The ground state energy of the frustrated ferromagnetic spin chain near the transition point

Ren-Gui Zhu

College of physics and electronic information,
Anhui Normal University, Wuhu, 241000, P. R. China

Abstract

The one-dimensional quantum spin-1/2 model with nearest-neighbor ferromagnetic and next-nearest-neighbor antiferromagnetic interaction is considered. The Hamiltonian is first bosonized by using the linear spin wave approximation, and then is treated by using the Green’s function approach. An integral expression of the quantum correction to the classical ground state energy is derived. The critical behavior of the ground state energy in the vicinity of the transition point from the ferromagnetic to the singlet ground state is analyzed by numerical calculation, and the result is $-8\gamma^2$.

PACS numbers: 75.10.Jm, 75.10.Pq, 75.10.Hk
I. INTRODUCTION

Low-dimensional frustrated spin models have been intensively investigated both theoretically and experimentally[1, 2]. The one-dimensional (1D) quantum spin-1/2 model with nearest-neighbor ferromagnetic interaction $J_1$ and next-nearest-neighbor antiferromagnetic interactions $J_2$ has attracted much attention in recent years[3–12]. The growing interest was triggered by experimental studies of various quasi-1D edge-sharing cuprates[13–27], which can be described by this so-called 1D F-AF model. Its Hamiltonian has a form:

$$H = J_1 \sum_{n=1}^{N} \left( S_n \cdot S_{n+1} - \frac{1}{4} \right) + J_2 \sum_{n=1}^{N} \left( S_n \cdot S_{n+2} - \frac{1}{4} \right),$$  \hspace{1cm} (1)

where $J_1 < 0, J_2 > 0$, and the constant shifts $1/4$ is added to secure the energy of the fully polarized state to be zero.

It is known that there is a ground state phase transition at the point $\alpha \equiv J_2/|J_1| = 1/4$[28–30]. For $\alpha < 1/4$, the ground state is ferromagnetic. For $\alpha > 1/4$, the ground state is an incommensurate singlet with spiral spin correlations. At $\alpha = 1/4$, the ferromagnetic state is degenerate with the singlet state.

One of the interesting problems in ground state properties is the critical behavior of the ground state energy at this transition point, which can be described by $E/N = -a \gamma^\beta$ with $\gamma = \alpha - 1/4$ and $0 < \gamma << 1$. The coupled cluster method gave $E/N \sim \gamma^2$[31]. The perturbation theory based on the classical approximation gave $E/N = -4\gamma^2$[32]. However, by using Jordan-Wigner mean field theory, Dmitriev and Krivnov[33] found recently that the critical exponent $\beta$ should be less than $12/7$. Later, they confirmed that $\beta = 5/3$ by using scaling estimates of perturbation theory[34].

According to the previous results, it seems that the critical behavior of the ground state energy in the vicinity of the transition point is still a controversial problem, and more elaborate methods are needed to obtain a definitive result. As an important method in quantum magnetism, the spin wave theory often gives out significant reference results. To our knowledge, however, the spin wave theory in a regular way has not been applied to this problem. In this paper, we try to make up this blank. Compared with previous work, our following treatment is easier and straightforward, and the final results have also some difference.
II. THE BOSONIZATION OF THE HAMILTONIAN

In the classical picture of the ground state of the 1D F-AF model, the spins are vectors which form the spiral structure with a pitch angle \( \varphi \) between neighboring spins in the \( xy \) plane, and all spin vectors have the same canted angle \( \theta \) from the \( z \) axis. We choose a reference state for the spin wave theory with all spin vectors point along the \( z \) axis. So we define the new spin operators \( \eta_n \)'s, which are related to the original ones by the following rotational transformation:

\[ S_n = R_z(n\varphi)R_y(\theta)\eta_n, \]

(2)

where \( R_y(\theta) \) is the rotational operator about the \( y \) axis by an angle \( \theta \), and \( R_z(n\varphi) \) is the rotational operator about the \( z \) axis by an angle \( n\varphi \).

