J$ (and notice that the non-zero gap below $2J$ is a result of the limited accuracy of the extrapolation).

5 Competition with Frustration

We now consider the frustrated model (where J and J' have different signs). Due to the incommensurate classical spiral state the ED technique for finite-size systems is less appropriate. The CCM intrinsically considers the limit $N \rightarrow \infty$ from the outset and thus has no problems in dealing with incommensurate states. Hence the CCM appears to be particularly suitable to attack the frustrated quantum model. We choose the classical state to be our CCM model state, although quantum fluctuations may change the pitch angle of the spiral phase. Hence, we determine the 'quantum pitch angle' Φ by minimizing $E_{\text{LSUB}n}(\Phi)$ with respect to Φ .

Néel versus Spiral. We consider (antiferromagnetic) $J = +1$ and (ferromagnetic) $J' < 0$. Results for $E(\Phi)$ and $\Phi(J')$ are shown in Fig. 4. The main results are

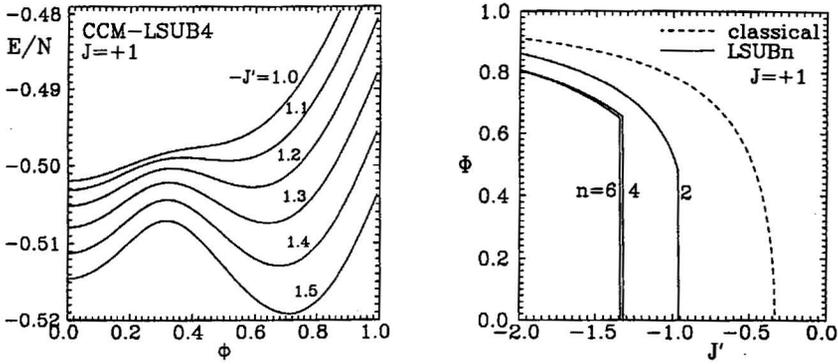


Figure 4. Energy versus quantum pitch angle for LSUB4 (left graph) and quantum pitch angle versus J' (right graph). Note, that $\Phi = 0$ corresponds to the Néel state.

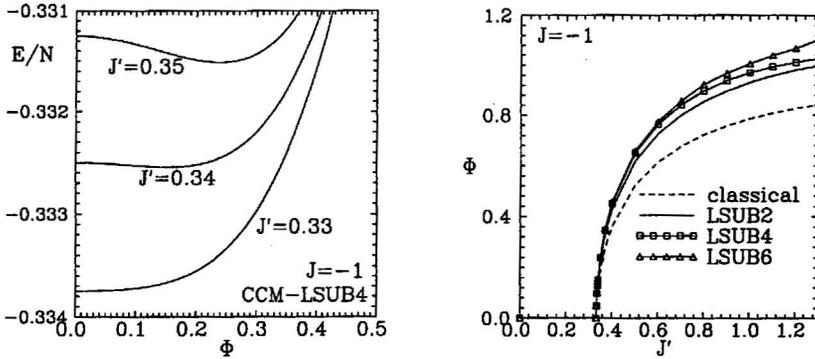


Figure 5. Energy versus quantum pitch angle for LSUB4 (left graph) and quantum pitch angle versus J' (right graph). Note, that $\Phi = 0$ corresponds to the fully polarized ferromagnetic state.

that: (i) In the quantum case the quantum Néel state remains the GS up to much stronger frustration than in the classical case. Indeed, it is generally found for spin systems, that quantum fluctuations favour collinear spin structures as opposed to noncollinear ones. (ii) The quantum fluctuations change the phase transition from second order to first order. (iii) The CCM yields a consistent description of the collinear and the spiral phases.

