Quantum Critical Points in Ising Systems with a Transverse Crystal Field

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We study a ferromagnetic Ising model with a transverse single-ion crystal field for various spins $S > 1/2$. The $S = 1$ model is mapped to the spin-1/2 transverse Ising model, allowing the $T = 0$ quantum critical point to be located exactly in 1-dimension and accurately in higher dimensions. The nature of the excited states of this model is also discussed. Generalisations to the models with $S = 3/2$ and $S = 2$ are developed.

Single-ion anisotropy generated by crystal fields plays an essential role in determining the properties of magnetic materials with spin $S > ½$ [1]. Ising models with longitudinal crystals fields, particularly variants of the Blume-Capel model [2], have been widely investigated in the literature, and have successfully described a range of physical phenomena. Recently, the ferromagnetic spin-S Ising model with a transverse crystal field has been studied by a number of authors [3,4].

Eddeqaqi et al. [3] have studied the spin-1 Ising model with a transverse crystal field, described by the Hamiltonian

$$H = -J\sum_{\langle i,j\rangle} S_i^z S_j^z - \Delta\sum_i \left(S_i^x\right)^2 \tag{1}$$

where the first sum is over nearest neighbour pairs, and Δ represents the strength of the crystal field. Using a generalised cluster mean-field method, they have calculated the phase diagram in the temperature-Δ/J plane for a number of lattices. They found that a critical line separates a magnetically ordered phase (low T, small Δ) from a disordered phase. They also computed the quantum critical points (QCP's) where this critical line meets the $T = 0$ axis.

We show here that the ground state properties of Hamiltonian (1) can be directly related to those of the famous spin-1/2 transverse Ising model, described by the Hamiltonian

$$H_{TIM} = -J\sum_{\langle i,j\rangle} \sigma_i^z \sigma_j^z - \Gamma\sum_i \sigma_i^x . \tag{2}$$

where Γ represents the strength of the transverse field that breaks the long range order. Hence, we are able to obtain the quantum critical points exactly in one-dimension, and considerably more accurately than [3] in higher dimensions. A more detailed description of this work is to be given in a forthcoming paper [5].

Let us choose z as the quantisation axis and take as the basis for the Hilbert space the usual product basis, $\{|m_1 m_2 \ldots m_N\rangle; m_i = -1,0,1\}$, where N is the number of sites in the lattice. The first step in establishing the correspondence between the ground states of Hamiltonians (1) and (2) is to note that the operator

$$N_0 = N - \sum_i \left(S_i^z\right)^2 \tag{3}$$

commutes with H. The eigenvalues of N_0 are the number of sites in the lattice with $m = 0$. Consequently, the Hamiltonian does not couple states with $m_i = 0$ to those with $m_i = \pm 1$, and the Hilbert space separates into disjoint sectors containing the states with particular values of $N_0 = 1, \ldots, N$.

In our forthcoming paper [5], it is formally proved that the ground state of Hamiltonian (1) always lies in the $N_0 = 0$ sector of the Hilbert space. Then, for the ground state, it suffices to consider just two states per site ($m = \pm 1$), and the Hamiltonian can be mapped to an equivalent spin-1/2 model. The formal mapping is

$$\begin{aligned} S_i^z &\to \sigma_i^z \\ S_i^+ S_i^+ &\to 2\sigma_i^+ \\ S_i^- S_i^- &\to 2\sigma_i^- \\ S_i^+ S_i^- &\to 1+\sigma_i^z \\ S_i^- S_i^+ &\to 1-\sigma_i^z \end{aligned} \tag{4}$$

where the σ_i are Pauli operators. The Hamiltonian (1) becomes

$$H \to H_{eff} = -\tfrac{1}{2} N\Delta - J\sum_{\langle i,j\rangle} \sigma_i^z \sigma_j^z - \tfrac{1}{2}\Delta \sum_i \sigma_i^x \tag{5}$$

which, to within a constant, is just H_{TIM}. Thus the quantum critical points of (1) can be immediately determined from those of H_{TIM}. The quantum critical points of the spin-1/2 transverse Ising model can be obtained exactly in 1-dimension [6], and in higher dimensions accurate results are available from linked-cluster expansions [7-9]. In Table 1 we give these values, and compare them with the results of Eddeqaqi et al. [3].

Table 1. Location of quantum critical points for Hamiltonian (1) for various lattices.

