Modified spin-wave theory of low-dimensional quantum spiral magnets

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A general spin-wave theory for the low-dimensional quantum spiral magnets with a constraint introduced by Takahashi is presented. We show that this theory can reproduce the main results of the conventional spin-wave theory for Heisenberg magnetic systems without frustrations. For the triangular lattice spin-$\frac{1}{2}$ Heisenberg antiferromagnet and the frustrated square lattice Heisenberg models, the present theory yields results different from those of the conventional spin-wave theory but in agreement with those of recent numerical simulations for small lattices.

Recently there has been a resurgence of interest in the low-dimensional quantum Heisenberg (LDQH) model in connection with the mechanism of the high-T_c superconductivity. The conventional spin-wave (CSW) method is inapplicable when global spin-rotation invariance is not broken, and to proceed we must develop a spin-rotation unbroken approach to study the magnetism. A great advance has been made in this direction. Takahashi has formulated a modified spin-wave (MSW) theory for both LDQH ferromagnets and antiferromagnets that yields excellent results.[1,2] His ideal was to supplement the CSW theory with an additional constraint that the magnetization of each site is zero, which enforces the condition that the spin rotation symmetry is not broken.

In this paper we formulate, along the same line, a general MSW theory for the quantum twisted magnets. It is known that arbitrary magnetic configurations can be described by the action of one or more twists applied to a ferromagnetic configuration. We can perform all calculations very easily in twisted coordinates where the spin correlations are locally ferromagnetic. We derive a set of self-consistent equations which permit us to calculate the physical quantities very conveniently for a LDQH system. It will be shown that this theory can reproduce the main results of the CSW theory for the LDQH model without frustrations. For the triangular lattice antiferromagnet, we obtain the ground-state energy $E_0=-0.181$ J/bond and the staggered magnetization $M_0=0.375$ in agreement with the variational values for small lattices[3] $E_0=-0.1789$ and $M_0=0.34$. Our result for E_0 is also consistent with $E_0-0.183\pm0.0003$ obtained from the exact diagonalization of small clusters.[4] This suggests that the ground state of the triangular lattice antiferromagnetic has long-range Neél order. While for the frustrated Heisenberg magnetic systems, the present theory gives the different phase diagrams from the CSW theory.

Let us consider the frustrated LDQH model described by the following generalized Heisenberg Hamiltonian:

$$H=\sum_{\langle ij\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j \ . \tag{1}$$

The summation over $\langle ij\rangle$ in the above equation including all possible spin-spin interactions. For example, $J_{ij}=J_1, J_2, \ldots,$ and J_n if $\langle ij\rangle$, respectively, represents first-, second-,..., and nth-nearest-neighboring pairs. When $\langle ij\rangle$ denotes the nearest-neighboring pair, $J_1=J\neq0$, $J_2=J_3=\cdots=J_n=0$ the above Hamiltonian reduces back to the standard Heisenberg model. Generally, the ground state of Hamiltonian (1) has a spiral spin configuration which can be characterized by a twisted vector $\mathbf{Q}$. We introduce twisted coordinates (ξ,η,ζ) at each site

$$\begin{aligned} S_i^{\xi}&=-S_i^{z} \ ,\\ S_i^{\eta}&=-S_i^{x}\sin\mathbf{Q}\cdot\mathbf{r}_i+S_i^{y}\cos\mathbf{Q}\cdot\mathbf{r}_i \ ,\\ S_i^{\zeta}&=S_i^{x}\cos\mathbf{Q}\cdot\mathbf{r}_i+S_i^{y}\sin\mathbf{Q}\cdot\mathbf{r}_i \ , \end{aligned} \tag{2}$$

such that the equilibrium direction of each spin is along its ζ direction. Now we introduce the Dyson-Maleev (DM) transformation[5] for $S_i^{+}\equiv S_i^{\xi}+iS_i^{\eta}$, $S_i^{-}\equiv S_i^{\xi}-iS_i^{\eta}$, and S_i^{ζ} instead of Holstein-Promakoff (HP) transformation[6]

$$\begin{aligned} S_i^{-}&=(2S-a_i^{\dagger}a_i)a_i \ ,\\ S_i^{+}&=a_i^{\dagger} \ ,\\ S_i^{\zeta}&=-S+a_i^{\dagger}a_i \ , \end{aligned} \tag{3}$$

