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1995 J. Phys.: Condens. Matter 7 7991

(http://iopscience.iop.org/0953-8984/7/41/008)

J. Phys.: Condens. Matter 7 (1995) 7991–7996. Printed in the UK

Estimation of the critical magnetic field of the phase transition for an $S = 1$ quantum spin chain

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Received 30 May 1995, in final form 1 August 1995

Abstract. It has been shown that there exists an additional magnetic phase transition of the magnetization curve for the $S = 1$ SU(3) antiferromagnetic spin chain at zero temperature. As a the magnetic field decreases from the saturation field, there is a phase change at a critical field h_c, where the magnetization curve versus the magnetic field has a cusp. The critical field is a boundary between two states, one of which contains the particles with the spin $+1$ and 0 and the other with the spin $+1$, 0 and -1. In this paper we estimate the critical field h_c of the phase transition by examining the stability of these states.

Low-dimensional quantum systems have attracted much attention for a long time. One of the most interesting studies is that of Haldane's conjecture [1] on the excitation gap between the singlet and triplet ground-state energies for the spin-1 Heisenberg quantum spin chain. The ground state is theoretically shown to consist of the valence-bond-solid state and have an energy gap and an exponentially decaying correlation function [2]. On the other hand, as a result of experimental techniques such as the generation of high magnetic field and the production of quasi-one dimensional systems being developed, many experiments have been performed on $S = 1$ Heisenberg antiferromagnets and they have given experimental evidence for Haldane's conjecture [3, 4]. So far most studies on quantum spin chains have been carried out for systems at low magnetic field, so the behaviour of quantum spin systems in the high-magnetic-field region has not yet been fully examined. However, very recently detailed magnetic properties near the saturation field for quasi-one-dimensional systems such as NENP and $CsNiCl_3$ were observed by Nojiri *et al* [5]; moreover, interesting theoretical work on quantum systems in the high-magnetic-field region has been done and curious phenomena have been found [6, 7]. It is important to investigate magnetic properties of low-dimensional systems in high magnetic fields.

Several years ago, Parkinson [8] showed that the magnetic field dependence of the magnetization curve for the SU(3) antiferromagnetic quantum spin chain at zero temperature has a cusp which corresponds to the discontinuity of the magnetic susceptibility in the finite-magnetic-field region. We extended his result and pointed out that the integrable SU(M) and SU$_q$(M) spin chains undergo $M - 1$ phase transitions [9]. The SU(M) quantum spin chain has already been solved by Sutherland [10] using the Bethe *ansatz* method. The original eigenvalue problem is reduced to a set of integral equations. We solved these integral equations numerically and estimated the critical magnetic field from figures showing the magnetization curve versus the magnetic field. In this paper, we estimate the critical field by examining the stability of the states.

0953-8984/95/417991+06$19.50

The Hamiltonian of the SU(3) quantum spin chain of N sites in an external magnetic field h is given by

$$H = \sum_{i=1}^{N}[S_i \cdot S_{i+1} + (S_i \cdot S_{i+1})^2] - h\sum_{i=1}^{N} S_i^z \tag{1}$$

where the S_i are the spin operators for $S = 1$. In the S_i^z-diagonal representations, the operator $S_i \cdot S_{i+1} + (S_i \cdot S_{i+1})^2$ conserves the number of sites with 'spin' (value of S_i^z) of each of the three possible types $+1$, 0 and -1. We define the number of particles with 'spin' $+1$, 0 and -1 as n_{+1}, n_0 and n_{-1}, respectively. Imposing the periodic boundary condition, the eigenvalue problem of the above Hamiltonian (1) is reduced to a set of transcendental equations for rapidities α and β by the Bethe *ansatz* method [10]. These equations are the following ones

$$(-1)^N \left(\frac{\alpha_a - \mathrm{i}/2}{\alpha_a + \mathrm{i}/2}\right)^N = \prod_{b=1}^{n_0}\left(\frac{\alpha_a - \beta_b + \mathrm{i}/2}{\alpha_a - \beta_b - \mathrm{i}/2}\right)\prod_{a'=1}^{n_0+n_{-1}}\left(\frac{\alpha_a - \alpha_{a'} - \mathrm{i}}{\alpha_a - \alpha_{a'} + \mathrm{i}}\right) \tag{2}$$

$$\prod_{b'=1}^{n_{-1}}\left(\frac{\beta_b - \beta_{b'} - \mathrm{i}}{\beta_b - \beta_{b'} + \mathrm{i}}\right) = \prod_{a=1}^{n_0+n_{-1}}\left(\frac{\beta_b - \alpha_a - \mathrm{i}/2}{\beta_b - \alpha_a + \mathrm{i}/2}\right). \tag{3}$$

