A solvable quantum antiferromagnet model

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Abstract

We introduce a quantum antiferromagnet model, having exactly soluble thermodynamic properties. It is an infinite range antiferromagnetic Ising model put in a transverse field. The free energy gives the ground state energy in the zero temperature limit and it also gives the low temperature behaviour of the specific heat, the exponential variation of which gives the precise gap magnitude in the excitation spectrum of the system. The detailed behaviour of the (random sublattice) staggered magnetisation and susceptibilities are obtained and studied near the Néel temperature and the zero temperature quantum critical point.

With the realisation in the mid last century, that the Néel state can not be the ground state, or even an eigenstate, of the quantum Heisenberg antiferromagnets, considerable efforts have gone in search for the nature of the ground state for such quantum antiferromagnets. Searches have also been made for low lying eigen states of Heisenberg antiferromagnets even in the semi-classical limits, or in some other variants of the model where exact ground state and other eigenstates are available [1,2]. In particular, the exact dimerised (two-fold degenerate; disordered) ground state in the one dimensional next nearest neighbour interacting Heisenberg antiferromagnet (having strength ratio 1/2 between the next nearest and nearest neighbours) has been found out [3] and this observation has attracted considerable attention in the context of high temperature superconductors occurring in materials having antiferromagnetic properties [1,2]. Regarding the excited states in such quantum antiferromagnets, the Haldane conjecture [2,4] states that the integer spin systems are massive (have a gap), while the half-integer ones are massless.

The low temperature limit of the exact free energy obtained here for the (spin-$\frac{1}{2}$) long-range interacting transverse Ising model shows that the specific heat has an exponential (in gap and inverse temperature) variation, giving the precise magnitude of the gap in the model. The order-disorder transition, driven both by temperature and the tunneling or transverse field, are investigated studying the ordering and susceptibility behaviours.

The model we study here has the Hamiltonian

$$H = \frac{J}{N}\sum_{i,j} S_i^z S_j^z - h\sum_i S_i^z - \Gamma \sum_i S_i^x, \tag{1}$$

where J denotes the long-range antiferromagnetic ($J>0$) exchange constant and S^x and S^z denote the x and z components of the N Pauli spins ($S=1/2$):

$$S_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \ S_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\ \ i=1,2,...,N.$$

Denoting half of the randomly chosen lattice sites as members of sublattice A and the rest of B, and expressing the cooperative term in Hamiltonian (1) as the difference of two quadratics, the Hamiltonian can be rewritten as

$$\begin{aligned} H &= \frac{J}{2N}\left(\left[\sum_i S_{i(A)}^z + \sum_i S_{i(B)}^z\right]^2 - \left[\sum_i S_{i(A)}^z - \sum_i S_{i(B)}^z\right]^2\right) \\ &\quad -h\sum_i (S_{i(A)}^z + S_{i(B)}^z) - \Gamma\sum_i (S_{i(A)}^x + S_{i(B)}^x). \end{aligned}$$

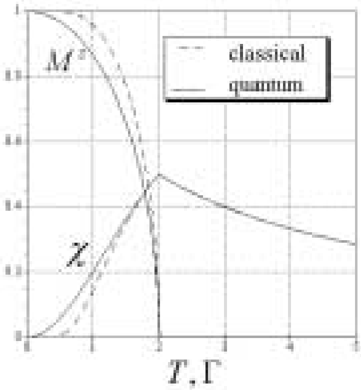

Figure 1: Variations of longitudinal sublattice magnetization and susceptibilities in the classical and quantum cases ($J = 1$).

In fact, the Hamiltonian (1) is meaningful when the spins in the cooperative term there belongs to two different (though randomly defined) sublattices, each consisting of $N/2$ spins. Using the Hubbard-Stratonovich transformation, the partition function can be expressed as

$$\begin{aligned} Z &= \mathrm{Tr}_{\,S_A,\,S_B} \int_{-\infty}^{\infty}\int_{-i\infty}^{+i\infty} \frac{idm_+ dm_-}{(2\pi/N\beta J)} \exp\left[\frac{N\beta J}{2}(m_+^2 - m_-^2)\right] \\ &\times \exp\Bigg[(\beta J m_+)\sum_i (S^z_{i(A)} + S^z_{i(B)}) + (\beta J m_-)\sum_i (S^z_{i(A)} - S^z_{i(B)}) \\ &+ \beta h \sum_i (S^z_{i(A)} + S^z_{i(B)}) + \beta\Gamma \sum_i (S^x_{i(A)} + S^x_{i(B)})\Bigg], \end{aligned} \tag{2}$$