Ferro versus Spiral: We now consider the model for (ferromagnetic) $J = -1$ and (antiferromagnetic) $J' > 0$. In the classical model we again have a second-order transition from a collinear to a spiral state (see section 3). In the quantum model the situation is quite different. Although the collinear antiferromagnetic state possesses strong quantum fluctuations, the collinear, fully polarized, ferromagnetic state possesses no such quantum fluctuations. The corresponding results for $E(\Phi)$ and $\Phi(J')$ are shown in Fig. 5. By contrast to the situation at $J = +1$, the transition from the ferromagnetic to the noncollinear spiral is now of second order, the same as for the classical model. Furthermore, the classical critical point $J'/J = -1/3$

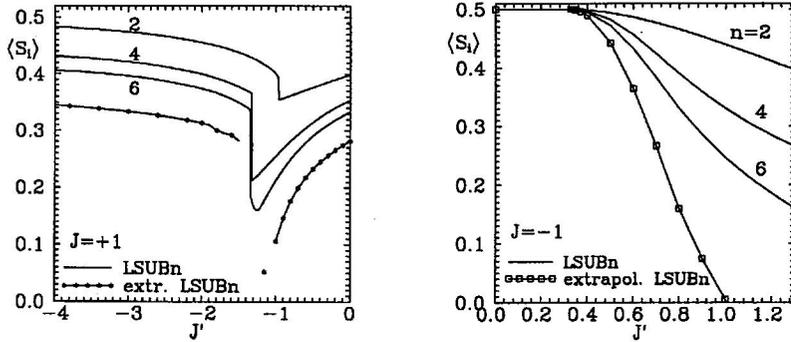


Figure 6. On-site magnetic moment versus J' for $J = +1$ (left graph) and $J = -1$ (right graph).

also holds for the quantum case. The difference between both cases also becomes evident when the order parameter $\langle S_i \rangle$ is considered (Fig. 6). For $J = +1$ there is a discontinuity in $\langle S_i \rangle$ at every level of LSUBn approximation. However, the extrapolation to $n \rightarrow \infty$ becomes imprecise close to the phase transition point. We cannot therefore decide whether the order parameter vanishes near to the transition point. For $J = -1$ there is a smooth change in $\langle S_i \rangle$ at the critical point. Increasing the antiferromagnetic J' the spiral magnetic order becomes weaker and vanishes at $J' \approx 1$. The underlying reason for that is local singlet formation, as discussed in section 4, and the continuous vanishing of the spiral order is therefore very similar to this second-order transition. However, the strength of J' needed for local singlet formation is much smaller due to the assisting effects of frustration (c.f., Ref. 15).

6 Conclusions

In this article we have investigated the zero-temperature phase transitions of a spin-half Heisenberg system on the square lattice. The main results of our treatment are: (i) Quantum fluctuations plus competition without frustration are able to destroy Néel LRO by local singlet formation. This is a pure quantum effect and has no classical counterpart. The control parameter is the strength of the competition and the breakdown of Néel ordering is accompanied by the opening of a spin gap. Standard SWT (even to higher orders) fails to describe this transition, whereas the CCM describes both the order parameter and the gap satisfactorily. Since we have no frustration, most standard techniques (e.g., QMC) are applicable and a quantitative description is possible. As was discussed in Ref. 17, the critical properties seem to correspond to the 3D classical Heisenberg model. (ii) Competition due to frustration was found to give more complex magnetic properties. In the model considered we have a second-order transition between collinear (antiferro- or ferro-magnetic) and noncollinear (spiral) states driven by frustration in the classical case. In the quantum spin-half model, standard techniques (e.g., QMC) are not applicable due to the violation of Marshall's sign rule. By contrast, the CCM provides a consistent description of collinear, noncollinear, and disordered phases.

Furthermore, we find a strong influence of quantum fluctuations on the nature of the collinear-noncollinear transition, and quantum fluctuations (which favour collinear ordering) may change the second-order classical transition to a first-order quantum transition. If quantum fluctuations are suppressed in the collinear phase, the transition to the spiral phase is similar for the quantum and classical models.

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