PHYSICAL REVIEW B VOLUME 34, NUMBER 1 1 JULY 1986

Anisotropic Heisenberg chain with composite spin

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(Received 31 March 1986)

A family of one-dimensional magnetic Hamiltonians is introduced, where at each site there are n spin-S operators. It is shown that, for special couplings between spins and for $S=\frac{1}{2}$, the model contains the complete spectrum of the Heisenberg chain with spins $\frac{1}{2}$, 1, $\frac{3}{2}$, etc., and the ground state is that of the corresponding Heisenberg chain. By the varying of a single parameter the model allows continuous transitions between chains with different spin. We map the spin-$(S+S)$ model onto the nonlinear σ model and discuss the possibility of a finite gap in the spin-$(\frac{1}{2}+\frac{1}{2})$ model.

The spin-$\frac{1}{2}$ Heisenberg chain admits of an exact solution via the Bethe ansatz[1] or the quantum inverse method.[2] The latter method can be generalized[2] to solve exactly spin systems of higher spin length with specific nonlinear interactions. All of these solvable (integrable) spin systems have[2] a similar ground state and a spectrum which is gapless around the isotropic antiferromagnetic point. It is expected also from $1/S$-expansion results[3] or from variational calculations[4] that increasing spin length does not give rise to any drastic changes in the behavior of the system.

However, by mapping a nonintegrable spin Hamiltonian onto the O(3) nonlinear σ model, Haldane argued[5] that integer and half-integer spin systems may have a different ground state at the isotropic antiferromagnetic point, such that the excitation spectrum has a gap in the integer-spin case, but not in the half-integer case. Much computer time has since been devoted[6] to this question, resulting in considerable numerical evidence for the existence of the gap in the spectrum of the $S=1$ antiferromagnet, but definite answers are still lacking.

In this Rapid Communication we propose a new kind of spin system with variable spin length, which thus provides a totally new way of looking for effects of spin length: We consider a system of n spin-S operators at each lattice site. Note that in earlier work,[7] where the spin-1 operator was approximated by two spin-$\frac{1}{2}$ operators in the continuum limit, the philosophy was very different. A special case of the spin-$(S+S)$ model to be introduced below has been considered in Ref. 8.

In fact, we have a whole family of models depending on the number n of spins, the spin length S, and the kind of interactions we assume. In this Rapid Communication we only consider the cases $n=2$ and 3 with nearest-neighbor exchange interactions, and we study the model by two methods, finite-size scaling and mapping to the nonlinear σ model. In a general form the Hamiltonian can be written as

$$H=\sum_{\alpha,\beta} H_{\alpha\beta},\ \alpha,\beta=\sigma,\rho,(\tau)\ , \tag{1}$$

where σ, ρ, and τ are spin-S operators, and by (τ) we mean that τ spins are included only in the $n=3$ case. Each term $H_{\alpha\beta}$ in Eq. (1) is of the form

$$H_{\alpha\beta}=-\tfrac{1}{2}J_{xy}^{\alpha\beta}\sum_i(\alpha_i^+\beta_{i+1}^-+\alpha_i^-\beta_{i+1}^+)-J_z^{\alpha\beta}\sum_i\alpha_i^z\beta_{i+1}^z, \tag{2}$$

and $J_{xy}^{\alpha\beta}$, $J_z^{\alpha\beta}$, respectively, are the transverse and longitudinal exchange coupling of α and β spins. We allow for different coupling for each pair of spins, and therefore the phase space is very large: $d=7$ for $n=2$ and $d=17$ for $n=3$. We shall show below that the (local) spin length of the system (1) with (2) takes different values in different regions of the phase space.

For simplicity we consider here only two-dimensional (2D) surfaces in the phase space and use in particular the parametrization

$$\begin{aligned} J_j^{\alpha\beta}&=J_j,\ \alpha=\beta \\ &=\lambda J_j,\ \alpha\neq\beta \end{aligned}\ (j=xy,z)\ , \tag{3}$$

where α and β take the values indicated in Eq. (1), and λ is a free parameter. The Hamiltonian (1) now contains terms like

$$H_{\alpha\alpha}=-\tfrac{1}{2}J_{xy}\sum_i(\alpha_i^+\alpha_{i+1}^-+\alpha_i^-\alpha_{i+1}^+)-J_z\sum_i\alpha_i^z\alpha_{i+1}^z, \tag{4a}$$

