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Fluid–dimer critical point in $S=\frac{1}{2}$ antiferromagnetic Heisenberg chain with next nearest neighbor interactions

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We numerically investigate the critical value α_c of the fluid–dimer transition in the ground state of the $S=\frac{1}{2}$ antiferromagnetic Heisenberg chain with next nearest neighbor interactions, $H=J\Sigma\ (\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1}+\alpha\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+2})$ with $J>0$ and $\alpha>0$. With the help of the conformal field theory, we can estimate $\alpha_c=0.2411\pm0.0001$.

The $S=\frac{1}{2}$ antiferromagnetic Heisenberg chain with next nearest neighbor interactions is one of the typical models for competing interactions. Our Hamiltonian in this paper is expressed as

$$H=J\sum_{j=1}^{N}\ (\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1}+\alpha\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+2})\ ,$$

$$J>0\ ,\quad \alpha>0\ , \tag{1}$$

where we assume the periodic boundary condition $\boldsymbol{S}_{N+1}=\boldsymbol{S}_1$ and N is the number of spins which is assumed to be even. We are interested only in the ground state.

When $\alpha=0$, as is well known, the ground state of the Hamiltonian (1) is the spin fluid state, which is characterized by the gapless excitation and the power decay of the spin correlation.

In the case of $\alpha=\frac{1}{2}$, the exact ground state has been obtained [1–4]. If we introduce the notation for the singlet pair as

$$[l,m]\equiv\frac{1}{\sqrt{2}}\ (\uparrow_l\downarrow_m-\downarrow_l\uparrow_m)\ , \tag{2}$$

and define $\Phi_1(N)$ and $\Phi_2(N)$ as

$$\Phi_1(N)\equiv[1,2][3,4][5,6]\ldots[N-1,N]\ , \tag{3}$$

$$\Phi_2(N)\equiv[2,3][4,5][6,7]\ldots[N,1]\ , \tag{4}$$

we can see that both $\Phi_1(N)$ and $\Phi_2(N)$ are the eigenstates of the Hamiltonian (1) having the energy

$$E_g(N)=-\tfrac{3}{8}NJ\ , \tag{5}$$

when $\alpha=\frac{1}{2}$. The energy $E_g(N)$ in eq. (5) was proved to be the ground state energy by van den Broek [3], and Shastry and Sutherland [4]. Affleck, Kennedy, Lieb and Tasaki [5] proved that only the states of eqs. (3) and (4) are the ground states and there is an energy gap between the ground state and the first excited state. Therefore the ground state is the dimer state when $\alpha=\frac{1}{2}$. The dimer state is characterized by the excitation gap and the exponential decay of the spin correlation.

From the above facts, the fluid–dimer transition in the ground state will be observed at $\alpha=\alpha_c$, if we run from $\alpha=0$ to $\alpha=\frac{1}{2}$. Haldane [6] transformed the spin Hamiltonian (1) into the effective Hamiltonian via the Jordan–Wigner transformation and taking the continuum limit. By the use of this effective Hamiltonian and the renormalization group (RG) method, he discussed the fluid–dimer transition and stated that this transition occurs at $\alpha_c=\frac{1}{6}$. Kuboki and Fukuyama [7] (KF) rewrote Haldane's effective Hamiltonian into the phase Hamiltonian form

$$H=\int \mathrm{d}z\ \{A[\nabla\theta(z)]^2+C[P(z)]^2$$
$$-D\cos[2\theta(z)]\}\ , \tag{6}$$

where the commutation relation $[\theta(z_1), P(z_2)] = i\delta(z_1 - z_2)$ holds, the coefficients A and C are smooth functions of α, and

$$D = \frac{J}{2a_0}(1-3\alpha), \tag{7}$$

where a_0 is the spacing between neighboring spins. KF stated that the fluid–dimer transition occurs at $D=0$ by the use of the RG equations and the isotropic nature of the original spin Hamiltonian. Then the conclusion of KF is

$$\alpha_c = \tfrac{1}{3}. \tag{8}$$

The reason for the difference between Haldane's value $\alpha_c = \frac{1}{6}$ and KF's value $\alpha_c = \frac{1}{3}$ is given by KF.

Of course, the above estimations of α_c are not exact. For instance, the expression for D in eq. (7) is valid only in the limit $\alpha \to 0$. Although the picture that the fluid–dimer transition occurs at $D=0$ may hold, the exact value of α_c itself cannot be obtained from the above discussion. Then, if we want to know α_c, there seems to be no other way than the numerical method.

