RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 31, NUMBER 11 1 JUNE 1985

Symmetry and boundary condition of planar spin systems

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(Received 18 May 1984; revised manuscript received 14 January 1985)

For finite quantum systems, the boundary condition has physical as well as computational significance. Here planar spin chains are investigated with the use of a boundary condition that differs from the most commonly used periodic boundary condition. The symmetry properties then explicitly distinguish between even and odd half-integer spins. Finite-size scaling performs better with the use of this boundary.

The study of finite systems is motivated both by the fact that physical systems are finite, and because frequently they are easier to investigate than infinite systems. In either case, the boundary condition is important for the following: to describe the physical properties of real systems correctly and as a tool to obtain the best finite-size estimate for the infinite system. For the purpose of minimizing finite-size corrections the preferred choice is the periodic boundary condition (in some cases antiperiodic, respectively, open boundaries are appropriate).

Here, I wish to show that for planar systems physical insight can be gained and at the same time the numerical convergence can be improved by appropriately choosing the boundary. The system considered is the anisotropic spin-S Heisenberg model in one dimension. The approach, however, can be generalized to more complicated interactions and higher dimensions. The spin-S Heisenberg model has been studied extensively and there are a number of exact results available. The $S=\frac{1}{2}$ Heisenberg chain has been solved a long time ago[1] and renewed interest produced exact results for specific generalizations for $S>\frac{1}{2}$.[2,3] A global picture developed recently[4] distinguishes between odd and even half-integer spins. The symmetry properties investigated here support this description in a natural way.

The idea to vary the boundary condition has been used numerically for spinless fermions[5] and to study confinement in field theory.[6]

The anisotropic spin-S Heisenberg chain is defined by the following Hamiltonian in terms of the spin operators $\mathbf{S}$,

$$H=\sum_{n=1}^{N}(S_n^xS_{n+1}^x+S_n^yS_{n+1}^y)+\lambda\sum_{n=1}^{N}S_n^zS_{n+1}^z \quad . \tag{1}$$

For $\lambda=1(-1)\,H$ reduces to the isotropic antiferromagnetic (ferromagnetic) case with full rotational symmetry. The discussion will be restricted to N even, which is appropriate to the antiferromagnetic case, as can be seen most clearly in the Ising limit $\lambda\rightarrow\infty$. The periodic (antiperiodic) boundary condition identifies $\mathbf{S}_{N+1}\equiv\mathbf{S}_1$ ($\mathbf{S}_{N+1}\equiv-\mathbf{S}_1$) and the open boundary condition restricts the sums in (1) to $N-1$. Here, I study the situation when the planar term $S_N^xS_1^x+S_N^yS_1^y$ coupling the last and the first spin in the chain is replaced by

$$(S_N^xS_1^x+S_N^yS_1^y)\cos(N\theta)-(S_N^xS_1^y-S_N^yS_1^x)\sin(N\theta) \quad . \tag{2}$$

The angle θ can be restricted to $0\leq\theta<2\pi/N$. Applying the transformation

$$S_n^{\pm}\rightarrow S_n^{\pm}e^{\pm i\theta n},\quad S_n^{\pm}\equiv S_n^x\pm iS_n^y \tag{3}$$

leads to the equivalent, periodically bounded Hamiltonian

$$\begin{aligned}H(\theta)&=\sum_{n=1}^{N}(S_n^xS_{n+1}^x+S_n^yS_{n+1}^y)\cos\theta\\&\quad-\sum_{n=1}^{N}(S_n^xS_{n+1}^y-S_n^yS_{n+1}^x)\sin\theta+\lambda\sum_{n=1}^{N}S_n^zS_{n+1}^z\\&=\frac{1}{2}\sum_{n=1}^{N}(S_n^-S_{n+1}^+e^{i\theta}+S_n^+S_{n+1}^-e^{-i\theta})+\lambda\sum_{n=1}^{N}S_n^zS_{n+1}^z \quad ,\end{aligned} \tag{4}$$

which is explicitly translationally invariant and shows that the new boundary corresponds to a planar twist of the chain. The previous case is recovered for $\theta=0$.