where $a^{\dagger}$ and a are the spin-wave operators and satisfy the boson commutation relations. It should be pointed out that DM transformation violates the Hermitian conjugate relationship $S_i^{+}=(S_i^{-})^{\dagger}$, which is different from HP transformation. It is expected that this will not affect the ground-state properties.[2,7] In fact, this Hermitian can be recovered by an additional nonunitary transformation.[8] Next we introduce the ideal spin-wave density matrix $\rho=\exp(-\sum_k \varepsilon_k\alpha_k^{\dagger}\alpha_k/T)$ with Bogoliubov transformation $\alpha_k=\cosh\theta_k a_k-\sinh\theta_k a_{-k}^{\dagger}$. Substituting the relations in Eqs. (2) and (3) into Eq. (1) and using this density matrix and the Wick's theorem[9] for the interaction terms between spin waves, we can compute the expectation value of the energy $E=\langle H\rangle$. At zero external magnetic field, the spin rotation symmetry requires that the magnetization of each site should be zero:[1,2] $\langle S_i^{\zeta}\rangle=0$.

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Under this constraint, minimizing the free energy of the system, we obtain

$$\tanh 2\theta_k = A_k / B_k \ , \tag{4}$$

$$A_k = \frac{1}{2} \sum_{\langle ij \rangle} J_{ij}(1-\cos\mathbf{Q}\cdot\mathbf{r}_{ij}) g(\mathbf{r}_{ij}) e^{-i\mathbf{k}\cdot\mathbf{r}_{ij}} \ , \tag{5}$$

$$\begin{aligned} B_k = \frac{1}{2} \sum_{\langle ij \rangle} J_{ij}[& (1-\cos\mathbf{Q}\cdot\mathbf{r}_{ij}) g(\mathbf{r}_{ij}) \\ & -(1+\cos\mathbf{Q}\cdot\mathbf{r}_{ij}) f(\mathbf{r}_{ij}) \\ & \times(1-e^{-i\mathbf{k}\cdot\mathbf{r}_{ij}})] + \mu \ , \end{aligned} \tag{6}$$

$$g(\mathbf{r}_{ij}) = M_0 + \frac{1}{N} \sum_k {}' \sinh 2\theta_k (n_k + \tfrac{1}{2}) e^{-i\mathbf{k}\cdot\mathbf{r}_{ij}} \ , \tag{7}$$

$$f(\mathbf{r}_{ij}) = M_0 + \frac{1}{N} \sum_k {}' \cosh 2\theta_k (n_k + \tfrac{1}{2}) e^{-i\mathbf{k}\cdot\mathbf{r}_{ij}} \ . \tag{8}$$

Here $n_k = \langle \alpha_k^\dagger \alpha_k \rangle = 1/(e^{\varepsilon_k/T}-1)$, μ is the Lagrange multiplier introduced by the constraint, M_0 is the number of the zero-energy spin waves which represents the long-range order of the system, and $\sum_k'$ denotes the sum excluding the zero-energy modes. While the spin-wave spectrum is given by

$$\varepsilon_k = (B_k^2 - A_k^2)^{1/2} \ , \tag{9}$$

and the ground-state energy is obtained as

$$E_0 = -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \{ (1-\cos\mathbf{Q}\cdot\mathbf{r}_{ij}) [g(\mathbf{r}_{ij})]^2 - (1+\cos\mathbf{Q}\cdot\mathbf{r}_{ij}) [f(\mathbf{r}_{ij})]^2 \} \ . \tag{10}$$

From the constraint $\langle S_l^\xi \rangle = 0$, M_0 has the expression

$$M_0 = S + \frac{1}{2} - \frac{1}{N} \sum_k {}' \cosh 2\theta_k (n_k + \tfrac{1}{2}) \ . \tag{11}$$

From the above equation, the Lagrange multiplier μ in Eq. (6) can be determined. M_0 here is in fact equivalent to the staggered magnetization in the CSW theory.[10] Thus a set of self-consistent equations (4)–(11) which govern the basic magnetic properties of the spiral Heisenberg magnets are obtained. In a system with a long-range magnetic order and from Eqs. (7) and (8), one has $g(\mathbf{r}_{ij}) \sim f(\mathbf{r}_{ij}) \sim S$ for $S \to \infty$. In the classical limit ($S \to \infty$) we obtain the spin-wave spectrum from Eq. (9)

$$\varepsilon_k = S \{ (J_k - J_Q) [(J_{k+Q} + J_{k-Q})/2 - J_Q] \}^{1/2} \ , \tag{12}$$

which is exactly the result of the CSW theory for a spiral magnetic system[10] with $J_k = \sum_{\langle ij \rangle} J_{ij} \exp(i\mathbf{k}\cdot\mathbf{r}_{ij})$. It should be emphasized here that for finite S or for the case close to the critical transition boundary even in large S limit where the staggered magnetization is vanishing, $g(\mathbf{r}_{ij})$ and $f(\mathbf{r}_{ij})$ in Eqs. (7) and (8) are quite different from S. Therefore, it is expected that the present theory will yield different results from the CSW theory.