Tonegawa and Harada [8] (TH) numerically diagonalized the finite size spin Hamiltonian. For the determination of α_c, TH used the singlet–triplet gap defined by

$$G_{st}(N, \alpha) \equiv E_1^{(0)}(N, \alpha) - E_0^{(0)}(N, \alpha), \tag{9}$$

where $E_m^{(0)}(N, \alpha)$ and $E_m^{(l)}(N, \alpha)$ are the ground state energy and the lth excited state energy in the $S_{total} = m$ subspace, respectively. TH's basic idea was that the ground state is either the spin fluid state or the dimer state depending upon whether $G_{st}(\infty, \alpha) = 0$ or $G_{st}(\infty, \alpha) > 0$. Generally speaking, however, it is difficult to judge whether the extrapolated value $G_{st}(\infty, \alpha)$ is zero or positive. Following Haldane [6], the excitation gap behaves as

$$G_{st}(\infty, \alpha) \sim \frac{1}{\sqrt{\alpha - \alpha_c}} \exp\left(-\frac{a}{\alpha - \alpha_c}\right), \tag{10}$$

near α_c, where a is some positive constant. Further, since the $D\cos[2\theta(x)]$ term is marginally irrelevant in the spin fluid state (see below), there appear logarithmic corrections added to the main contribution of the order of $1/N$. Due to such unfavorable conditions, the determination of α_c from the $N \to \infty$ extrapolation of $G_{st}(N, \alpha)$ is very difficult.

In spite of these unfavorable conditions, TH [8] tried to determine α_c from $G_{st}(\infty, \alpha)$ obtained by the use of the alternating $-\epsilon$ algorithm [9] to conclude $\alpha_c = 0.30 \pm 0.01$. The simple finite size scaling plot did not work well [10,11]. Although one of us (K.O.) and Inagaki [10,11] tried to apply the dimer field to this system to know the behavior of the dimer susceptibility, they could not obtain any definite conclusion on α_c. The main reason for this failure seems to be the existence of the logarithmic corrections.

The RG equations for the phase Hamiltonian (6) are [7]

$$\frac{dx}{dl} = 2y^2, \tag{11}$$

$$\frac{dy}{dl} = 2xy, \tag{12}$$

with

$$x \equiv 1 - \eta, \quad \eta \equiv \frac{1}{2\pi}\sqrt{C/A}, \quad y \propto \frac{D}{\sqrt{AC}}. \tag{13}$$

The flow diagram was discussed on the basis of eqs. (11) and (12) by Haldane [6] and KF [7]. The isotropic nature of our model requires $y = -x$ in the spin fluid region, which results in

$$\frac{dy}{dl} = -2y^2, \tag{14}$$

having the solution

$$y(N) = \frac{1}{2\log N + 1/y_0}. \tag{15}$$

Here we have set $l = \log N$ as usual and y_0 is the bare value of y. Thus y behaves as $1/\log N$ for large N, which explains why the logarithmic corrections appear in the isotropic spin fluid state.

Therefore the $D\cos[2\theta(z)]$ term produces the logarithmic corrections to the excitation gaps of the finite systems in the spin fluid region ($\alpha < \alpha_c$), whereas it generates the excitation gap of the infinite system in the dimer region ($\alpha > \alpha_c$). The quantity $y(N)$ ($= -x(N)$) measures the distance from the fixed point Hamiltonian. Then we can use the result of the conformal field theory [12–14], which pre-

dicts that the singlet–triplet excitation in the spin fluid region behaves as

$$G_{st}(N,\alpha)=\frac{2\pi v(\alpha)}{N}\left[\tfrac{1}{2}-\tfrac{1}{4}2y(N,\alpha)\right.$$
$$\left.+(\text{higher order corrections})\right], \qquad (16)$$

whereas the singlet–singlet excitation behaves as

$$G_{ss}(N,\alpha)=\frac{2\pi v(\alpha)}{N}\left[\tfrac{1}{2}+\tfrac{3}{4}2y(N,\alpha)\right.$$
$$\left.+(\text{higher order corrections})\right], \qquad (17)$$

where $G_{ss}(N,\alpha)$ is defined by $G_{ss}(N,\alpha)\equiv G_0^{(1)}(N,\alpha)-G_0^{(0)}(N,\alpha)$. Here $v(\alpha)$ is the spin wave velocity which is a smooth function of α and we have explicitly written the α-dependence of y. Further the ground state energy $E_g(N)$ is expressed as

$$E_g(N,\alpha)=e_g(\alpha)N-\frac{\pi v(\alpha)}{6N}\left[1+O(y^3(N,\alpha))\right.$$
$$\left.+(\text{higher order corrections})\right], \qquad (18)$$

$e_g(\alpha)$ being the ground state energy per spin of the infinite system.