$$H_{\alpha\beta}=-\frac{\lambda}{2}J_{xy}\sum_i(\alpha_i^+\beta_{i+1}^-+\alpha_i^-\beta_{i+1}^+)-\lambda J_z\sum_i\alpha_i^z\beta_{i+1}^z, \tag{4b}$$

with $\alpha\neq\beta$ in (4b). We now restrict ourselves to $S=\frac{1}{2}$ and will consider more general cases in a subsequent paper. In what follows we call the $n=2$ case the spin-$(\frac{1}{2}+\frac{1}{2})$ model and the $n=3$ case the spin-$(3\times\frac{1}{2})$ model. Note that λ provides an extra degree of freedom such that, by varying λ, we can have a continuous transition between chains with different spin, as we shall show below. At the same time λ provides another means of controlling the N^{-1} behavior of energy levels.

In the spin-$(\frac{1}{2}+\frac{1}{2})$ model the one-site Hilbert space of states is $\mathcal{D}_{1/2}\otimes\mathcal{D}_{1/2}=\mathcal{D}_0\oplus\mathcal{D}_1$, and thus it is useful to consider at each site the states

$$\begin{aligned} &|1\rangle\equiv|\uparrow,\uparrow\rangle,|-1\rangle\equiv|\downarrow,\downarrow\rangle, \\ &|0\rangle\equiv(1/\sqrt{2})(|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle), \\ &|0'\rangle\equiv(1/\sqrt{2})(|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle). \end{aligned} \tag{5}$$

The first three states constitute the three components of a spin-1 state, and $|0'\rangle$ is a spin-0 state. At $\lambda=0$ the length of $\sigma_n+\rho_n$ is not a good quantum number, and the system describes two independent spin-$\frac{1}{2}$ chains. For $0<\lambda<1$ the local spin length is not well defined either, and neighboring spins that are in $|1\rangle$ and $|-1\rangle$ states, respectively, can flip to state $|0\rangle|0\rangle$ or $|0'\rangle|0'\rangle$. At $\lambda=1$, however, $(\sigma_n+\rho_n)^2$ commutes with the Hamiltonian, and we can assign a definite value to the spin at each site. Furthermore, all the matrix elements between the $|0'\rangle$ state and all the other states vanish at this point, and hence the number and positions of spin-0 states in the chain are conserved. The Hilbert space of the system is sectorized into independent subspaces which include the complete spin-1 subspace, and all the other subspaces can be classified by a number ν, $\nu=1,\ldots,N$, which is the number of spin-0 states in the chain of N sites. The only effect of the immobile spin-0 states is to break the spin-1 chain, and thus appear as nonmagnetic "impurities." In principle, we could describe the model equivalently as a nonmagnetic chain diluted by spin-1 impurities, but as we shall show below, the ground state of the model is always in the spin-1 subspace.

If we increase λ beyond $\lambda=1$, we find in the spin-$(\frac{1}{2}+\frac{1}{2})$ model a simple duality property: All energy levels $E(\lambda)$ of the model satisfy

$$E(\lambda)=\lambda E(1/\lambda)\ . \tag{6}$$

This duality condition results from the decoupling of the system into two independent spin-$\frac{1}{2}$ chains, both at $\lambda=0$ and at $\lambda=\infty$. For $\lambda<0$, the model includes both ferromagnetic and antiferromagnetic couplings and the ground state differs from that in the positive λ case. Consequently, Eq. (6) only holds for $\lambda>0$. In any parametrization there is an analogous duality relation which is satisfied between two decoupling points, provided they exist, in the corresponding λ space.

To find the energy levels of the spin-$(\frac{1}{2}+\frac{1}{2})$ model, we have performed exact numerical calculations for periodic chains containing $N\leq 8$ sites. Figure 1 shows, at $\lambda=1$, the first two excited levels and the lowest level which contains spin-0 states. Close to the isotropic antiferromagnetic point, $J_z/J_{xy}=-1$, the first two excited levels are the $S^z_{\rm tot}=1$, $k=0$, and $S^z_{\rm tot}=0$, $k=\pi$ levels of the spin-1 Heisenberg chain; the ground state is the $S^z_{\rm tot}=0$, $k=0$ state of the same subspace. The first impurity level is much higher in energy, and the gap to this level remains definitely finite for $N\rightarrow\infty$. Therefore, the ground state of the spin-$(\frac{1}{2}+\frac{1}{2})$ model is always in the spin-1 subspace.