An an example, we first apply the present theory to study the ground-state properties of the LDQH bipartite lattice antiferromagnets with the nearest-neighbor coupling ($J_1 = J$) only. Using the mean-field approximation as in Ref. 2 and from Eqs. (4)–(6), one has

$$\tanh 2\theta_k = \frac{A_k}{B_k} = \frac{zJg(\delta)\gamma_k}{zJg(\delta)+\mu} \ , \tag{13}$$

with $\gamma_k = \sum_\delta \exp(i\mathbf{k}\cdot\boldsymbol{\delta})/z$, where $\boldsymbol{\delta}$ is the vector to the nearest neighbors and z is the coordination number. For 1D, Rezende[11] has used this theory to predict the existence of a Haldane gap.[12] In fact, we know that there is no long-range order in the ground state for 1D antiferromagnet. Solving Eqs. (9) and (11) with $M_0 = 0$ at large S limit, we obtain the spin-wave gap $\varepsilon_0 \sim zSJe^{-\pi S}$, which is essentially the same result obtained by Haldane[12] from the nonlinear σ-model mapping. Of course, like Schwinger boson approach,[13] the present theory is unable to predict the absence of a gap in half-odd-integer spin systems. For 2D antiferromagnet, Eqs. (13) and (9)–(11) give the exact same equations obtained by Takahashi,[2] which lead to a quantitative agreement with the CSW approach[2] and the renormalization group theory.[14]

The more powerful aspect of our theory is for a frustrated Heisenberg system. Recently, the square lattice Heisenberg antiferromagnet (HAF) with first- and second-nearest-neighbor couplings J_1 and J_2 that we will call the J_1-J_2 model have been studied by various approaches.[15–18] The advantage of this model is that it retains the square lattice symmetry while simultaneously exhibiting frustrations. In fact, for very small J_2/J_1 the ground state has the Néel order, while at large J_2/J_1 limit, the system decouples into two unfrustrated sublattices each one with its own Néel order, and the dominant configurations have alternating rows (or columns) of spin up and down that we will call collinear state.[15–18] All previous methods[15–18] for this model only consider the small and large J_2/J_1 limit, i.e., they only study the Néel state and the collinear state. Here we give a unified picture for arbitrary values of J_2/J_1 based upon our Eqs. (4)–(11). Generally, this model has a spiral spin structure which can be described by a twisted vector $\mathbf{Q} = Q(1,1)$, where Q satisfies

$$\begin{aligned} J_2 \{ [g(\delta')]^2 + [f(\delta')]^2 \} \sin 2Q + J_1 \{ & [g(\delta)]^2 \\ & + [f(\delta)]^2 \} \sin Q = 0 \ , \end{aligned} \tag{14}$$

which corresponds to the minimal energy of Eq. (10). δ' is the vector to the next-nearest-neighbors. Equations (14) and (15) has the solution

$$\begin{aligned} & Q = \pi, \quad \text{for } \alpha > 1 \ , \\ & Q = \cos^{-1}(-\alpha), \quad \text{for } \alpha < 1 \ , \end{aligned} \tag{15}$$

where

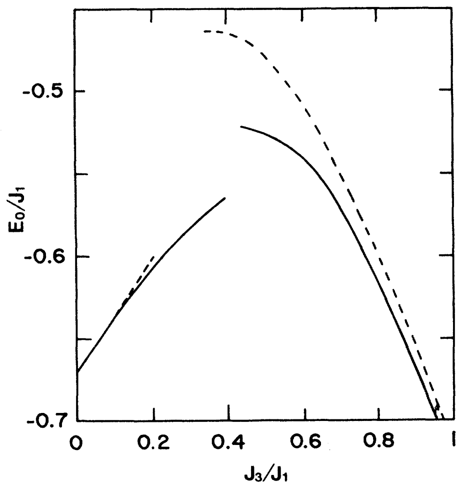

FIG. 1. Energy of the ground state vs J_3/J_1 for the J_1-J_3 model with $S=\frac{1}{2}$. The solid and the dashed lines are the results of the present theory and those of the linear CSW theory, respectively.