Using the new spin operators, the Hamiltonian (1) can be rewritten as

\[
H = \sum_{m=1}^{2} \sum_{n=1}^{N} J_m \left[ F_{++}(\theta, m\varphi)(\eta_n^+ \eta_{n+m}^+ + \eta_n^- \eta_{n+m}^-)
 + F_{+-}(\theta, m\varphi)\eta_n^+ \eta_{n+m}^- + F_{-+}(\theta, m\varphi)\eta_n^- \eta_{n+m}^+
 + F_{zz}(\theta, m\varphi)(\eta_n^z \eta_{n+m}^z + \eta_n^{-z} \eta_{n+m}^{-z})
 + F^+_{zz}(\theta, m\varphi)(\eta_n^z \eta_{n+m}^- + \eta_n^{-z} \eta_{n+m}^z) \right] - \frac{N(J_1 + J_2)}{4},
\]

(3)

where \( \eta_n^\pm = \eta_n^x \pm i \eta_n^y \), and the coefficient functions are

\[
F_{++}(\theta, \varphi) := \frac{1}{4} \sin^2 \theta (1 - \cos \varphi),
\]

(4)

\[
F_{+-}(\theta, \varphi) := \frac{1}{4} (\cos \varphi \cos^2 \theta + \sin^2 \theta + \cos \varphi - 2i \sin \varphi \cos \theta),
\]

(5)

\[
F_{zz}(\theta, \varphi) := \cos \varphi \sin^2 \theta + \cos^2 \theta,
\]

(6)

\[
F^+_{zz}(\theta, \varphi) := \left[ \frac{1}{4} \sin 2\theta (\cos \varphi - 1) - \frac{i}{2} \sin \varphi \sin \theta \right].
\]

(7)

Taking the linear spin-wave approximation\[35\]: \( \eta_n^+ = \sqrt{2S}a_n, \eta_n^- = \sqrt{2S}a_n^\dagger, \eta_n^z = S - a_n^\dagger a_n \), and then the Fourier transformation: \( a_n = \frac{1}{\sqrt{N}} \sum_k b_k e^{i kn} \), we obtain the bosonic Hamiltonian:

\[
H = E_0(\theta, \varphi) + \sum_k A(\theta, \varphi, k) b_k^\dagger b_k + \sum_k B(\theta, \varphi, k)(b_k b_{-k} + b_k^\dagger b_{-k}^\dagger),
\]

(8)
where
\[
A(\theta, \varphi, k) = \sum_{m=1}^{2} 4S J_m \text{Re}[F_{+\pm}(\theta, m\varphi) \cos mk] - \sum_m 2SJ_m F_{zz}(\theta, m\varphi),
\]

(9)
\[
B(\theta, \varphi, k) = \sum_{m=1}^{2} 2SJ_m F_{++}(\theta, m\varphi) \cos mk,
\]

(10)
\[
E_0(\theta, \varphi) = N\left[\sum_{m=1}^{2} S^2 J_m F_{zz}(\theta, m\varphi) - \frac{1}{4}(J_1 + J_2)\right].
\]

(11)

We note here that the terms containing four Bose-operators have been neglected as usually. The terms containing odd number of Bose operators have been neglected as well according to the treatment in Ref. [33], because they have no contribution to the energy in the mean-field approximation. It is only based on these approximations that we can obtain the above regular bosonic Hamiltonian, and its effectiveness can be demonstrated by the results derived from it.

### III. THE CRITICAL BEHAVIOR OF THE GROUND STATE ENERGY

In the following, we take \(S = 1/2, J_1 = -1\) and \(J_2 = \alpha\). The energy function \(E_0(\varphi, \theta)\) is minimized at
\[
\varphi = \cos^{-1} \frac{1}{4\alpha}, \quad \theta = \pi/2
\]

(12)
The minimum of \(E_0(\varphi, \theta)\) is just the classical ground state energy:
\[
\epsilon_{cl} \equiv \frac{E_{cl}}{N} = -\frac{(\alpha - 1/4)^2}{2\alpha},
\]

(13)
which gives the critical behavior: \(\epsilon_{cl} = -2\gamma^2\) as \(\gamma \to 0\).

