Scaling of Critical Temperature and Ground State Magnetization near a Quantum Phase Transition

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We investigate a simple model antiferromagnet which shows a Quantum Phase Transition between a conventional Néel antiferromagnetic phase and a dimerized 'Valence Bond Solid' phase. Both the critical temperature and the ground state magnetization in the Néel phase approach zero at the critical point, and are found to scale according to power laws, with exponents 0.5, as expected from general considerations.

1. Introduction

The subject of Quantum Phase Transitions (QPT's) in condensed matter systems remains a frontier area of research [1]. These are transitions, at temperature $T = 0$, in the nature of the ground state of a strongly correlated quantum system. At QPT's large quantum fluctuations play the same role as do large thermal fluctuations at normal phase transitions, and analogous universal scaling laws are to be expected. In real materials QPT's can be induced by pressure, by applied magnetic fields, or by disorder.

Theoretical studies of QPT's are largely based on various simplified models, particularly low dimensional antiferromagnets, where the system can be tuned through a QPT by varying a particular parameter g in the Hamiltonian. Most of the models hereto studied have been two-dimensional. Examples include antiferromagnets with strong and weak bonds, with or without frustration, and bilayer systems, where the QPT separates a conventional Néel antiferromagnetic phase from a dimerized phase with only short-range correlations and no magnetic order. In such systems the magnetic order present in the ground state does not extend to finite temperatures.

In the present work we study a three-dimensional model where magnetic order persists to some critical temperature $T_c(g)$. We expect $T_c(g)$ to vanish as $g \rightarrow g_c$, and we are interested in comparing the vanishing of T_c with the vanishing of the ground state magnetization M_0. The magnetization is expected to vanish as $(g_c - g)^{\beta}$, where the critical exponent β is expected to have the value 0.5, corresponding to a classical thermally driven transition in four spatial dimensions, which is mean-field like (with possible logarithmic corrections). Does $T_c(g)$ scale with $(g_c - g)$ in the same way?

2. The model and results

Our model, shown in Fig. 1(a), is a spin-½ tetragonal antiferromagnet with bonds of strength J and gJ. For $g = 1$ we have an isotropic cubic antiferromagnet, which will have reduced Néel order in the ground state ($M_0 = 0.42$) and a critical temperature $k_B T_c/J = 1.89$. On the other hand, for $g >> 1$, the strong bonds will form spin-singlet dimers, leading to a phase with short-range correlations and no magnetic order. A QPT will separate these two phases, as shown schematically in Fig. 1(b).

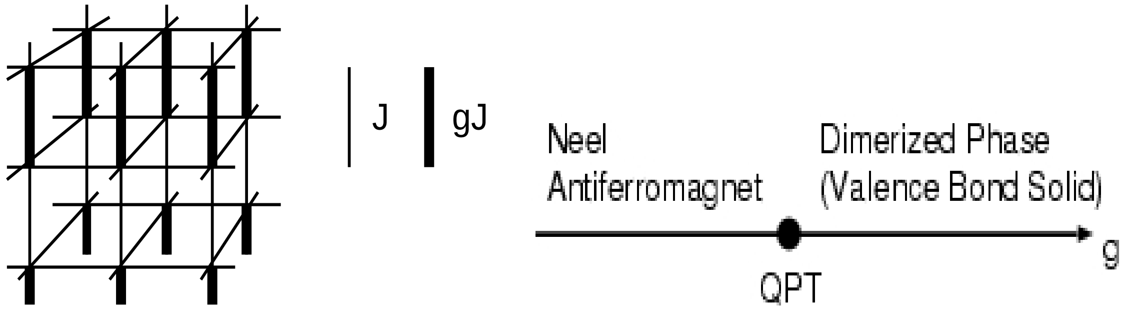

Fig. 1. (a) The model, with thin lines denoting J bonds and thick lines denoting gJ bonds;
(b) Schematic phase diagram for the model at temperature $T = 0$.

This model has been studied previously [2], in connection with magnetic-field induced QPT's, and the critical point located at $g_c = 4.013 \pm 0.003$ (in our units), using Quantum Monte Carlo (QMC) methods. However, the critical temperature in the Néel phase has not, to our knowledge, been previously studied.

Our calculations are based on series expansion methods [3], and involve a number of separate parts:

- In the ground state we compute the energy, starting from both Néel and dimer limits. The crossing point will determine the position of the QPT. The energy curves are shown in Fig. 2. As is apparent, the two curves meet smoothly, as expected for a second-order QPT, or Quantum Critical Point (QCP). It is not possible to locate g_c accurately from this crossing.
- We compute the magnetization at $T = 0$, in the Néel phase. This is also shown in Fig. 2. As is again apparent, the magnetization decreases rather sharply to zero near $g \sim 4.0$. Although the error bars become rather large near the QCP, from a Padé approximant analysis we estimate the critical point at $g_c = 4.05 \pm 0.05$, consistent with, but less precise than the QMC result. The merging of the energy curves is consistent with this value.
- Finally we compute high-temperature expansions for the Néel susceptibility. This is not the physical susceptibility, but the response to a 'staggered' field. This susceptibility is expected to have a strong divergence at the critical point, and can be used to estimate the critical temperature $T_c(g)$. This curve is also shown in Fig. 2. It is clear that the critical temperature also drops sharply to zero at the QCP. However, these series are rather short and, consequently, the error bars near the QCP large.