Let $\psi(q)$ be an eigenvector of (4) with wave vector q and energy E,

$$H(\theta)\psi(q)=E\psi(q) \quad . \tag{5}$$

The q dependence of ψ can be made explicit by writing

$$\psi(q)=\sum_{\mathbf{n}}a_{\mathbf{n}}\sum_{m=1}^{N}e^{iqm}S_{n_1+m}^+\cdots S_{n_r+m}^+|0\rangle \quad , \tag{6}$$

where $|0\rangle$ is the fully aligned state, $\mathbf{n}=(n_1,\ldots,n_r)$ denotes the distinct configurations of (conserved) total spin $S_{\text{tot}}^z=r-NS$, and the $a_{\mathbf{n}}$ are determined by (5). It is understood that the indices n_K+m are periodically brought back into the interval $1\ldots N$. First, using Eq. (6) and the standard Pauli matrix representation of the spin operators (where all the matrix elements for S^+ are real), the complex conjugate of (5) changes θ into $-\theta$ and q into $-q$. Then the transformation of Eq. (3) with an angle θ' is applied, changing $-\theta$ into $\theta'-\theta$ and multiplying $S_{n_1+m}^+\cdots S_{n_r+m}^+|0\rangle$ by l^{χ}, where

$$\chi=i(mr\theta'+lN\theta'+(n_1+\cdots+n_r)\theta') \quad ,$$

and l is an integer. The boundary condition, Eq. (2), is unchanged if $\theta'=(2\pi/N)k,k$ integer. The wave vector of ψ then changes into $q'=rk(2\pi/N)-q$. I now fix θ and θ' at $\theta=\pi/N$ and $\theta'=2\pi/N$. The Hamiltonian

$$H(2\pi/N-\pi/N)=H(\pi/N)$$

and the boundary condition then do not change, but

$$q\rightarrow q'=2\pi S+(2\pi/N)S_{\text{tot}}^z-q$$

and

$$E(q)=E\left(2\pi S+\frac{2\pi}{N}S_{\text{tot}}^z-q\right) \quad . \tag{7}$$

This result shows clearly that odd and even half-integer spins have different symmetry properties. The spectrum is symmetric with respect to $q=m\pi+\pi/2$ ($q=m\pi$), m integer, for odd (even) half-integer spin. Finite-size calculations up to $S=3$ indicate that the ground state, for any S and $\lambda>0$, has $S^z_{\text{tot}}=0$ and $q=0$. Equation (7) says that the ground state is exactly degenerate with a state with $q=\pi$, for odd half-integer S only. Note that the spectra of Eqs. (1), (2), and (4) are identical, but with a wave vector shifted by $S\pi+(\pi/N)S^z_{\text{tot}}$. These results favor the distinction between even and odd half-integer spins. One expects that modifying the boundary can render pseudodegenerate states truly degenerate for finite N. On the other hand, if the ground state is a singlet, as conjectured for the integer S case ($\lambda=1$), a change of the boundary does not alter this fact. Equation (7) holds for any planar system, no matter how complicated the Hamiltonian. The derivation is based solely on its planar character.

It is illustrative to consider the exactly soluble $S=\frac{1}{2}$ case. For $\theta=0$, it can be demonstrated[7] that the ($q=0$) ground state for finite N is nondegenerate in contradistinction to the present result for $\theta=(\pi/N)$. The Hamiltonian $H(\theta)$ [Eq. (4)] can also be solved by the Bethe ansatz. The generalized equations corresponding to the original isotropic solution (Bethe) are

$$2\cot\frac{\phi_{ij}}{2}=\cot\frac{(k_i-\theta)}{2}-\cot\frac{(k_j-\theta)}{2}\ ,$$
$$Nk_i=2\pi\lambda_i+\sum_{j\neq i}\phi_{ij},\quad \lambda_i \text{ integer}\ , \tag{8}$$

and the energy and wave vector are given by

$$E=\sum_{i=1}^{r}[1-\cos(k_i-\theta)]\ ,\quad k=\sum_{i=1}^{r}k_i=\frac{2\pi}{N}\sum_{i=1}^{r}\lambda_i\ .$$

For $\theta=0$, these equations reduce to Bethe's result and for $\theta=(\pi/N)$ and $r=(N/2)$, the transformation

$$k_i\to(2\pi/N)-k_i,\quad \phi_{ij}\to-\phi_{ij}\ ,$$

and $\lambda_i\to1-\lambda_i$ produces a solution with the same energy and wave vector $\pi-k$, in accordance with (7).

Let us test the consequences of the modified boundary on finite-size scaling. Varying the boundary can give clues as to how the results should converge as $N\to\infty$. While the most interesting cases are $\theta=0$ and $\theta=(\pi/N)$, θ can of course be varied continuously.

In Fig. 1 the low-lying spectrum of the isotropic, antiferromagnetic $S=\frac{1}{2}$ model for $N=8$ is compared with the exact ($N\to\infty$) result. The $\theta=0$ points, degenerate for $S^z_{\text{tot}}=0$, ±1 deviate much more from the exact result than the $\theta=(\pi/N)$ spectrum, which is symmetric with respect to $q=(\pi/2)$. In addition, the $S^z_{\text{tot}}=\pm1$ points provide estimates for intermediate q values, otherwise inaccessible for $N=8$ [this is due to the shift of the wave vector by (π/N) when passing from (1), (2) to (4)].