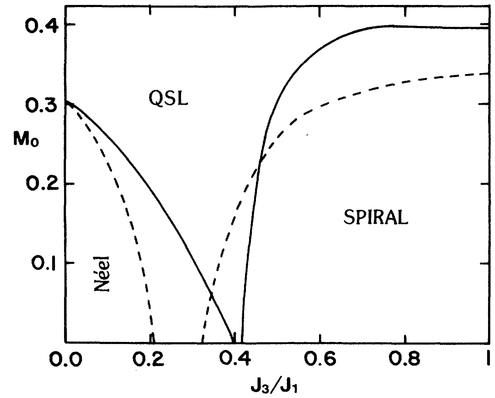

FIG. 2. Staggered magnetization vs J_3/J_1 for the J_1-J_3 model with $S=\frac{1}{2}$. The solid and the dashed lines corresponding to the results of the present theory and those of the linear CSW theory, respectively.

$$\alpha=\frac{J_1}{2J_2}\frac{[f(\delta)]^2+[g(\delta)]^2}{[f(\delta')]^2+[g(\delta')]^2} . \tag{16}$$

We can see from the above equations that for small J_2/J_1, $\alpha>1$ and $Q=\pi$, which corresponds to the Néel state. While at very large J_2/J_1 limit, $\alpha\to 0$ and $Q\to\pi/2$, which gives the collinear state. In the general case of $\alpha<1$, the incommensurate spiral phase with $Q=\cos^{-1}(-\alpha)$ is the ground state.

In Ref. 15 we performed a self-consistent calculation only for small and large J_2/J_1 limit, i.e., for the Néel state and the collinear state. The lower ground-state energy than that obtained from the CSW theory has been obtained.[15,16] Our results agree well with those of the recent numerical simulation for small lattices.[17,18] Here we present a general expression for the twisted vector **Q** in the whole parameter region. We show that at both small J_2/J_1 limit (corresponding to the Néel state) and large J_2/J_1 limit (corresponding to the collinear state), our general results can automatically return back to those obtained previously.[15]

Now we study the square lattice HAF with first- and third-nearest-neighbor couplings J_1 and J_3 that we will call the J_1-J_3 model. Generally, the ground state of this model has a spiral spin structure which can be characterized by a wave vector $\mathbf{Q}=Q(1,1)$, where Q satisfies

$$J_1\{[f(\delta_1)]^2+[g(\delta_1)]^2\}\sin Q+2J_3\{[f(\delta_3)]^2+[g(\delta_3)]^2\}\sin 2Q=0 , \tag{17}$$

which corresponds to the minimal energy of Eq. (10). δ_1 and δ_3 here are the vectors to the first- and third-nearest-neighbors, respectively. Equation (17) has a solution

$$\begin{aligned} &Q=\pi, \quad \text{for } \alpha>1 , \\ &Q=\cos^{-1}(-\alpha), \quad \text{for } \alpha<1 , \end{aligned} \tag{18}$$

where

$$\alpha=\frac{J_1}{4J_3}\frac{[f(\delta_1)]^2+[g(\delta_1)]^2}{[f(\delta_3)]^2+[g(\delta_3)]^2} . \tag{19}$$

We note that at the classical limit ($S\to\infty$), $f(\delta_{1,3})$ and $g(\delta_{1,3})\sim S$, Eqs. (17) and (19) reduce back to $J_1\sin Q+2J_3\sin 2Q=0$ and $\alpha=J_1/4J_3$ which are just the results of linear CSW theory.[19] We have performed the self-consistent calculations for this model with $S=\frac{1}{2}$. The results for the ground-state energy E_0 and the staggered magnetization M_0 are shown in Figs. 1 and 2, respectively. It is clear from Fig. 1 that the present result for E_0 is lower than that obtained from the CSW theory. In Fig. 2, the result for M_0 show that for small value of J_3/J_1 the Néel state is the ground state, while for the large enough frustrations the incommensurate spiral phase with $Q=\cos^{-1}(-\alpha)$ becomes stable. The change from one state to the other occurs around $J_3/J_1=0.4$. There exists a narrow region around $J_3/J_1=0.4$ to accommodate the nonmagnetic quantum spin liquid (QSL) phase. An investigation with other analytical or numerical methods would be necessary to characterize the true ground state around $J_3/J_1=0.4$. This picture is qualitatively similar to that of the CSW theory,[19] but a significant quantitative different exists between these two results.

