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LETTER TO THE EDITOR

The $s = \frac{1}{2}$ spin chain with interactions to third neighbours

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Abstract. We have investigated the phase diagram of the $s = \frac{1}{2}$ J_1 – J_2 – J_3 chain using finite-lattice techniques. The location of the boundary between spin-liquid and dimer phases has been estimated, and the characterization of these phases via correlation functions is presented.

In classical systems with competing interactions, such as the ANNNI model [1], it is well known that the combined effect of frustration and thermal fluctuations can result in a rich phase diagram, incorporating a finite or infinite set of modulated phases. The corresponding quantum systems are less well understood, and are the subject of much recent and current research. In low-dimensional systems strong quantum fluctuations, even at $T = 0$, may play a role somewhat like thermal fluctuations. When frustration is also present a rich structure of ground-state phases may be possible.

We consider in this letter the $s = \frac{1}{2}$ quantum spin chain with Hamiltonian

$$H = 2J_1 \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1} + 2J_2 \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+2} + 2J_3 \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+3} \quad (1)$$

with periodic boundary conditions. The nearest-neighbour interaction is antiferromagnetic and, without loss of generality, we choose its magnitude to be $J_1 = 1$. The other interactions may be of either sign although, in this work, we choose $J_2 > 0$ to frustrate the nearest-neighbour exchange.

It is well known [2] that when $J_2 = J_3 = 0$ the ground-state properties can be obtained exactly, via the Bethe *ansatz*. The ground state is gapless, with algebraic decay of correlations, and is often termed a ‘spin-liquid’ phase. When $J_2 \neq 0$ but still $J_3 = 0$, the model is no longer solvable except at the special point $J_2 = \frac{1}{2}$ where the ground-state wavefunction is a simple product of pair singlet states [3]. This point lies in the ‘dimer’ phase, which has a finite gap between ground and excited states and exponential decay of correlations. The general J_2 case has been extensively studied via numerical finite-lattice methods [4, 5] and approximate field-theoretic mappings [6, 7]. All of these studies predict a transition from a spin-liquid ground state to a dimer ground state at a critical value J_{2c} , which the most recent numerical work estimates to be $J_{2c} = 0.2411$.

Since the Hamiltonian (1) is isotropic in spin space the total spin s_{tot} is a good quantum number. The ground state, in the parameter regime of interest, is found to be a singlet ($s_{\text{tot}} = 0$) whereas the first excited state may be a triplet ($s_{\text{tot}} = 1$) or another singlet. Tonegawa and Harada [4] attempt to determine J_{2c} from a finite-size scaling analysis of the singlet–triplet gap

$$\Delta_{\text{st}} = E_0(s_{\text{tot}} = 1) - E_0(s_{\text{tot}} = 0)$$

where the terms on the right are, respectively, the lowest energies in the sector with $s_{\text{tot}} = 0$ (the ground state) and in the sector with $s_{\text{tot}} = 1$. In the dimer phase Δ_{st} tends to a finite gap in the thermodynamic limit $N \rightarrow \infty$, whereas in the spin-liquid phase, according to conformal field theory [8], the gap should vanish according to

$$\Delta_{\text{st}} = (\pi v/N)[1 - y(N, J_2) + \dots]. \quad (2)$$

Here v is the J_2 -dependent spin-wave velocity and $y(N, J_2)$ is the leading logarithmic correction term. Okamoto and Nomura [5] proposed an alternative method, based on a simultaneous consideration of Δ_{st} and the singlet–singlet gap

$$\Delta_{\text{ss}} = E_1(s_{\text{tot}} = 0) - E_0(s_{\text{tot}} = 0)$$

which will vanish in the spin liquid according to

$$\Delta_{\text{st}} = (\pi v/N)[1 + 3y(N, J_2) + \dots]. \quad (3)$$

At the critical coupling J_{2c} the logarithmic corrections vanish, i.e. $y(N, J_{2c}) = 0$ and hence $\Delta_{\text{ss}} = \Delta_{\text{st}}$. A plot of Δ_{ss} and Δ_{st} versus J_2 for a finite chain will show a crossing at some J_{2c} and extrapolation of this sequence of crossing points will yield an accurate estimate of J_{2c} in the thermodynamic limit.

It is of some interest to investigate the stability of the dimer phase when further perturbations are included, and this is our primary reason for studying the full Hamiltonian (1) which includes third-neighbour interactions. For classical Ising spins it is clear that $J_3 > 0$ (antiferromagnetic) will enhance the stability of the classical Néel state while $J_3 < 0$ (ferromagnetic) will act to destabilize the Néel state. The quantum case is more subtle but, qualitatively, we might expect J_{2c} to be an increasing function of J_3 . Our approach is similar to that of Okamoto and Nomura [5]. We use the standard Lanczos method to obtain the lowest few eigenvalues for finite chains of $N = 8$ –18 spins. In practice it is tedious to consider basis states labelled by the total spin s_{tot} . Rather we consider sectors labelled by s_{tot}^z . Singlet states can then be readily identified by energies that occur in the $s_{\text{tot}}^z = 0$ sector but not in the $s_{\text{tot}}^z = 1$ sector, whereas triplet states occur in both sectors. We again use the equality of Δ_{st} and Δ_{ss} to locate the phase boundary between spin-liquid and dimer phases.

Table 1. Values of critical coupling J_{2c} for various J_3 obtained from equality of the singlet–triplet and singlet–singlet gaps. Results are shown for finite chains with $N = 10, 12, 14, 16, 18$ as well as estimates for the thermodynamic limit $N = \infty$.

