

# Mixed Spin Chains of Spins with Magnitudes $\frac{1}{2}$ and 1

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## Abstract

Periodic mixed spin chains consisting of spins with magnitudes  $\frac{1}{2}$  and 1 are studied. A nonlinear  $\sigma$  model method provides equations which determine gapless phase boundaries separating gapful disordered phases. Phase diagrams in the space of exchange constants are shown in the cases of periods 6 and 8.

*Key words:* mixed spin chain; spin gap; disordered state; nonlinear  $\sigma$  model

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One-dimensional quantum spin models have been investigated to understand disordered states with spin gap. For a uniform spin chain, a disordered state appears if the spin magnitude is an integer and does not if it is a half-odd-integer [1]. This result is found by mapping the spin Hamiltonian into a nonlinear  $\sigma$  model (NLSM). The NLSM method has been developed to be applicable to inhomogeneous spin chains [2–6]. In particular an unambiguous NLSM method derived a general equation to determine phase boundaries for mixed spin chains with finite period [4].

Among various possibilities, mixed spin chains consisting of spins with magnitudes  $\frac{1}{2}$  and 1 are mostly expected to be synthesized. We obtain phase diagrams in cases of several combinations of  $\frac{1}{2}$ 's and 1's by applying the general NLSM formula. The Hamiltonian is

$$H = \sum_j J_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}, \quad (1)$$

where  $\mathbf{S}_j$  is the spin with magnitude  $s_j$  ( $= \frac{1}{2}$  or 1) at site  $j$  and  $J_j (> 0)$  is the nearest-neighbor exchange constant. We consider the case that  $J_j$  is 1 between spin  $\frac{1}{2}$ 's,  $J$  between spin 1's, and  $J'$  between spin  $\frac{1}{2}$  and spin 1. We restrict ourselves to the case of even period  $2b$ .

The magnetization of the system is determined by the condition

$$\sum_{j=1}^b s_{2j} = \sum_{j=1}^b s_{2j-1}, \quad (2)$$

following Lieb-Mattis theorem [7]. If the condition is not satisfied, the ground state is ferrimagnetic and the magnetization is  $\sum s_{2j} - \sum s_{2j-1}$ .

If the condition (2) is satisfied, the ground state is singlet and Eq. (1) is mapped into an NLSM [4] with effective action

$$S_{\text{eff}} = \iint d\tau dx \left[ -i \frac{J^{(0)}}{J^{(1)}} \mathbf{m} \cdot (\partial_\tau \mathbf{m} \times \partial_x \mathbf{m}) + \frac{1}{2J^{(1)}} \left( \frac{J^{(1)}}{J^{(2)}} - \frac{J^{(0)}}{J^{(1)}} \right) (\partial_\tau \mathbf{m})^2 + \frac{J^{(0)}}{2} (\partial_x \mathbf{m})^2 \right], \quad (3)$$

where

$$\frac{1}{J^{(n)}} = \frac{1}{2b} \sum_{j=1}^{2b} \frac{(\tilde{s}_j)^n}{J_j s_j s_{j+1}} \quad (n = 0, 1, 2) \quad (4)$$

with  $\tilde{s}_j = \sum_{k=1}^j (-1)^{k+1} s_k$ . The coefficient of the topological term gives the *gapless equation*, which determines gapless phase boundaries separating gapful phases:

$$\frac{J^{(0)}}{J^{(1)}} = \frac{h}{2}. \quad (h : \text{half odd integer}) \quad (5)$$

In the case of period 4, only the possible array satisfying Eq. (2) is  $(s_1, s_2, s_3, s_4) = (\frac{1}{2}, \frac{1}{2}, 1, 1)$ . The phase

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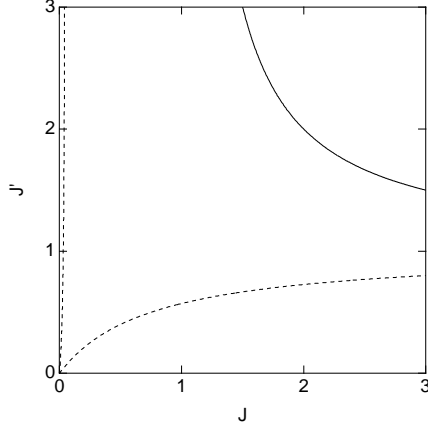


Fig. 1. Phase diagrams for the period 6 case. Two phase diagrams are drawn in a single graph. The solid line is the phase boundary for  $(\frac{1}{2}, \frac{1}{2}, 1, 1, 1, 1)$  and the two dashed lines are those for  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1, 1)$ .

diagram for the system has been discussed in detail by the NLSM method [5].