Consider next the behavior of the lowest-lying levels as a function of λ, in particular at the isotropic antiferromagnetic point. Note that by going from $\lambda=0$ to $\lambda=1$ we interpolate smoothly between $S=\frac{1}{2}$ and $S=1$, respectively, and return to $S=\frac{1}{2}$ at $\lambda=\infty$. Figure 2 shows the primary gap for periodic chains having up to 10 sites. A finite-size scaling estimate for the infinite chain gap, satisfying the self-duality condition (6), is also shown. Finite-size scaling indicates that the gap scales to zero only at $\lambda=0$, which becomes a singular point: The gap behaves as $|\lambda|^{\alpha}$ with $\alpha<1$ ($\lambda<0$), $\alpha\simeq 1$ ($\lambda>0$). A linearly increasing gap close to the origin (spin $\frac{1}{2}$) implies, through Eq. (6), a finite gap at $\lambda=\infty$ (spin $\frac{1}{2}$ with infinite coupling).

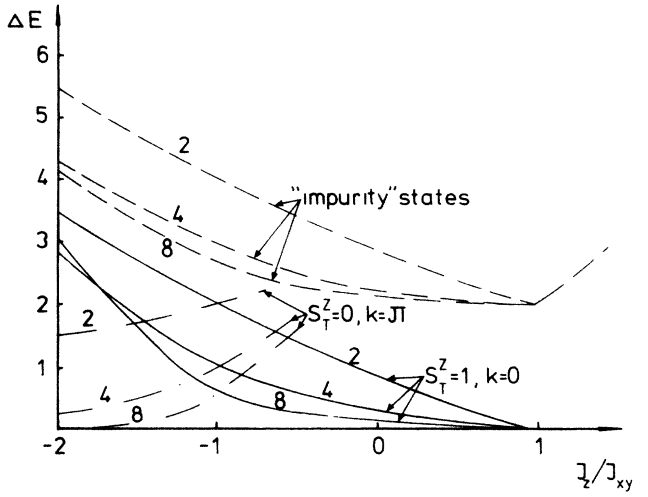

FIG. 1. Energy difference of the ground state and the lowest two excited states in the spin-$(\frac{1}{2}+\frac{1}{2})$ model. The difference from the lowest impurity level including spin-0 states is also shown. Figures attached to each line indicate the number of lattice points used in the finite-size calculation.

From Fig. 2 we are tempted to conclude that Haldane's conjecture[5] is correct. Moreover, in our model the gap is finite for any finite λ. For comparison we have done the same calculations for the spin-$(3\times\frac{1}{2})$ model. This model has eight spin states per site, four of which constitute a spin-$\frac{3}{2}$ multiplet and the other four two spin-$\frac{1}{2}$ multiplets. The Hilbert space of the model, at $\lambda=1$, is again sectorized into a complete spin-$\frac{3}{2}$ subspace and subspaces la-

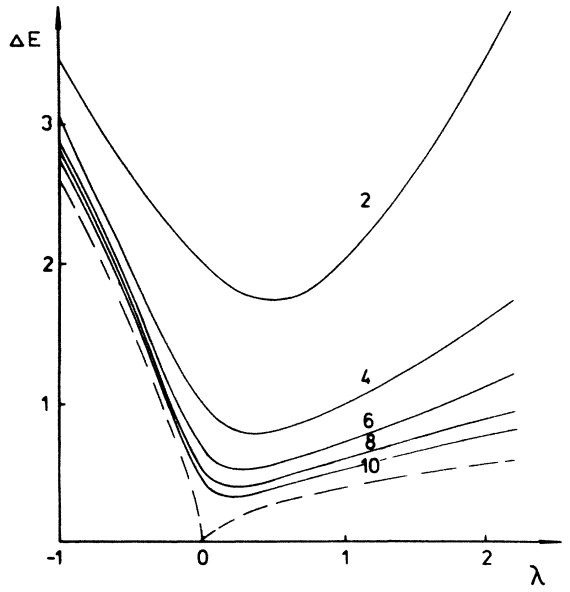

FIG. 2. Primary gap of the spin-$(\frac{1}{2}+\frac{1}{2})$ model at the isotropic antiferromagnetic point for $N=2$, 4, 6, 8, and 10. The dashed line is an estimate for the finite-size scaling result which would satisfy the self-duality relation (6).

beled by two "spin-$\frac{1}{2}$–impurity" numbers. There is no decoupling at $\lambda=\infty$.