When $\alpha=\alpha_c$, there appear no logarithmic corrections in the excitation gaps because the bare coupling y_0 is zero. In this way, Affleck, Gepner, Schulz and Ziman [13] stated that $\alpha_c\simeq 0.25$ from their numerical data for the excitation gaps of the $N=20$ system. Here we perform a more detailed analysis than Affleck et al. The critical value α_c will be determined by

$$\alpha_c=\lim_{N\to\infty}\alpha_c(N), \qquad (19)$$

where $\alpha_c(N)$ is obtained from

$$G_{st}(N,\alpha_c(N))=G_{ss}(N,\alpha_c(N)). \qquad (20)$$

This is our basic idea to determine α_c.

We have numerically calculated $G_{st}(N,\alpha)\equiv E_1^{(0)}(N,\alpha)-E_0^{(0)}(N,\alpha)$ and $G_{ss}(N,\alpha)\equiv E_0^{(1)}(N,\alpha)-E_0^{(0)}(N,\alpha)$ for the finite systems $N=8$, 10, ..., 24 by the use of TITPACK ver. 2 developed by Nishimori. Figure 1 shows $G_{st}(N,\alpha)$ and $G_{ss}(N,\alpha)$ as a function of α when $N=10$ and 20. We can see that the crossing points of $G_{st}(N,\alpha)$ and $G_{ss}(N,\alpha)$ are almost independent of N as expected. In table 1, we list the values of $\alpha_c(N)$ calculated through eq. (20) by the use of the numerical data with a 0.01 step of α and linear interpolation. For the $N\to\infty$ extrapolation of $\alpha_c(N)$, we have used the so-called alternating-ϵ algorithm [9] defined by the equations

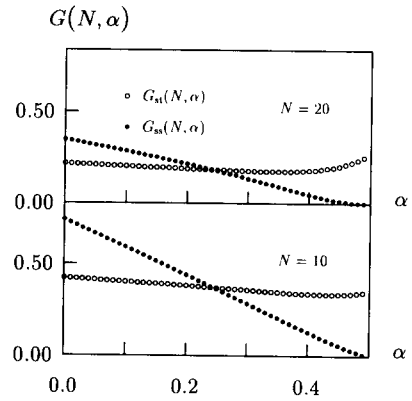

Fig. 1. Singlet–triplet gap $E_{st}(N,\alpha)$ (open circles) and singlet–singlet gap $E_{ss}(N,\alpha)$ (closed circles) for $N=10$ and 20. The gaps are measured in units of J. In both cases, $E_{st}(N,\alpha)=E_{ss}(N,\alpha)$ occurs for $0.24<\alpha<0.25$.

$$\alpha_c^{(m+1)}(N)=\alpha_c^{(m)}(N)$$
$$+\frac{1}{Q^{(m)}(N)-Q^{(m)}(N-2)}, \qquad (21)$$

$$Q^{(m)}(N)=a_m Q^{(m-1)}(N)$$
$$+\frac{1}{\alpha_c^{(m)}(N+2)-\alpha_c^{(m)}(N)}, \qquad (22)$$

where $Q^{(-1)}(N)=0$, $\alpha_c^{(0)}(N)\equiv\alpha_c(N)$ and

$$a_m\equiv-\tfrac{1}{2}[1-(-1)^m]. \qquad (23)$$

The extrapolation procedure is shown in table 1, from which we obtain

$$\alpha_c=0.24112218 \quad (\text{alternating-}\epsilon\text{ algorithm}). \qquad (24)$$

Setting $a_m=0$, eqs. (21) and (22) are equivalent to Shanks' transformation [9]. Shanks' transformation yields

$$\alpha_c=0.24117290 \quad (\text{Shanks' transformation}). \qquad (25)$$

Next we consider the origin of the N-dependence of

Table 1
The values of $\alpha_c(N)$ and the VBS extrapolation procedure.