where β denotes the inverse temperature T and m_+, m_- are related to the (uniform; z-component) magnetisation M_A^z and M_B^z of the sublattices A and B respectively: $m_+ = -(M_A^z + M_B^z)$ and $m_- = (M_A^z - M_B^z)$. The trace in (2) can now be easily performed [5] as each spin $\vec{S}$ can now be imagined to be isolated and present only in a vector field $\vec{h}$ having both z and x components: $h^x = \Gamma$ and $h^z \sim \beta J m$. In the $N \to \infty$ limit, the free energy f per spin can be obtained from

$$\begin{aligned} Z &= \exp[-N\beta f], \\ f &= \frac{J}{2}\left[(M_A^z + M_B^z)^2 - (M_A^z - M_B^z)^2\right] \\ &+ \frac{1}{2\beta}\log\left[\cosh\beta\sqrt{(2JM_B^z - h)^2 + \Gamma^2}\right] + \frac{1}{2\beta}\log\left[\cosh\beta\sqrt{(2JM_A^z - h)^2 + \Gamma^2}\right], \end{aligned} \tag{3}$$

where the sublattice magnetisations M_A^z and M_B^z are given by the (self-consistent) saddle point equations:

$$\begin{aligned} M_A^z &= \frac{(-2JM_B^z + h)}{\sqrt{(-2JM_B^z + h)^2 + \Gamma^2}} \tanh\beta\sqrt{(-2JM_B^z + h)^2 + \Gamma^2} \\ M_B^z &= \frac{(-2JM_A^z + h)}{\sqrt{(-2JM_A^z + h)^2 + \Gamma^2}} \tanh\beta\sqrt{(-2JM_A^z + h)^2 + \Gamma^2}. \end{aligned} \tag{4}$$

The spontaneous sublattice order M_A^z or M_B^z vanishes at the Néel phase boundary $T_N(\Gamma)$; see Fig. 1. It may be noted that the choice of sublattices here is purely random and the sublattice order therefore looks like that of a glass. Also, deep inside the antiferromagnetic phase (at $\beta \to \infty, \Gamma \to 0, h = 0$), $M_A^z = 1 = -M_B^z$, so that the free energy f can be expressed as $f \sim (1/\beta)\log[1 + \exp(-2\beta\Delta)]$ and the specific heat $\partial^2 f/\partial T^2$ will have a variation like $\exp[-2\beta\Delta(\Gamma)]$, similar to those of a two level system with

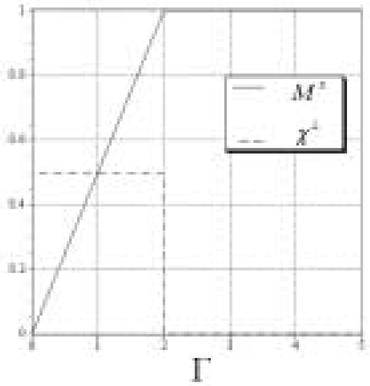

Figure 2: Variations of transverse magnetisation and susceptibility in the quantum case ($J = 1$).

a gap $\Delta(\Gamma) = \sqrt{4J^2 + \Gamma^2}$. This is the exact magnitude of the gap in the magnon spectrum of this long range transverse Ising antiferromagnet. Actually, the above result for the gap can be seen directly from the effective Hamiltonian in (2) having a simple $\begin{pmatrix} a & b \\ b & -a \end{pmatrix}$ matrix form where $a = 2\beta J m$ and $b = \Gamma$, giving the eigen values $\pm\beta\sqrt{4J^2m^2 + \Gamma^2}$. This gives the gap $\beta\Delta$ at $T = 0 = \Gamma$, where the magnetisation m becomes equal to unity.

