Summary of Dissertation "Quantum phase transitions in magnetic systems: Application of coupled cluster method"
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We present in this thesis theoretical investigation of quantum spin systems with competing interactions, quantum phase transitions in magnetic system and various problems concerned with and without frustrated magnetism, employing the coupled cluster method (CCM) for high orders of approximation, exact diagonalization (ED), and variational mean-field approach (MFA). In particular, we discuss the ground-state properties of different quantum spin models at zero temperature. In Chap. 3 we investigate the ground-state order-disorder transition for the square lattice spin-1/2 XXZ model with two different nearest-neighbor couplings J and J' using the CCM, ED and MFA. We study the influence of the anisotropy parameter Δ and spin quantum number s on this phase transition. We present evidence that the critical value J'_c increases with growing Δ and s according to $J'_c(\Delta) \propto \alpha\Delta$ ($\Delta \geq 1$) with $\alpha \sim 2.3 \ldots 3.0$ and $J'_c \propto s(s+1)$, i.e. the transition disappears in the Ising limit $\Delta \to \infty$ and in the limit $s \to \infty$. In Chap. 4 we study the ground state and the magnetization process of the spin-1/2 two-dimensional Shastry-Sutherland antiferromagnet. For the critical point J_2^c/J_1 where the semi-classical Néel order disappears we obtain a significantly lower value than J_2^d/J_1, namely, J_2^c/J_1 in the range $[1.14, 1.39]$. We therefore conclude that an intermediate phase exists between the Néel and the dimer phases. In Chap. 5 we present a method for the direct calculation of the spin stiffness by means of the CCM. For the spin-half Heisenberg antiferromagnet on the square, the triangular and the cubic lattices we calculate the stiffness in high orders of approximation. For the square and the cubic lattices our results are in very good agreement with the best results available in the literature. For the triangular lattice our result is more precise than any other result obtained so far by other approximate method. In Chap. 6 we investigate the phase diagram of the frustrated Heisenberg antiferromagnet, the J_1–J_2 model, in two dimensions. We have found that the quantum critical points for both the Néel and collinear order are $J_2^{c1} \approx 0.44 \ldots 0.45 J_1$ and $J_2^{c2} \approx 0.58 \ldots 0.59 J_1$ respectively, which are in good agreement with the results obtained by other approximations. We use the CCM and ED to analyse the generalized susceptibilities. We find that the phase transition from the Néel to the paramagnetic state at J_2^{c1} is second order. In Chap. 7 we also discuss the influence of interlayer coupling ($J_\perp$) on the quantum paramagnetic ground-state phase. We demonstrate that increasing the interlayer coupling $J_\perp > 0$ the parameter region of this phase decreases, and finally the quantum paramagnetic phase disappears for quite small $J_\perp \sim 0.2 - 0.3 J_1$. In Chap. 8 we use the CCM to investigate the GS phase diagram of the 2D J_1–J_1'–J_2 spin-1/2 and spin-1 Heisenberg model, where the nearest-neighbour bonds have different strengths J_1 and J_1' in, say, the x (intrachain) and y (interchain) directions respectively. In particular, we study the effect of the coupling J_1' on the Néel and stripe states. We found that for the spin-1/2 case there exists a quantum triple point (QTP) below which there is a second-order phase transition between the quasiclassical Néel and stripe-ordered phase with magnetic LRO, whereas only above this point are these two phases separated by the intermediate magnetically disordered phase seen in the pure spin-1/2 J_1–J_2 model ($J_1' = J_1$). The QTP was found to occur at $J_1'/J_1 \approx 0.60 \pm 0.03$, $J_2/J_1 \approx 0.33 \pm 0.02$. By contrast with the $s = 1/2$ case, we found for the spin-1 no evidence for a magnetically disordered state between the Néel and stripe states. However, for the $s = 1$ case we found instead strong evidence for the QTP at $J_1'/J_1 = 0.66 \pm 0.03$, $J_2/J_1 = 0.35 \pm 0.02$, where a line of second-order phase transitions between the quasiclassical Néel and columnar stripe-ordered phases (for $J_1'/J_1 \lesssim 0.66$) meets a line of first-order phase transitions between the same two phases (for $J_1'/J_1 \gtrsim 0.66$). In Chap. 9 we discuss the influence of an exchange anisotropy Δ on the zero-temperature phase transition of the spin-1/2 and spin-1 frustrated J_1–J_2 XXZ antiferromagnet on the square lattice. We find for spin-1/2 case strong evidence for two QTP's at ($\Delta^c = -0.10 \pm 0.15$, $J_2^c/J_1 = 0.505 \pm 0.015$) and ($\Delta^c = 2.05 \pm 0.15$, $J_2^c/J_1 = 0.530 \pm 0.015$), between which an intermediate magnetically-disordered phase emerges to separate the quasiclassical Néel and stripe collinear phases. Above the upper QTP ($\Delta \gtrsim 2.0$) we find a direct first-order phase transition between the Néel and stripe phases, exactly as for the classical case. The z-aligned and xy-planar-aligned phases meet precisely at $\Delta = 1$, also as for the classical case. For all values of the anisotropy parameter between those of the two QTP's there exists a narrow range of values of J_2/J_1, $\alpha^{c_1}(\Delta) < J_2/J_1 < \alpha^{c_2}(\Delta)$, centered near the point of maximum classical frustration, $J_2/J_1 = \frac{1}{2}$, for which the intermediate phase exists. This range is widest precisely at the isotropic point, $\Delta = 1$, where $\alpha^{c_1}(1) = 0.44 \pm 0.01$ and $\alpha^{c_2}(1) = 0.59 \pm 0.01$. The two QTP's are characterized by values $\Delta = \Delta^c$ at which $\alpha^{c_1}(\Delta^c) = \alpha^{c_2}(\Delta^c)$. For spin-1 we predict no intermediate disordered phase between the Néel and collinear stripe phases, for any value of the frustration J_2/J_1, for either the z-aligned ($\Delta > 1$) or xy-planar-aligned ($0 \leq \Delta < 1$) states. The quantum phase transition is determined to be first-order for all values of J_2/J_1 and Δ. The position of the phase boundary $J_2^c(\Delta)$ is determined accurately. It is observed to deviate most from its classical position $J_2^c = \frac{1}{2}$ (for all values of $\Delta > 0$) at the Heisenberg isotropic point ($\Delta = 1$), where $J_2^c(1) = 0.55 \pm 0.01$. By contrast, at the XY isotropic point ($\Delta = 0$), we find $J_2^c(0) = 0.50 \pm 0.01$. In the Ising limit ($\Delta \to \infty$) $J_2^c \to 0.5$ as expected.