In order to obtain the quantum correction to the classical ground state energy, we use the double-time Green’s function approach [36, 37] to derive the zero-temperature average \(\langle b_k^\dagger b_k \rangle_0, \langle b_k b_{-k} \rangle_0\) and \(\langle b_k^\dagger b_{-k}^\dagger \rangle_0\). By solving the group of equations of motion for the four Green’s functions: \(\langle \langle b_k; b_k^\dagger \rangle \rangle_\omega, \langle b_{-k}^\dagger; b_k^\dagger \rangle_\omega, \langle \langle b_{-k}; b_k \rangle \rangle_\omega\) and \(\langle \langle b_k^\dagger; b_k \rangle \rangle_\omega\), and using the spectral theorem and taking the zero-temperature limit, we finally get:
\[
\langle b_k^\dagger b_k \rangle_0 = \frac{1}{2} \left( \frac{A}{C} - 1 \right),
\]

(14)
and
\[
\langle b_k b_{-k} \rangle_0 = \langle b_k^\dagger b_{-k}^\dagger \rangle_0 = -\frac{B}{C},
\]

(15)
FIG. 1: (Color online) The dependence of the ground state energy on \( \gamma \) given by Eq.(17) (solid line), \( E/N = -4\gamma^2 \) of Ref. [32] (short-dashed line), and \( E/N = -1.585\gamma^{12/7} \) of Ref. [33] (long-dashed line).

where \( C = \sqrt{A^2 - 4B^2} \) is the pole of the above green’s functions.

By taking Eq.(14) and Eq.(15) into the bosonic Hamiltonian (8), we obtain the energy function per site including the quantum correction:

\[
\epsilon = \epsilon_0 - \frac{1}{2\pi} \int_{k \in D} dk (A - \sqrt{A^2 - 4B^2}),
\]

where \( \epsilon = \frac{E}{N} \), \( \epsilon_0 = \frac{E_0}{N} \), and the quasimomentums \( k \) is restricted in the region \( D = \{ k | 0 \leq k \leq \pi \text{ and } A^2 - 4B^2 \geq 0 \} \).

The integral expression on the right side of Eq.(16) is the quantum correction to the classical energy. Based on this expression the critical behavior of the total ground state energy can be analyzed as follows. Considering the values of \( \theta \) and \( \varphi \) in the classical ground state, we take \( \theta = \pi/2 \) in Eq.(16) and obtain the energy function \( \epsilon(\varphi, \alpha) \). Furthermore, from the relation \( \cos \varphi = \frac{1}{4\alpha} \), we get \( \varphi = \sqrt{8\gamma} \) for \( \gamma \to 0 \). Finally, the critical behavior of the total ground state energy can be described by the function:

\[
\frac{E(\gamma)}{N} = \epsilon(\sqrt{8\gamma}, \gamma + \frac{1}{4}), \text{ for } 0 < \gamma << 1.
\]

Fig.1 shows that in the quite low region of \( \gamma \) our result calculated from Eq.(17) is close to \(-4\gamma^2\) of Ref. [32]. While in the most part of the region \( \gamma \in (0, 0.02) \) our result is close
FIG. 2: The curve of the function $a(\gamma)$ calculated from $E(\gamma)/N = -a\gamma^2$ predicts the limit value $a(\gamma \to 0) \approx 8.0$

to $-1.585\gamma^{12/7}$ of Ref. [33]. So from the calculation result, we can predict that the critical behavior of the ground state energy given by Eq. (17) is $E(\gamma)/N = -a\gamma^2$. The coefficient $a$ is given by $a(\gamma) = -E(\gamma)\gamma^{-2}/N$ with the limit $\gamma \to 0$. From Fig. 2, one can predict that $a \approx 8.0$.