Lattice	$(\Delta/J)_c$	Result of [3]
Linear chain	±2	
Honeycomb lattice	±4.256	-3.65, 3.78
Square lattice	±6.088	-5.54, 5.81
Triangular lattice	±9.536	
Simple cubic lattice	±10.317	-9.436, 9.73

We note that there is small asymmetry in the mean field result for positive and negative values of Δ, which is an artefact of the approximation in [3]. We also note that the mean-field only involves the lattice structure through the coordination number *z*, and hence would give the same results for simple cubic and triangular lattices, whereas there is a clear difference. Notwithstanding this, the results of [3] are semi-quantitatively accurate, lying some 10-15% below our more accurate figures.

We also consider the more general Hamiltonian,

$$H = -J\sum_{\langle i,j\rangle} S_i^z S_j^z - \Delta_x \sum_i \left(S_i^x\right)^2 - \Delta_y \sum_i \left(S_i^y\right)^2 . \tag{6}$$

Much of the above analysis applies to this case. The mapping (4) yields

$$H \to H_{eff} = -\tfrac{1}{2} N\left(\Delta_x + \Delta_y\right) - J\sum_{\langle i,j\rangle} \sigma_i^z \sigma_j^z - \tfrac{1}{2}\left(\Delta_x - \Delta_y\right)\sum_i \sigma_i^x \tag{7}$$

This model has quantum critical points at $\tfrac{1}{2}\left(\Delta_x - \Delta_y\right) = \pm\Gamma_c$ for any ratio of Δ_x/Δ_y except 1. In that special case, the Hamiltonian (6) can be seen to reduce to the classical Blume-Capel model [2].

Next, consider the sectors of the Hilbert space of Hamiltonian (1) with $N_0 = 1,2,3,\ldots$. The Hamiltonian, acting on a state with some particular set of sites with $m = 0$, leaves these sites fixed. Referring to these sites as "holes", we note the bonds connecting holes to other sites in the lattice contain no energy, and hence can be deleted. The remaining network of sites with $m = \pm 1$ and connecting bonds can again be mapped to a transverse Ising model. For *p* holes, this mapping gives

$$H = H_{TIM} - \tfrac{1}{2}\Delta(N+p) \tag{8}$$

where H_{TIM} is defined on the (irregular) cluster of remaining sites and bonds. Each hole configuration is decoupled from the other configurations, implying that the levels in the sectors with $N_0 > 0$ will be highly degenerate.

For the case of the linear chain the analysis may be carried further. The ground state energy in the $N_0 = 0$ sector is [6]

$$E_0^{(0)} = -N(\varepsilon_\infty + \tfrac{1}{2}\Delta) + O(N^{-1}) \tag{9}$$

where $\varepsilon_\infty = \frac{2}{\pi}(1+\Gamma)E(\frac{\pi}{2}, m)$ with $m = 4\Gamma/(1+\Gamma)^2$ and $E(\frac{\pi}{2}, m)$ is the complete elliptic integral of the second kind. The lowest energy in the $N_0 = 1$ sector is

$$E_0^{(1)} = -(N-1)\varepsilon_\infty + \varepsilon_s - \tfrac{1}{2}\Delta(N+p) + O(N^{-1}) \tag{10}$$

where ε_s is the surface energy for a transverse Ising chain with free ends [10]. Hence we find

$$E_0^{(1)} - E_0^{(0)} = \varepsilon_\infty + \varepsilon_s - \tfrac{1}{2} + O(N^{-1}) \tag{11}$$

which is always positive. Thus, there is a gap to the lowest excitation with $N_0 > 0$.

Finally, we consider the Hamiltonian (1) for higher spin values, in particular for $S = \frac{3}{2}$ and *S* = 2. For the spin-3/2 case, a mapping of the ground state can be constructed to the spin-1/2 Hamiltonian (*z* is the lattice coordination number),

$$H \to H_{eff} = Const. - J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z - \tfrac{1}{2}(zJ - \Delta)\sum_i \sigma_i^z - \frac{\sqrt{3}}{2}\Delta\sum_i \sigma_i^x\,. \tag{12}$$

This is an Ising model with both transverse and longitudinal fields, which does not have a phase transition. The *S* = 2 Hamiltonian can be mapped to an effective Hamiltonian expressed in terms of the pseudospin-1 operators τ,

$$H \to H_{eff} = Const. - 4J\sum_{\langle i,j\rangle}\tau_i^z\tau_j^z + 2\Delta\sum_i(\tau_i^z)^2 - \sqrt{3}\Delta\sum_i \tau_i^x \tag{13}$$

the properties of which remain unexplored.

Further details of this work will appear in the forthcoming paper [5].

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