All discussions above are confined to the bipartite lattice models. Our theory can be also applied to the nonbipartite lattice systems. As an example of the nonbipartite lattice, we consider here the triangular lattice HAF with $S=\frac{1}{2}$. The triangular lattice HAF with $S=\frac{1}{2}$ is the simplest frustrated system with the nearest-neighbor coupling only. The ground state of this system consists of three sublattices, A, B, and C, with spins on each sublattice at an angle of $2\pi/3$ to those on the other two sublattices, i.e., $\mathbf{Q}\cdot\delta_{AB}=2\pi/3$ and $\mathbf{Q}\cdot\delta_{AC}=4\pi/3$. Thus, from Eqs. (4)–(6) we obtain

$$\tanh 2\theta_k=\frac{A_k}{B_k}=\frac{3zJg(\delta)\gamma_k}{3zJg(\delta)-zJf(\delta)(1-\gamma_k)+\mu} . \tag{20}$$

Substituting the above relation into Eqs. (10) and (11), and performing the self-consistent calculation, we obtain the ground-state energy $E_0=-0.181J$/bond and the staggered magnetization $M_0=0.375$. The diagonalization of small clusters[4] has led to an estimate for the ground-state energy which is $E_0=-0.183\pm0.003$, but with no information on the staggered magnetization. Recently, Huse and Elser[3] have performed a variational calculation for small lattices with an ordered trial wave function including three parameters. They got $E_0=-0.1789$ and $M_0=0.34$. These values are very close to our MSW results. The CSW results of Jolicoeur and Guillou[20] lead to a slightly higher energy $E_0=-0.1796$ than our result. But they obtained $M_0=0.239$ which is much smaller than our result and that of Ref. 3. It is interesting to note that our value for E_0 is much lower than the $E_0=-0.158\pm0.005$ estimated from various RVB-type wave functions.[21,22] This suggests that the situation of the triangular lattice HAF is quite similar to that of the square lattice: a ground state with long-range Néel order exists in both cases.

The theory discussed here is of rather general utility and can be easily applied to other LDQH models with complicated magnetic structures. It is also convenient to use this theory to calculate the other physical quantities. For example, the spin-spin correlation function can be computed by evaluating $\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle$ in the ground state, which yields the result

$$\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle=\tfrac{1}{2}(1+\cos\mathbf{Q}\cdot\mathbf{r}_{ij})[f(\mathbf{r}_{ij})]^2 -\tfrac{1}{2}(1-\cos\mathbf{Q}\cdot\mathbf{r}_{ij})[g(\mathbf{r}_{ij})]^2-\tfrac{1}{4}\delta_{ij} \ . \tag{21}$$

The details of the calculations together with the finite-temperature results are planned to be presented elsewhere.

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[1]M. Takahashi, Prog. Theor. Phys. Suppl. **87**, 233 (1986); Phys. Rev. Lett. **58**, 168 (1987).

[2]M. Takahashi, Phys. Rev. B **40**, 2491 (1989); J. E. Hirsch and S. Tang, *ibid*. **40**, 4769 (1989).

[3]D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988).

[4]H. Nishimori and N. Nakanishi, J. Phys. Soc. Jpn. **57**, 626 (1988).

[5]F. J. Dyson, Phys. Rev. **102**, 1217 (1956); **102**, 1230 (1956); S. V. Maleev, Zh. Eksp. Teor. Fiz. **33**, 1010 (1958) [Sov. Phys. JETP **6**, 776 (1958)].

[6]T. Holstein and H. Primakoff, Phys. Rev. **59**, 1098 (1940).

[7]S. Tyĉ and B. I. Halperin, Phys. Rev. B **42**, 2096 (1990).

[8]T. Oguchi and A. Homma, J. Appl. Phys. **34**, 1153 (1963).

[9]A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971), Chap. 7.

[10]F. Keffer, in *Ferromagnetismus*, edited by S. Flugge (Springer, New York, 1966), Handbuch der Physik, Vol. 18, Part 2.

[11]S. M. Rezende, Phys. Rev. B **42**, 2589 (1990).

[12]F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).

[13]D. P. Arovas and A. Auerbach, Phys. Rev. Lett. **61**, 617 (1988); Phys. Rev. B **38**, 316 (1988).

[14]S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B **39**, 2344 (1989).

[15]J. H. Xu and C. S. Ting, Phys. Rev. B **42**, 6861 (1990).

[16]P. Chandra and B. Doucot, Phys. Rev. B **38**, 9335 (1988).

[17]E. Dagotto and A. Moreo, Phys. Rev. B **39**, 4744 (1989); Phys. Rev. Lett. **63**, 2148 (1989).

[18]E. Dagotto (unpublished); A. Moreo, E. Dagotto, T. Jolicoeur, and J. Riera, Phys. Rev. B **42**, 6283 (1990).

[19]P. Locher, Phys. Rev. B **41**, 2537 (1990).

[20]Th. Jolicoeur and J. C. Le Guillou, Phys. Rev. B **40**, 2727 (1989).

[21]V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987), and references therein.

[22]T. K. Lee and Shiping Feng, Phys. Rev. B **41**, 11 110 (1990).