On the other hand, doing a regular expansion in powers of small parameter $\varphi$ to the fourth order, and taking $\alpha \to 1/4$, we obtain $A - C = F_2(k)\varphi^2 + F_4(k)\varphi^4$ with the coefficients:

$$F_2(k) = 0, \quad F_4(k) = \frac{(\cos 2k - \cos k)^2}{8(3 - 4\cos k + \cos 2k)}.$$  \hspace{1cm} (18)

The quantum correction to the classical part of the ground state energy is

$$-\frac{\varphi^4}{2\pi} \int_0^\pi F_4(k)dk = -\frac{3\varphi^4}{32} = -6\gamma^2, \text{ for } \varphi = \sqrt{8\gamma}, \gamma \to 0,$$  \hspace{1cm} (19)

which is consistent with the above numerical calculation. However, if we do the expansion to the sixth order, the integral for the coefficient $F_6$ is infrared-divergent. This fact may implicit the restriction on the effectiveness of our treatment to this model. Nevertheless, our calculations and results derived from Eq. (16) and Eq. (17) seem reasonable, and the whole treatment is straightforward and easier than previous treatments.
IV. CONCLUSION

In this paper, the ground state energy of 1D F-AF model (1) in the vicinity of the transition point \( \alpha = 1/4 \) is considered. Using the linear spin-wave approximation and the green’s function approach in a very regular way, we obtain an integral expression Eq.(16) for the ground state energy including the quantum correction. The critical behavior of the ground state energy is described by the function \( \epsilon(\sqrt{8\gamma}, \gamma + 1/4) \) in Eq.(17), and the result is \( E(\gamma)/N = -8\gamma^2 \) which is compared with the previous results in Fig.1.

It is known that the total energy of the \( M \)-magnon state of the model (1) is \( E_M = -8M\gamma^2 \) [32, 38]. The critical behavior of the ground state energy \( E/N = -8\gamma^2 \) means that \( N \) noninteracting magnons are created in the ground state.

Acknowledgments

This work belongs to the collegial key project of natural science research funded by Anhui province in China under Grant No. KJ2010A131, and is partly supported by the National Natural Science Foundation of China under Grant No.10947138.

[1] Frustrated Spin Systems, edited by H. T. Diep (World Scientific, Singapore, 2004).
[2] H.-J. Mikeska and A. K. Kolezhuk, in Quantum magnetism, Lecture Notes in Physics Vol. 645, edited by U. Schollwöck, J. Richter, D. J. J. Farnell, and R. F. Bishop (Springer, Berlin, 2004), p.1.
[3] H. T. Lu, Y. J. Wang, S. Qin and T. Xiang, Phys. Rev. B 74, 134425 (2006).
[4] M. Härtel, J. Richter, D. Ihle, S.-L. Drechsler, Phys. Rev. B 78, 174412 (2008).
[5] D. V. Dmitriev and V. Ya. Krivnov, Phys. Rev. B 77, 024401 (2008).
[6] R. Zinke, S. L. Drechsler and J. Richter, Phys. Rev. B 79, 094425 (2009).
[7] J. Richter, M. Härtel, D. Ihle, and S.-L. Drechsler, J. Phys.: Conf. Ser. 145, 012064 (2009).
[8] D. V. Dmitriev and V. Ya. Krivnov, Phys. Rev. B 79, 054421 (2009).
[9] S. Furukawa, M. Sato and A. Furusaki, Phys. Rev. B 81, 094430 (2010).
[10] D. V. Dmitriev and V. Ya. Krivnov, Phys. Rev. B 81, 054408 (2010).
[11] R. Zinke, J. Richter and S. L. Drechsler, J. Phys.: condens. Matt. 22, 446002 (2010).
[12] M. Enderle, B. Fäk, H.-J. Mikeska, R. K. Kremer, A. Prokofiev, W. Assmus, Phys. Rev. Lett. 104, 237207 (2010).

[13] Y. Mizuno, T. Tohyama, S. Maekawa, T. Osafune, N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. B 57, 5326 (1998).

[14] T. Masuda, A. Zheludev, A. Bush, M. Markina, and A. Vasiliev, Phys. Rev. Lett. 92, 177201 (2004).

[15] B. J. Gibson, R. K. Kremer, A. V. Prokofiev, W. Assmus, and G. J. McIntyre, Physica B 350, E253 (2004).