Taking the logarithm of equations (2) and (3), and taking the limit $N \to \infty$ with the ratio $(n_0 + n_{-1})/N$ and n_{-1}/N kept finite, we have a set of integral equations for root-density distribution functions $\rho_1(k)$ and $\rho_2(k)$

$$2\pi\rho_1(\alpha) = g(\alpha) + \int_{-B_1}^{B_1} K_1(\alpha - \alpha')\rho_1(\alpha')\,\mathrm{d}\alpha' + \int_{-B_2}^{B_2} K_2(\alpha - \beta')\rho_2(\beta')\,\mathrm{d}\beta' \tag{4}$$

$$2\pi\rho_2(\beta) = \int_{-B_1}^{B_1} K_2(\beta - \alpha')\rho_1(\alpha')\,\mathrm{d}\alpha' + \int_{-B_2}^{B_2} K_1(\beta - \beta')\rho_2(\beta')\,\mathrm{d}\beta' \tag{5}$$

where

$$g(x) = K_2(x) = \frac{4}{1+4x^2} \tag{6}$$

$$K_1(x) = -\frac{2}{1+x^2}. \tag{7}$$

The integration bounds $\{B_i\}$ are related to $\{n_j\}$ by the following equations,

$$\frac{n_0 + n_{-1}}{N} = \int_{-B_1}^{B_1} \rho_1(\alpha)\,\mathrm{d}\alpha \tag{8}$$

$$\frac{n_{-1}}{N} = \int_{-B_2}^{B_2} \rho_2(\beta)\,\mathrm{d}\beta. \tag{9}$$

The magnetization per site $\sigma = \sum_i S_i^z/N$ and the energy per site ϵ are given by

$$\sigma = 1 - \int_{-B_1}^{B_1} \rho_1(\alpha)\,\mathrm{d}\alpha - \int_{-B_2}^{B_2} \rho_2(\beta)\,\mathrm{d}\beta \tag{10}$$

$$\epsilon = \epsilon_0 - h\sigma = -\int_{-B_1}^{B_1} g(\alpha)\rho_1(\alpha)\,\mathrm{d}\alpha - h\left[1 - \int_{-B_1}^{B_1}\rho_1(\alpha)\,\mathrm{d}\alpha - \int_{-B_2}^{B_2}\rho_2(\beta)\,\mathrm{d}\beta\right] \tag{11}$$

where, for simplicity, we have taken the energy of the ferromagnetic state as zero energy. Parkinson solved these equations, (4), (5), (10) and (11), numerically for various values of B_1 and B_2, so that he obtained the lowest energy ϵ_0 for a given σ. The magnetic field for a given magnetization can be calculated from the derivative of the energy with respect to the magnetization:

$$h = \frac{\partial \epsilon_0}{\partial \sigma}. \tag{12}$$

In the high-magnetic-field region the integral set of equations for the ground state becomes

$$2\pi\rho_1(\alpha) = g(\alpha) + \int_{-B_1}^{B_1} K_1(\alpha - \alpha')\rho_1(\alpha')\, \mathrm{d}\alpha' \tag{13}$$

$$\sigma = 1 - \int_{-B_1}^{B_1} \rho_1(\alpha)\, \mathrm{d}\alpha. \tag{14}$$

These equations correspond to the case $\rho_2 = 0$ (namely, $n_{-1} = 0$) in equations (4) and (10), and are the same as the integral equations of the $S = 1/2$ isotropic antiferromagnetic Heisenberg model. On decreasing the magnetic field from the saturation field, the value of ρ_2 in the integral equations for the ground state becomes non-zero at the critical magnetic field h_c. The ground state in the finite magnetic field has a phase change from a state which consists of particles with spins $+1$ and 0 in the higher-magnetic-field region to one with spins $+1$, 0 and -1 in the lower-magnetic-field region. At the critical field h_c the magnetization curve as a function of the external magnetic field has a cusp, which corresponds to the discontinuity of the magnetic susceptibility.

