Magnetic and Critical Properties of Alternating Spin Chain with $S = 1/2$, 1 in Magnetic Fields

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We study an integrable spin chain with an alternating array of spins $S = 1/2$, 1 in external magnetic fields using the Bethe ansatz exact solution. The calculated magnetization possesses a cusp structure at a critical magnetic field $H = H_C$, at which the specific heat shows a divergence property. We also calculate finite-size corrections to the energy spectrum, and obtain the critical exponents of correlation functions with the use of conformal field theory (CFT). Low-energy properties of the model are described by two $c = 1$ $U(1)$ CFTs in $H < H_C$ and one $c = 1$ $U(1)$ CFT in $H > H_C$.

KEYWORDS: alternating spin chain, exact solution, conformal field theory

It is now well established that the antiferromagnetic quantum spin chains with half-integer spins have massless excitations, whereas those with integer spins have massive ones (Haldane gap), although the ground state of both cases are known to be singlet. Experimentally, the spin systems with an alternating array of integer and half-integer spins both for ferromagnetic and antiferromagnetic cases have been found, i.e. the spin systems with an alternating array of spins $S = 1/2$ and $S = 1$ in external magnetic fields are known to be singlet. In this paper, we study the integrable alternating spin model of

$$\sigma_1 \sigma_2 \sigma_3 \sigma_4 \cdots \sigma_{2N},$$

where

$$L = 2N$$

is assumed to be a multiple of 4. Here we have taken the fully polarized state as a reference state, and denotes the number of “particles” by $M$, which are created by the spin-lowering operator. So, the $z$-component of the total spin is to be $S^z = 3N/2 - M$. One can see two kinds of phase factors reflecting the mixture of spin 1 and 1/2 in $S^z$ in the left-hand side of (2). The total energy is

$$E = \frac{7}{6}N - \sum_{j=1}^{M} \left( \frac{1}{\lambda_j^2 + \frac{1}{4}} + \frac{2}{\lambda_j^2 + 1} \right) - HS^z$$

and the total momentum is given by $P = \text{Im} \sum_{j=1}^{M} \log[(\lambda_j - \frac{1}{2})(\lambda_j + \frac{1}{2})]$. So far, thermodynamic properties of the model have been investigated, revealing some properties distinct from those of the ordinary Heisenberg spin chain. Also, conformal properties have been discussed to some extent: the system at zero field is classified as
CFT of central charge $c = \frac{3}{2}$, and is conjectured to be described by level-1 SU(2) Wess-Zumino-Witten model. In what follows, we systematically study the model in the presence of magnetic fields, and show that below a certain critical field $H_C$, low-energy properties of the model are described by two $c = 1$ U(1) CFTs, while for $H > H_C$ by one $c = 1$ U(1) CFT. Accordingly, the system shows quite different critical behaviors for low fields $H < H_C$ and high fields $H > H_C$.

We start with the calculation of the magnetization curve. To this end we need the Bethe equations in the thermodynamic limit. For large enough $L$, the ground state properties can be described by $M_R$, $2$-string complex rapidities $\lambda_R^\alpha$, and $2$-string complex rapidities $\lambda_C^\alpha$:

$$\lambda_R^\alpha = \lambda_C^\alpha + \frac{1}{2} i (3 - 2 \alpha) \quad (\alpha = 1, 2),$$

where $\lambda_C^\alpha (j = 1, 2, \cdots, M_C)$ is a real number which labels the center of the $2$-string $\lambda_C^\alpha$. The Bethe equation (4) is thus converted into integral equations for the density functions $\rho^R(\lambda^R)$ and $\rho^C(\lambda^C)$ for these rapidities:

$$\begin{pmatrix} \rho^R \\ \rho^C \end{pmatrix} = \begin{pmatrix} \rho^R_0 \\ \rho^C_0 \end{pmatrix} - \begin{pmatrix} K^{RR} & K^{RC} \\ K^{RC} & K^{CC} \end{pmatrix} \otimes \begin{pmatrix} \rho^R \\ \rho^C \end{pmatrix},$$

where the integral kernels are given by $K^{RR}(\lambda) = K_R(\lambda)$, $K^{CC}(\lambda) = \{2K_1(\lambda) + K_2(\lambda)\}$, $K^{CR}(\lambda) = K_R(\lambda) = \{K_{1/2}(\lambda) + K_{3/2}(\lambda)\}$, respectively, in terms of the function $K_\alpha(x) = (x/\pi)[x^2 + 1]^{-1}$. The driving terms read

$$\begin{pmatrix} \rho^R_0 \\ \rho^C_0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} K_1 + K_{1/2} \\ K_{1/2} + K_1 + K_{3/2} \end{pmatrix},$$

and the symbol $\otimes$ denotes the convolution integral in the finite range of $[\Delta^+_\alpha, \Delta^-_\alpha]$ respectively for the sectors of $\alpha = R, C$.