In the classical case, near the Néel temperature $T_N^0 \equiv T_N(\Gamma = 0)$, we expand the equations (4) around $M_A \simeq 0, M_B \simeq 0$ for $h = 0$ and obtain $M_A^z \simeq -2J\beta M_B^z + \mathcal{O}((M_B^z)^3), M_B^z \simeq -2J\beta M_A^z + \mathcal{O}((M_A^z)^3)$. The only possible solutions for these linearized equations are $M_A^z = -M_B^z = M^z = 0$ and $M_A^z = -M_B^z = M^z \sim (T - T_N^0)^{1/2}$, where $T_N^0 = 2J$. The longitudinal linear susceptibilities $\chi_{A/B}$ are given by $\chi_{A/B} = \lim_{h\to 0} \partial M_{A/B}^z/\partial h = \beta(1 - 2J\chi_{B/A})\cosh^2\beta(-2JM_{B/A}^z)$. Hence, $\chi = \chi_A + \chi_B$ behaves as

$$\chi \quad = \quad \frac{2}{T_N^0 + T\cosh^2(2JM^z)/T}. \tag{5}$$

This gives $\chi = 2/(T + T_N^0)$ for high temperatures $T > T_N^0$ (where $M_A = -M_B = M^z = 0$) and at T_N^0 it grows upto a value $1/2J$ and drops down again to 0 as $T \to 0$, giving the well known cusp behaviour (see e.g., [6]) for the classical antiferromagnets.

In the pure quantum case ($T = 0$, $\Gamma \neq 0$), the tanh term in (4) equals to unity and with a similar expansion near the quantum critical point $\Gamma_N = 2J$, one gets the longitudinal susceptibility $\chi = \chi_A + \chi_B$; $\chi_{A/B} = \lim_{h\to 0} \partial M_{A/B}^z/\partial h = \Gamma^2(1 - 2J\chi_{B/A})/[(2JM_{B/A}^z)^2 + \Gamma^2]^{3/2}$. We then have

$$\chi \quad = \quad \frac{2\Gamma^2}{[(\Gamma_N M^z)^2 + \Gamma^2]^{3/2} + \Gamma_N\Gamma^2}, \tag{6}$$

giving $\chi = 2/(\Gamma + \Gamma_N)$ for $\Gamma > \Gamma_N$ and growing upto a value $1/2J$ at $\Gamma = \Gamma_N$ and then decreasing eventually to a value $\chi = \Gamma^2/4J^3$ as $\Gamma \to 0$. Again a cusp behaviour is seen for the susceptibility at the quantum critical point Γ_N for such a quantum antiferromagnet (see Fig. 1). The behaviour is of course qualitatively similar to that the classical critical (Néel) point. One can also study the transverse susceptibility $\chi^{\perp}(= dM^x/d\Gamma)$ behaviour. One finds $\chi_A^{\perp} = 0 = \chi_B^{\perp}$ for $\Gamma > \Gamma_N$ and $\chi_A^{\perp} = 1/2J = \chi_B^{\perp}$ for the ordered phase (see Fig. 2).

In view of the intriguing ground state properties of quantum antiferromagnets [2], indications coming often only from approximate theories (see e.g., [7] for a long range quantum Heisenberg antiferromagnet) or numerical simulations (see e.g., [8] and references therein), our proposed quantum antiferromagnetic model, having exactly soluble thermodynamic properties, should be of some interest. The model consists of an infinite range antiferromagnetic Ising system, put in a transverse field. The classical ground state of the model is highly degenerate. Although no signature of slow dynamics, like in glasses, can be seen here, the ordered state in the system corresponds to (quantum) glass-like system as well. The number of degenerate states can be estimated to be $\mathcal{O}(2^{N/2})$, which is larger than that for the Sherrington-Kirkpatrick model ($\sim \mathcal{O}(2^{0.28743N})$) [9]. This may be compared and contrasted with the transverse Ising antiferromagnets on topologically frustrated triangular lattices studied extensively in the last few years [10]. The free energy in (3) gives the ground state energy in the zero temperature limit and it also gives the low temperature behaviour of the specific heat, the exponential variation of which gives the precise gap magnitude $\Delta (= \sqrt{4J^2 + \Gamma^2})$ in the excitation spectrum of the system. It may be noted that although it is a spin-1/2 system, because of the restricted (Ising) symmetry and the infinite dimensionality (long range interaction) involved, there need not be any conflict with the Haldane conjecture. Although our entire analysis has been for spin-1/2 (Ising) case, because of the reduction of the effective Hamiltonian in (2) to that of a single spin in an effective vector field, the results can be easily generalised for higher values of the spin S. No qualitative change is observed. The order-disorder transition in the model can be driven both by thermal fluctuations (increasing T) or by the quantum fluctuations (increasing Γ). These transitions in the model have been investigated here studying the behaviours of the (random sublattice) magnetisation and the (longitudinal and transverse) susceptibilities. No quantum phase transition, where the gap Δ vanishes, is observed in the model, unlike in the one dimensional transverse Ising antiferromagnets [1,5].

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