In order to calculate the critical magnetic field h_c, we compare the stability of the states in the subspace $n_{-1} = 1$ with ones in the subspace $n_{-1} = 0$. In the case of the states in the subspace $n_{-1} = 0$, a set of the integral equations leads to (13) and (14) as mentioned the above. On the other hand, in the case of the states in the subspace $n_{-1} = 1$, we recall the set of the transcendental equations (2) and (3), which becomes

$$(-1)^N \left(\frac{\alpha_a - \mathrm{i}/2}{\alpha_a + \mathrm{i}/2}\right)^N = \left(\frac{\alpha_a - \beta + \mathrm{i}/2}{\alpha_a - \beta - \mathrm{i}/2}\right) \prod_{a'=1}^{n_0+1} \left(\frac{\alpha_a - \alpha_{a'} - \mathrm{i}}{\alpha_a - \alpha_{a'} + \mathrm{i}}\right) \tag{15}$$

$$1 = \prod_{a=1}^{n_0+1} \left(\frac{\beta - \alpha_a - \mathrm{i}/2}{\beta - \alpha_a + \mathrm{i}/2}\right) \tag{16}$$

where β is the rapidity of the particle with spin -1. We take the logarithm of these equations:

$$2N \tan^{-1}(2\alpha_a) = 2\pi I_a - 2\tan^{-1} 2(\alpha_a - \beta) + \sum_{a'} 2\tan^{-1}(\alpha_a - \alpha_{a'}) \tag{17}$$

$$0 = 2\pi J - \sum_{a'} 2\tan^{-1} 2(\beta - \alpha_{a'}). \tag{18}$$

Hence we set $\beta = 0$, which corresponds to the long-wavelength limit of the -1 excitation with spin and realizes the lowest-energy state in the subspace $n_{-1} = 1$. Even if there exists an external magnetic field, the values of the rapidities α are distributed symmetrically with respect to the origin. Setting $J = 0$, equation (18) is satisfied. In the limit of $N \to \infty$ and $n_0 \to \infty$ with the ratio n_0/N kept finite, we have the $1/N$ expansion of the root-density distribution function $\tilde{\rho}_1(\alpha)$:

$$g(\alpha) = 2\pi\tilde{\rho}_1(\alpha) - \frac{1}{N}g(\alpha) - \int_{-\tilde{B}_1}^{\tilde{B}_1} K_1(\alpha - \alpha')\tilde{\rho}_1(\alpha')\, \mathrm{d}\alpha' + \mathrm{O}\left(\frac{1}{N^2}\right). \tag{19}$$

The magnetization and the energy in the subspace $n_{-1} = 1$ lead to

$$\tilde{\sigma} = 1 - \int_{-\tilde{B}_1}^{\tilde{B}_1} \tilde{\rho}_1(\alpha)\, \mathrm{d}\alpha - \frac{1}{N} \tag{20}$$

$$\tilde{\epsilon} = - \int_{-\tilde{B}_1}^{\tilde{B}_1} g(\alpha)\tilde{\rho}_1(\alpha)\, \mathrm{d}\alpha - h\tilde{\sigma}. \tag{21}$$

Our aim is to compare the value of (11) with that of (21). For the purpose of this comparison, manipulations used in [11, 12] are very useful. In order to examine the energy difference of $1/N$ order, we introduce the distribution function $\rho_1^{(1)}(\alpha)$:

$$\tilde{\rho}_1(\alpha) = \rho_1(\alpha) + \frac{1}{N}\rho_1^{(1)}(\alpha) \tag{22}$$

where $\rho_1(\alpha)$ is the distribution function in the integral equation (13). Putting formula (22) into the integral equation (19). It is easy to show that the distribution function $\rho_1^{(1)}(\alpha)$ satisfies the same equation as (13), that is, $\rho_1^{(1)}(\alpha) = \rho_1(\alpha)$. In order to indicate the dependence on the integration bound B of the magnetization and the energy, we rewrite the magnetization and the energy as follows:

$$\sigma^{(0)}(B) = 1 - \int_{-B}^{B} \rho_1(\alpha)\, \mathrm{d}\alpha \tag{23}$$

$$\epsilon^{(0)}(B) = - \int_{-B}^{B} g(\alpha)\rho_1(\alpha)\, \mathrm{d}\alpha. \tag{24}$$

Since we are investigating the stability of the energy with fixed magnetization, the magnetization (14) is equal to (20).

$$1 - \int_{-B_1}^{B_1} \rho_1(\alpha)\, \mathrm{d}\alpha = 1 - \int_{-\tilde{B}_1}^{\tilde{B}_1} \tilde{\rho}_1(\alpha)\, \mathrm{d}\alpha - \frac{1}{N}. \tag{25}$$