By calculating the above integral equations (5) numerically, we have computed the magnetization $M(\equiv S^z)$ as a function of the magnetic field. The results are shown in Fig.1. We can see that the magnetization begins linearly in magnetic fields (finite spin susceptibility) since the ground state is singlet, and increases smoothly up to the critical field $H_C$, where we encounter a characteristic cusp structure. The existence of the cusp at $H = H_C$ indicates that the magnetization for $H < H_C$ consists of two contributions, i.e. $M = M_R + M_C$, and one of them, $M_C$, saturates at $H = H_C$. For $H > H_C$, the remaining massless spin excitations still contribute to the magnetization, and then at $H = 6$ the system is completely polarized. These characteristic properties directly reflect that the system consists of two kinds of different spins. The anomaly at $H = H_C$ also appears in the specific heat. We show the computed results for the coefficient $\gamma$ of the $T$-linear specific heat in Fig.2. The divergence property for $H \rightarrow H_C$ implies that the velocity for one of spin excitations tends to zero when the system approaches the critical field $H_C$, since the specific heat coefficient $\gamma$ is inversely proportional to the velocity. To see this point clearly, we have plotted two velocities $v_R$ and $v_C$ in Fig.3. It is seen that $v_C$ indeed vanishes at $H = H_C$. Therefore, we can say that there exist two species of spin excitations which behave differently in magnetic fields. They have the distinct pseudo-Fermi surfaces $p_F^R$ and $p_F^C$, both of them decrease with the increase of magnetic fields. In particular, at $H = H_C$, $p_F^C$ vanishes and the corresponding spin excitation becomes massive. In what follows we refer to these spin excitations as spinons in the R- and C-sectors respectively.

In order to further study critical properties of the model in magnetic fields, we now calculate the finite-size corrections. Following a standard technique, we obtain the corrections to the energy

$$E = \lambda_{\infty}(\pm \lambda_0^R, \pm \lambda_0^C) - \frac{\pi v_R}{6L} - \frac{\pi v_C}{6L} + \frac{2\pi v_R}{L}(\Delta^+_R + \Delta^-_R) + \frac{2\pi v_C}{L}(\Delta^+_C + \Delta^-_C).$$

where $\lambda_{\infty}$ is the bulk energy density in the thermodynamic limit. Also, the finite-size corrections to the momentum are

$$P = \sum_{\alpha = R, C} [-2\pi f_\alpha \Delta D_\alpha - \frac{2\pi}{L}(\Delta^+_\alpha - \Delta^-_\alpha)]$$

where “the Fermi momenta” for two spinons are given by $p_F^R = \pi/4 - \pi M_R/L$ and $p_F^C = \pi/2 - \pi M_C/L$ with $M_R = L/4 - M_R$ and $M_C = L/2 - 2M_C$. Here $\Delta D_\alpha$ labels an excitation across the two Fermi points, which carries the large momentum transfer $2\pi f_\alpha \Delta D_\alpha$.

We note that both of the above expressions (7) and (8) completely fit in with the finite-size scaling formu-

lae in CFT. Namely, the corrections $-\pi v_\alpha/(6L)$ to the ground state energy in (7) indicate that two kinds of spinons are described by two $c = 1$ CFTs. Also, the conformal dimensions $\Delta_{\pm}$, which enter the excitation energy as well as the momentum are of desirable forms predicted by CFT.

$$\Delta_{\pm} = \frac{1}{2} \left\{ \frac{\xi_{\alpha}}{2\Delta D_\alpha} \pm (\xi_{\alpha} \Delta D_\alpha + \xi_{\alpha} \Delta D_\beta) \right\}^2 + \xi_{\alpha}$$

for $\alpha = R, C$. Here the so-called dressed charge matrix $\xi_{\alpha}$ is determined by the following integral equations,

$$\xi = I - K \otimes \xi,$$

where $K$ is the $2 \times 2$ matrix of integral kernels which has appeared in eq.(5), and $I$ is the identity matrix. The above dressed charge matrix determines the critical exponents of the present model in magnetic fields. Note that the conformal dimensions (9) both for R- and C-sectors have a typical form inherent in $c = 1$ Gaussian CFT with U(1) symmetry, which has previously appeared in various contexts, for instance, in the analysis of interacting electron systems. Recall here that for $H > H_C$, spinons of the C-sector become massive with vanishing $v_C$. Therefore we can see that low-energy properties of the present model in magnetic fields are described by two $c = 1$ CFTs for $0 < H < H_C$ and one $c = 1$ CFT for $H \geq H_C$.