In the case of period 6, possible arrays satisfying Eq. (2) are  $(\frac{1}{2}, \frac{1}{2}, 1, 1, 1, 1)$  and  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1, 1)$  [8]. Correspondingly, Eq. (5) reduces to

$$J' = \frac{hJ}{(1-h)J + (1-3h)}, \quad \left(h = \frac{1}{2}\right) \quad (6)$$

$$J' = \frac{4hJ}{4(2-3h)J + (2-h)}, \quad \left(h = \frac{1}{2}, \frac{3}{2}\right) \quad (7)$$

respectively. These phase boundaries provide the phase diagrams shown in Fig. 1. Here a few values of  $h$  are allowed because of  $J > 0$  and  $J' > 0$ . There are two gapful phases in the former, and three in the latter. Each phase is explained by a VBS picture [9] or its extension, a singlet cluster picture [5]. For example, in the former the phase of large  $J$  and large  $J'$  is explained by Fig. 2(a) and the other phase is explained by Fig. 2(b).

In the case of period 8, arrays  $(\frac{1}{2}, \frac{1}{2}, 1, 1, 1, 1, 1, 1)$ ,  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1, 1, 1, 1)$  and  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1, 1)$  satisfy Eq. (2) [10]. Equation (5) reduces to

$$J' = \frac{4hJ}{4(1-h)J + (6-5h)}, \quad \left(h = \frac{1}{2}\right) \quad (8)$$

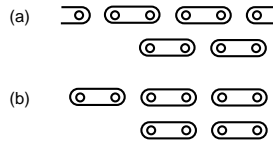


Fig. 2. VBS pictures for the phases of  $(\frac{1}{2}, \frac{1}{2}, 1, 1, 1, 1)$  chain: (a) the phase of large  $J$  and large  $J'$  and (b) the other phase. A small circle represents a spin  $\frac{1}{2}$  and an oval does a singlet. A spin 1 is decomposed into two spin  $\frac{1}{2}$ 's.

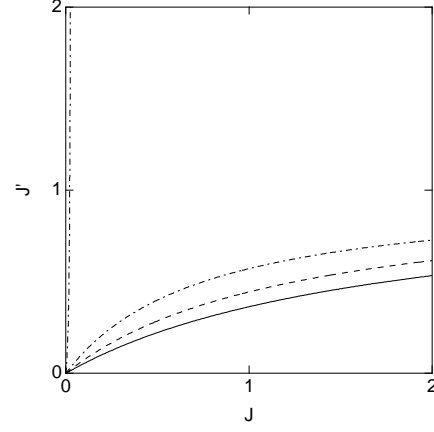


Fig. 3. Phase diagrams for the period 8 case. Three phase diagrams are drawn in a single graph. The solid line is the phase boundary for  $(\frac{1}{2}, \frac{1}{2}, 1, 1, 1, 1, 1, 1)$ , the dashed line is that for  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1, 1, 1, 1)$  and the two dash-dotted lines are those for  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1, 1)$ .

$$J' = \frac{4hJ}{4(2-3h)J + (4-3h)}, \quad \left(h = \frac{1}{2}\right) \quad (9)$$

$$J' = \frac{4hJ}{4(3-5h)J + (2-h)}, \quad \left(h = \frac{1}{2}, \frac{3}{2}\right) \quad (10)$$

correspondingly. The phase diagrams are shown in Fig. 2. There are two gapful phases in the first and the second cases, and three in the third.

In summary, we studied mixed spin chains consisting of spins with magnitudes  $\frac{1}{2}$  and 1 by the nonlinear  $\sigma$  model method. We provided ground-state phase diagrams in the space of exchange constants for the cases of periods 6 and 8. It is expected that real mixed spin chains are synthesized, examined experimentally and compared to the present theory.

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