[16] A. A. Gippius, E. N. Morozova, A. S. Moskvin, A. V. Zalessky, A. A. Bush, M. Baenitz, H. Rosner, and S.-L. Drechsler, Phys. Rev. B 70, 020406(R) (2004).

[17] M. Hase, H. Kuroe, K. Ozawa, O. Suzuki, H. Kitazawa, G. Kido and T. Sekine. Phys. Rev. B 70, 104426 (2004).

[18] T. Masuda, A. Zheludev, B. Roessli, A. Bush, M. Markina, and A. Vasiliev, Phys. Rev. B 72, 014405 (2005).

[19] M. Enderle, C. Mukherjee, B. Fäk, R. K. Kremer, J.-M. Broto, H. Rosner, S.-L. Drechsler, J. Richter, J. Malek, A. Prokofiev, W. Assmus, P. Pujol, J.-L. Raggazzoni, H. Rakoto, M. Rheinstädter, and H. M. Rønnow, Europhys. Lett. 70, 237 (2005).

[20] S. L. Drechsler, J. Málek, J. Richter, A. S. Moskvin, A. A. Gippius, and H. Rosner, Phys. Rev. Lett. 94, 039705 (2005).

[21] L. Capogna, M. Mayr, P. Horsch, M. Raichle, R. K. Kremer, M. Sofin, A. Maljuk, M. Jansen, and B. Keimer, Phys. Rev. B 71, 140402(R) (2005).

[22] S.-L. Drechsler, J. Richter, A. A. Gippius, A. Vasiliev, A. S. Moskvin, J. Málek, Y. Prots, W. Schnelle, and H. Rosner, Europhys. Lett. 73, 83 (2006).

[23] S.-L. Drechsler, J. Richter, R. Kuzian, J. Málek, N. Tristan, B. Büchner, A. S. Moskvin, A. A. Gippius, A. Vasiliev, O. Volkova, A. Prokofiev, H. Rakato, J.-M. Broto, W. Schnelle, M. Schmitt, A. Ormeci, C. Loison, and H. Rosner, J. Magn. Magn. Mater. 316, 306 (2007).

[24] S.-L. Drechsler, O. Volkova, A. N. Vasiliev, N. Tristan, J. Richter, M. Schmitt, H. Rosner, J. Málek, R. Klingeler, A. A. Zvyagin, and B. Büchner, Phys. Rev. Lett. 98, 077202 (2007).

[25] S. Park, Y. J. Choi, C. L. Zhang, and S.-W. Cheong, Phys. Rev. Lett. 98, 057601 (2007).

[26] J. Malek, S.-L. Drechsler, U. Nitzsche, H. Rosner, and H. Eschrig, Phys. Rev. B 78, 060508(R) (2008).
[27] Y. Tarui, Y. Kobayashi, M. Sato, J. Phys. Soc. Jpn. 77, 043703 (2008).
[28] H. P. Bader and R. Schilling, Phys. Rev. B 19, 3556 (1979).
[29] T. Hamada, J. Kane, S. Nakagawa, and Y. Natsume, J. Phys. Soc. Jpn. 57, 1891 (1988); 58, 3869 (1989).
[30] T. Tonegawa and I. Harada, J. Phys. Soc. Jpn. 58, 2902 (1989).
[31] R. Bursill, G. A. Gehring, D. J. J. Farnell, J. B. Parkinson, T. Xiang, and C. Zeng, J. Phys.: condens. Mater. 7, 8605 (1995).
[32] V. Ya. Krivnov and A. A. Ovchinnikov, Phys. Rev. B 53, 6435 (1996).
[33] D. V. Dmitriev and V. Ya. Krivnov, Phys. Rev. B 73, 024402 (2006).
[34] D. V. Dmitriev, V. Ya. Krivnov and J. Richter, Phys. Rev. B 75, 014424 (2007).
[35] T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940).
[36] S. V. Tyablikov, Methods in the Quantum Theory of Magnetism (Plenum, New York, 1967).
[37] P. Fröbrich and P. J. Kuntz, Phys. Rep. 432, 223 (2006).
[38] A. A. Ovchinnikov, JETP Lett. 5, 48 (1967).