Having specified the critical behavior in magnetic fields by CFT, we now read critical exponents of correlation functions from the conformal dimensions (9) by
suitably choosing the quantum numbers. For this purpose, we should note that the quantum numbers in (9) are subject to the selection rules

$$\Delta D_R = \frac{\Delta M_R}{2}, \quad \Delta D_C = \frac{\Delta M_C}{2} \pmod{1}, \quad (11)$$

which directly reflect that spinons can be regarded as interacting bosons.

For $H < H_C$ both of two kinds of spinons control the long-distance behavior of correlation functions, since $\gamma_R$ and $\gamma_C$ have finite values. Thus choosing the quantum numbers as

$$(\Delta M_R, \Delta M_C, \Delta D_R, \Delta D_C) = \begin{cases} (0,0,1,0) \\ (0,0,0,1) \end{cases}, \quad (12)$$

we find the spin-spin correlation function to have the asymptotic form,

$$\chi_s(x) \sim \frac{a_0}{x^2} + \frac{a_1 \cos(2p^R_C x)}{x^{\alpha_s^R}} + \frac{a_2 \cos(2p^C_C x)}{x^{\alpha_s^C}}. \quad (13)$$

Note that the spin-spin correlation function has two oscillating terms, reflecting the presence of two-types of spinons. By inserting (12) into (9), and using the formula $\alpha = 2 \sum_{p=1}^{\infty} [\Delta s^p + \Delta C^p]$, we obtain critical exponents for the oscillating parts,

$$\alpha_s^R = 2(\xi^2_{RR} + \xi^2_{RC}), \quad \alpha_s^C = 2(\xi^2_{CR} + \xi^2_{CC}). \quad (14)$$

The numerical results for $\alpha_s^R$ and $\alpha_s^C$ are plotted as a function of the magnetic field in Fig.4. In weak magnetic fields, $\alpha_s^C$ represents how dominant the antiferromagnetic fluctuations are, because $p_C^C \sim \pi/2$. Since the value of $\alpha_s^C$ is close to unity in weak fields, we can see that the antiferromagnetic correlation is indeed dominant there, but is gradually suppressed with the increase of the magnetic filed. For $H \geq H_C$, spinons of the C-sector become massive, and remaining massless spinons in the R-sector solely determine the critical behavior of the system. Accordingly, the third term of the right-hand side in eq.(13) vanishes. Also, the critical exponent $\alpha_s^R$ exhibits a discontinuity at $H = H_C$. This decrease in the critical exponent $\alpha_s^R$ may imply that the corresponding spin correlation may be enhanced to some extent in magnetic fields. Similar phenomena have been indeed observed in a different context where spin correlations are enhanced by decreasing the multiplicity of bands.

As seen from Fig.4, however, the corresponding exponent is larger than unity, so this fluctuation may not become dominant. We note here that a logarithmic correction should enter the correlation functions at $H = 0$ since the symmetry of the system is enhanced from $U(1)$ to $SU(2)$ at $H = 0$, although it does not appear in the present case with finite magnetic fields.

Here, following the arguments of Sachdev [3], we would like to briefly discuss the temperature dependence of nuclear magnetic relaxation rates which may be an experimental probe to study low-energy properties of the system. Since the low-temperature behavior of the model is mainly determined by spinons mentioned above, we can obtain the leading temperature dependence of the nuclear spin-lattice relaxation rates $1/T_1$ and the nuclear spin-spin relaxation rates $1/T_2$ from eq.(13) [4],

$$\frac{1}{T_1} \sim \frac{C_1}{T^{1-\alpha_s^R}} + \frac{C_2}{T^{1-\alpha_s^C}} + C_3 T, \quad (15)$$

$$\left(\frac{1}{T_2 G} \right)^2 \sim \frac{D_1}{T^{3-2\alpha_s^R}} + \frac{D_2}{T^{3-2\alpha_s^C}}. \quad (16)$$