J_3	N					
	10	12	14	16	18	∞
–0.1	0.1612	0.1576	0.1554	0.1541	0.1532	0.150
0.0	0.2444	0.2433	0.2426	0.2420	0.2420	0.242
0.1	0.3215	0.3233	0.3243	0.3249	0.3257	0.345
0.2	0.3942	0.3986	0.4018	0.4039	0.4055	0.417
0.4	0.5330	0.5385	0.5480	0.5533	0.5576	0.598

We now turn to the results. In table 1 we give values of J_{2c} for chains of various lengths, for a selection of values of J_3 . The last column shows our estimates in the thermodynamic limit, which have been obtained from a fit to the last three points of the form

$$J_N = J_\infty + \alpha/N + \beta/N^2.$$

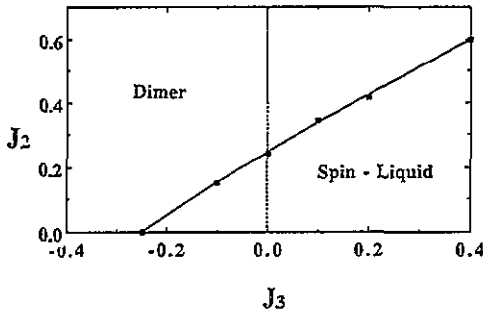


Figure 1. The boundary between spin-liquid and dimer phases for the J_1 - J_2 - J_3 spin chain.

More sophisticated sequence extrapolation methods can be used but will not affect the estimates significantly. These results are then used to plot the boundary between spin-liquid and dimer phases, shown in figure 1. It should be noted that even when $J_2 = 0$ the presence of third-neighbour interactions can induce a liquid-dimer transition.

In order to explore the nature of the phases we have investigated spin-spin correlations. Following Tonegawa and Harada [4] we define a two-spin correlation function

$$C(l) = 4\langle S_1^z S_l^z \rangle_g \tag{4}$$

and a dimer correlation function

$$D(l) = \langle T_1 T_l \rangle_g - \langle T_1 \rangle_g \langle T_l \rangle_g \tag{5}$$

with

$$T_l = S_l^+ S_{l+1}^- + S_l^- S_{l+1}^+ \tag{6}$$

where the angular brackets denote a ground-state average. In the spin-liquid phase $C(l)$ should alternate in sign and decrease in magnitude according to a power law. In the dimer phase $C(l)$ should decrease more rapidly and show more complex sign variation, whereas $D(l)$ should alternate in sign and have roughly constant magnitude. For the special case $J_2 = \frac{1}{2}$, $J_3 = 0$, which lies within the dimer phase, it can be shown that

$$C(l) = 1, -\frac{1}{2}, 0, 0, 0, 0, \dots \quad D(l) = -\frac{1}{2}, -\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}, \dots$$

for $l = 1, 2, 3, 4, \dots$

Figure 2 shows the form of these correlations at four points in the phase diagram. The expected behaviour is clearly seen. We have obtained similar results at other points in the phase diagram and conclude that the nature of the spin-liquid phase is essentially unchanged throughout the region shown in figure 1, and likewise the dimer phase forms an extended phase in the diagram. It is possible that for larger values of J_2 and/or J_3 other phases may occur, and this is presently under investigation.

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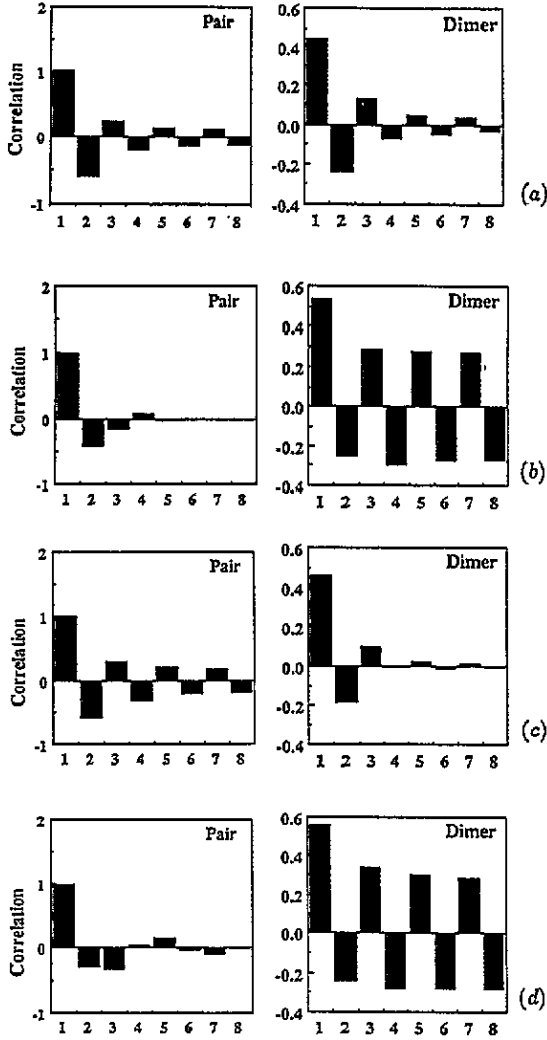


Figure 2. Pair and dimer correlations (4,5) for four points in the phase diagram for $N = 16$: (a) $J_2 = 0.1$, $J_3 = 0.0$ (liquid phase); (b) $J_2 = 0.6$, $J_3 = 0.0$ (dimer phase); (c) $J_2 = 0.1$, $J_3 = 0.4$ (liquid phase); (d) $J_2 = 0.8$, $J_3 = 0.4$ (dimer phase).

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