We substitute formulas (22) and (23) into the above identity (25), so that we obtain

$$\sigma^{(0)}(B_1) = \sigma^{(0)}(\tilde{B}_1) - \frac{1}{N}\left[\int_{-B_1}^{B_1} \rho_1^{(1)}(\alpha)\, \mathrm{d}\alpha + 1\right] \tag{26}$$

where we replaced the integration bound $\tilde{B}_1$ by B_1, since this equation is an approximation of order $1/N$. From the relation (26), we can obtain the difference between B_1 and $\tilde{B}_1$,

$$\tilde{B}_1 - B_1 = \left[\frac{\partial\sigma^{(0)}(B_1)}{\partial B_1}\right]^{-1} \frac{1}{N}\left[\int_{-B_1}^{B_1} \rho_1^{(1)}(\alpha)\, \mathrm{d}\alpha + 1\right] \tag{27}$$

where we have taken the difference between B_1 and $\tilde{B}_1$ up to the order of $1/N$. As for the difference between the energies, we obtain

$$\begin{aligned}
\tilde{\epsilon}'(\tilde{B}_1) - \epsilon^{(0)}(B_1) &= - \int_{-\tilde{B}_1}^{\tilde{B}_1} g(\alpha)\tilde{\rho}_1(\alpha)\, \mathrm{d}\alpha - \epsilon^{(0)}(B_1) \\
&= \epsilon^{(0)}(\tilde{B}_1) - \epsilon^{(0)}(B_1) - \frac{1}{N}\int_{-B_1}^{B_1} g(\alpha)\rho_1^{(1)}(\alpha)\, \mathrm{d}\alpha \\
&= \frac{\partial\epsilon^{(0)}(B_1)}{\partial B_1}(\tilde{B}_1 - B_1) - \frac{1}{N}\int_{-B_1}^{B_1} g(\alpha)\rho_1^{(1)}(\alpha)\, \mathrm{d}\alpha \\
&= \frac{\partial\epsilon^{(0)}(B_1)}{\partial B_1}\left[\frac{\partial\sigma^{(0)}(B_1)}{\partial B_1}\right]^{-1} \frac{1}{N}\left[\int_{-B_1}^{B_1} \rho_1^{(1)}(\alpha)\, \mathrm{d}\alpha + 1\right]
\end{aligned}$$

$$-\frac{1}{N}\int_{-B_1}^{B_1} g(\alpha)\rho_1^{(1)}(\alpha)\,\mathrm{d}\alpha. \tag{28}$$

In order to derive the energy difference, we need to calculate the derivation of the magnetization and the energy with respect to the integration bound B_1. For simplicity, we introduce a short-hand vector–matrix notation of the integral equation (13):

$$2\pi\rho_1(\alpha) = g(\alpha) + K_{1:\alpha,\alpha'} * \rho_1(\alpha') \tag{29}$$

where the symbol $*$ represents the usual matrix product and integration over α' from $-B_1$ to B_1 [13, 14]. The derivation of ρ_1 with respect to the integration bound B_1 leads to

$$\frac{\partial\rho_1(\alpha)}{\partial B_1} = -\frac{\rho_1(B_1)}{\pi}[1+K_{1:\alpha,\alpha'}]^{-1} * \left[\frac{1}{1+(\alpha'+B_1)^2} + \frac{1}{1+(\alpha'-B_1)^2}\right] \tag{30}$$

where ρ_1 is even function. Taking the derivatives (23) and (24) with respect to B_1, we obtain

$$\frac{\partial\sigma^{(0)}(B_1)}{\partial B_1} = -2\rho_1(B_1) - \int_{-B_1}^{B_1}\frac{\partial\rho_1(\alpha)}{\partial B_1}\,\mathrm{d}\alpha$$

$$\frac{\partial\epsilon^{(0)}(B_1)}{\partial B_1} = -2g(B_1)\rho_1(B_1) - \int_{-B_1}^{B_1} g(\alpha)\frac{\partial\rho_1(\alpha)}{\partial B_1}\,\mathrm{d}\alpha.$$

Using (30), we find that

$$\frac{\partial\sigma^{(0)}(B_1)}{\partial B_1} = -\rho_1(B_1)\left\{2 - \frac{1}{\pi}\int_{-B_1}^{B_1}[1+K_{1:\alpha,\alpha'}]^{-1} * \left[\frac{1}{1+(\alpha'+B_1)^2} + \frac{1}{1+(\alpha'-B_1)^2}\right]\mathrm{d}\alpha\right\} \tag{31}$$

$$\frac{\partial\epsilon^{(0)}(B_1)}{\partial B_1} = -\rho_1(B_1)\left\{2g(B_1) - \frac{1}{\pi}\int_{-B_1}^{B_1} g(\alpha)[1+K_{1:\alpha,\alpha'}]^{-1} * \left[\frac{1}{1+(\alpha'+B_1)^2} + \frac{1}{1+(\alpha'-B_1)^2}\right]\mathrm{d}\alpha\right\}. \tag{32}$$