N	$\alpha_c(N)$	$\alpha_c^{(1)}(N)$	$\alpha_c^{(2)}(N)$	$\alpha_c^{(3)}(N)$	$\alpha_c^{(4)}$
8	0.24630338				
10	0.24449187	0.24220936			
12	0.24348191	0.24190605	0.24104429		
14	0.24286642	0.24170966	0.24111223	0.24112389	
16	0.24246468	0.24157860	0.24112235	0.24112205	0.24112218
18	0.24218827	0.24148728	0.24112204	0.24112231	
20	0.24199002	0.24142112	0.24112416		
22	0.24184301	0.24137172			
24	0.24173095				

$\alpha_c(N)$. Besides the logarithmic corrections by the marginal term, there exist contributions from the irrelevant terms which are not explicitly shown in the phase Hamiltonian. Among them, the most important one should be $O(N^{-3})$ [12,14]. Taking account of this term, eqs. (16) and (17) should be rewritten as

$$G_{st}(N,\alpha)=\frac{2\pi v(\alpha)}{N}\left(\frac{1}{2}-\frac{1}{4}\frac{2}{2\log N+1/y_0}+\frac{C_1}{N^2}\right), \tag{26}$$

$$G_{ss}(N,\alpha)=\frac{2\pi v(\alpha)}{N}\left(\frac{1}{2}+\frac{3}{4}\frac{2}{2\log N+1/y_0}+\frac{C_2}{N^2}\right), \tag{27}$$

respectively. Since y_0 is proportional to $\alpha_c-\alpha$ near α_c, we can write $y_0=p(\alpha_c-\alpha)$ with a positive constant p. The solution of $G_{st}(N,\ \alpha(N))=G_{ss}(N,\ \alpha(N))$ is

$$\alpha_c(N)-\alpha_c=\frac{C_2-C_1}{2pN^2}+O\left(\frac{\log N}{N^4}\right), \tag{28}$$

Strictly speaking, there are $\log(\log N)$ and $(\log N)^2$ terms [14], but the main point of the above argument still holds. Therefore $\alpha_c(N)$ can be approximated as

$$\alpha_c(N)=\alpha_c+\frac{\text{const}}{N^2}. \tag{29}$$

In fact, we can see a very good linearity when we plot $\alpha_c(N)$ versus $1/N^2$. The least-squares fitting to eq. (29) yields

$$\alpha_c=0.241155\pm0.000003, \tag{30}$$

and we can reproduce the data of $\alpha_c(N)$ by eq. (29) within 0.03% accuracy. The very small error in eq. (30) ensures the above consideration.

Thus we can safely conclude that

$$\alpha_c=0.2411\pm0.0001. \tag{31}$$

As a check of the conformal invariance in the spin fluid region, we try to calculate the spin wave velocity $v(\alpha)$ from

$$E_g(N,\alpha)=e_g(\alpha)N-\frac{\pi v_0(\alpha)}{6N} \tag{32}$$

(see eq. (18)), and

$$\tfrac{1}{4}[3G_{st}(N,\alpha)+G_{ss}(N,\alpha)]=\frac{\pi v_1(\alpha)}{N}\left(1+\frac{\text{const}}{(\log N)^2}\right) \tag{33}$$

(see eqs. (16) and (17)). Figure 2 shows the ratio $R(\alpha)\equiv v_0(\alpha)/v_1(\alpha)$ versus α. From the relation $R(\alpha)\simeq 1$ in the spin fluid region, we can say that conformal invariance holds in this region.

Recently Tonegawa and Harada [15] have stated that $\alpha_c=0.25\pm0.01$ from the re-analysis of their data by the use of the phenomenological renormalization group.

In conclusion, we have determined the critical value $\alpha_c=0.2411\pm0.0001$ from the numerical data of the finite size systems with the help of conformal field theory.

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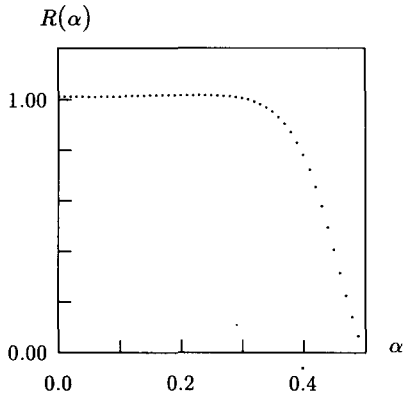

Fig. 2. Plot of $R(\alpha) \equiv v_0(\alpha)/v_1(\alpha)$ versus α.

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