We have made finite-size calculations for periodic chains with $N\leq 6$ sites, the maximum we could achieve with our computer facilities. The first two excited (spin-$\frac{3}{2}$) levels have the same quantum numbers as the corresponding levels in the spin-$(\frac{1}{2}+\frac{1}{2})$ model, and impurity levels have a finite gap everywhere. In the planar phase, $-J_{xy}+\varepsilon<J_z<J_{xy}$ (we do not specify the size of ε here), the impurity levels become degenerate, as they do in the spin-$(\frac{1}{2}+\frac{1}{2})$ model with a gap $\Delta E_I=n$. We conclude that the ground state of the spin-$(3\times\frac{1}{2})$ model is always in the spin-$\frac{3}{2}$ subspace; at $\lambda=0$ it describes three independent spin-$\frac{1}{2}$ chains.

We find that the primary gap of the spin-$(3\times\frac{1}{2})$ model behaves at $J_z/J_{xy}=-1$ much as that of the spin-$(\frac{1}{2}+\frac{1}{2})$ model, except perhaps for $\lambda<0$. If Haldane's conjecture was correct, we would expect that the gap in this case remains zero for all $\lambda\geq 0$, in contrast with what seems to be the result from finite-size scaling. Considering the chain lengths we could handle, finite-size results do not yet warrant definite conclusions. Notice, however, that we always get a vanishing gap at $\lambda=0$, which is known to be correct in the spin-$\frac{1}{2}$ limit.

Haldane's arguments are based on the mapping onto the O(3) nonlinear σ model, so we consider here the same mapping for our spin-$(S+S)$ model. Indeed, the Hilbert space of the σ model rather resembles that of the spin-$(S+S)$ model,[8] and we find that the mapping becomes exact in the scaling limit g, $a\rightarrow 0$ (a is the lattice spacing) with the σ model coupling constant g,

$$g^{-2}=S(1-\lambda)^{1/2}\ . \tag{7}$$

In the scaling limit the σ model is known[9] to have a dynamic generation of mass $m\sim a^{-1}\exp[-2\pi S(1-\lambda)^{1/2}]$, and for $\lambda=0$ we recover the results of Ref. 8. Our spin-$(\frac{1}{2}+\frac{1}{2})$ lattice model at $\lambda=0$ is certainly far from the scaling limit, and finite-size scaling gives a vanishing mass (gap) as expected.[1,2]

The $\lambda=1$ case is quite different, however. Then the spin-$(S+S)$ model maps onto a particular limit of the σ model where the gradient of the field term vanishes, and in the remaining time derivative term the coupling g' is independent of the spin S. This problem is equivalent to a classical 1D Heisenberg chain at temperature $T=g'$ and has mass $m\sim g'$. We conclude that if $S=\frac{1}{2}$ is not a singular point in the mapping, there is a finite mass even in the spin-$(\frac{1}{2}+\frac{1}{2})$ model, and thus in the spin-1 Heisenberg chain.

In conclusion, we have introduced a family of Hamiltonians having n spin-S operators at each lattice site. With an appropriate choice of interaction for $S=\frac{1}{2}$, $n=2,3$, the model includes the complete spectra of spin-$\frac{1}{2}$, -1, and -$\frac{3}{2}$ Heisenberg chains as special cases and allows continuous transitions between different spin lengths. Under "symmetric" parametrizations, the energy levels are shown to satisfy a self-duality relation.

We have shown that the spin-$(\frac{1}{2}+\frac{1}{2})$ and spin-$(3\times\frac{1}{2})$ models display, in many respects, a similar behavior, although for the latter model the results are not yet decisive. In the spin-$(\frac{1}{2}+\frac{1}{2})$ model the self-duality relation (6) provides an increased accuracy of the finite-size scaling results for the energy levels. The mapping of the spin-$(S+S)$ model onto the O(3) nonlinear σ model suggests that the gap at $S=\frac{1}{2}$, $\lambda=1$, is indeed finite, as indicated by finite-size scaling. We have also used parametrizations different from Eq. (3), but the results are qualitatively the same.

Other aspects of the model, for example, the possibility of novel phases compared with those of the Heisenberg model when extra interactions are included, will be treated in a more detailed paper.

The authors are grateful to NORDITA and to Professor Alan Luther for hospitality accorded them during their stay in Copenhagen. One of us (J.T.) acknowledges useful discussions with Antti Kupiainen on the nonlinear σ model. This research has been supported in part by the Swiss National Science Foundation through Grant No. 2.847-0.83.

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