These equations, (31) and (32), yield the energy difference (28):

$$\Delta\epsilon(B_1) = \tilde{\epsilon}'(\tilde{B}_1) - \epsilon^{(0)}(B_1). \tag{33}$$

We solve the equation $\Delta\epsilon(B_1) = 0$ numerically by converting the integral equation into a matrix equation for various integration bounds B_1 and obtain $B_c = 0.709\,28\cdots$. On increasing the integration limit B_1 from 0 to ∞, the states in the subspace $n_{-1} = 0$ are more stable than those in the subspace $n_{-1} \neq 0$ in the region $0 < B_1 < B_c$. When B_1 is in the region $B_c < B_1 < \infty$, the states in the subspace $n_{-1} \neq 0$ are more stable than those in the subspace $n_{-1} = 0$. In order to obtain the critical field, we use (12), (31) and (32) (cf. [15]).

$$h = \frac{\partial\epsilon^{(0)}}{\partial\sigma^{(0)}} = \frac{\partial\epsilon^{(0)}(B_1)}{\partial B_1}\frac{\partial B_1}{\partial\sigma^{(0)}(B_1)} = \frac{(\text{numerator})}{(\text{denominator})} \tag{34}$$

where

$$(\text{numerator}) = 2g(B_1) - \frac{1}{\pi}\int_{-B_1}^{B_1} g(\alpha)[1+K_{1:\alpha,\alpha'}]^{-1} * \left[\frac{1}{1+(\alpha'+B_1)^2} + \frac{1}{1+(\alpha'-B_1)^2}\right]\mathrm{d}\alpha$$

$$(\text{denominator}) = 2 - \frac{1}{\pi}\int_{-B_1}^{B_1}[1+K_{1:\alpha,\alpha'}]^{-1} * \left[\frac{1}{1+(\alpha'+B_1)^2} + \frac{1}{1+(\alpha'-B_1)^2}\right]\mathrm{d}\alpha.$$

Putting $B_c = 0.709\,28\cdots$ into (23) and (34), we obtain the magnetization $\sigma_c = 0.556\,20\cdots$ and the critical field $h_c = 0.941\,38\cdots$, which are in agreement with the Parkinson's results [8].

It has been already shown that the $S = 1$ $SU(3)$ quantum antiferromagnetic spin chain undergoes a phase transition in the finite-magnetic-field region. The transition is of second order with a cusp in the magnetization curve. This new phase change marks the boundary between two states, one of which contains the particles with the spin $+1$ and 0 and the other with the spin $+1$, 0 and -1. In this paper the critical magnetic field h_c is obtained accurately by comparing the stability of the two states.

The Hamiltonian (1) is easily generalized to the following one:

$$H = \sum_{i=1}^{N}[S_i \cdot S_{i+1} + \beta(S_i \cdot S_{i+1})^2] - h\sum_{i=1}^{N} S_i^z \tag{35}$$

where β ranges from $-\infty$ to $+\infty$. We have only discussed the case of $\beta = 1$. When $\beta \neq 1$, it is interesting to investigate the possibility of this phase change, which corresponds to the cusp of the magnetization curve. For the $S = 1$ Heisenberg spin chain (namely, $\beta = 0$), Yamamoto and Miyashita [7] performed a quantum Monte Carlo calculation for both the open and the periodic boundary condition and investigated the magnetization curve at finite temperature. Comparing the result under the periodic boundary condition with the open one, they have shown that as the magnetic field increases, the state of the system changes from the Haldane phase to a different phase. It is very interesting to investigate whether this phase change corresponds to the cusp of the magnetization curve or not.

We point out that our approach is valid for non-integral systems which are integrable in the high-magnetic-field region. In this paper we utilize the integrability of the system in high-magnetic-field region and exactly calculated two-body S-matrices. If a set of the equations which correspond to (15) and (16) are derived exactly, the critical field is calculated by the method in this paper.

Acknowledgment

We are grateful to Professor Y Akutsu for introducing us to this problem and for critical reading of the manuscript.

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