According to the distinction between odd and even half-integer S the isotropic, antiferromagnetic Heisenberg model should have a finite gap between the ground state and the lowest excitation for integer S.[4] Recent numerical results up to $S=2$ support this,[8] whereby the most conclusive evidence is obtained from comparing $S=1$ with $S=\frac{1}{2},\frac{3}{2}$. The conclusion that the gap remains finite asymptotically as $N\to\infty$ can be strengthened by considering different values of θ. The gap has been evaluated as a function of N and θ, and it never vanishes for any θ (up to $N=12$) in contrast with half-integer S. Figure 2 shows results for $\theta=0$,

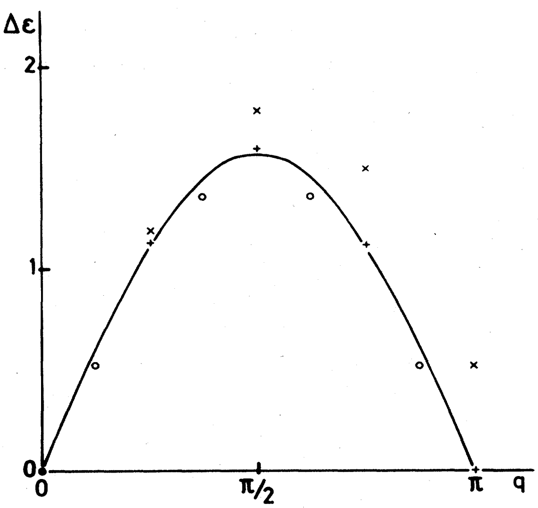

FIG. 1. Spectrum $\Delta\epsilon(q)=E_0(q)-E_0$ for isotropic, antiferromagnetic $S=\frac{1}{2}$ Heisenberg chain. The $\theta=0$, $S^z_{\text{tot}}=0$, ±1 gaps (×) are compared with the $\theta=(\pi/N)$ gaps for $S^z_{\text{tot}}=0$ (+) and for $S^z_{\text{tot}}=\pm1$ (○), with q values shifted by (π/N). The common ground state has $q=0$ (●). The $\theta=(\pi/N)$ points lie much closer to the exact spectrum (curve). There are $N=8$ spins in the chain.

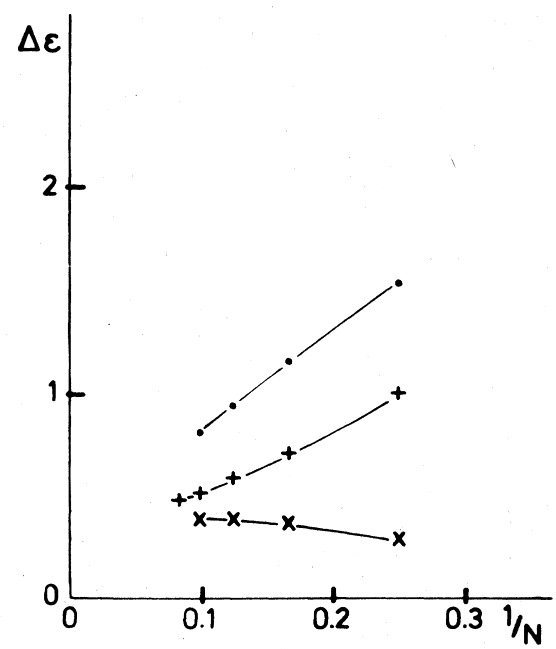

FIG. 2. Energy gap $\Delta\epsilon=E_1-E_0$ of isotropic, antiferromagnetic $S=1$ Heisenberg chain of length N, up to $N=12$. The $\theta=0$, $S^z_{\text{tot}}=0$, ±1 (+), $\theta=(\pi/N)$, $S^z_{\text{tot}}=0$ (×), and $\theta=(\pi/N)$, $S^z_{\text{tot}}=\pm1$ (○) gaps all converge towards the same finite value as $1/N$ decreases. The three series combined give a more reliable estimate of the asymptotic behavior.

(π/N), and $S^z_{tot}=0$, ± 1. Clearly, the results for varying θ are consistent with a finite gap and they are more reliable when considered together. Note that the modified boundary breaks the full rotational symmetry in spin space ($\lambda=\pm 1$). Figure 2 indicates that it is restored as $N\rightarrow\infty$.

Analogous modifications of the boundary can be used in other cases. For example, the $S=1$ models which have been solved by the Bethe ansatz[2,3] [including a $(\mathbf{S}\cdot\mathbf{S})^2$ term] can be approached in a similar way. For other cases, such as fermions, similar procedures apply.

Laboratoire de Physique des Solides is Laboratoire associé au CNRS. I have benefited from discussions with R. Botet, D. Haldane, R. Jullien, and K. A. Penson and from the support of the Deutsche Forschungsgemeinschaft during the final stages of this work.

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