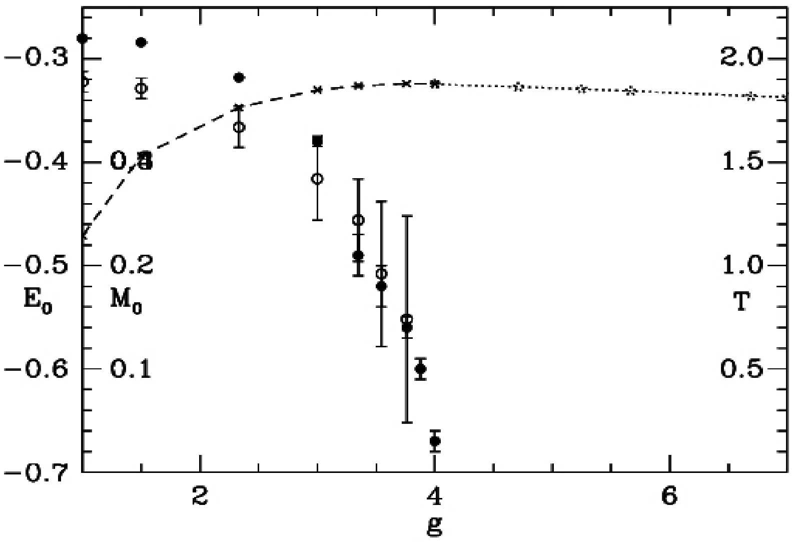

Fig. 2. Variation of the ground state energy E_0 in the Néel and dimer phases (dashed and dotted lines – left scale), the ground state magnetization M_0 in the Néel phase (solid circles – inner left scale), and the critical temperature T_c (open circles – inner right scale) with the tuning parameter g. The 'temperature' T plotted is the dimensionless quantity $k_B T_c / J_{av}$.

To investigate the scaling behaviour of M_0 and T_c in more detail, we first plot M_0^2 versus g. This is shown in Fig. 3 (left). Within the error limits the points lie on a straight line, confirming the scaling law $M_0 \sim (g_c - g)^{0.5}$, and yielding the more precise estimate $g_c = 4.02 \pm 0.02$. In Fig. 3 (right) we show log-log plots of both M_0 and T_c versus $(g_c - g)$. From the figure we see that the M_0 data fall well on a straight line with slope 0.5, consistent with the plot in Fig. 3 (left). It is not possible to estimate T_c as close to the QCP, and consequently there are fewer points and larger error bars. However, the points are also consistent with a power law, with the same exponent 0.5.

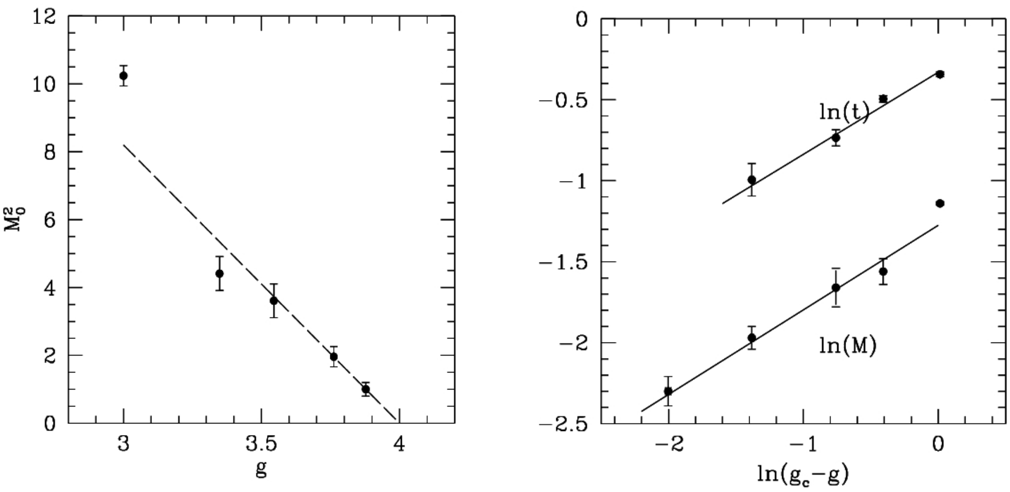

Fig. 3. (Left) Plot of M_0^2 versus g; (Right) Log – log plots of magnetization M_0 and critical temperature T_c versus $(g_c - g)$. The solid lines have slope 0.5.

3. Discussion

We have studied a three-dimensional spin model which has a Quantum Phase Transition between a conventional Néel ordered antiferromagnetic phase and a dimerized 'valence bond solid' phase which has no long-range magnetic order. The quantum critical point is located at $g_c = 4.01 \pm 0.01$. The ground state magnetization in the Néel phase is found to vanish as

$g \rightarrow g_c$ with a power law with exponent ½, as expected from general considerations. The critical temperature also vanishes as $g \rightarrow g_c$, and, within the limited precision of our results, appears to follow a power law with the same exponent ½.

Our model is not directly applicable to any real physical system. However, we believe that the results are universal. Recent work [4] on the material $TlCuCl_3$, where the QPT is induced by pressure, shows precisely the same kind of behaviour.

Acknowledgments

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References

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