Combining these expressions with the numerical results for the critical exponents shown in Fig.4, we see that $1/T_1$ behaves like $1/T^{1-\alpha_s^R}$ at low temperatures for $H < H_C$. However for $H \geq H_C$ this term vanishes and the low temperature behavior of $1/T_1$ is determined by the term $1/T^{1-\alpha_s^C}$. The temperature dependence of $1/T_2$ for $H < H_C$ is also governed by spinons in the C-sector and given by $1/T^{3/2-\alpha_s^C}$. For $H \geq H_C$ $1/T_2$ behaves like $1/T^{3/2-\alpha_s^C}$.

We have been concerned with the rather special model with alternating spins in this paper. Before concluding the paper, we wish to briefly mention what would be expected if the system were away from the solvable point with coupling constants being changed. Unfortunately there have not been systematic attempts to this problem so far, so that we summarize here two possible disordered ground states predicted by the present analysis. (i) A possibility is that one of the $c = 1$ fields becomes massive in the presence of some relevant perturbations. In this case, we can see from the present results that low-field properties are classified by $c = 1$ CFT, and then the magnetization begins linearly. What is characteristic for this case is that a cusp structure in Fig.1 may not be observed. (ii) Another interesting possibility may be that both of two spinons become massive, and hence the system shows properties like a Haldane-gap system, for which there is no magnetization in low fields. These states, as well as the present massless state, should compete with the magnetically ordered state. In order to fully understand these problems, an extensive study with the aid of bosonization methods and numerical methods would be quite helpful. This issue is now under consideration.

In summary we have investigated magnetic and critical properties of an integrable alternating spin chain in external magnetic fields. The critical properties in magnetic fields are classified in terms of CFT. Although the present analysis is based on a rather special model, it would provide a plausible guideline to systematically explore characteristic properties of this new class of quantum spin chains.

[1] G. T. Yee, J. M. Manriquez, D. A Dixon, R. S. McLean, D. M. Groski, R. B. Flippen, K. S. Narayan, A. J. Epstein, and J. S. Miller: Adv. Mater. 3 (1991) 309; Inorg. Chem. 22 (1983) 2324; ibid. 26 (1987) 136.
[2] J. H. de Vega and F. Wodnarovich: J. Phys. A 25 (1992) 4499.
[3] J. H. de Vega, L. Mezincescu, and R. I. Nepomechie: Phys. Rev. B 49 (1994) 13223; Int. J. Mod. Phys. B 8 (1994) 3473.
[4] S. R. Adams and M. J. Martins: J. Phys. A 26 (1993) L529.
[5] M. J. Martins: J. Phys. A 26 (1993) 7301.
[6] The cut-off parameters $\Lambda^\pm$ are determined so as to minimize the free energy.
[7] We note that a similar cusp structure has been found for the

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related spin model in which different spins are randomly distributed. See P. Schlottmann, Phys. Rev. B 49 (1994) 9202.
[8] H. J. de Vega and F. Woynarovich: Nucl. Phys. B 251 (1985) 439 (1985); F. Woynarovich, J. Phys. A 22 (1989) 4243.
[9] J.L. Cardy: Nucl. Phys. B 270 [FS16] (1986) 186; H. W. Bröte, J. L. Cardy and M. P. Nightingale: Phys. Rev. Lett. 56 (1986) 742; I. Affleck, Phys. Rev. Lett. 56 (1986) 746.
[10] A.G. Izergin, V.E. Korepin and N.Y. Reshetikhin: J. Phys. A22 (1989) 2615.
[11] H.Frahm and V.E. Korepin: Phys. Rev. B. 42, (1990) 10553; N.Kawakami and S.K. Yang: Phys. Rev. Lett. 65 (1990) 2309.
[12] T. Itakura and N. Kawakami: J. Phys. Soc. Jpn. 64 (1995) 2321.
[13] S. Sachdev: Phys. Rev. B 50 (1994) 13006.

Fig. 1. Magnetization as a function of the magnetic field.

Fig. 2. Specific-heat coefficient as a function of the magnetic field.

Fig. 3. Velocities of spin excitations as a function of the magnetic field.

Fig. 4. Critical exponents $\alpha_R$ and $\alpha_C$ for oscillating sectors in the spin correlator as a function of the magnetic field.